



## Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:41 AM UTC

PDB ID : 6KMX / pdb\_00006kmx  
EMDB ID : EMD-0727  
Title : Structure of PSI from *H. hongdechloris* grown under far-red light condition  
Authors : Kato, K.; Nagao, R.; Shen, J.R.; Miyazaki, N.; Akita, F.  
Deposited on : 2019-08-01  
Resolution : 2.41 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:

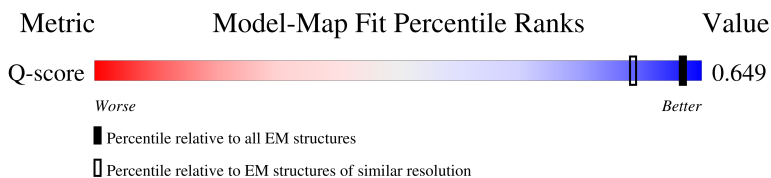
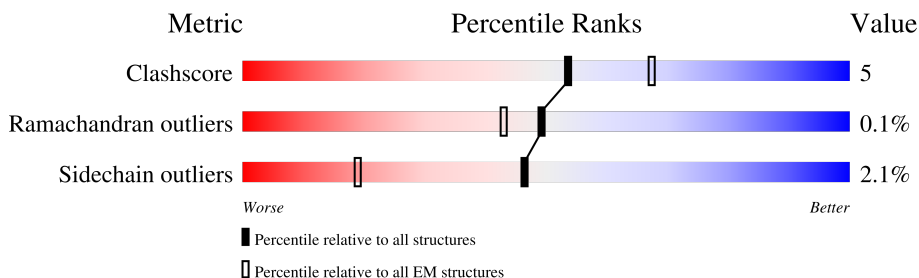
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01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

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.41 Å.

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



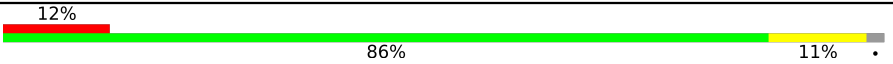
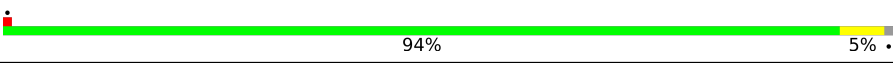
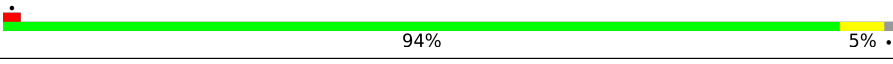
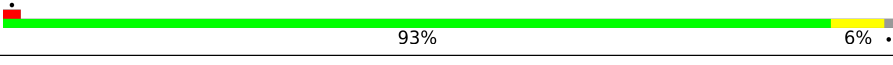
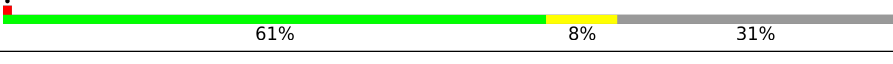
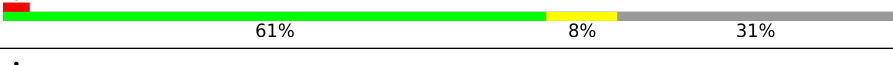
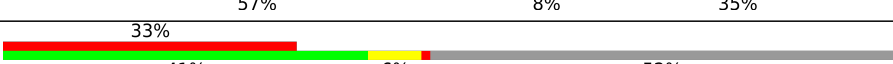
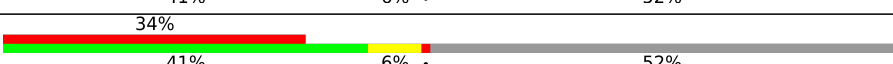
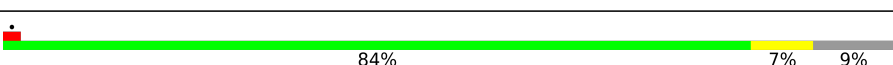
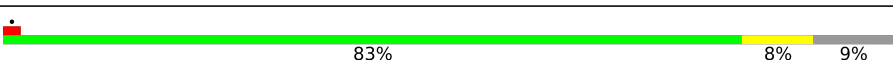
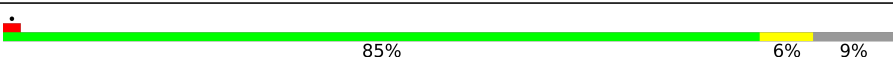
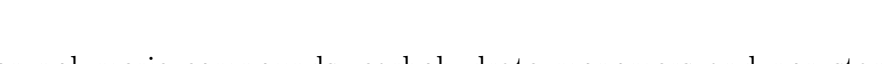
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 5662 ( 1.92 - 2.91 )                                     |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | aA    | 784    |                  |
| 1   | bA    | 784    |                  |
| 1   | cA    | 784    |                  |
| 2   | aB    | 743    |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 2   | bB    | 743    |    |
| 2   | cB    | 743    |    |
| 3   | aC    | 81     |    |
| 3   | bC    | 81     |    |
| 3   | cC    | 81     |    |
| 4   | aD    | 142    |    |
| 4   | bD    | 142    |    |
| 4   | cD    | 142    |    |
| 5   | aE    | 68     |    |
| 5   | bE    | 68     |    |
| 5   | cE    | 68     |    |
| 6   | aI    | 63     |   |
| 6   | bI    | 63     |  |
| 6   | cI    | 63     |  |
| 7   | aK    | 96     |  |
| 7   | bK    | 96     |  |
| 7   | cK    | 96     |  |
| 8   | aL    | 189    |  |
| 8   | bL    | 189    |  |
| 8   | cL    | 189    |  |
| 9   | aM    | 31     |  |
| 9   | bM    | 31     |  |
| 9   | cM    | 31     |  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 10  | CL0  | aA    | 801 | X         | -        | -       | -                |
| 10  | CL0  | bA    | 801 | X         | -        | -       | -                |
| 10  | CL0  | cA    | 801 | X         | -        | -       | -                |
| 11  | CLA  | aA    | 802 | X         | -        | -       | -                |
| 11  | CLA  | aA    | 803 | X         | -        | -       | -                |
| 11  | CLA  | aA    | 804 | X         | -        | -       | -                |
| 11  | CLA  | aA    | 805 | X         | -        | -       | -                |
| 11  | CLA  | aA    | 806 | X         | -        | -       | -                |
| 11  | CLA  | aA    | 807 | X         | -        | -       | -                |
| 11  | CLA  | aA    | 808 | X         | -        | -       | -                |
| 11  | CLA  | aA    | 809 | X         | -        | -       | -                |
| 11  | CLA  | aA    | 810 | X         | -        | -       | -                |
| 11  | CLA  | aA    | 811 | X         | -        | -       | -                |
| 11  | CLA  | aA    | 812 | X         | -        | -       | -                |
| 11  | CLA  | aA    | 813 | X         | -        | -       | -                |
| 11  | CLA  | aA    | 814 | X         | -        | -       | -                |
| 11  | CLA  | aA    | 815 | X         | -        | -       | -                |
| 11  | CLA  | aA    | 816 | X         | -        | -       | -                |
| 11  | CLA  | aA    | 817 | X         | -        | -       | -                |
| 11  | CLA  | aA    | 818 | X         | -        | -       | -                |
| 11  | CLA  | aA    | 819 | X         | -        | -       | -                |
| 11  | CLA  | aA    | 820 | X         | -        | -       | -                |
| 11  | CLA  | aA    | 821 | X         | -        | -       | -                |
| 11  | CLA  | aA    | 822 | X         | -        | -       | -                |
| 11  | CLA  | aA    | 823 | X         | -        | -       | -                |
| 11  | CLA  | aA    | 824 | X         | -        | -       | -                |
| 11  | CLA  | aA    | 825 | X         | -        | -       | -                |
| 11  | CLA  | aA    | 828 | X         | -        | -       | -                |
| 11  | CLA  | aA    | 829 | X         | -        | -       | -                |
| 11  | CLA  | aA    | 831 | X         | -        | -       | -                |
| 11  | CLA  | aA    | 833 | X         | -        | -       | -                |
| 11  | CLA  | aA    | 834 | X         | -        | -       | -                |
| 11  | CLA  | aA    | 835 | X         | -        | -       | -                |
| 11  | CLA  | aA    | 836 | X         | -        | -       | -                |
| 11  | CLA  | aA    | 837 | X         | -        | -       | -                |
| 11  | CLA  | aA    | 838 | X         | -        | -       | -                |
| 11  | CLA  | aA    | 839 | X         | -        | -       | -                |
| 11  | CLA  | aA    | 840 | X         | -        | -       | -                |
| 11  | CLA  | aA    | 841 | X         | -        | -       | -                |
| 11  | CLA  | aA    | 842 | X         | -        | -       | -                |
| 11  | CLA  | aA    | 843 | X         | -        | -       | -                |
| 11  | CLA  | aB    | 801 | X         | -        | -       | -                |
| 11  | CLA  | aB    | 802 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 11  | CLA  | aB    | 803 | X         | -        | -       | -                |
| 11  | CLA  | aB    | 804 | X         | -        | -       | -                |
| 11  | CLA  | aB    | 805 | X         | -        | -       | -                |
| 11  | CLA  | aB    | 806 | X         | -        | -       | -                |
| 11  | CLA  | aB    | 807 | X         | -        | -       | -                |
| 11  | CLA  | aB    | 808 | X         | -        | -       | -                |
| 11  | CLA  | aB    | 809 | X         | -        | -       | -                |
| 11  | CLA  | aB    | 810 | X         | -        | -       | -                |
| 11  | CLA  | aB    | 811 | X         | -        | -       | -                |
| 11  | CLA  | aB    | 812 | X         | -        | -       | -                |
| 11  | CLA  | aB    | 813 | X         | -        | -       | -                |
| 11  | CLA  | aB    | 814 | X         | -        | -       | -                |
| 11  | CLA  | aB    | 815 | X         | -        | -       | -                |
| 11  | CLA  | aB    | 816 | X         | -        | -       | -                |
| 11  | CLA  | aB    | 817 | X         | -        | -       | -                |
| 11  | CLA  | aB    | 818 | X         | -        | -       | -                |
| 11  | CLA  | aB    | 819 | X         | -        | -       | -                |
| 11  | CLA  | aB    | 820 | X         | -        | -       | -                |
| 11  | CLA  | aB    | 821 | X         | -        | -       | -                |
| 11  | CLA  | aB    | 823 | X         | -        | -       | -                |
| 11  | CLA  | aB    | 825 | X         | -        | -       | -                |
| 11  | CLA  | aB    | 826 | X         | -        | -       | -                |
| 11  | CLA  | aB    | 827 | X         | -        | -       | -                |
| 11  | CLA  | aB    | 828 | X         | -        | -       | -                |
| 11  | CLA  | aB    | 829 | X         | -        | -       | -                |
| 11  | CLA  | aB    | 830 | X         | -        | -       | -                |
| 11  | CLA  | aB    | 831 | X         | -        | -       | -                |
| 11  | CLA  | aB    | 832 | X         | -        | -       | -                |
| 11  | CLA  | aB    | 833 | X         | -        | -       | -                |
| 11  | CLA  | aB    | 834 | X         | -        | -       | -                |
| 11  | CLA  | aB    | 835 | X         | -        | -       | -                |
| 11  | CLA  | aB    | 836 | X         | -        | -       | -                |
| 11  | CLA  | aB    | 837 | X         | -        | -       | -                |
| 11  | CLA  | aB    | 838 | X         | -        | -       | -                |
| 11  | CLA  | aB    | 839 | X         | -        | -       | -                |
| 11  | CLA  | aB    | 840 | X         | -        | -       | -                |
| 11  | CLA  | aK    | 101 | X         | -        | -       | -                |
| 11  | CLA  | aL    | 204 | X         | -        | -       | -                |
| 11  | CLA  | aL    | 205 | X         | -        | -       | -                |
| 11  | CLA  | aL    | 206 | X         | -        | -       | -                |
| 11  | CLA  | bA    | 802 | X         | -        | -       | -                |
| 11  | CLA  | bA    | 803 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 11  | CLA  | bA    | 804 | X         | -        | -       | -                |
| 11  | CLA  | bA    | 805 | X         | -        | -       | -                |
| 11  | CLA  | bA    | 806 | X         | -        | -       | -                |
| 11  | CLA  | bA    | 807 | X         | -        | -       | -                |
| 11  | CLA  | bA    | 808 | X         | -        | -       | -                |
| 11  | CLA  | bA    | 809 | X         | -        | -       | -                |
| 11  | CLA  | bA    | 810 | X         | -        | -       | -                |
| 11  | CLA  | bA    | 811 | X         | -        | -       | -                |
| 11  | CLA  | bA    | 812 | X         | -        | -       | -                |
| 11  | CLA  | bA    | 813 | X         | -        | -       | -                |
| 11  | CLA  | bA    | 814 | X         | -        | -       | -                |
| 11  | CLA  | bA    | 815 | X         | -        | -       | -                |
| 11  | CLA  | bA    | 816 | X         | -        | -       | -                |
| 11  | CLA  | bA    | 817 | X         | -        | -       | -                |
| 11  | CLA  | bA    | 818 | X         | -        | -       | -                |
| 11  | CLA  | bA    | 819 | X         | -        | -       | -                |
| 11  | CLA  | bA    | 820 | X         | -        | -       | -                |
| 11  | CLA  | bA    | 821 | X         | -        | -       | -                |
| 11  | CLA  | bA    | 822 | X         | -        | -       | -                |
| 11  | CLA  | bA    | 823 | X         | -        | -       | -                |
| 11  | CLA  | bA    | 824 | X         | -        | -       | -                |
| 11  | CLA  | bA    | 825 | X         | -        | -       | -                |
| 11  | CLA  | bA    | 828 | X         | -        | -       | -                |
| 11  | CLA  | bA    | 829 | X         | -        | -       | -                |
| 11  | CLA  | bA    | 831 | X         | -        | -       | -                |
| 11  | CLA  | bA    | 833 | X         | -        | -       | -                |
| 11  | CLA  | bA    | 834 | X         | -        | -       | -                |
| 11  | CLA  | bA    | 835 | X         | -        | -       | -                |
| 11  | CLA  | bA    | 836 | X         | -        | -       | -                |
| 11  | CLA  | bA    | 837 | X         | -        | -       | -                |
| 11  | CLA  | bA    | 838 | X         | -        | -       | -                |
| 11  | CLA  | bA    | 839 | X         | -        | -       | -                |
| 11  | CLA  | bA    | 840 | X         | -        | -       | -                |
| 11  | CLA  | bA    | 841 | X         | -        | -       | -                |
| 11  | CLA  | bA    | 842 | X         | -        | -       | -                |
| 11  | CLA  | bA    | 843 | X         | -        | -       | -                |
| 11  | CLA  | bB    | 801 | X         | -        | -       | -                |
| 11  | CLA  | bB    | 802 | X         | -        | -       | -                |
| 11  | CLA  | bB    | 803 | X         | -        | -       | -                |
| 11  | CLA  | bB    | 804 | X         | -        | -       | -                |
| 11  | CLA  | bB    | 805 | X         | -        | -       | -                |
| 11  | CLA  | bB    | 806 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 11  | CLA  | bB    | 807 | X         | -        | -       | -                |
| 11  | CLA  | bB    | 808 | X         | -        | -       | -                |
| 11  | CLA  | bB    | 809 | X         | -        | -       | -                |
| 11  | CLA  | bB    | 810 | X         | -        | -       | -                |
| 11  | CLA  | bB    | 811 | X         | -        | -       | -                |
| 11  | CLA  | bB    | 812 | X         | -        | -       | -                |
| 11  | CLA  | bB    | 813 | X         | -        | -       | -                |
| 11  | CLA  | bB    | 814 | X         | -        | -       | -                |
| 11  | CLA  | bB    | 815 | X         | -        | -       | -                |
| 11  | CLA  | bB    | 816 | X         | -        | -       | -                |
| 11  | CLA  | bB    | 817 | X         | -        | -       | -                |
| 11  | CLA  | bB    | 818 | X         | -        | -       | -                |
| 11  | CLA  | bB    | 819 | X         | -        | -       | -                |
| 11  | CLA  | bB    | 820 | X         | -        | -       | -                |
| 11  | CLA  | bB    | 821 | X         | -        | -       | -                |
| 11  | CLA  | bB    | 823 | X         | -        | -       | -                |
| 11  | CLA  | bB    | 825 | X         | -        | -       | -                |
| 11  | CLA  | bB    | 826 | X         | -        | -       | -                |
| 11  | CLA  | bB    | 827 | X         | -        | -       | -                |
| 11  | CLA  | bB    | 828 | X         | -        | -       | -                |
| 11  | CLA  | bB    | 829 | X         | -        | -       | -                |
| 11  | CLA  | bB    | 830 | X         | -        | -       | -                |
| 11  | CLA  | bB    | 831 | X         | -        | -       | -                |
| 11  | CLA  | bB    | 832 | X         | -        | -       | -                |
| 11  | CLA  | bB    | 833 | X         | -        | -       | -                |
| 11  | CLA  | bB    | 834 | X         | -        | -       | -                |
| 11  | CLA  | bB    | 835 | X         | -        | -       | -                |
| 11  | CLA  | bB    | 836 | X         | -        | -       | -                |
| 11  | CLA  | bB    | 837 | X         | -        | -       | -                |
| 11  | CLA  | bB    | 838 | X         | -        | -       | -                |
| 11  | CLA  | bB    | 839 | X         | -        | -       | -                |
| 11  | CLA  | bB    | 840 | X         | -        | -       | -                |
| 11  | CLA  | bK    | 101 | X         | -        | -       | -                |
| 11  | CLA  | bL    | 204 | X         | -        | -       | -                |
| 11  | CLA  | bL    | 205 | X         | -        | -       | -                |
| 11  | CLA  | bL    | 206 | X         | -        | -       | -                |
| 11  | CLA  | cA    | 802 | X         | -        | -       | -                |
| 11  | CLA  | cA    | 803 | X         | -        | -       | -                |
| 11  | CLA  | cA    | 804 | X         | -        | -       | -                |
| 11  | CLA  | cA    | 805 | X         | -        | -       | -                |
| 11  | CLA  | cA    | 806 | X         | -        | -       | -                |
| 11  | CLA  | cA    | 807 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 11  | CLA  | cA    | 808 | X         | -        | -       | -                |
| 11  | CLA  | cA    | 809 | X         | -        | -       | -                |
| 11  | CLA  | cA    | 810 | X         | -        | -       | -                |
| 11  | CLA  | cA    | 811 | X         | -        | -       | -                |
| 11  | CLA  | cA    | 812 | X         | -        | -       | -                |
| 11  | CLA  | cA    | 813 | X         | -        | -       | -                |
| 11  | CLA  | cA    | 814 | X         | -        | -       | -                |
| 11  | CLA  | cA    | 815 | X         | -        | -       | -                |
| 11  | CLA  | cA    | 816 | X         | -        | -       | -                |
| 11  | CLA  | cA    | 817 | X         | -        | -       | -                |
| 11  | CLA  | cA    | 818 | X         | -        | -       | -                |
| 11  | CLA  | cA    | 819 | X         | -        | -       | -                |
| 11  | CLA  | cA    | 820 | X         | -        | -       | -                |
| 11  | CLA  | cA    | 821 | X         | -        | -       | -                |
| 11  | CLA  | cA    | 822 | X         | -        | -       | -                |
| 11  | CLA  | cA    | 823 | X         | -        | -       | -                |
| 11  | CLA  | cA    | 824 | X         | -        | -       | -                |
| 11  | CLA  | cA    | 825 | X         | -        | -       | -                |
| 11  | CLA  | cA    | 828 | X         | -        | -       | -                |
| 11  | CLA  | cA    | 829 | X         | -        | -       | -                |
| 11  | CLA  | cA    | 831 | X         | -        | -       | -                |
| 11  | CLA  | cA    | 833 | X         | -        | -       | -                |
| 11  | CLA  | cA    | 834 | X         | -        | -       | -                |
| 11  | CLA  | cA    | 835 | X         | -        | -       | -                |
| 11  | CLA  | cA    | 836 | X         | -        | -       | -                |
| 11  | CLA  | cA    | 837 | X         | -        | -       | -                |
| 11  | CLA  | cA    | 838 | X         | -        | -       | -                |
| 11  | CLA  | cA    | 839 | X         | -        | -       | -                |
| 11  | CLA  | cA    | 840 | X         | -        | -       | -                |
| 11  | CLA  | cA    | 841 | X         | -        | -       | -                |
| 11  | CLA  | cA    | 842 | X         | -        | -       | -                |
| 11  | CLA  | cA    | 843 | X         | -        | -       | -                |
| 11  | CLA  | cB    | 801 | X         | -        | -       | -                |
| 11  | CLA  | cB    | 802 | X         | -        | -       | -                |
| 11  | CLA  | cB    | 803 | X         | -        | -       | -                |
| 11  | CLA  | cB    | 804 | X         | -        | -       | -                |
| 11  | CLA  | cB    | 805 | X         | -        | -       | -                |
| 11  | CLA  | cB    | 806 | X         | -        | -       | -                |
| 11  | CLA  | cB    | 807 | X         | -        | -       | -                |
| 11  | CLA  | cB    | 808 | X         | -        | -       | -                |
| 11  | CLA  | cB    | 809 | X         | -        | -       | -                |
| 11  | CLA  | cB    | 810 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 11  | CLA  | cB    | 811 | X         | -        | -       | -                |
| 11  | CLA  | cB    | 812 | X         | -        | -       | -                |
| 11  | CLA  | cB    | 813 | X         | -        | -       | -                |
| 11  | CLA  | cB    | 814 | X         | -        | -       | -                |
| 11  | CLA  | cB    | 815 | X         | -        | -       | -                |
| 11  | CLA  | cB    | 816 | X         | -        | -       | -                |
| 11  | CLA  | cB    | 817 | X         | -        | -       | -                |
| 11  | CLA  | cB    | 818 | X         | -        | -       | -                |
| 11  | CLA  | cB    | 819 | X         | -        | -       | -                |
| 11  | CLA  | cB    | 820 | X         | -        | -       | -                |
| 11  | CLA  | cB    | 821 | X         | -        | -       | -                |
| 11  | CLA  | cB    | 823 | X         | -        | -       | -                |
| 11  | CLA  | cB    | 825 | X         | -        | -       | -                |
| 11  | CLA  | cB    | 826 | X         | -        | -       | -                |
| 11  | CLA  | cB    | 827 | X         | -        | -       | -                |
| 11  | CLA  | cB    | 828 | X         | -        | -       | -                |
| 11  | CLA  | cB    | 829 | X         | -        | -       | -                |
| 11  | CLA  | cB    | 830 | X         | -        | -       | -                |
| 11  | CLA  | cB    | 831 | X         | -        | -       | -                |
| 11  | CLA  | cB    | 832 | X         | -        | -       | -                |
| 11  | CLA  | cB    | 833 | X         | -        | -       | -                |
| 11  | CLA  | cB    | 834 | X         | -        | -       | -                |
| 11  | CLA  | cB    | 835 | X         | -        | -       | -                |
| 11  | CLA  | cB    | 836 | X         | -        | -       | -                |
| 11  | CLA  | cB    | 837 | X         | -        | -       | -                |
| 11  | CLA  | cB    | 838 | X         | -        | -       | -                |
| 11  | CLA  | cB    | 839 | X         | -        | -       | -                |
| 11  | CLA  | cB    | 840 | X         | -        | -       | -                |
| 11  | CLA  | cK    | 101 | X         | -        | -       | -                |
| 11  | CLA  | cL    | 204 | X         | -        | -       | -                |
| 11  | CLA  | cL    | 205 | X         | -        | -       | -                |
| 11  | CLA  | cL    | 206 | X         | -        | -       | -                |
| 12  | F6C  | aA    | 826 | X         | -        | -       | -                |
| 12  | F6C  | aA    | 827 | X         | -        | -       | -                |
| 12  | F6C  | aA    | 830 | X         | -        | -       | -                |
| 12  | F6C  | aA    | 832 | X         | -        | -       | -                |
| 12  | F6C  | aA    | 844 | X         | -        | -       | -                |
| 12  | F6C  | aB    | 824 | X         | -        | -       | -                |
| 12  | F6C  | aL    | 202 | X         | -        | -       | -                |
| 12  | F6C  | bA    | 826 | X         | -        | -       | -                |
| 12  | F6C  | bA    | 827 | X         | -        | -       | -                |
| 12  | F6C  | bA    | 830 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 12  | F6C  | bA    | 832 | X         | -        | -       | -                |
| 12  | F6C  | bA    | 844 | X         | -        | -       | -                |
| 12  | F6C  | bB    | 824 | X         | -        | -       | -                |
| 12  | F6C  | bL    | 202 | X         | -        | -       | -                |
| 12  | F6C  | cA    | 826 | X         | -        | -       | -                |
| 12  | F6C  | cA    | 827 | X         | -        | -       | -                |
| 12  | F6C  | cA    | 830 | X         | -        | -       | -                |
| 12  | F6C  | cA    | 832 | X         | -        | -       | -                |
| 12  | F6C  | cA    | 844 | X         | -        | -       | -                |
| 12  | F6C  | cB    | 824 | X         | -        | -       | -                |
| 12  | F6C  | cL    | 202 | X         | -        | -       | -                |

## 2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 65112 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | aA    | 717      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5669  | 3724 | 966 | 950 | 29 |         |       |
| 1   | bA    | 717      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5669  | 3724 | 966 | 950 | 29 |         |       |
| 1   | cA    | 717      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5669  | 3724 | 966 | 950 | 29 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | aB    | 727      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5783  | 3786 | 976 | 996 | 25 |         |       |
| 2   | bB    | 727      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5783  | 3786 | 976 | 996 | 25 |         |       |
| 2   | cB    | 727      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5783  | 3786 | 976 | 996 | 25 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 3   | aC    | 80       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 596   | 366 | 102 | 117 | 11 |         |       |
| 3   | bC    | 80       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 596   | 366 | 102 | 117 | 11 |         |       |
| 3   | cC    | 80       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 596   | 366 | 102 | 117 | 11 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | aD    | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 768   | 492 | 130 | 143 | 3 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | bD    | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 768   | 492 | 130 | 143 | 3 |         |       |
| 4   | cD    | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 768   | 492 | 130 | 143 | 3 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |  | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|--|---------|-------|
| 5   | aE    | 61       | Total | C   | N  | O  |  | 0       | 0     |
|     |       |          | 499   | 317 | 87 | 95 |  |         |       |
| 5   | bE    | 61       | Total | C   | N  | O  |  | 0       | 0     |
|     |       |          | 499   | 317 | 87 | 95 |  |         |       |
| 5   | cE    | 61       | Total | C   | N  | O  |  | 0       | 0     |
|     |       |          | 499   | 317 | 87 | 95 |  |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 6   | aI    | 41       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 349   | 247 | 48 | 52 | 2 |         |       |
| 6   | bI    | 41       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 349   | 247 | 48 | 52 | 2 |         |       |
| 6   | cI    | 41       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 349   | 247 | 48 | 52 | 2 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 7   | aK    | 46       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 317   | 206 | 55 | 54 | 2 |         |       |
| 7   | bK    | 46       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 317   | 206 | 55 | 54 | 2 |         |       |
| 7   | cK    | 46       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 317   | 206 | 55 | 54 | 2 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | aL    | 172      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1303  | 838 | 223 | 239 | 3 |         |       |
| 8   | bL    | 172      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1303  | 838 | 223 | 239 | 3 |         |       |

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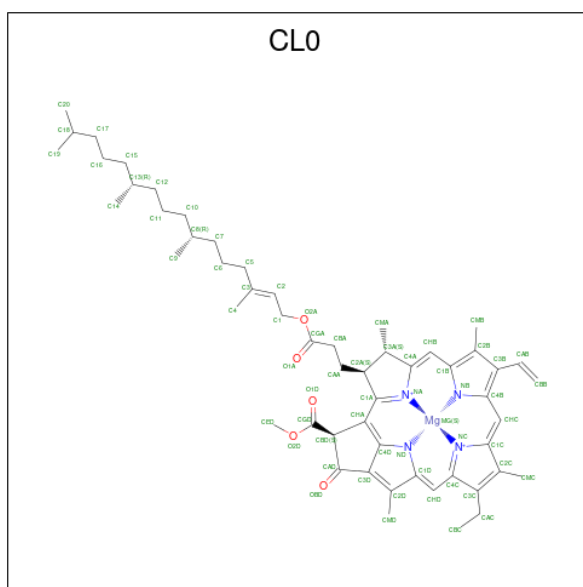
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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | cL    | 172      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1303  | 838 | 223 | 239 | 3 |         |       |

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

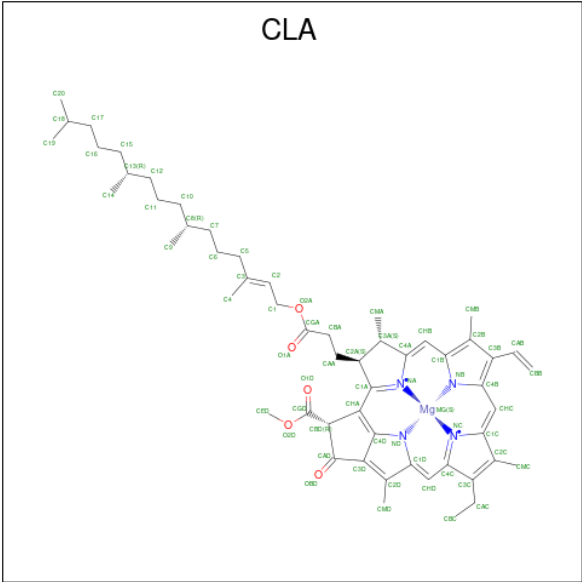
| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 9   | aM    | 31       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 241   | 162 | 36 | 42 | 1 |         |       |
| 9   | bM    | 31       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 241   | 162 | 36 | 42 | 1 |         |       |
| 9   | cM    | 31       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 241   | 162 | 36 | 42 | 1 |         |       |

- Molecule 10 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula:  $C_{55}H_{72}MgN_4O_5$ ).



| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 10  | aA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 10  | bA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 10  | cA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |

- Molecule 11 is CHLOROPHYLL A (CCD ID: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ).



| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 11  | aA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | aA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 46 | 1  | 4 | 5 |         |
| 11  | aA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | aA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | aA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | aA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | aA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |
| 11  | aA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | aA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | aA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | aA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | aA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 11  | aA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | aA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 11  | aA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | aA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 49    | 39 | 1  | 4 | 5 |         |
| 11  | aA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 11  | aA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 11  | aA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | aA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 61    | 51 | 1  | 4 | 5 |         |
| 11  | aA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | aA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | aA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |
| 11  | aA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | aA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 11  | aA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | aA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | aA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | aA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | aA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | aA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | aA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |
| 11  | aA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | aA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 11  | aA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 11  | aA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | aA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |
| 11  | aB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | aB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 57    | 47 | 1  | 4 | 5 |         |
| 11  | aB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 61    | 51 | 1  | 4 | 5 |         |
| 11  | aB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 11  | aB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | aB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | aB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 61    | 51 | 1  | 4 | 5 |         |
| 11  | aB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | aB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 37 | 1  | 4 | 5 |         |
| 11  | aB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | aB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | aB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | aB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 46 | 1  | 4 | 5 |         |
| 11  | aB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | aB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 11  | aB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 59    | 49 | 1  | 4 | 5 |         |
| 11  | aB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 11  | aB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 11  | aB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 37 | 1  | 4 | 5 |         |
| 11  | aB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | aB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 11  | aB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | aB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 11  | aB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | aB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 61    | 51 | 1  | 4 | 5 |         |
| 11  | aB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | aB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 11  | aB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | aB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 49    | 39 | 1  | 4 | 5 |         |
| 11  | aB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 46 | 1  | 4 | 5 |         |
| 11  | aB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | aB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | aB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | aB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |
| 11  | aB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 11  | aB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 37 | 1  | 4 | 5 |         |
| 11  | aB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | aB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 11  | aK    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 38    | 32 | 1  | 4 | 1 |         |
| 11  | aK    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |
| 11  | aL    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | aL    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | aL    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | bA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | bA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 46 | 1  | 4 | 5 |         |
| 11  | bA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | bA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | bA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | bA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | bA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |
| 11  | bA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | bA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | bA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | bA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | bA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 11  | bA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | bA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | bA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | bA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 49    | 39 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 11  | bA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 11  | bA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 11  | bA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | bA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 61    | 51 | 1  | 4 | 5 |         |
| 11  | bA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | bA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | bA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |
| 11  | bA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | bA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 11  | bA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | bA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | bA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | bA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | bA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | bA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | bA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |
| 11  | bA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | bA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | bA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 11  | bA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 11  | bA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |
| 11  | bB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | bB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 57    | 47 | 1  | 4 | 5 |         |
| 11  | bB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 61    | 51 | 1  | 4 | 5 |         |
| 11  | bB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 11  | bB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | bB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | bB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 61    | 51 | 1  | 4 | 5 |         |
| 11  | bB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | bB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 37 | 1  | 4 | 5 |         |
| 11  | bB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | bB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | bB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | bB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 46 | 1  | 4 | 5 |         |
| 11  | bB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | bB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 11  | bB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 59    | 49 | 1  | 4 | 5 |         |
| 11  | bB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 11  | bB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | bB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 37 | 1  | 4 | 5 |         |
| 11  | bB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 11  | bB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 11  | bB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | bB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 11  | bB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | bB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 61    | 51 | 1  | 4 | 5 |         |
| 11  | bB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | bB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 11  | bB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | bB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 49    | 39 | 1  | 4 | 5 |         |
| 11  | bB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 46 | 1  | 4 | 5 |         |
| 11  | bB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | bB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | bB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | bB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | bB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |
| 11  | bB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 11  | bB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 37 | 1  | 4 | 5 |         |
| 11  | bB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | bB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | bK    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 38    | 32 | 1  | 4 | 1 |         |
| 11  | bK    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 11  | bL    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 11  | bL    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 11  | bL    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 11  | cA    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 11  | cA    | 1        | Total<br>56 | C<br>46 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 11  | cA    | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 11  | cA    | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 11  | cA    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 11  | cA    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 11  | cA    | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 11  | cA    | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 11  | cA    | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 11  | cA    | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 11  | cA    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 11  | cA    | 1        | Total<br>54 | C<br>44 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 11  | cA    | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 11  | cA    | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 11  | cA    | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 11  | cA    | 1        | Total<br>49 | C<br>39 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 11  | cA    | 1        | Total<br>54 | C<br>44 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 11  | cA    | 1        | Total<br>54 | C<br>44 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 11  | cA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | cA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 61    | 51 | 1  | 4 | 5 |         |
| 11  | cA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | cA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | cA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |
| 11  | cA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | cA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 11  | cA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | cA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | cA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | cA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | cA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | cA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | cA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | cA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |
| 11  | cA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | cA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | cA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 11  | cA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | cA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |
| 11  | cB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 11  | cB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 57    | 47 | 1  | 4 | 5 |         |
| 11  | cB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 61    | 51 | 1  | 4 | 5 |         |
| 11  | cB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 11  | cB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | cB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | cB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 61    | 51 | 1  | 4 | 5 |         |
| 11  | cB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | cB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 37 | 1  | 4 | 5 |         |
| 11  | cB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | cB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | cB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | cB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 46 | 1  | 4 | 5 |         |
| 11  | cB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | cB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 11  | cB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 59    | 49 | 1  | 4 | 5 |         |
| 11  | cB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 11  | cB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | cB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 37 | 1  | 4 | 5 |         |
| 11  | cB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | cB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 11  | cB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |

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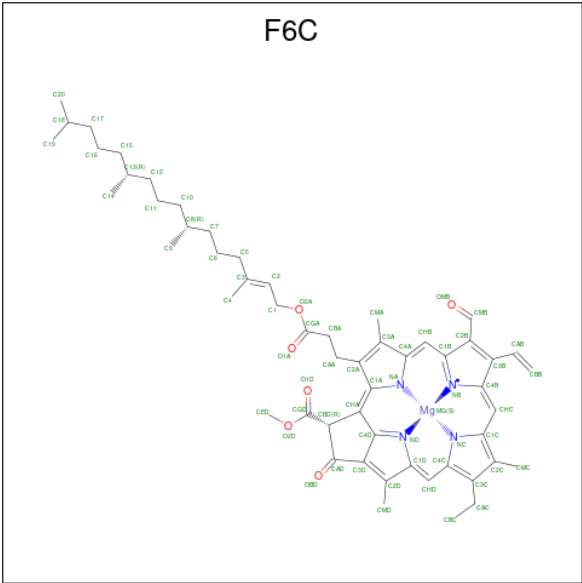
| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 11  | cB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 11  | cB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | cB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 61    | 51 | 1  | 4 | 5 |         |
| 11  | cB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | cB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 11  | cB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | cB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 49    | 39 | 1  | 4 | 5 |         |
| 11  | cB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 46 | 1  | 4 | 5 |         |
| 11  | cB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | cB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | cB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | cB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | cB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |
| 11  | cB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 11  | cB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 37 | 1  | 4 | 5 |         |
| 11  | cB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | cB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 11  | cK    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 38    | 32 | 1  | 4 | 1 |         |
| 11  | cK    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |
| 11  | cL    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 11  | cL    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 11  | cL    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |

- Molecule 12 is Chlorophyll F (CCD ID: F6C) (formula: C<sub>55</sub>H<sub>68</sub>MgN<sub>4</sub>O<sub>6</sub>).



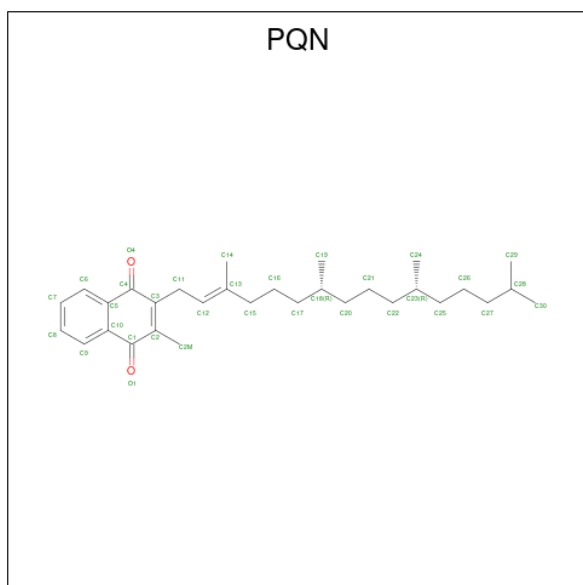
| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 12  | aA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 12  | aA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 45 | 1  | 4 | 6 |         |
| 12  | aA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 12  | aA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 40 | 1  | 4 | 6 |         |
| 12  | aA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 12  | aB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 58    | 47 | 1  | 4 | 6 |         |
| 12  | aL    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 12  | bA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 12  | bA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 45 | 1  | 4 | 6 |         |
| 12  | bA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |

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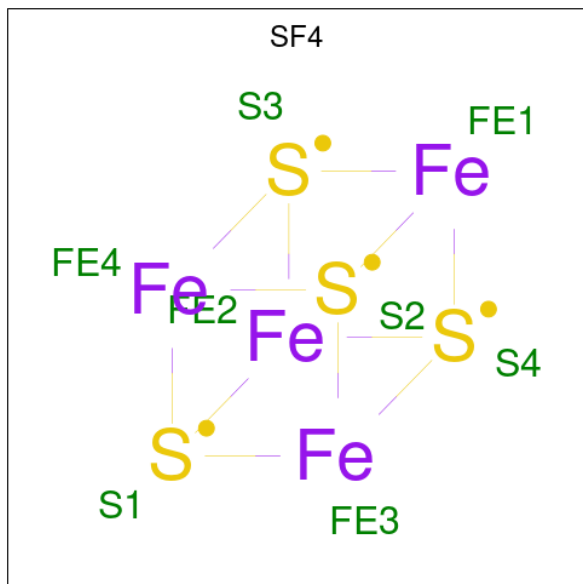
| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 12  | bA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 40 | 1  | 4 | 6 |         |
| 12  | bA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 12  | bB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 58    | 47 | 1  | 4 | 6 |         |
| 12  | bL    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 12  | cA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 12  | cA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 45 | 1  | 4 | 6 |         |
| 12  | cA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 12  | cA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 40 | 1  | 4 | 6 |         |
| 12  | cA    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 12  | cB    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 58    | 47 | 1  | 4 | 6 |         |
| 12  | cL    | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |

- Molecule 13 is PHYLLOQUINONE (CCD ID: PQN) (formula:  $C_{31}H_{46}O_2$ ).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 13  | aA    | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |
| 13  | aB    | 1        | Total | C  | O | 0       |
|     |       |          | 28    | 26 | 2 |         |
| 13  | bA    | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |
| 13  | bB    | 1        | Total | C  | O | 0       |
|     |       |          | 28    | 26 | 2 |         |
| 13  | cA    | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |
| 13  | cB    | 1        | Total | C  | O | 0       |
|     |       |          | 28    | 26 | 2 |         |

- Molecule 14 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 14  | aA    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 14  | aC    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 14  | aC    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 14  | bA    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 14  | bC    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 14  | bC    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |

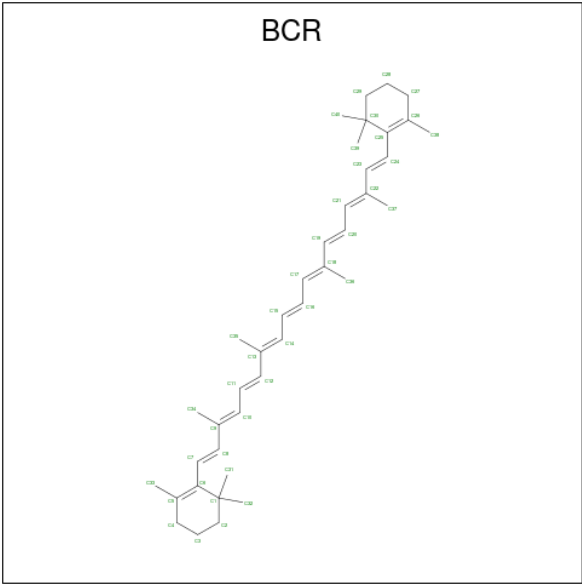
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| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 14  | cA    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 14  | cC    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 14  | cC    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |

- Molecule 15 is BETA-CAROTENE (CCD ID: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 15  | aA    | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 15  | aA    | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 15  | aA    | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 15  | aA    | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 15  | aA    | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 15  | aB    | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 15  | aB    | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 15  | aB    | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |

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| Mol | Chain | Residues | Atoms            | AltConf |
|-----|-------|----------|------------------|---------|
| 15  | aB    | 1        | Total C<br>40 40 | 0       |
| 15  | aB    | 1        | Total C<br>40 40 | 0       |
| 15  | aB    | 1        | Total C<br>40 40 | 0       |
| 15  | aI    | 1        | Total C<br>40 40 | 0       |
| 15  | aK    | 1        | Total C<br>40 40 | 0       |
| 15  | aL    | 1        | Total C<br>40 40 | 0       |
| 15  | aL    | 1        | Total C<br>40 40 | 0       |
| 15  | aL    | 1        | Total C<br>40 40 | 0       |
| 15  | aM    | 1        | Total C<br>40 40 | 0       |
| 15  | bA    | 1        | Total C<br>40 40 | 0       |
| 15  | bA    | 1        | Total C<br>40 40 | 0       |
| 15  | bA    | 1        | Total C<br>40 40 | 0       |
| 15  | bA    | 1        | Total C<br>40 40 | 0       |
| 15  | bA    | 1        | Total C<br>40 40 | 0       |
| 15  | bB    | 1        | Total C<br>40 40 | 0       |
| 15  | bB    | 1        | Total C<br>40 40 | 0       |
| 15  | bB    | 1        | Total C<br>40 40 | 0       |
| 15  | bB    | 1        | Total C<br>40 40 | 0       |
| 15  | bB    | 1        | Total C<br>40 40 | 0       |
| 15  | bB    | 1        | Total C<br>40 40 | 0       |
| 15  | bI    | 1        | Total C<br>40 40 | 0       |

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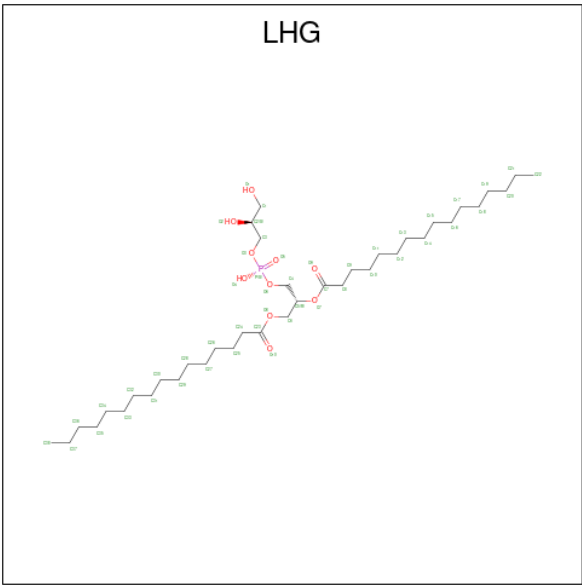
| Mol | Chain | Residues | Atoms            | AltConf |
|-----|-------|----------|------------------|---------|
| 15  | bK    | 1        | Total C<br>40 40 | 0       |
| 15  | bL    | 1        | Total C<br>40 40 | 0       |
| 15  | bL    | 1        | Total C<br>40 40 | 0       |
| 15  | bL    | 1        | Total C<br>40 40 | 0       |
| 15  | bM    | 1        | Total C<br>40 40 | 0       |
| 15  | cA    | 1        | Total C<br>40 40 | 0       |
| 15  | cA    | 1        | Total C<br>40 40 | 0       |
| 15  | cA    | 1        | Total C<br>40 40 | 0       |
| 15  | cA    | 1        | Total C<br>40 40 | 0       |
| 15  | cA    | 1        | Total C<br>40 40 | 0       |
| 15  | cB    | 1        | Total C<br>40 40 | 0       |
| 15  | cB    | 1        | Total C<br>40 40 | 0       |
| 15  | cB    | 1        | Total C<br>40 40 | 0       |
| 15  | cB    | 1        | Total C<br>40 40 | 0       |
| 15  | cB    | 1        | Total C<br>40 40 | 0       |
| 15  | cB    | 1        | Total C<br>40 40 | 0       |
| 15  | cI    | 1        | Total C<br>40 40 | 0       |
| 15  | cK    | 1        | Total C<br>40 40 | 0       |
| 15  | cL    | 1        | Total C<br>40 40 | 0       |
| 15  | cL    | 1        | Total C<br>40 40 | 0       |
| 15  | cL    | 1        | Total C<br>40 40 | 0       |

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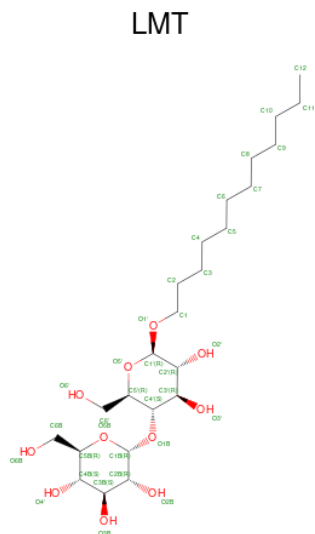
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 15  | cM    | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |

- Molecule 16 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



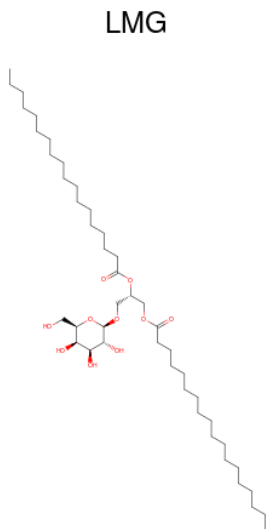
| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 16  | aA    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 16  | bA    | 1        | Total | C  | O  | P | 0       |
|    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

- Molecule 17 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



| Mol | Chain | Residues | Atoms       |         |         | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 17  | aA    | 1        | Total<br>35 | C<br>24 | O<br>11 | 0       |
| 17  | bA    | 1        | Total<br>35 | C<br>24 | O<br>11 | 0       |
| 17  | cA    | 1        | Total<br>35 | C<br>24 | O<br>11 | 0       |

- Molecule 18 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 18  | aB    | 1        | Total | C  | O  | 0       |
|     |       |          | 46    | 36 | 10 |         |
| 18  | bB    | 1        | Total | C  | O  | 0       |
|     |       |          | 46    | 36 | 10 |         |
| 18  | cB    | 1        | Total | C  | O  | 0       |
|     |       |          | 46    | 36 | 10 |         |

- Molecule 19 is UNKNOWN LIGAND (CCD ID: UNL) (formula: ).

| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 19  | aI    | 1        | Total | C  |   | 0       |
|     |       |          | 9     | 9  |   |         |
| 19  | aL    | 4        | Total | C  | O | 0       |
|     |       |          | 56    | 52 | 4 |         |
| 19  | bI    | 1        | Total | C  |   | 0       |
|     |       |          | 9     | 9  |   |         |
| 19  | bL    | 4        | Total | C  | O | 0       |
|     |       |          | 56    | 52 | 4 |         |
| 19  | cI    | 2        | Total | C  | O | 0       |
|     |       |          | 25    | 23 | 2 |         |
| 19  | cL    | 3        | Total | C  | O | 0       |
|     |       |          | 40    | 38 | 2 |         |

- Molecule 20 is CALCIUM ION (CCD ID: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 20  | aL    | 1        | Total | Ca | 0       |
|     |       |          | 1     | 1  |         |
| 20  | bL    | 1        | Total | Ca | 0       |
|     |       |          | 1     | 1  |         |
| 20  | cL    | 1        | Total | Ca | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 21 is water.

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 21  | aA    | 72       | Total | O  | 0       |
|     |       |          | 72    | 72 |         |
| 21  | aB    | 72       | Total | O  | 0       |
|     |       |          | 72    | 72 |         |
| 21  | aC    | 21       | Total | O  | 0       |
|     |       |          | 21    | 21 |         |

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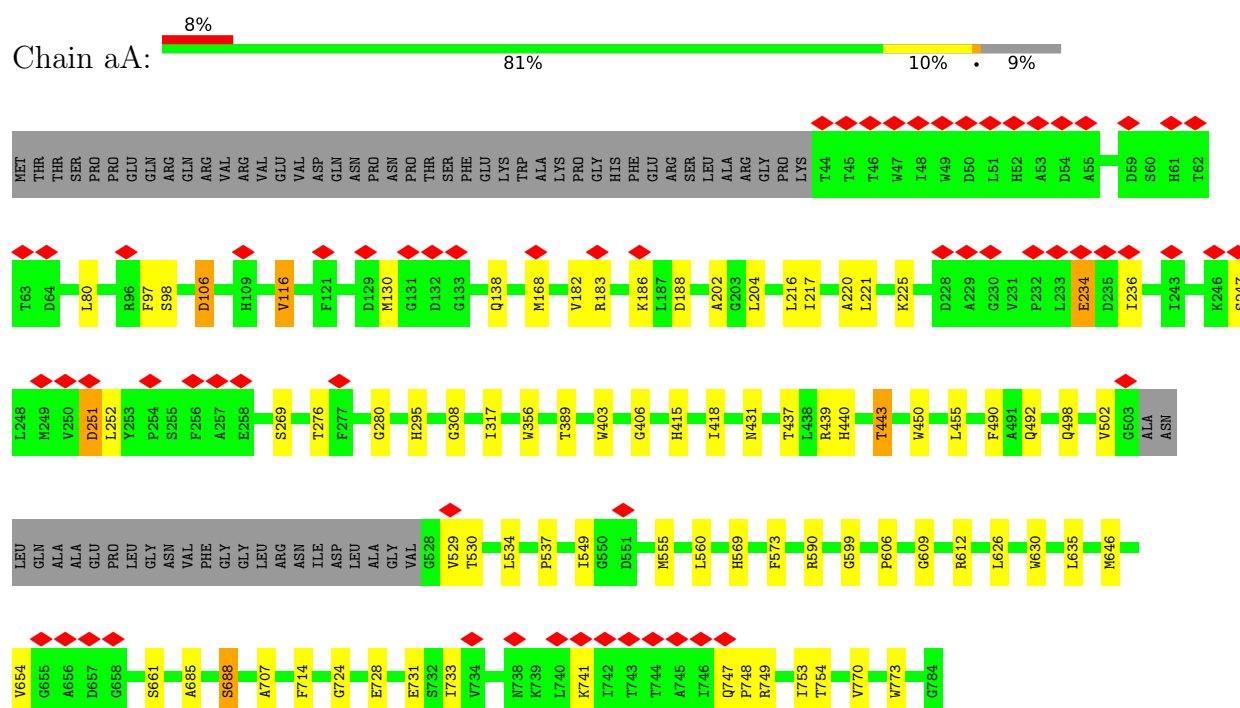
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| Mol | Chain | Residues | Atoms       |         | AltConf |
|-----|-------|----------|-------------|---------|---------|
| 21  | aD    | 15       | Total<br>15 | O<br>15 | 0       |
| 21  | aI    | 5        | Total<br>5  | O<br>5  | 0       |
| 21  | aK    | 1        | Total<br>1  | O<br>1  | 0       |
| 21  | aL    | 25       | Total<br>25 | O<br>25 | 0       |
| 21  | aM    | 1        | Total<br>1  | O<br>1  | 0       |
| 21  | bA    | 72       | Total<br>72 | O<br>72 | 0       |
| 21  | bB    | 72       | Total<br>72 | O<br>72 | 0       |
| 21  | bC    | 20       | Total<br>20 | O<br>20 | 0       |
| 21  | bD    | 16       | Total<br>16 | O<br>16 | 0       |
| 21  | bI    | 6        | Total<br>6  | O<br>6  | 0       |
| 21  | bK    | 1        | Total<br>1  | O<br>1  | 0       |
| 21  | bL    | 24       | Total<br>24 | O<br>24 | 0       |
| 21  | bM    | 1        | Total<br>1  | O<br>1  | 0       |
| 21  | cA    | 72       | Total<br>72 | O<br>72 | 0       |
| 21  | cB    | 72       | Total<br>72 | O<br>72 | 0       |
| 21  | cC    | 21       | Total<br>21 | O<br>21 | 0       |
| 21  | cD    | 15       | Total<br>15 | O<br>15 | 0       |
| 21  | cI    | 6        | Total<br>6  | O<br>6  | 0       |
| 21  | cK    | 1        | Total<br>1  | O<br>1  | 0       |
| 21  | cL    | 24       | Total<br>24 | O<br>24 | 0       |
| 21  | cM    | 1        | Total<br>1  | O<br>1  | 0       |

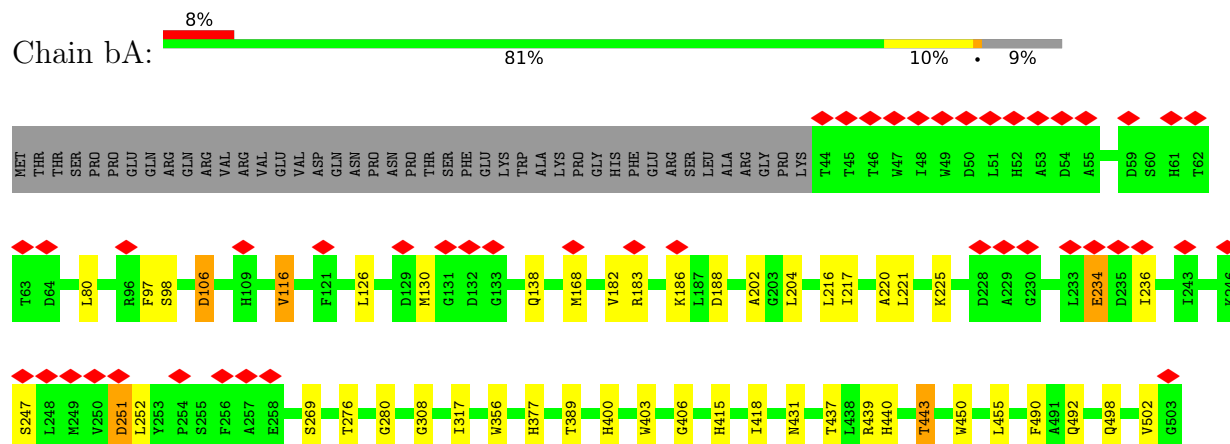
### 3 Residue-property plots

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

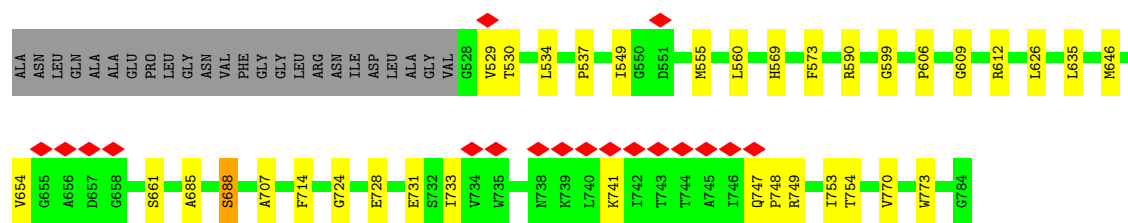
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



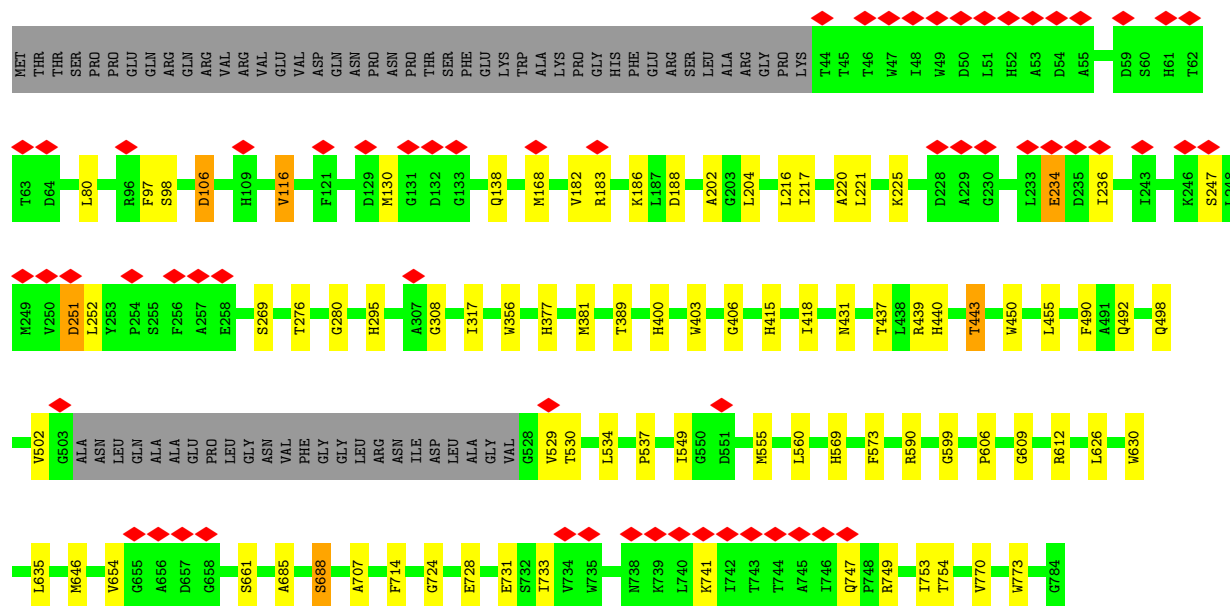
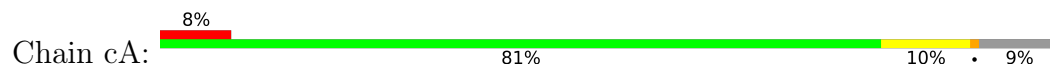
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



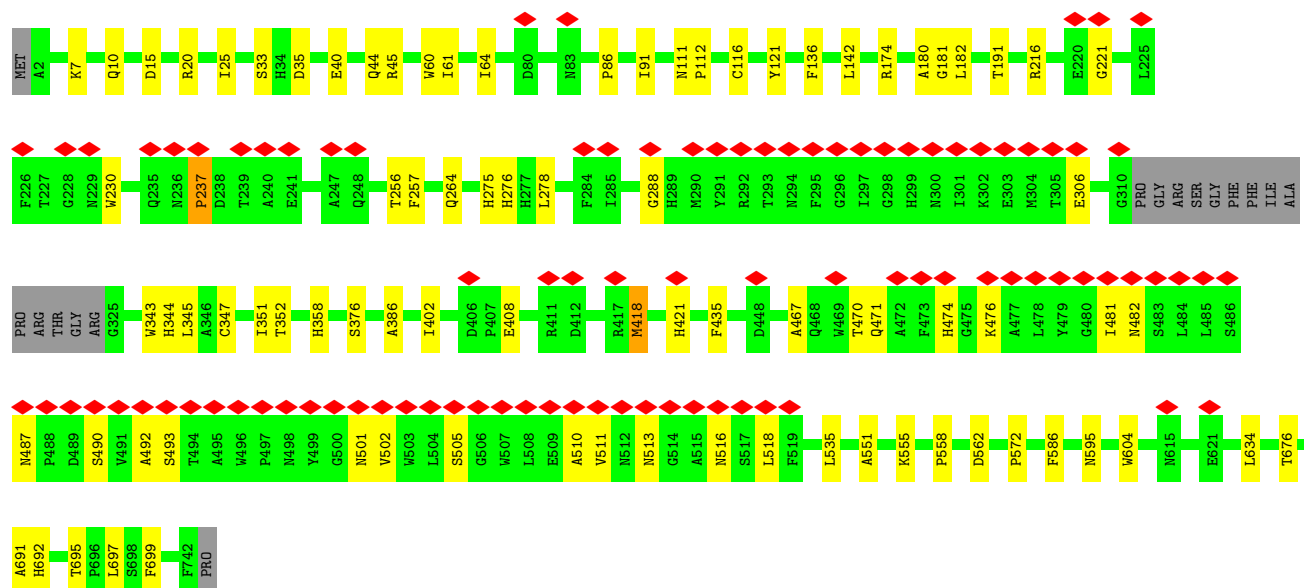
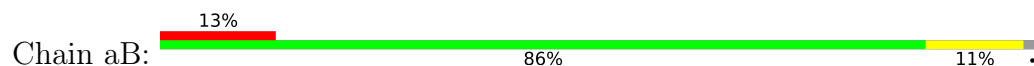




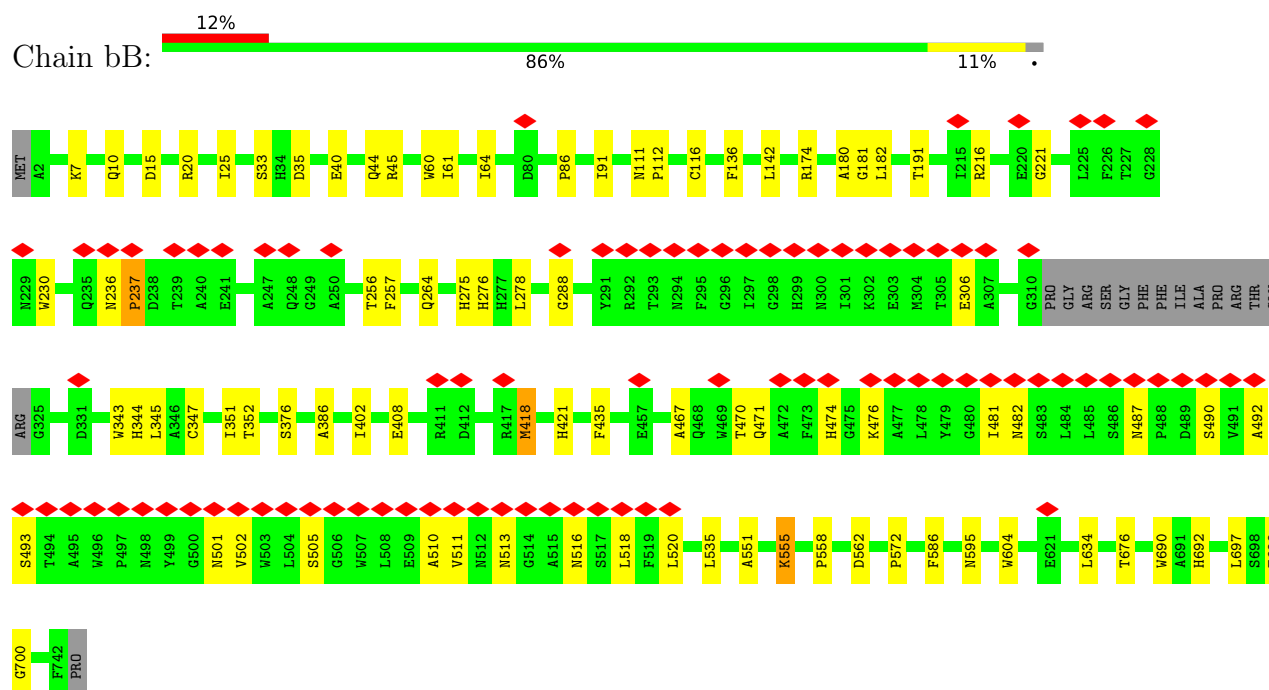
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



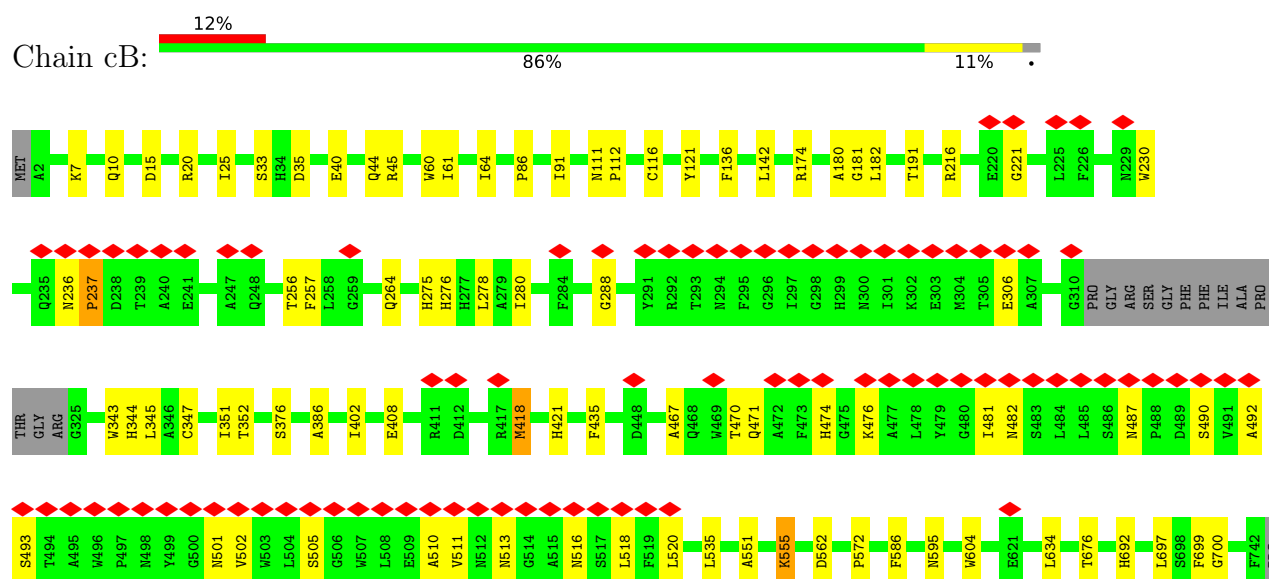
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



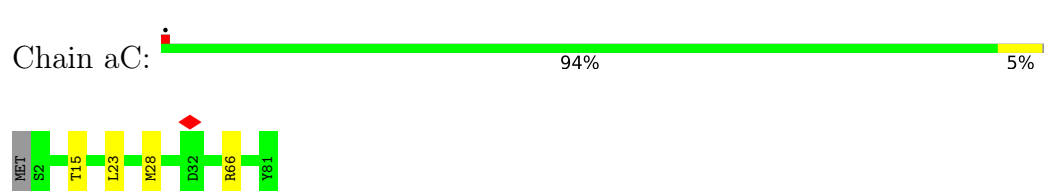
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



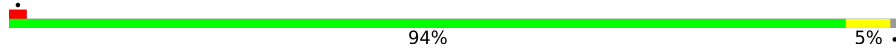
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

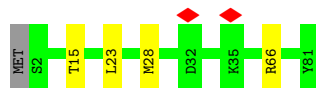


- Molecule 3: Photosystem I iron-sulfur center

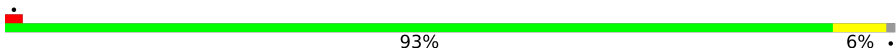


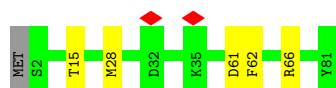
- Molecule 3: Photosystem I iron-sulfur center

Chain bC:  94% 5%



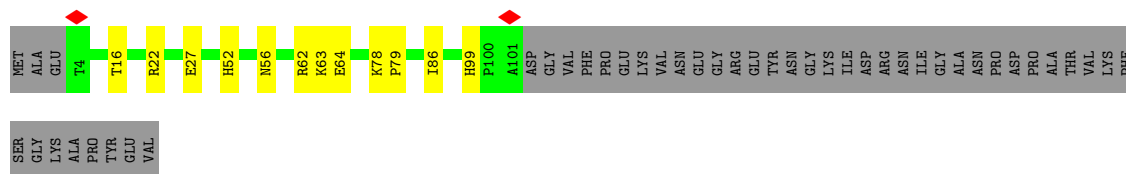
- Molecule 3: Photosystem I iron-sulfur center

Chain cC:  93% 6%



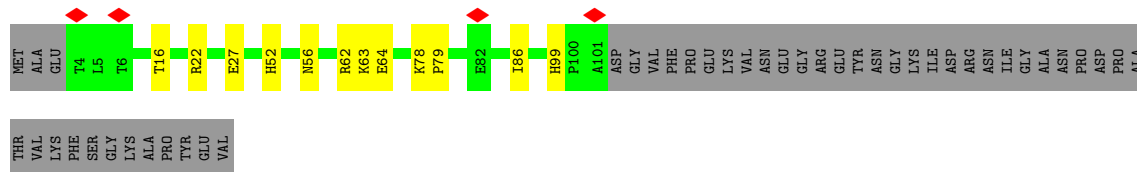
- Molecule 4: Photosystem I reaction center subunit II

Chain aD:  61% 8% 31%



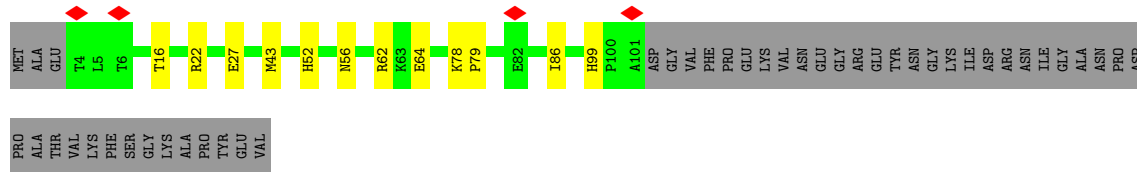
- Molecule 4: Photosystem I reaction center subunit II

Chain bD:  61% 8% 31%



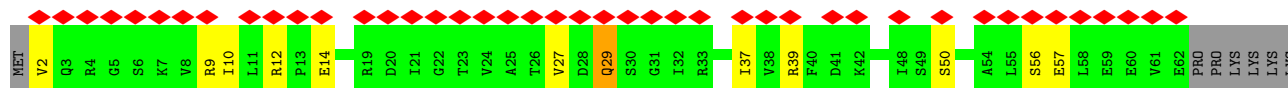
- Molecule 4: Photosystem I reaction center subunit II

Chain cD:  61% 8% 31%

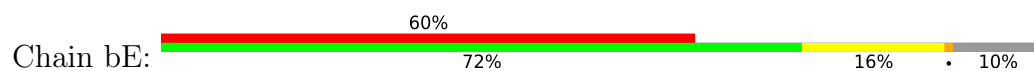


- Molecule 5: Photosystem I reaction center subunit IV

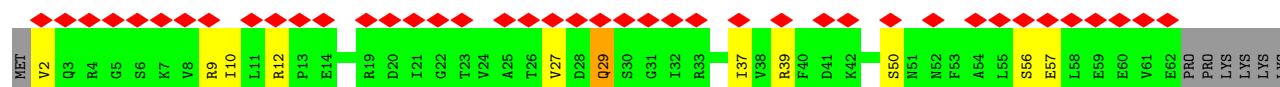
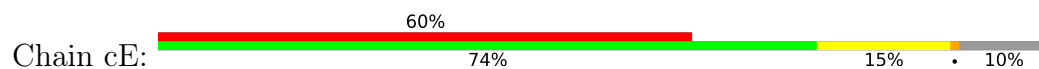
Chain aE:  63% 72% 16% 10%



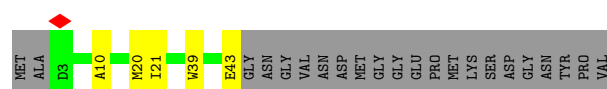
- Molecule 5: Photosystem I reaction center subunit IV



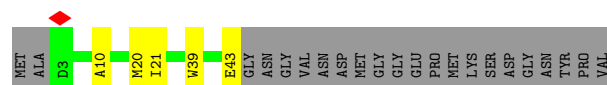
- Molecule 5: Photosystem I reaction center subunit IV



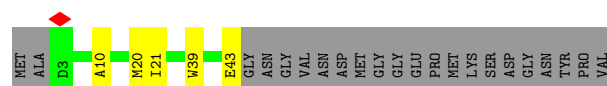
- Molecule 6: Photosystem I reaction center subunit VIII



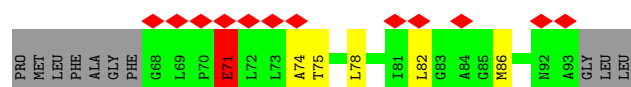
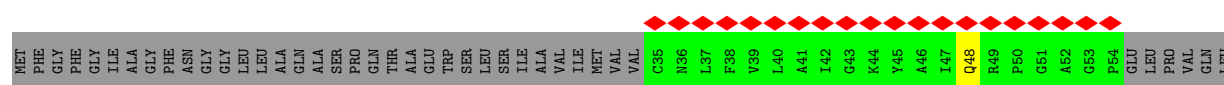
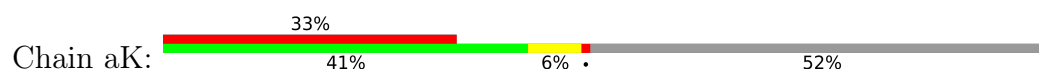
- Molecule 6: Photosystem I reaction center subunit VIII



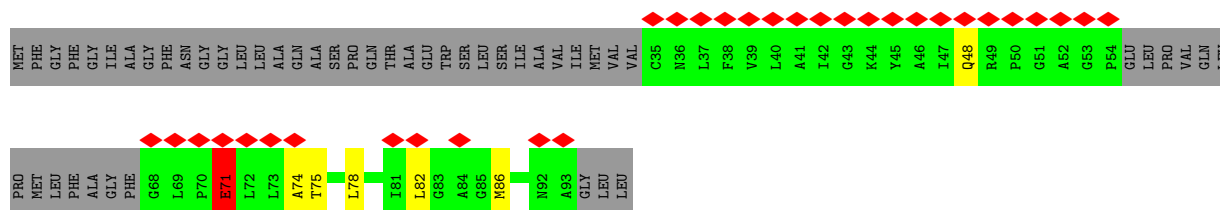
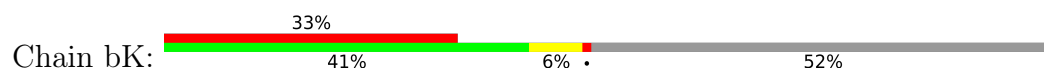
- Molecule 6: Photosystem I reaction center subunit VIII



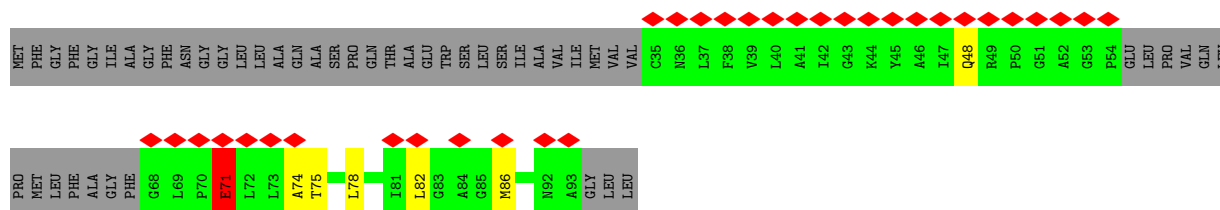
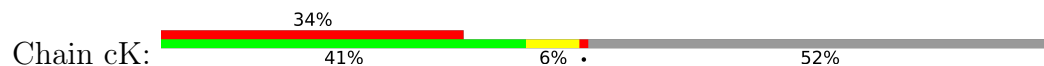
- Molecule 7: Photosystem I reaction center subunit PsaK



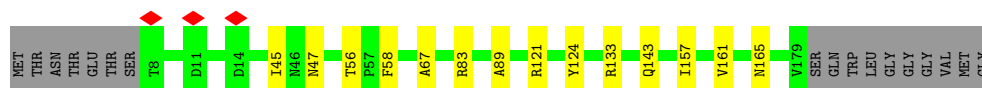
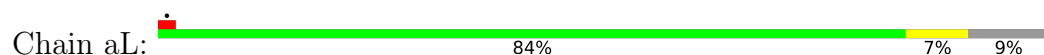
- Molecule 7: Photosystem I reaction center subunit PsaK



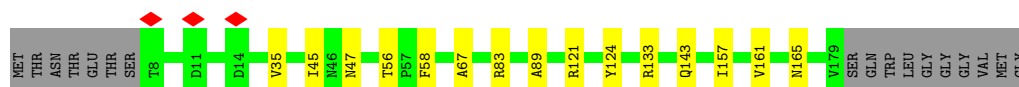
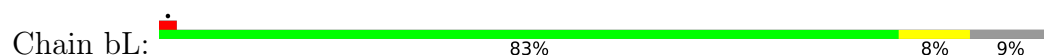
- Molecule 7: Photosystem I reaction center subunit PsaK



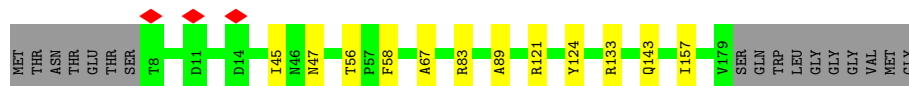
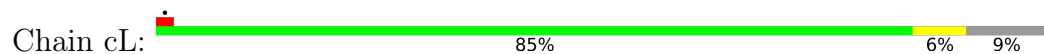
- Molecule 8: Photosystem I reaction center subunit XI



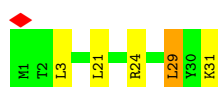
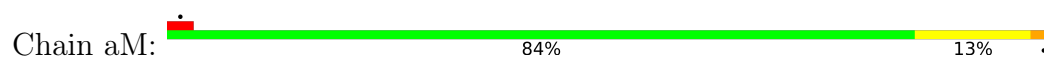
- Molecule 8: Photosystem I reaction center subunit XI



- Molecule 8: Photosystem I reaction center subunit XI

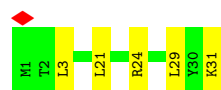


- Molecule 9: Photosystem I reaction center subunit XII



- Molecule 9: Photosystem I reaction center subunit XII

Chain bM:  84% 16%



- Molecule 9: Photosystem I reaction center subunit XII

Chain cM:  84% 13% .



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C3                               | Depositor |
| Number of particles used             | 311993                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 47                                      | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | FEI FALCON III (4k x 4k)                | Depositor |
| Maximum map value                    | 0.915                                   | Depositor |
| Minimum map value                    | -0.310                                  | Depositor |
| Average map value                    | 0.001                                   | Depositor |
| Map value standard deviation         | 0.013                                   | Depositor |
| Recommended contour level            | 0.06                                    | Depositor |
| Map size ( $\text{\AA}$ )            | 313.2, 313.2, 313.2                     | wwPDB     |
| Map dimensions                       | 360, 360, 360                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 0.87, 0.87, 0.87                        | 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, UNL, SF4, LMG, LMT, BCR, LHG, CLA, PQN, CA, F6C

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

| Mol | Chain | Bond lengths |             | Bond angles |                 |
|-----|-------|--------------|-------------|-------------|-----------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$     |
| 1   | aA    | 0.20         | 0/5868      | 0.47        | 3/7993 (0.0%)   |
| 1   | bA    | 0.20         | 0/5868      | 0.47        | 3/7993 (0.0%)   |
| 1   | cA    | 0.20         | 0/5868      | 0.47        | 2/7993 (0.0%)   |
| 2   | aB    | 0.20         | 0/5993      | 0.49        | 1/8185 (0.0%)   |
| 2   | bB    | 0.20         | 0/5993      | 0.49        | 1/8185 (0.0%)   |
| 2   | cB    | 0.20         | 0/5993      | 0.49        | 1/8185 (0.0%)   |
| 3   | aC    | 0.18         | 0/606       | 0.49        | 0/820           |
| 3   | bC    | 0.18         | 0/606       | 0.49        | 0/820           |
| 3   | cC    | 0.18         | 0/606       | 0.49        | 0/820           |
| 4   | aD    | 0.17         | 0/785       | 0.43        | 0/1061          |
| 4   | bD    | 0.17         | 0/785       | 0.43        | 0/1061          |
| 4   | cD    | 0.17         | 0/785       | 0.43        | 0/1061          |
| 5   | aE    | 0.31         | 0/509       | 0.71        | 1/689 (0.1%)    |
| 5   | bE    | 0.31         | 0/509       | 0.71        | 1/689 (0.1%)    |
| 5   | cE    | 0.31         | 0/509       | 0.71        | 1/689 (0.1%)    |
| 6   | aI    | 0.30         | 0/365       | 0.64        | 0/503           |
| 6   | bI    | 0.30         | 0/365       | 0.64        | 0/503           |
| 6   | cI    | 0.30         | 0/365       | 0.64        | 0/503           |
| 7   | aK    | 0.23         | 0/321       | 0.71        | 1/433 (0.2%)    |
| 7   | bK    | 0.24         | 0/321       | 0.71        | 1/433 (0.2%)    |
| 7   | cK    | 0.24         | 0/321       | 0.71        | 1/433 (0.2%)    |
| 8   | aL    | 0.19         | 0/1334      | 0.45        | 0/1819          |
| 8   | bL    | 0.19         | 0/1334      | 0.45        | 0/1819          |
| 8   | cL    | 0.20         | 0/1334      | 0.45        | 0/1819          |
| 9   | aM    | 0.23         | 0/244       | 0.61        | 0/332           |
| 9   | bM    | 0.23         | 0/244       | 0.60        | 0/332           |
| 9   | cM    | 0.23         | 0/244       | 0.60        | 0/332           |
| All | All   | 0.21         | 0/48075     | 0.50        | 17/65505 (0.0%) |

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 |
|-----|-------|---------------------|---------------------|
| 2   | aB    | 0                   | 1                   |
| 2   | bB    | 0                   | 1                   |
| 2   | cB    | 0                   | 1                   |
| 9   | aM    | 0                   | 1                   |
| 9   | bM    | 0                   | 1                   |
| 9   | cM    | 0                   | 1                   |
| All | All   | 0                   | 6                   |

There are no bond length outliers.

All (17) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | cA    | 234 | GLU  | CA-CB-CG | 7.39  | 128.89      | 114.10   |
| 1   | bA    | 234 | GLU  | CA-CB-CG | 7.37  | 128.84      | 114.10   |
| 1   | aA    | 234 | GLU  | CA-CB-CG | 7.35  | 128.79      | 114.10   |
| 7   | aK    | 71  | GLU  | CA-CB-CG | 6.70  | 127.49      | 114.10   |
| 7   | cK    | 71  | GLU  | CA-CB-CG | 6.69  | 127.48      | 114.10   |
| 7   | bK    | 71  | GLU  | CA-CB-CG | 6.67  | 127.44      | 114.10   |
| 1   | bA    | 106 | ASP  | CB-CA-C  | 6.50  | 119.98      | 111.01   |
| 1   | aA    | 106 | ASP  | CB-CA-C  | 6.49  | 119.96      | 111.01   |
| 1   | cA    | 106 | ASP  | CB-CA-C  | 6.47  | 119.94      | 111.01   |
| 2   | bB    | 482 | ASN  | N-CA-CB  | -5.45 | 103.86      | 112.63   |
| 2   | aB    | 482 | ASN  | N-CA-CB  | -5.45 | 103.86      | 112.63   |
| 2   | cB    | 482 | ASN  | N-CA-CB  | -5.43 | 103.88      | 112.63   |
| 5   | aE    | 29  | GLN  | CB-CG-CD | 5.16  | 121.37      | 112.60   |
| 5   | bE    | 29  | GLN  | CB-CG-CD | 5.15  | 121.36      | 112.60   |
| 5   | cE    | 29  | GLN  | CB-CG-CD | 5.14  | 121.34      | 112.60   |
| 1   | aA    | 234 | GLU  | CB-CA-C  | -5.03 | 101.02      | 110.67   |
| 1   | bA    | 234 | GLU  | CB-CA-C  | -5.01 | 101.05      | 110.67   |

There are no chirality outliers.

All (6) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 2   | aB    | 481 | ILE  | Peptide |
| 9   | aM    | 29  | LEU  | Peptide |
| 2   | bB    | 481 | ILE  | Peptide |
| 9   | bM    | 29  | LEU  | Peptide |
| 2   | cB    | 481 | ILE  | Peptide |

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| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 9   | cM    | 29  | LEU  | Peptide |

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | aA    | 5669  | 0        | 5487     | 49      | 0            |
| 1   | bA    | 5669  | 0        | 5487     | 50      | 0            |
| 1   | cA    | 5669  | 0        | 5487     | 51      | 0            |
| 2   | aB    | 5783  | 0        | 5519     | 59      | 0            |
| 2   | bB    | 5783  | 0        | 5519     | 59      | 0            |
| 2   | cB    | 5783  | 0        | 5519     | 59      | 0            |
| 3   | aC    | 596   | 0        | 576      | 3       | 0            |
| 3   | bC    | 596   | 0        | 576      | 3       | 0            |
| 3   | cC    | 596   | 0        | 576      | 3       | 0            |
| 4   | aD    | 768   | 0        | 774      | 8       | 0            |
| 4   | bD    | 768   | 0        | 774      | 7       | 0            |
| 4   | cD    | 768   | 0        | 774      | 8       | 0            |
| 5   | aE    | 499   | 0        | 488      | 4       | 0            |
| 5   | bE    | 499   | 0        | 488      | 4       | 0            |
| 5   | cE    | 499   | 0        | 488      | 3       | 0            |
| 6   | aI    | 349   | 0        | 353      | 5       | 0            |
| 6   | bI    | 349   | 0        | 353      | 4       | 0            |
| 6   | cI    | 349   | 0        | 353      | 5       | 0            |
| 7   | aK    | 317   | 0        | 336      | 5       | 0            |
| 7   | bK    | 317   | 0        | 336      | 5       | 0            |
| 7   | cK    | 317   | 0        | 336      | 5       | 0            |
| 8   | aL    | 1303  | 0        | 1301     | 14      | 0            |
| 8   | bL    | 1303  | 0        | 1301     | 15      | 0            |
| 8   | cL    | 1303  | 0        | 1301     | 13      | 0            |
| 9   | aM    | 241   | 0        | 266      | 6       | 0            |
| 9   | bM    | 241   | 0        | 266      | 4       | 0            |
| 9   | cM    | 241   | 0        | 266      | 6       | 0            |
| 10  | aA    | 65    | 0        | 72       | 0       | 0            |
| 10  | bA    | 65    | 0        | 72       | 0       | 0            |
| 10  | cA    | 65    | 0        | 72       | 0       | 0            |
| 11  | aA    | 2112  | 0        | 1999     | 48      | 0            |
| 11  | aB    | 2116  | 0        | 1932     | 53      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 11  | aK    | 89    | 0        | 68       | 1       | 0            |
| 11  | aL    | 195   | 0        | 216      | 6       | 0            |
| 11  | bA    | 2112  | 0        | 1999     | 46      | 0            |
| 11  | bB    | 2116  | 0        | 1932     | 48      | 0            |
| 11  | bK    | 89    | 0        | 68       | 1       | 0            |
| 11  | bL    | 195   | 0        | 216      | 8       | 0            |
| 11  | cA    | 2112  | 0        | 1999     | 53      | 0            |
| 11  | cB    | 2116  | 0        | 1932     | 54      | 0            |
| 11  | cK    | 89    | 0        | 68       | 1       | 0            |
| 11  | cL    | 195   | 0        | 216      | 5       | 0            |
| 12  | aA    | 305   | 0        | 0        | 0       | 0            |
| 12  | aB    | 58    | 0        | 0        | 1       | 0            |
| 12  | aL    | 66    | 0        | 0        | 0       | 0            |
| 12  | bA    | 305   | 0        | 0        | 0       | 0            |
| 12  | bB    | 58    | 0        | 0        | 0       | 0            |
| 12  | bL    | 66    | 0        | 0        | 0       | 0            |
| 12  | cA    | 305   | 0        | 0        | 0       | 0            |
| 12  | cB    | 58    | 0        | 0        | 1       | 0            |
| 12  | cL    | 66    | 0        | 0        | 0       | 0            |
| 13  | aA    | 33    | 0        | 46       | 0       | 0            |
| 13  | aB    | 28    | 0        | 33       | 3       | 0            |
| 13  | bA    | 33    | 0        | 46       | 1       | 0            |
| 13  | bB    | 28    | 0        | 33       | 2       | 0            |
| 13  | cA    | 33    | 0        | 46       | 1       | 0            |
| 13  | cB    | 28    | 0        | 33       | 1       | 0            |
| 14  | aA    | 8     | 0        | 0        | 0       | 0            |
| 14  | aC    | 16    | 0        | 0        | 0       | 0            |
| 14  | bA    | 8     | 0        | 0        | 0       | 0            |
| 14  | bC    | 16    | 0        | 0        | 0       | 0            |
| 14  | cA    | 8     | 0        | 0        | 0       | 0            |
| 14  | cC    | 16    | 0        | 0        | 0       | 0            |
| 15  | aA    | 200   | 0        | 280      | 16      | 0            |
| 15  | aB    | 240   | 0        | 336      | 9       | 0            |
| 15  | aI    | 40    | 0        | 56       | 2       | 0            |
| 15  | aK    | 40    | 0        | 56       | 2       | 0            |
| 15  | aL    | 120   | 0        | 168      | 7       | 0            |
| 15  | aM    | 40    | 0        | 56       | 0       | 0            |
| 15  | bA    | 200   | 0        | 280      | 18      | 0            |
| 15  | bB    | 240   | 0        | 336      | 7       | 0            |
| 15  | bI    | 40    | 0        | 56       | 0       | 0            |
| 15  | bK    | 40    | 0        | 56       | 2       | 0            |
| 15  | bL    | 120   | 0        | 168      | 7       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 15  | bM    | 40    | 0        | 56       | 2       | 0            |
| 15  | cA    | 200   | 0        | 280      | 15      | 0            |
| 15  | cB    | 240   | 0        | 336      | 10      | 0            |
| 15  | cI    | 40    | 0        | 56       | 0       | 0            |
| 15  | cK    | 40    | 0        | 56       | 2       | 0            |
| 15  | cL    | 120   | 0        | 168      | 9       | 0            |
| 15  | cM    | 40    | 0        | 56       | 0       | 0            |
| 16  | aA    | 49    | 0        | 74       | 1       | 0            |
| 16  | bA    | 49    | 0        | 74       | 1       | 0            |
| 16  | cA    | 49    | 0        | 74       | 1       | 0            |
| 17  | aA    | 35    | 0        | 46       | 2       | 0            |
| 17  | bA    | 35    | 0        | 46       | 2       | 0            |
| 17  | cA    | 35    | 0        | 46       | 2       | 0            |
| 18  | aB    | 46    | 0        | 65       | 1       | 0            |
| 18  | bB    | 46    | 0        | 65       | 1       | 0            |
| 18  | cB    | 46    | 0        | 65       | 1       | 0            |
| 19  | aI    | 9     | 0        | 0        | 0       | 0            |
| 19  | aL    | 56    | 0        | 0        | 0       | 0            |
| 19  | bI    | 9     | 0        | 0        | 0       | 0            |
| 19  | bL    | 56    | 0        | 0        | 0       | 0            |
| 19  | cI    | 25    | 0        | 0        | 0       | 0            |
| 19  | cL    | 40    | 0        | 0        | 0       | 0            |
| 20  | aL    | 1     | 0        | 0        | 0       | 0            |
| 20  | bL    | 1     | 0        | 0        | 0       | 0            |
| 20  | cL    | 1     | 0        | 0        | 0       | 0            |
| 21  | aA    | 72    | 0        | 0        | 1       | 0            |
| 21  | aB    | 72    | 0        | 0        | 1       | 0            |
| 21  | aC    | 21    | 0        | 0        | 0       | 0            |
| 21  | aD    | 15    | 0        | 0        | 0       | 0            |
| 21  | aI    | 5     | 0        | 0        | 0       | 0            |
| 21  | aK    | 1     | 0        | 0        | 0       | 0            |
| 21  | aL    | 25    | 0        | 0        | 0       | 0            |
| 21  | aM    | 1     | 0        | 0        | 0       | 0            |
| 21  | bA    | 72    | 0        | 0        | 1       | 0            |
| 21  | bB    | 72    | 0        | 0        | 1       | 0            |
| 21  | bC    | 20    | 0        | 0        | 0       | 0            |
| 21  | bD    | 16    | 0        | 0        | 0       | 0            |
| 21  | bI    | 6     | 0        | 0        | 0       | 0            |
| 21  | bK    | 1     | 0        | 0        | 0       | 0            |
| 21  | bL    | 24    | 0        | 0        | 0       | 0            |
| 21  | bM    | 1     | 0        | 0        | 0       | 0            |
| 21  | cA    | 72    | 0        | 0        | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 21  | cB    | 72    | 0        | 0        | 1       | 0            |
| 21  | cC    | 21    | 0        | 0        | 0       | 0            |
| 21  | cD    | 15    | 0        | 0        | 0       | 0            |
| 21  | cI    | 6     | 0        | 0        | 0       | 0            |
| 21  | cK    | 1     | 0        | 0        | 0       | 0            |
| 21  | cL    | 24    | 0        | 0        | 0       | 0            |
| 21  | cM    | 1     | 0        | 0        | 0       | 0            |
| All | All   | 65112 | 0        | 61809    | 653     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (653) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:aD:52:HIS:H      | 4:aD:56:ASN:HD21   | 1.33                     | 0.76              |
| 4:cD:52:HIS:H      | 4:cD:56:ASN:HD21   | 1.34                     | 0.76              |
| 4:bD:52:HIS:H      | 4:bD:56:ASN:HD21   | 1.34                     | 0.75              |
| 11:aB:840:CLA:HAC2 | 15:aB:846:BCR:H21C | 1.69                     | 0.73              |
| 11:cB:840:CLA:HAC2 | 15:cB:846:BCR:H21C | 1.69                     | 0.73              |
| 11:bB:840:CLA:HAC2 | 15:bB:846:BCR:H21C | 1.69                     | 0.72              |
| 7:aK:78:LEU:HB2    | 15:aK:102:BCR:H24C | 1.74                     | 0.69              |
| 1:bA:707:ALA:HB1   | 15:bA:851:BCR:H15C | 1.75                     | 0.69              |
| 7:bK:78:LEU:HB2    | 15:bK:102:BCR:H24C | 1.74                     | 0.69              |
| 8:aL:143:GLN:HE22  | 8:bL:58:PHE:HB3    | 1.58                     | 0.68              |
| 1:aA:707:ALA:HB1   | 15:aA:851:BCR:H15C | 1.75                     | 0.67              |
| 2:bB:7:LYS:HD2     | 9:bM:31:LYS:HB3    | 1.76                     | 0.67              |
| 1:cA:707:ALA:HB1   | 15:cA:851:BCR:H15C | 1.75                     | 0.67              |
| 7:cK:78:LEU:HB2    | 15:cK:102:BCR:H24C | 1.74                     | 0.67              |
| 11:aA:825:CLA:HAC1 | 15:aA:849:BCR:HC8  | 1.79                     | 0.65              |
| 11:bA:825:CLA:HAC1 | 15:bA:849:BCR:HC8  | 1.79                     | 0.64              |
| 11:cA:806:CLA:H72  | 15:cA:848:BCR:H24C | 1.80                     | 0.64              |
| 8:bL:143:GLN:HE22  | 8:cL:58:PHE:HB3    | 1.62                     | 0.64              |
| 11:aA:806:CLA:H72  | 15:aA:848:BCR:H24C | 1.80                     | 0.64              |
| 2:cB:25:ILE:HD11   | 15:cL:207:BCR:H322 | 1.80                     | 0.63              |
| 11:aB:818:CLA:HAA2 | 11:aB:823:CLA:HAB  | 1.80                     | 0.63              |
| 2:bB:25:ILE:HD11   | 15:bL:207:BCR:H322 | 1.80                     | 0.63              |
| 11:aA:822:CLA:H2   | 11:aA:824:CLA:HBC1 | 1.81                     | 0.63              |
| 1:bA:770:VAL:HG22  | 15:bA:851:BCR:H323 | 1.81                     | 0.63              |
| 11:bA:806:CLA:H72  | 15:bA:848:BCR:H24C | 1.79                     | 0.63              |
| 1:bA:502:VAL:HG12  | 1:bA:534:LEU:HD13  | 1.81                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:cB:818:CLA:HAA2 | 11:cB:823:CLA:HAB  | 1.80                     | 0.63              |
| 2:cB:7:LYS:HD2     | 9:cM:31:LYS:HB3    | 1.81                     | 0.63              |
| 2:aB:25:ILE:HD11   | 15:aL:207:BCR:H322 | 1.81                     | 0.62              |
| 11:bA:822:CLA:H2   | 11:bA:824:CLA:HBC1 | 1.81                     | 0.62              |
| 11:cA:825:CLA:HAC1 | 15:cA:849:BCR:HC8  | 1.79                     | 0.62              |
| 11:bB:818:CLA:HAA2 | 11:bB:823:CLA:HAB  | 1.80                     | 0.62              |
| 1:cA:770:VAL:HG22  | 15:cA:851:BCR:H323 | 1.81                     | 0.62              |
| 2:aB:7:LYS:HD2     | 9:aM:31:LYS:HB3    | 1.81                     | 0.61              |
| 1:aA:502:VAL:HG12  | 1:aA:534:LEU:HD13  | 1.81                     | 0.61              |
| 1:aA:770:VAL:HG22  | 15:aA:851:BCR:H323 | 1.81                     | 0.61              |
| 11:cA:822:CLA:H2   | 11:cA:824:CLA:HBC1 | 1.81                     | 0.61              |
| 11:bB:806:CLA:H162 | 11:bB:827:CLA:HBB2 | 1.82                     | 0.61              |
| 8:aL:58:PHE:HB3    | 8:cL:143:GLN:HE22  | 1.64                     | 0.61              |
| 1:cA:502:VAL:HG12  | 1:cA:534:LEU:HD13  | 1.81                     | 0.61              |
| 11:aB:825:CLA:HED1 | 11:aB:833:CLA:HAB  | 1.83                     | 0.61              |
| 5:aE:10:ILE:HG22   | 5:aE:12:ARG:H      | 1.66                     | 0.60              |
| 11:bB:825:CLA:HED1 | 11:bB:833:CLA:HAB  | 1.83                     | 0.60              |
| 2:cB:493:SER:O     | 2:cB:501:ASN:ND2   | 2.35                     | 0.60              |
| 11:cB:806:CLA:H162 | 11:cB:827:CLA:HBB2 | 1.82                     | 0.60              |
| 5:cE:10:ILE:HG22   | 5:cE:12:ARG:H      | 1.66                     | 0.60              |
| 11:aB:806:CLA:H162 | 11:aB:827:CLA:HBB2 | 1.82                     | 0.60              |
| 2:bB:15:ASP:HB3    | 2:bB:20:ARG:HB2    | 1.84                     | 0.60              |
| 2:bB:64:ILE:HG23   | 11:bB:808:CLA:HED2 | 1.84                     | 0.60              |
| 2:bB:351:ILE:HD12  | 11:bB:817:CLA:H71  | 1.84                     | 0.60              |
| 5:bE:10:ILE:HG22   | 5:bE:12:ARG:H      | 1.66                     | 0.60              |
| 11:cB:825:CLA:HED1 | 11:cB:833:CLA:HAB  | 1.83                     | 0.60              |
| 2:aB:15:ASP:HB3    | 2:aB:20:ARG:HB2    | 1.84                     | 0.59              |
| 2:aB:493:SER:O     | 2:aB:501:ASN:ND2   | 2.35                     | 0.59              |
| 11:bA:814:CLA:H161 | 15:bA:848:BCR:H353 | 1.85                     | 0.59              |
| 2:bB:493:SER:O     | 2:bB:501:ASN:ND2   | 2.35                     | 0.59              |
| 11:aA:814:CLA:H161 | 15:aA:848:BCR:H353 | 1.85                     | 0.59              |
| 11:bA:820:CLA:H8   | 11:bA:820:CLA:HAB  | 1.85                     | 0.59              |
| 1:aA:317:ILE:HD13  | 7:aK:74:ALA:HB2    | 1.85                     | 0.59              |
| 2:aB:510:ALA:O     | 2:aB:516:ASN:ND2   | 2.36                     | 0.59              |
| 2:cB:15:ASP:HB3    | 2:cB:20:ARG:HB2    | 1.84                     | 0.59              |
| 2:aB:64:ILE:HG23   | 11:aB:808:CLA:HED2 | 1.84                     | 0.59              |
| 11:cA:820:CLA:HAB  | 11:cA:820:CLA:H8   | 1.85                     | 0.59              |
| 11:cB:807:CLA:H43  | 6:cI:20:MET:HE2    | 1.85                     | 0.59              |
| 11:aA:820:CLA:HAB  | 11:aA:820:CLA:H8   | 1.85                     | 0.59              |
| 15:aA:851:BCR:H362 | 11:aB:802:CLA:H52  | 1.84                     | 0.59              |
| 1:cA:490:PHE:HB3   | 11:cA:838:CLA:H11  | 1.85                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:bB:807:CLA:H43  | 6:bI:20:MET:HE2    | 1.85                     | 0.58              |
| 15:cA:851:BCR:H362 | 11:cB:802:CLA:H52  | 1.84                     | 0.58              |
| 2:cB:64:ILE:HG23   | 11:cB:808:CLA:HED2 | 1.84                     | 0.58              |
| 3:aC:23:LEU:O      | 4:aD:63:LYS:NZ     | 2.35                     | 0.58              |
| 11:cA:833:CLA:H42  | 8:cL:45:ILE:HD11   | 1.85                     | 0.58              |
| 2:cB:351:ILE:HD12  | 11:cB:817:CLA:H71  | 1.84                     | 0.58              |
| 1:cA:186:LYS:NZ    | 1:cA:188:ASP:OD2   | 2.36                     | 0.58              |
| 1:bA:317:ILE:HD13  | 7:bK:74:ALA:HB2    | 1.85                     | 0.58              |
| 11:bA:833:CLA:H42  | 8:bL:45:ILE:HD11   | 1.85                     | 0.58              |
| 2:bB:510:ALA:O     | 2:bB:516:ASN:ND2   | 2.36                     | 0.58              |
| 11:cA:814:CLA:H161 | 15:cA:848:BCR:H353 | 1.85                     | 0.58              |
| 8:aL:56:THR:HG21   | 8:cL:143:GLN:HG2   | 1.85                     | 0.58              |
| 11:aB:804:CLA:HBC3 | 11:aB:828:CLA:H41  | 1.86                     | 0.58              |
| 1:bA:490:PHE:HB3   | 11:bA:838:CLA:H11  | 1.85                     | 0.58              |
| 2:cB:510:ALA:O     | 2:cB:516:ASN:ND2   | 2.36                     | 0.58              |
| 2:aB:351:ILE:HD12  | 11:aB:817:CLA:H71  | 1.84                     | 0.57              |
| 11:cA:820:CLA:H101 | 11:cA:822:CLA:H142 | 1.86                     | 0.57              |
| 1:aA:490:PHE:HB3   | 11:aA:838:CLA:H11  | 1.85                     | 0.57              |
| 2:aB:86:PRO:HB2    | 2:aB:116:CYS:HB3   | 1.86                     | 0.57              |
| 11:aB:807:CLA:H43  | 6:aI:20:MET:HE2    | 1.85                     | 0.57              |
| 2:bB:276:HIS:HE1   | 11:bB:816:CLA:ND   | 2.03                     | 0.57              |
| 11:cB:804:CLA:HBC3 | 11:cB:828:CLA:H41  | 1.86                     | 0.57              |
| 1:cA:317:ILE:HD13  | 7:cK:74:ALA:HB2    | 1.85                     | 0.57              |
| 2:cB:86:PRO:HB2    | 2:cB:116:CYS:HB3   | 1.86                     | 0.57              |
| 11:aA:833:CLA:H42  | 8:aL:45:ILE:HD11   | 1.85                     | 0.57              |
| 2:aB:276:HIS:HE1   | 11:aB:816:CLA:ND   | 2.03                     | 0.57              |
| 15:bA:851:BCR:H362 | 11:bB:802:CLA:H52  | 1.84                     | 0.57              |
| 8:aL:143:GLN:HG2   | 8:bL:56:THR:HG21   | 1.85                     | 0.57              |
| 2:cB:276:HIS:HE1   | 11:cB:816:CLA:ND   | 2.03                     | 0.56              |
| 11:aA:820:CLA:H101 | 11:aA:822:CLA:H142 | 1.87                     | 0.56              |
| 11:bA:820:CLA:H101 | 11:bA:822:CLA:H142 | 1.87                     | 0.56              |
| 8:bL:47:ASN:HB3    | 11:bL:204:CLA:HAC1 | 1.88                     | 0.56              |
| 1:aA:186:LYS:NZ    | 1:aA:188:ASP:OD2   | 2.36                     | 0.56              |
| 8:aL:47:ASN:HB3    | 11:aL:204:CLA:HAC1 | 1.88                     | 0.56              |
| 2:bB:86:PRO:HB2    | 2:bB:116:CYS:HB3   | 1.86                     | 0.56              |
| 11:bB:804:CLA:HBC3 | 11:bB:828:CLA:H41  | 1.86                     | 0.56              |
| 1:bA:186:LYS:NZ    | 1:bA:188:ASP:OD2   | 2.36                     | 0.56              |
| 8:cL:47:ASN:HB3    | 11:cL:204:CLA:HAC1 | 1.88                     | 0.56              |
| 1:aA:217:ILE:HA    | 1:aA:221:LEU:HD12  | 1.87                     | 0.56              |
| 1:cA:406:GLY:HA3   | 1:cA:635:LEU:HD11  | 1.87                     | 0.56              |
| 1:bA:356:TRP:HB3   | 11:bA:806:CLA:HAC1 | 1.88                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:cA:217:ILE:HA    | 1:cA:221:LEU:HD12  | 1.87                     | 0.55              |
| 1:bA:217:ILE:HA    | 1:bA:221:LEU:HD12  | 1.87                     | 0.55              |
| 2:bB:595:ASN:HB2   | 11:bB:802:CLA:HBC2 | 1.89                     | 0.55              |
| 1:bA:406:GLY:HA3   | 1:bA:635:LEU:HD11  | 1.87                     | 0.55              |
| 1:aA:356:TRP:HB3   | 11:aA:806:CLA:HAC1 | 1.88                     | 0.55              |
| 1:aA:406:GLY:HA3   | 1:aA:635:LEU:HD11  | 1.87                     | 0.55              |
| 2:aB:595:ASN:HB2   | 11:aB:802:CLA:HBC2 | 1.89                     | 0.55              |
| 1:aA:216:LEU:HA    | 1:aA:220:ALA:HB3   | 1.89                     | 0.55              |
| 2:cB:595:ASN:HB2   | 11:cB:802:CLA:HBC2 | 1.89                     | 0.55              |
| 1:cA:225:LYS:HD3   | 1:cA:252:LEU:HB3   | 1.90                     | 0.54              |
| 1:aA:225:LYS:HD3   | 1:aA:252:LEU:HB3   | 1.90                     | 0.54              |
| 1:cA:356:TRP:HB3   | 11:cA:806:CLA:HAC1 | 1.88                     | 0.54              |
| 1:cA:216:LEU:HA    | 1:cA:220:ALA:HB3   | 1.89                     | 0.53              |
| 2:bB:180:ALA:HB2   | 2:bB:288:GLY:HA3   | 1.91                     | 0.53              |
| 11:bB:810:CLA:HBD  | 15:bB:848:BCR:HC7  | 1.91                     | 0.53              |
| 11:cB:810:CLA:HBD  | 15:cB:848:BCR:HC7  | 1.90                     | 0.53              |
| 1:bA:216:LEU:HA    | 1:bA:220:ALA:HB3   | 1.89                     | 0.53              |
| 2:aB:237:PRO:HB3   | 2:aB:256:THR:HG21  | 1.91                     | 0.53              |
| 11:aB:810:CLA:HBD  | 15:aB:848:BCR:HC7  | 1.91                     | 0.53              |
| 1:bA:225:LYS:HD3   | 1:bA:252:LEU:HB3   | 1.90                     | 0.53              |
| 2:bB:237:PRO:HB3   | 2:bB:256:THR:HG21  | 1.91                     | 0.53              |
| 8:bL:143:GLN:HG2   | 8:cL:56:THR:HG21   | 1.91                     | 0.53              |
| 2:aB:180:ALA:HB2   | 2:aB:288:GLY:HA3   | 1.91                     | 0.53              |
| 4:cD:86:ILE:HB     | 4:cD:99:HIS:HB3    | 1.91                     | 0.53              |
| 11:aA:820:CLA:H191 | 11:aA:822:CLA:H52  | 1.91                     | 0.53              |
| 2:bB:174:ARG:HB2   | 11:bB:812:CLA:HBC2 | 1.91                     | 0.52              |
| 6:aI:43:GLU:OE1    | 8:aL:121:ARG:NH2   | 2.43                     | 0.52              |
| 1:cA:443:THR:CG2   | 4:cD:16:THR:HG21   | 2.39                     | 0.52              |
| 4:bD:86:ILE:HB     | 4:bD:99:HIS:HB3    | 1.91                     | 0.52              |
| 6:bI:43:GLU:OE1    | 8:bL:121:ARG:NH2   | 2.43                     | 0.52              |
| 2:cB:180:ALA:HB2   | 2:cB:288:GLY:HA3   | 1.90                     | 0.52              |
| 11:aA:804:CLA:HBB2 | 11:aA:812:CLA:H112 | 1.92                     | 0.52              |
| 2:aB:174:ARG:HB2   | 11:aB:812:CLA:HBC2 | 1.91                     | 0.52              |
| 4:aD:86:ILE:HB     | 4:aD:99:HIS:HB3    | 1.91                     | 0.52              |
| 11:bA:820:CLA:H191 | 11:bA:822:CLA:H52  | 1.91                     | 0.52              |
| 6:cI:43:GLU:OE1    | 8:cL:121:ARG:NH2   | 2.43                     | 0.52              |
| 2:aB:470:THR:O     | 2:aB:474:HIS:ND1   | 2.37                     | 0.52              |
| 11:cA:820:CLA:H191 | 11:cA:822:CLA:H52  | 1.91                     | 0.52              |
| 2:cB:237:PRO:HB3   | 2:cB:256:THR:HG21  | 1.91                     | 0.52              |
| 2:cB:174:ARG:HB2   | 11:cB:812:CLA:HBC2 | 1.91                     | 0.52              |
| 11:cB:839:CLA:HBB2 | 13:cB:841:PQN:H141 | 1.92                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:aB:839:CLA:HBB2 | 13:aB:841:PQN:H141 | 1.92                     | 0.51              |
| 11:bB:839:CLA:HBB2 | 13:bB:841:PQN:H141 | 1.92                     | 0.51              |
| 2:aB:61:ILE:HG23   | 2:aB:142:LEU:HD13  | 1.93                     | 0.51              |
| 2:bB:470:THR:O     | 2:bB:474:HIS:ND1   | 2.37                     | 0.51              |
| 11:cA:821:CLA:H122 | 11:cA:821:CLA:HBB1 | 1.93                     | 0.51              |
| 2:cB:61:ILE:HG23   | 2:cB:142:LEU:HD13  | 1.93                     | 0.51              |
| 1:aA:612:ARG:NH1   | 21:aA:908:HOH:O    | 2.44                     | 0.51              |
| 1:cA:251:ASP:OD1   | 1:cA:251:ASP:N     | 2.44                     | 0.51              |
| 2:bB:487:ASN:HB3   | 2:bB:490:SER:HB2   | 1.93                     | 0.50              |
| 2:cB:470:THR:O     | 2:cB:474:HIS:ND1   | 2.37                     | 0.50              |
| 1:aA:529:VAL:HG13  | 1:aA:530:THR:HG23  | 1.94                     | 0.50              |
| 1:bA:529:VAL:HG13  | 1:bA:530:THR:HG23  | 1.94                     | 0.50              |
| 11:bA:804:CLA:HBB2 | 11:bA:812:CLA:H112 | 1.92                     | 0.50              |
| 11:cA:804:CLA:HBB2 | 11:cA:812:CLA:H112 | 1.92                     | 0.50              |
| 11:aA:821:CLA:HBB1 | 11:aA:821:CLA:H122 | 1.93                     | 0.50              |
| 2:aB:487:ASN:HB3   | 2:aB:490:SER:HB2   | 1.93                     | 0.50              |
| 1:cA:529:VAL:HG13  | 1:cA:530:THR:HG23  | 1.94                     | 0.49              |
| 2:cB:487:ASN:HB3   | 2:cB:490:SER:HB2   | 1.93                     | 0.49              |
| 2:bB:45:ARG:HH22   | 11:bB:804:CLA:HED2 | 1.77                     | 0.49              |
| 1:aA:251:ASP:OD1   | 1:aA:251:ASP:N     | 2.44                     | 0.49              |
| 1:bA:443:THR:HG22  | 2:bB:690:TRP:CH2   | 2.48                     | 0.49              |
| 1:cA:747:GLN:OE1   | 1:cA:749:ARG:NH2   | 2.46                     | 0.49              |
| 11:cA:814:CLA:H41  | 15:cA:848:BCR:H19C | 1.94                     | 0.49              |
| 1:bA:251:ASP:OD1   | 1:bA:251:ASP:N     | 2.44                     | 0.49              |
| 11:bA:821:CLA:HBB1 | 11:bA:821:CLA:H122 | 1.93                     | 0.49              |
| 2:bB:61:ILE:HG23   | 2:bB:142:LEU:HD13  | 1.93                     | 0.49              |
| 2:cB:45:ARG:HH22   | 11:cB:804:CLA:HED2 | 1.77                     | 0.49              |
| 2:cB:111:ASN:HD22  | 6:cI:10:ALA:H      | 1.61                     | 0.49              |
| 2:cB:692:HIS:O     | 8:cL:133:ARG:NH2   | 2.42                     | 0.49              |
| 1:aA:443:THR:CG2   | 4:aD:16:THR:HG21   | 2.42                     | 0.48              |
| 1:bA:747:GLN:OE1   | 1:bA:749:ARG:NH2   | 2.46                     | 0.48              |
| 7:bK:71:GLU:O      | 7:bK:75:THR:OG1    | 2.25                     | 0.48              |
| 2:aB:45:ARG:HH22   | 11:aB:804:CLA:HED2 | 1.77                     | 0.48              |
| 2:cB:471:GLN:HB3   | 2:cB:476:LYS:HD3   | 1.96                     | 0.48              |
| 2:aB:344:HIS:CG    | 11:aB:823:CLA:HAA1 | 2.49                     | 0.48              |
| 2:bB:344:HIS:CG    | 11:bB:823:CLA:HAA1 | 2.49                     | 0.48              |
| 5:cE:39:ARG:HG3    | 5:cE:50:SER:HB2    | 1.96                     | 0.48              |
| 1:aA:747:GLN:OE1   | 1:aA:749:ARG:NH2   | 2.46                     | 0.48              |
| 11:aB:816:CLA:H3A  | 11:aB:816:CLA:HBA2 | 1.61                     | 0.48              |
| 7:bK:86:MET:HG3    | 11:bK:103:CLA:HAB  | 1.96                     | 0.48              |
| 1:aA:443:THR:HG22  | 4:aD:16:THR:HG21   | 1.94                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:bA:840:CLA:HBA1 | 11:bA:840:CLA:HBD  | 1.96                     | 0.48              |
| 1:cA:431:ASN:OD1   | 1:cA:439:ARG:NH2   | 2.47                     | 0.48              |
| 1:bA:443:THR:CG2   | 4:bD:16:THR:HG21   | 2.43                     | 0.48              |
| 1:bA:612:ARG:NH1   | 21:bA:907:HOH:O    | 2.46                     | 0.48              |
| 2:bB:111:ASN:HD22  | 6:bI:10:ALA:H      | 1.61                     | 0.48              |
| 1:aA:555:MET:HE1   | 1:aA:646:MET:HE1   | 1.96                     | 0.48              |
| 11:aA:814:CLA:H41  | 15:aA:848:BCR:H19C | 1.94                     | 0.48              |
| 11:bA:814:CLA:H41  | 15:bA:848:BCR:H19C | 1.94                     | 0.48              |
| 1:aA:492:GLN:NE2   | 1:aA:560:LEU:O     | 2.42                     | 0.47              |
| 7:aK:86:MET:HG3    | 11:aK:103:CLA:HAB  | 1.96                     | 0.47              |
| 1:bA:431:ASN:OD1   | 1:bA:439:ARG:NH2   | 2.47                     | 0.47              |
| 1:cA:276:THR:HA    | 11:cA:818:CLA:HED1 | 1.96                     | 0.47              |
| 2:aB:91:ILE:HB     | 2:aB:112:PRO:HB2   | 1.96                     | 0.47              |
| 2:aB:136:PHE:HB2   | 9:aM:3:LEU:HD21    | 1.96                     | 0.47              |
| 2:bB:471:GLN:HB3   | 2:bB:476:LYS:HD3   | 1.96                     | 0.47              |
| 1:aA:276:THR:HA    | 11:aA:818:CLA:HED1 | 1.96                     | 0.47              |
| 1:bA:773:TRP:NE1   | 11:bA:829:CLA:O1A  | 2.45                     | 0.47              |
| 2:aB:471:GLN:HB3   | 2:aB:476:LYS:HD3   | 1.96                     | 0.47              |
| 2:cB:586:PHE:HZ    | 18:cB:847:LMG:H362 | 1.80                     | 0.47              |
| 11:aA:840:CLA:HBA1 | 11:aA:840:CLA:HBD  | 1.96                     | 0.47              |
| 2:bB:275:HIS:HB3   | 11:bB:816:CLA:HMB1 | 1.97                     | 0.47              |
| 6:aI:39:TRP:HE1    | 9:aM:31:LYS:HE2    | 1.79                     | 0.47              |
| 1:bA:276:THR:HA    | 11:bA:818:CLA:HED1 | 1.96                     | 0.47              |
| 2:cB:40:GLU:OE2    | 2:cB:44:GLN:NE2    | 2.48                     | 0.47              |
| 1:aA:590:ARG:O     | 1:aA:599:GLY:N     | 2.45                     | 0.47              |
| 2:aB:111:ASN:HD22  | 6:aI:10:ALA:H      | 1.61                     | 0.47              |
| 2:aB:586:PHE:HZ    | 18:aB:847:LMG:H362 | 1.80                     | 0.47              |
| 11:cA:840:CLA:HBD  | 11:cA:840:CLA:HBA1 | 1.96                     | 0.47              |
| 2:cB:344:HIS:CG    | 11:cB:823:CLA:HAA1 | 2.49                     | 0.47              |
| 11:cB:804:CLA:HAA2 | 9:cM:29:LEU:HB3    | 1.97                     | 0.47              |
| 5:aE:39:ARG:HG3    | 5:aE:50:SER:HB2    | 1.96                     | 0.47              |
| 9:aM:21:LEU:HD23   | 9:aM:24:ARG:HD3    | 1.97                     | 0.47              |
| 1:cA:612:ARG:NH1   | 21:cA:908:HOH:O    | 2.46                     | 0.47              |
| 2:cB:91:ILE:HB     | 2:cB:112:PRO:HB2   | 1.96                     | 0.47              |
| 2:cB:136:PHE:HB2   | 9:cM:3:LEU:HD21    | 1.96                     | 0.47              |
| 2:cB:216:ARG:HD3   | 2:cB:221:GLY:HA3   | 1.97                     | 0.47              |
| 2:cB:501:ASN:OD1   | 2:cB:501:ASN:N     | 2.48                     | 0.47              |
| 1:bA:492:GLN:NE2   | 1:bA:560:LEU:O     | 2.42                     | 0.47              |
| 1:bA:590:ARG:O     | 1:bA:599:GLY:N     | 2.45                     | 0.47              |
| 2:bB:586:PHE:HZ    | 18:bB:847:LMG:H362 | 1.80                     | 0.47              |
| 1:cA:492:GLN:NE2   | 1:cA:560:LEU:O     | 2.42                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:cA:555:MET:HE1   | 1:cA:646:MET:HE1   | 1.96                     | 0.47              |
| 6:cI:39:TRP:HE1    | 9:cM:31:LYS:HE2    | 1.79                     | 0.47              |
| 11:aB:804:CLA:HAA2 | 9:aM:29:LEU:HB3    | 1.97                     | 0.47              |
| 13:bA:845:PQN:H241 | 13:bA:845:PQN:H262 | 1.79                     | 0.47              |
| 5:bE:39:ARG:HG3    | 5:bE:50:SER:HB2    | 1.96                     | 0.47              |
| 1:aA:431:ASN:OD1   | 1:aA:439:ARG:NH2   | 2.47                     | 0.46              |
| 1:bA:555:MET:HE1   | 1:bA:646:MET:HE1   | 1.96                     | 0.46              |
| 11:cB:821:CLA:H41  | 11:cB:821:CLA:H62  | 1.68                     | 0.46              |
| 11:cB:829:CLA:HBA2 | 11:cB:829:CLA:H3A  | 1.49                     | 0.46              |
| 7:cK:86:MET:HG3    | 11:cK:103:CLA:HAB  | 1.96                     | 0.46              |
| 2:aB:40:GLU:OE2    | 2:aB:44:GLN:NE2    | 2.48                     | 0.46              |
| 11:aB:806:CLA:H143 | 11:aB:827:CLA:HBB2 | 1.97                     | 0.46              |
| 11:bA:823:CLA:HBA1 | 7:bK:48:GLN:HB3    | 1.97                     | 0.46              |
| 1:cA:773:TRP:NE1   | 11:cA:829:CLA:O1A  | 2.45                     | 0.46              |
| 1:aA:773:TRP:NE1   | 11:aA:829:CLA:O1A  | 2.45                     | 0.46              |
| 2:aB:275:HIS:HB3   | 11:aB:816:CLA:HMB1 | 1.97                     | 0.46              |
| 2:bB:40:GLU:OE2    | 2:bB:44:GLN:NE2    | 2.48                     | 0.46              |
| 2:bB:91:ILE:HB     | 2:bB:112:PRO:HB2   | 1.96                     | 0.46              |
| 2:cB:257:PHE:HD2   | 2:cB:502:VAL:HB    | 1.80                     | 0.46              |
| 2:bB:264:GLN:NE2   | 21:bB:909:HOH:O    | 2.47                     | 0.46              |
| 11:cA:809:CLA:H3A  | 11:cA:809:CLA:HBA2 | 1.54                     | 0.46              |
| 11:aA:813:CLA:HHC  | 11:aA:813:CLA:HBB1 | 1.98                     | 0.46              |
| 11:bA:813:CLA:HHC  | 11:bA:813:CLA:HBB1 | 1.98                     | 0.46              |
| 11:bA:821:CLA:H3A  | 11:bA:821:CLA:HBA2 | 1.66                     | 0.46              |
| 2:bB:257:PHE:HD2   | 2:bB:502:VAL:HB    | 1.80                     | 0.46              |
| 2:bB:558:PRO:HB2   | 5:bE:14:GLU:HG3    | 1.96                     | 0.46              |
| 2:bB:692:HIS:O     | 8:bL:133:ARG:NH2   | 2.42                     | 0.46              |
| 1:cA:437:THR:HA    | 1:cA:440:HIS:CE1   | 2.51                     | 0.46              |
| 11:cB:806:CLA:H143 | 11:cB:827:CLA:HBB2 | 1.97                     | 0.46              |
| 1:bA:724:GLY:O     | 1:bA:728:GLU:HG3   | 2.16                     | 0.46              |
| 11:bB:806:CLA:H143 | 11:bB:827:CLA:HBB2 | 1.97                     | 0.46              |
| 11:bB:821:CLA:H41  | 11:bB:821:CLA:H62  | 1.69                     | 0.46              |
| 11:cA:813:CLA:HHC  | 11:cA:813:CLA:HBB1 | 1.98                     | 0.46              |
| 2:cB:264:GLN:NE2   | 21:cB:909:HOH:O    | 2.47                     | 0.46              |
| 2:cB:275:HIS:HB3   | 11:cB:816:CLA:HMB1 | 1.97                     | 0.46              |
| 9:cM:21:LEU:HD23   | 9:cM:24:ARG:HD3    | 1.97                     | 0.46              |
| 1:aA:724:GLY:O     | 1:aA:728:GLU:HG3   | 2.16                     | 0.46              |
| 11:aA:823:CLA:HBA1 | 7:aK:48:GLN:HB3    | 1.97                     | 0.46              |
| 3:bC:15:THR:HG22   | 3:bC:28:MET:HG3    | 1.98                     | 0.46              |
| 2:aB:558:PRO:HB2   | 5:aE:14:GLU:HG3    | 1.98                     | 0.46              |
| 11:bA:833:CLA:HAC2 | 11:bL:205:CLA:H18  | 1.98                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:bA:839:CLA:H191 | 11:bL:205:CLA:H71  | 1.98                     | 0.46              |
| 11:bB:804:CLA:HMB2 | 15:bM:101:BCR:HC21 | 1.98                     | 0.46              |
| 11:bB:819:CLA:HBA2 | 11:bB:819:CLA:H3A  | 1.64                     | 0.46              |
| 1:aA:130:MET:HE1   | 1:aA:138:GLN:HB2   | 1.98                     | 0.46              |
| 11:aA:833:CLA:HAC2 | 11:aL:205:CLA:H18  | 1.98                     | 0.46              |
| 2:aB:692:HIS:O     | 8:aL:133:ARG:NH2   | 2.42                     | 0.46              |
| 11:bA:809:CLA:HAB  | 11:bA:829:CLA:H152 | 1.98                     | 0.46              |
| 8:bL:161:VAL:O     | 8:bL:165:ASN:ND2   | 2.44                     | 0.46              |
| 1:aA:437:THR:HA    | 1:aA:440:HIS:CE1   | 2.51                     | 0.45              |
| 2:aB:60:TRP:HB2    | 11:aB:808:CLA:H192 | 1.98                     | 0.45              |
| 4:aD:22:ARG:NH2    | 4:aD:27:GLU:OE2    | 2.49                     | 0.45              |
| 11:bA:823:CLA:H3A  | 11:bA:823:CLA:HBA2 | 1.61                     | 0.45              |
| 2:aB:257:PHE:HD2   | 2:aB:502:VAL:HB    | 1.80                     | 0.45              |
| 2:aB:435:PHE:CD2   | 11:aB:837:CLA:HAB  | 2.52                     | 0.45              |
| 1:bA:130:MET:HE1   | 1:bA:138:GLN:HB2   | 1.98                     | 0.45              |
| 2:bB:191:THR:HG21  | 2:bB:278:LEU:HB2   | 1.98                     | 0.45              |
| 2:bB:216:ARG:HD3   | 2:bB:221:GLY:HA3   | 1.97                     | 0.45              |
| 11:bB:829:CLA:H3A  | 11:bB:829:CLA:HBA2 | 1.49                     | 0.45              |
| 2:cB:435:PHE:CD2   | 11:cB:837:CLA:HAB  | 2.52                     | 0.45              |
| 15:cB:848:BCR:H382 | 15:cB:848:BCR:H371 | 1.99                     | 0.45              |
| 11:bA:806:CLA:HBA1 | 11:bA:806:CLA:H3A  | 1.73                     | 0.45              |
| 4:bD:22:ARG:NH2    | 4:bD:27:GLU:OE2    | 2.49                     | 0.45              |
| 1:cA:450:TRP:HH2   | 11:cA:839:CLA:H151 | 1.82                     | 0.45              |
| 11:cA:823:CLA:HBA1 | 7:cK:48:GLN:HB3    | 1.97                     | 0.45              |
| 2:aB:216:ARG:HD3   | 2:aB:221:GLY:HA3   | 1.97                     | 0.45              |
| 1:bA:437:THR:HA    | 1:bA:440:HIS:CE1   | 2.51                     | 0.45              |
| 1:cA:724:GLY:O     | 1:cA:728:GLU:HG3   | 2.16                     | 0.45              |
| 17:cA:853:LMT:H6'2 | 8:cL:83:ARG:HH11   | 1.82                     | 0.45              |
| 2:cB:492:ALA:HB2   | 11:cB:834:CLA:HBC3 | 1.99                     | 0.45              |
| 2:aB:181:GLY:HA3   | 11:aB:812:CLA:HBB1 | 1.99                     | 0.45              |
| 15:bB:848:BCR:H382 | 15:bB:848:BCR:H371 | 1.99                     | 0.45              |
| 15:cL:207:BCR:H15C | 15:cL:207:BCR:H351 | 1.84                     | 0.45              |
| 11:aA:803:CLA:H102 | 15:aA:851:BCR:H24C | 1.99                     | 0.45              |
| 15:aB:848:BCR:H371 | 15:aB:848:BCR:H382 | 1.99                     | 0.45              |
| 1:bA:685:ALA:O     | 1:bA:688:SER:OG    | 2.35                     | 0.45              |
| 11:cA:840:CLA:H111 | 11:cA:840:CLA:H193 | 1.98                     | 0.45              |
| 11:aB:806:CLA:H72  | 11:aB:806:CLA:H111 | 1.50                     | 0.45              |
| 11:cA:809:CLA:HAB  | 11:cA:829:CLA:H152 | 1.98                     | 0.45              |
| 15:aA:847:BCR:H383 | 15:aK:102:BCR:H10C | 1.99                     | 0.45              |
| 3:aC:15:THR:HG22   | 3:aC:28:MET:HG3    | 1.98                     | 0.45              |
| 8:aL:161:VAL:O     | 8:aL:165:ASN:ND2   | 2.44                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:bA:202:ALA:HB2   | 1:bA:308:GLY:HA3   | 1.99                     | 0.45              |
| 11:bA:840:CLA:H111 | 11:bA:840:CLA:H193 | 1.98                     | 0.45              |
| 9:bM:21:LEU:HD23   | 9:bM:24:ARG:HD3    | 1.97                     | 0.45              |
| 11:aA:803:CLA:H92  | 11:aA:803:CLA:H61  | 1.83                     | 0.45              |
| 11:aA:840:CLA:H192 | 11:aA:840:CLA:H162 | 1.87                     | 0.45              |
| 17:aA:853:LMT:H6'2 | 8:aL:83:ARG:HH11   | 1.82                     | 0.45              |
| 2:bB:181:GLY:HA3   | 11:bB:812:CLA:HBB1 | 1.99                     | 0.45              |
| 2:cB:345:LEU:HD21  | 11:cB:828:CLA:HAB  | 1.99                     | 0.45              |
| 1:aA:280:GLY:N     | 1:aA:537:PRO:O     | 2.50                     | 0.45              |
| 2:aB:191:THR:HG21  | 2:aB:278:LEU:HB2   | 1.98                     | 0.45              |
| 15:aL:207:BCR:H20C | 15:aL:207:BCR:H361 | 1.85                     | 0.45              |
| 2:bB:345:LEU:HD21  | 11:bB:828:CLA:HAB  | 1.99                     | 0.45              |
| 1:cA:130:MET:HE1   | 1:cA:138:GLN:HB2   | 1.98                     | 0.45              |
| 13:cA:845:PQN:H241 | 13:cA:845:PQN:H262 | 1.79                     | 0.45              |
| 4:cD:22:ARG:NH2    | 4:cD:27:GLU:OE2    | 2.49                     | 0.45              |
| 11:aB:805:CLA:H192 | 11:aB:805:CLA:H162 | 1.85                     | 0.44              |
| 1:bA:747:GLN:HA    | 1:bA:748:PRO:HD3   | 1.86                     | 0.44              |
| 2:bB:435:PHE:CD2   | 11:bB:837:CLA:HAB  | 2.52                     | 0.44              |
| 3:bC:66:ARG:HA     | 3:bC:66:ARG:HD2    | 1.79                     | 0.44              |
| 11:cA:839:CLA:H191 | 11:cL:205:CLA:H71  | 1.98                     | 0.44              |
| 11:aA:809:CLA:HAB  | 11:aA:829:CLA:H152 | 1.98                     | 0.44              |
| 11:aA:839:CLA:H191 | 11:aL:205:CLA:H71  | 1.98                     | 0.44              |
| 15:bA:847:BCR:H20C | 15:bA:847:BCR:H361 | 1.86                     | 0.44              |
| 2:bB:60:TRP:HB2    | 11:bB:808:CLA:H192 | 1.98                     | 0.44              |
| 2:bB:555:LYS:HB2   | 2:bB:555:LYS:HE2   | 1.77                     | 0.44              |
| 1:cA:443:THR:HG22  | 4:cD:16:THR:HG21   | 1.99                     | 0.44              |
| 11:cA:819:CLA:HBA2 | 11:cA:819:CLA:H3A  | 1.72                     | 0.44              |
| 15:cA:847:BCR:H383 | 15:cK:102:BCR:H10C | 1.99                     | 0.44              |
| 2:cB:699:PHE:O     | 8:cL:124:TYR:OH    | 2.29                     | 0.44              |
| 1:aA:450:TRP:HH2   | 11:aA:839:CLA:H151 | 1.82                     | 0.44              |
| 11:aA:840:CLA:H111 | 11:aA:840:CLA:H193 | 1.98                     | 0.44              |
| 2:aB:345:LEU:HD21  | 11:aB:828:CLA:HAB  | 1.99                     | 0.44              |
| 11:cA:806:CLA:HBA1 | 11:cA:806:CLA:H3A  | 1.73                     | 0.44              |
| 1:aA:685:ALA:O     | 1:aA:688:SER:OG    | 2.35                     | 0.44              |
| 8:aL:67:ALA:HA     | 15:aL:208:BCR:H16C | 2.00                     | 0.44              |
| 15:bB:845:BCR:H15C | 15:bB:845:BCR:H351 | 1.85                     | 0.44              |
| 2:cB:60:TRP:HB2    | 11:cB:808:CLA:H192 | 1.98                     | 0.44              |
| 2:aB:264:GLN:NE2   | 21:aB:909:HOH:O    | 2.46                     | 0.44              |
| 2:aB:347:CYS:HB3   | 11:aB:823:CLA:H42  | 2.00                     | 0.44              |
| 15:bA:847:BCR:H383 | 15:bK:102:BCR:H10C | 1.99                     | 0.44              |
| 2:bB:467:ALA:HB1   | 11:bB:836:CLA:HBD  | 2.00                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:bB:492:ALA:HB2   | 11:bB:834:CLA:HBC3 | 1.98                     | 0.44              |
| 11:bB:805:CLA:H192 | 11:bB:805:CLA:H162 | 1.85                     | 0.44              |
| 11:cA:835:CLA:H61  | 11:cA:835:CLA:H92  | 1.86                     | 0.44              |
| 2:cB:181:GLY:HA3   | 11:cB:812:CLA:HBB1 | 1.99                     | 0.44              |
| 1:aA:182:VAL:HG12  | 1:aA:183:ARG:HG3   | 1.99                     | 0.44              |
| 11:aB:823:CLA:H62  | 11:aB:823:CLA:H41  | 1.83                     | 0.44              |
| 11:bA:803:CLA:H102 | 15:bA:851:BCR:H24C | 1.99                     | 0.44              |
| 2:cB:191:THR:HG21  | 2:cB:278:LEU:HB2   | 1.98                     | 0.44              |
| 11:cB:806:CLA:H72  | 11:cB:806:CLA:H111 | 1.50                     | 0.44              |
| 1:bA:182:VAL:HG12  | 1:bA:183:ARG:HG3   | 1.99                     | 0.44              |
| 1:bA:450:TRP:HH2   | 11:bA:839:CLA:H151 | 1.82                     | 0.44              |
| 1:cA:685:ALA:O     | 1:cA:688:SER:OG    | 2.35                     | 0.44              |
| 11:cA:833:CLA:HAC2 | 11:cL:205:CLA:H18  | 1.98                     | 0.44              |
| 11:bA:822:CLA:H51  | 11:bA:828:CLA:H61  | 2.00                     | 0.44              |
| 11:cB:805:CLA:H142 | 11:cB:805:CLA:H111 | 1.88                     | 0.44              |
| 11:aA:809:CLA:H3A  | 11:aA:809:CLA:HBA2 | 1.54                     | 0.44              |
| 2:aB:492:ALA:HB2   | 11:aB:834:CLA:HBC3 | 1.99                     | 0.44              |
| 1:bA:280:GLY:N     | 1:bA:537:PRO:O     | 2.50                     | 0.44              |
| 1:cA:182:VAL:HG12  | 1:cA:183:ARG:HG3   | 1.99                     | 0.44              |
| 11:cA:803:CLA:H102 | 15:cA:851:BCR:H24C | 1.99                     | 0.43              |
| 17:bA:853:LMT:H6'2 | 8:bL:83:ARG:HH11   | 1.81                     | 0.43              |
| 2:bB:343:TRP:HZ2   | 11:bB:823:CLA:HBB1 | 1.83                     | 0.43              |
| 4:bD:62:ARG:NH2    | 4:bD:64:GLU:OE2    | 2.51                     | 0.43              |
| 1:cA:280:GLY:N     | 1:cA:537:PRO:O     | 2.50                     | 0.43              |
| 2:cB:402:ILE:HD11  | 2:cB:551:ALA:HB1   | 2.00                     | 0.43              |
| 15:cB:845:BCR:H371 | 15:cB:845:BCR:H24C | 1.81                     | 0.43              |
| 3:cC:15:THR:HG22   | 3:cC:28:MET:HG3    | 1.98                     | 0.43              |
| 2:aB:697:LEU:HB2   | 15:aL:203:BCR:H282 | 2.01                     | 0.43              |
| 11:bB:816:CLA:H3A  | 11:bB:816:CLA:HBA2 | 1.61                     | 0.43              |
| 11:cA:831:CLA:H111 | 16:cA:852:LHG:H192 | 2.00                     | 0.43              |
| 2:cB:467:ALA:HB1   | 11:cB:836:CLA:HBD  | 2.00                     | 0.43              |
| 11:cB:827:CLA:HBA2 | 11:cB:827:CLA:H3A  | 1.64                     | 0.43              |
| 8:cL:67:ALA:HA     | 15:cL:208:BCR:H16C | 2.00                     | 0.43              |
| 2:aB:467:ALA:HB1   | 11:aB:836:CLA:HBD  | 2.00                     | 0.43              |
| 11:aB:837:CLA:HMA2 | 11:aB:838:CLA:HED2 | 2.01                     | 0.43              |
| 11:bB:806:CLA:H72  | 11:bB:806:CLA:H111 | 1.50                     | 0.43              |
| 15:cA:851:BCR:H403 | 15:cA:851:BCR:H371 | 2.01                     | 0.43              |
| 2:cB:343:TRP:HZ2   | 11:cB:823:CLA:HBB1 | 1.83                     | 0.43              |
| 8:cL:157:ILE:HG23  | 15:cL:208:BCR:H323 | 2.00                     | 0.43              |
| 11:aA:821:CLA:H3A  | 11:aA:821:CLA:HBA2 | 1.66                     | 0.43              |
| 15:bA:849:BCR:H20C | 15:bA:849:BCR:H361 | 1.87                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:bB:699:PHE:O     | 8:bL:124:TYR:OH    | 2.29                     | 0.43              |
| 3:cC:61:ASP:HA     | 3:cC:62:PHE:HA     | 1.89                     | 0.43              |
| 1:aA:415:HIS:HA    | 1:aA:418:ILE:HD12  | 2.00                     | 0.43              |
| 11:aA:822:CLA:H51  | 11:aA:828:CLA:H61  | 2.00                     | 0.43              |
| 2:aB:182:LEU:HD13  | 11:aB:812:CLA:HHB  | 2.00                     | 0.43              |
| 2:aB:699:PHE:O     | 8:aL:124:TYR:OH    | 2.29                     | 0.43              |
| 2:bB:10:GLN:N      | 2:bB:35:ASP:OD2    | 2.50                     | 0.43              |
| 2:bB:402:ILE:HD11  | 2:bB:551:ALA:HB1   | 2.00                     | 0.43              |
| 2:cB:182:LEU:HD13  | 11:cB:812:CLA:HHB  | 2.01                     | 0.43              |
| 11:cB:837:CLA:HMA2 | 11:cB:838:CLA:HED2 | 2.01                     | 0.43              |
| 1:aA:204:LEU:HD11  | 11:aA:814:CLA:H42  | 2.01                     | 0.43              |
| 15:bA:851:BCR:H403 | 15:bA:851:BCR:H371 | 2.01                     | 0.43              |
| 2:bB:136:PHE:HB2   | 9:bM:3:LEU:HD21    | 2.00                     | 0.43              |
| 8:bL:157:ILE:HG23  | 15:bL:208:BCR:H323 | 2.00                     | 0.43              |
| 1:cA:202:ALA:HB2   | 1:cA:308:GLY:HA3   | 1.99                     | 0.43              |
| 2:cB:634:LEU:HD11  | 11:cB:801:CLA:H72  | 2.01                     | 0.43              |
| 1:aA:202:ALA:HB2   | 1:aA:308:GLY:HA3   | 1.99                     | 0.43              |
| 8:bL:67:ALA:HA     | 15:bL:208:BCR:H16C | 2.00                     | 0.43              |
| 15:bL:203:BCR:H20C | 15:bL:203:BCR:H361 | 1.80                     | 0.43              |
| 11:aA:831:CLA:H111 | 16:aA:852:LHG:H192 | 2.00                     | 0.43              |
| 15:aA:850:BCR:H15C | 15:aA:850:BCR:H351 | 1.87                     | 0.43              |
| 2:bB:182:LEU:HD13  | 11:bB:812:CLA:HHB  | 2.00                     | 0.43              |
| 11:bB:837:CLA:HMA2 | 11:bB:838:CLA:HED2 | 2.01                     | 0.43              |
| 1:cA:590:ARG:O     | 1:cA:599:GLY:N     | 2.45                     | 0.43              |
| 2:cB:347:CYS:HB3   | 11:cB:823:CLA:H42  | 2.00                     | 0.43              |
| 15:cL:208:BCR:H20C | 15:cL:208:BCR:H361 | 1.87                     | 0.43              |
| 1:aA:269:SER:HA    | 11:aA:818:CLA:HAA2 | 2.01                     | 0.43              |
| 2:cB:510:ALA:HB1   | 2:cB:518:LEU:HD21  | 2.01                     | 0.43              |
| 11:aA:843:CLA:H3A  | 11:aA:843:CLA:HBA2 | 1.77                     | 0.42              |
| 1:bA:609:GLY:HA2   | 2:bB:572:PRO:HD3   | 2.01                     | 0.42              |
| 11:bA:831:CLA:H111 | 16:bA:852:LHG:H192 | 2.00                     | 0.42              |
| 2:bB:347:CYS:HB3   | 11:bB:823:CLA:H42  | 2.00                     | 0.42              |
| 11:cA:822:CLA:H51  | 11:cA:828:CLA:H61  | 2.00                     | 0.42              |
| 11:cB:805:CLA:HBA1 | 11:cB:805:CLA:H3A  | 1.71                     | 0.42              |
| 2:aB:402:ILE:HD11  | 2:aB:551:ALA:HB1   | 2.01                     | 0.42              |
| 1:bA:80:LEU:HD22   | 11:bA:806:CLA:H92  | 2.01                     | 0.42              |
| 1:bA:626:LEU:HD22  | 2:bB:676:THR:HG22  | 2.01                     | 0.42              |
| 2:bB:510:ALA:HB1   | 2:bB:518:LEU:HD21  | 2.01                     | 0.42              |
| 2:bB:697:LEU:HB2   | 15:bL:203:BCR:H282 | 2.01                     | 0.42              |
| 6:bI:39:TRP:HE1    | 9:bM:31:LYS:HE2    | 1.84                     | 0.42              |
| 1:aA:80:LEU:HD22   | 11:aA:806:CLA:H92  | 2.01                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:aA:403:TRP:CD1   | 11:aA:829:CLA:HAB  | 2.54                     | 0.42              |
| 2:aB:535:LEU:HD21  | 11:aB:802:CLA:HBB1 | 2.01                     | 0.42              |
| 13:aB:841:PQN:H172 | 13:aB:841:PQN:H212 | 1.76                     | 0.42              |
| 2:bB:352:THR:HB    | 2:bB:386:ALA:HB2   | 2.01                     | 0.42              |
| 15:bB:843:BCR:H20C | 15:bB:843:BCR:H361 | 1.91                     | 0.42              |
| 1:cA:403:TRP:CD1   | 11:cA:829:CLA:HAB  | 2.54                     | 0.42              |
| 1:cA:415:HIS:HA    | 1:cA:418:ILE:HD12  | 2.01                     | 0.42              |
| 11:cA:806:CLA:H151 | 15:cA:847:BCR:H323 | 2.01                     | 0.42              |
| 11:cB:816:CLA:H3A  | 11:cB:816:CLA:HBA2 | 1.60                     | 0.42              |
| 4:cD:62:ARG:NH2    | 4:cD:64:GLU:OE2    | 2.51                     | 0.42              |
| 3:aC:66:ARG:HD2    | 3:aC:66:ARG:HA     | 1.79                     | 0.42              |
| 15:bA:851:BCR:H15C | 15:bA:851:BCR:H351 | 1.91                     | 0.42              |
| 1:cA:269:SER:HA    | 11:cA:818:CLA:HAA2 | 2.01                     | 0.42              |
| 1:cA:626:LEU:HD22  | 2:cB:676:THR:HG22  | 2.01                     | 0.42              |
| 2:cB:10:GLN:N      | 2:cB:35:ASP:OD2    | 2.50                     | 0.42              |
| 2:cB:471:GLN:NE2   | 2:cB:520:LEU:O     | 2.50                     | 0.42              |
| 15:cL:208:BCR:H11C | 15:cL:208:BCR:H341 | 1.93                     | 0.42              |
| 11:aA:813:CLA:H2   | 11:aA:813:CLA:H62  | 1.80                     | 0.42              |
| 15:aA:851:BCR:H371 | 15:aA:851:BCR:H403 | 2.01                     | 0.42              |
| 2:aB:691:ALA:O     | 2:aB:695:THR:OG1   | 2.27                     | 0.42              |
| 11:bB:816:CLA:H72  | 11:bB:816:CLA:H111 | 1.84                     | 0.42              |
| 1:aA:609:GLY:HA2   | 2:aB:572:PRO:HD3   | 2.01                     | 0.42              |
| 1:aA:626:LEU:HD22  | 2:aB:676:THR:HG22  | 2.02                     | 0.42              |
| 8:aL:157:ILE:HG23  | 15:aL:208:BCR:H323 | 2.00                     | 0.42              |
| 1:bA:389:THR:HG21  | 1:bA:549:ILE:HB    | 2.02                     | 0.42              |
| 11:bB:832:CLA:H3A  | 11:bB:832:CLA:HBA2 | 1.70                     | 0.42              |
| 3:bC:23:LEU:O      | 4:bD:63:LYS:NZ     | 2.47                     | 0.42              |
| 15:bL:203:BCR:H11C | 15:bL:203:BCR:H341 | 1.92                     | 0.42              |
| 1:cA:773:TRP:CG    | 15:cA:851:BCR:HC22 | 2.55                     | 0.42              |
| 2:cB:697:LEU:HB2   | 15:cL:203:BCR:H282 | 2.01                     | 0.42              |
| 3:cC:66:ARG:HD2    | 3:cC:66:ARG:HA     | 1.79                     | 0.42              |
| 11:cL:206:CLA:HBA1 | 11:cL:206:CLA:H3A  | 1.76                     | 0.42              |
| 11:aA:836:CLA:HBB1 | 11:aA:838:CLA:HED2 | 2.02                     | 0.42              |
| 2:aB:343:TRP:HZ2   | 11:aB:823:CLA:HBB1 | 1.83                     | 0.42              |
| 1:bA:773:TRP:CG    | 15:bA:851:BCR:HC22 | 2.55                     | 0.42              |
| 2:bB:604:TRP:HB2   | 11:bB:836:CLA:HMC1 | 2.02                     | 0.42              |
| 2:bB:634:LEU:HD11  | 11:bB:801:CLA:H72  | 2.01                     | 0.42              |
| 15:bM:101:BCR:H20C | 15:bM:101:BCR:H361 | 1.92                     | 0.42              |
| 11:cB:832:CLA:HBA2 | 11:cB:832:CLA:H3A  | 1.70                     | 0.42              |
| 15:aA:847:BCR:H15C | 15:aA:847:BCR:H351 | 1.91                     | 0.42              |
| 11:aL:206:CLA:H141 | 11:aL:206:CLA:H161 | 1.84                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:bA:269:SER:HA    | 11:bA:818:CLA:HAA2 | 2.01                     | 0.42              |
| 15:bA:847:BCR:H15C | 15:bA:847:BCR:H351 | 1.91                     | 0.42              |
| 2:bB:418:MET:HA    | 2:bB:421:HIS:HB2   | 2.02                     | 0.42              |
| 1:cA:204:LEU:HD11  | 11:cA:814:CLA:H42  | 2.01                     | 0.42              |
| 1:cA:377:HIS:ND1   | 11:cA:819:CLA:OBD  | 2.53                     | 0.42              |
| 15:cB:845:BCR:H15C | 15:cB:845:BCR:H351 | 1.85                     | 0.42              |
| 11:aA:824:CLA:HBB1 | 11:aA:825:CLA:H3A  | 2.01                     | 0.42              |
| 2:aB:634:LEU:HD11  | 11:aB:801:CLA:H72  | 2.01                     | 0.42              |
| 1:bA:204:LEU:HD11  | 11:bA:814:CLA:H42  | 2.01                     | 0.42              |
| 2:bB:535:LEU:HD21  | 11:bB:802:CLA:HBB1 | 2.01                     | 0.42              |
| 11:bL:206:CLA:HBA1 | 11:bL:206:CLA:H3A  | 1.76                     | 0.42              |
| 1:cA:609:GLY:HA2   | 2:cB:572:PRO:HD3   | 2.01                     | 0.42              |
| 2:aB:10:GLN:N      | 2:aB:35:ASP:OD2    | 2.50                     | 0.42              |
| 11:aB:805:CLA:HBA1 | 11:aB:805:CLA:H3A  | 1.70                     | 0.42              |
| 11:aB:808:CLA:H202 | 11:aB:808:CLA:H162 | 1.93                     | 0.42              |
| 11:aL:205:CLA:H3A  | 11:aL:205:CLA:HBA2 | 1.66                     | 0.42              |
| 1:bA:400:HIS:HE1   | 11:bA:829:CLA:ND   | 2.15                     | 0.42              |
| 11:bA:824:CLA:HBB1 | 11:bA:825:CLA:H3A  | 2.01                     | 0.42              |
| 11:bA:836:CLA:HBB1 | 11:bA:838:CLA:HED2 | 2.02                     | 0.42              |
| 11:bL:206:CLA:H141 | 11:bL:206:CLA:H161 | 1.84                     | 0.42              |
| 1:cA:714:PHE:HZ    | 11:cA:843:CLA:HBC2 | 1.85                     | 0.42              |
| 11:cA:836:CLA:HBB1 | 11:cA:838:CLA:HED2 | 2.02                     | 0.42              |
| 11:cB:812:CLA:H111 | 11:cB:812:CLA:H71  | 1.86                     | 0.42              |
| 1:aA:773:TRP:CG    | 15:aA:851:BCR:HC22 | 2.55                     | 0.41              |
| 11:aA:825:CLA:H143 | 11:aA:825:CLA:H111 | 1.93                     | 0.41              |
| 11:aB:801:CLA:H62  | 11:aB:801:CLA:H102 | 1.88                     | 0.41              |
| 11:bA:843:CLA:HBA2 | 11:bA:843:CLA:H3A  | 1.77                     | 0.41              |
| 2:bB:692:HIS:NE2   | 2:bB:700:GLY:O     | 2.36                     | 0.41              |
| 4:bD:78:LYS:HD2    | 4:bD:79:PRO:HA     | 2.02                     | 0.41              |
| 11:cA:824:CLA:HBB1 | 11:cA:825:CLA:H3A  | 2.01                     | 0.41              |
| 11:aA:806:CLA:H151 | 15:aA:847:BCR:H323 | 2.01                     | 0.41              |
| 15:aA:849:BCR:H15C | 15:aA:849:BCR:H351 | 1.85                     | 0.41              |
| 4:aD:62:ARG:NH2    | 4:aD:64:GLU:OE2    | 2.51                     | 0.41              |
| 15:aI:101:BCR:H11C | 15:aI:101:BCR:H341 | 1.89                     | 0.41              |
| 1:cA:80:LEU:HD22   | 11:cA:806:CLA:H92  | 2.01                     | 0.41              |
| 15:cA:849:BCR:H20C | 15:cA:849:BCR:H361 | 1.87                     | 0.41              |
| 2:cB:535:LEU:HD21  | 11:cB:802:CLA:HBB1 | 2.01                     | 0.41              |
| 11:cB:823:CLA:H62  | 11:cB:823:CLA:H41  | 1.83                     | 0.41              |
| 1:aA:630:TRP:HE1   | 11:aB:803:CLA:C1D  | 2.34                     | 0.41              |
| 11:aA:803:CLA:H91  | 15:aA:851:BCR:H383 | 2.03                     | 0.41              |
| 2:aB:7:LYS:HE3     | 2:aB:7:LYS:HB2     | 1.86                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:aB:358:HIS:ND1   | 11:aB:816:CLA:OBD  | 2.51                     | 0.41              |
| 2:aB:510:ALA:HB1   | 2:aB:518:LEU:HD21  | 2.01                     | 0.41              |
| 2:aB:604:TRP:HB2   | 11:aB:836:CLA:HMC1 | 2.01                     | 0.41              |
| 11:aB:813:CLA:HBA1 | 15:aB:844:BCR:H383 | 2.02                     | 0.41              |
| 4:aD:78:LYS:HD2    | 4:aD:79:PRO:HA     | 2.02                     | 0.41              |
| 6:aI:39:TRP:NE1    | 9:aM:31:LYS:HE2    | 2.35                     | 0.41              |
| 15:aL:208:BCR:H20C | 15:aL:208:BCR:H361 | 1.87                     | 0.41              |
| 1:bA:377:HIS:ND1   | 11:bA:819:CLA:OBD  | 2.53                     | 0.41              |
| 1:bA:403:TRP:CD1   | 11:bA:829:CLA:HAB  | 2.54                     | 0.41              |
| 1:bA:415:HIS:HA    | 1:bA:418:ILE:HD12  | 2.01                     | 0.41              |
| 11:bB:805:CLA:H3A  | 11:bB:805:CLA:HBA1 | 1.71                     | 0.41              |
| 11:cA:813:CLA:H2   | 11:cA:813:CLA:H62  | 1.80                     | 0.41              |
| 1:bA:714:PHE:HZ    | 11:bA:843:CLA:HBC2 | 1.85                     | 0.41              |
| 15:bB:842:BCR:H20C | 15:bB:842:BCR:H361 | 1.90                     | 0.41              |
| 1:cA:389:THR:HG21  | 1:cA:549:ILE:HB    | 2.02                     | 0.41              |
| 11:cA:829:CLA:H3A  | 11:cA:829:CLA:HBA2 | 1.80                     | 0.41              |
| 2:cB:236:ASN:OD1   | 2:cB:236:ASN:N     | 2.54                     | 0.41              |
| 2:cB:352:THR:HB    | 2:cB:386:ALA:HB2   | 2.01                     | 0.41              |
| 2:cB:692:HIS:NE2   | 2:cB:700:GLY:O     | 2.36                     | 0.41              |
| 5:aE:2:VAL:HG12    | 5:aE:27:VAL:HG21   | 2.02                     | 0.41              |
| 1:bA:498:GLN:HE22  | 11:bA:836:CLA:C1A  | 2.33                     | 0.41              |
| 2:bB:7:LYS:HE3     | 2:bB:7:LYS:HB2     | 1.86                     | 0.41              |
| 13:bB:841:PQN:H212 | 13:bB:841:PQN:H172 | 1.76                     | 0.41              |
| 1:cA:400:HIS:HE1   | 11:cA:829:CLA:ND   | 2.15                     | 0.41              |
| 11:cB:815:CLA:H3A  | 11:cB:815:CLA:HBA2 | 1.76                     | 0.41              |
| 7:cK:71:GLU:O      | 7:cK:75:THR:OG1    | 2.25                     | 0.41              |
| 1:aA:97:PHE:HB3    | 1:aA:116:VAL:HG23  | 2.02                     | 0.41              |
| 1:aA:606:PRO:HB3   | 1:aA:753:ILE:HB    | 2.02                     | 0.41              |
| 1:aA:714:PHE:HZ    | 11:aA:843:CLA:HBC2 | 1.85                     | 0.41              |
| 15:aB:843:BCR:H11C | 15:aB:843:BCR:H341 | 1.97                     | 0.41              |
| 11:bL:204:CLA:H192 | 11:bL:204:CLA:H162 | 1.89                     | 0.41              |
| 11:bL:206:CLA:H202 | 11:bL:206:CLA:H162 | 1.89                     | 0.41              |
| 2:cB:418:MET:HA    | 2:cB:421:HIS:HB2   | 2.02                     | 0.41              |
| 2:cB:604:TRP:HB2   | 11:cB:836:CLA:HMC1 | 2.02                     | 0.41              |
| 11:cB:801:CLA:H102 | 11:cB:801:CLA:H62  | 1.87                     | 0.41              |
| 11:cB:808:CLA:O1A  | 11:cB:826:CLA:HBD  | 2.21                     | 0.41              |
| 11:cB:813:CLA:HBA1 | 15:cB:844:BCR:H383 | 2.03                     | 0.41              |
| 6:cI:39:TRP:NE1    | 9:cM:31:LYS:HE2    | 2.35                     | 0.41              |
| 1:aA:569:HIS:CD2   | 17:aA:853:LMT:H123 | 2.55                     | 0.41              |
| 11:aB:808:CLA:O1A  | 11:aB:826:CLA:HBD  | 2.21                     | 0.41              |
| 11:aB:815:CLA:H2   | 11:aB:815:CLA:H62  | 1.75                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:aB:817:CLA:H41  | 11:aB:817:CLA:H62  | 1.87                     | 0.41              |
| 15:aI:101:BCR:H20C | 15:aI:101:BCR:H361 | 1.91                     | 0.41              |
| 1:bA:606:PRO:HB3   | 1:bA:753:ILE:HB    | 2.03                     | 0.41              |
| 11:cA:807:CLA:H71  | 11:cA:807:CLA:H112 | 1.87                     | 0.41              |
| 11:cA:839:CLA:H203 | 11:cA:839:CLA:H162 | 1.91                     | 0.41              |
| 2:cB:230:TRP:HZ3   | 11:cB:815:CLA:H91  | 1.86                     | 0.41              |
| 11:cB:828:CLA:H61  | 11:cB:828:CLA:H2   | 1.86                     | 0.41              |
| 15:cL:203:BCR:H20C | 15:cL:203:BCR:H361 | 1.80                     | 0.41              |
| 11:cL:205:CLA:H3A  | 11:cL:205:CLA:HBA2 | 1.66                     | 0.41              |
| 1:aA:389:THR:HG21  | 1:aA:549:ILE:HB    | 2.02                     | 0.41              |
| 2:aB:352:THR:HB    | 2:aB:386:ALA:HB2   | 2.01                     | 0.41              |
| 2:aB:418:MET:HA    | 2:aB:421:HIS:HB2   | 2.02                     | 0.41              |
| 11:aB:801:CLA:H202 | 11:aB:802:CLA:HHB  | 2.03                     | 0.41              |
| 11:aB:815:CLA:H3A  | 11:aB:815:CLA:HBA2 | 1.76                     | 0.41              |
| 15:aL:203:BCR:H11C | 15:aL:203:BCR:H341 | 1.92                     | 0.41              |
| 11:aL:206:CLA:HBA1 | 11:aL:206:CLA:H3A  | 1.77                     | 0.41              |
| 1:bA:97:PHE:HB3    | 1:bA:116:VAL:HG23  | 2.02                     | 0.41              |
| 1:bA:569:HIS:CD2   | 17:bA:853:LMT:H123 | 2.56                     | 0.41              |
| 11:bA:839:CLA:H203 | 11:bA:839:CLA:H162 | 1.91                     | 0.41              |
| 2:bB:471:GLN:NE2   | 2:bB:520:LEU:O     | 2.50                     | 0.41              |
| 11:bB:808:CLA:H202 | 11:bB:808:CLA:H162 | 1.93                     | 0.41              |
| 11:bB:827:CLA:H3A  | 11:bB:827:CLA:HBA2 | 1.64                     | 0.41              |
| 1:cA:498:GLN:HE22  | 11:cA:836:CLA:C1A  | 2.33                     | 0.41              |
| 11:cB:805:CLA:H192 | 11:cB:805:CLA:H162 | 1.85                     | 0.41              |
| 1:aA:455:LEU:HB3   | 1:aA:573:PHE:HB2   | 2.03                     | 0.41              |
| 11:aB:827:CLA:H3A  | 11:aB:827:CLA:HBA2 | 1.64                     | 0.41              |
| 15:aB:845:BCR:H371 | 15:aB:845:BCR:H24C | 1.80                     | 0.41              |
| 1:bA:126:LEU:HD11  | 11:bA:810:CLA:HAC2 | 2.03                     | 0.41              |
| 11:bA:806:CLA:H151 | 15:bA:847:BCR:H323 | 2.01                     | 0.41              |
| 11:bL:205:CLA:HBA2 | 11:bL:205:CLA:H3A  | 1.66                     | 0.41              |
| 1:cA:97:PHE:HB3    | 1:cA:116:VAL:HG23  | 2.02                     | 0.41              |
| 11:cA:820:CLA:HBA2 | 11:cA:820:CLA:H3A  | 1.91                     | 0.41              |
| 11:cA:843:CLA:H3A  | 11:cA:843:CLA:HBA2 | 1.77                     | 0.41              |
| 2:cB:555:LYS:HB2   | 2:cB:555:LYS:HE2   | 1.77                     | 0.41              |
| 11:cB:812:CLA:H203 | 11:cB:812:CLA:H162 | 1.91                     | 0.41              |
| 15:cB:848:BCR:H20C | 15:cB:848:BCR:H361 | 1.93                     | 0.41              |
| 2:aB:230:TRP:HZ3   | 11:aB:815:CLA:H91  | 1.86                     | 0.41              |
| 1:bA:455:LEU:HB3   | 1:bA:573:PHE:HB2   | 2.03                     | 0.41              |
| 2:bB:230:TRP:HZ3   | 11:bB:815:CLA:H91  | 1.86                     | 0.41              |
| 1:cA:606:PRO:HB3   | 1:cA:753:ILE:HB    | 2.03                     | 0.41              |
| 2:cB:86:PRO:HB3    | 2:cB:121:TYR:CG    | 2.57                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:aB:841:PQN:H111 | 13:aB:841:PQN:H2M1 | 1.93                     | 0.40              |
| 15:aB:842:BCR:H351 | 15:aB:842:BCR:H15C | 1.85                     | 0.40              |
| 15:bA:849:BCR:H15C | 15:bA:849:BCR:H351 | 1.85                     | 0.40              |
| 1:cA:381:MET:HB2   | 1:cA:381:MET:HE3   | 1.88                     | 0.40              |
| 11:cA:822:CLA:H52  | 11:cA:822:CLA:H11  | 1.85                     | 0.40              |
| 8:cL:83:ARG:HA     | 8:cL:89:ALA:HB2    | 2.03                     | 0.40              |
| 1:aA:498:GLN:HE22  | 11:aA:836:CLA:C1A  | 2.33                     | 0.40              |
| 1:aA:747:GLN:HA    | 1:aA:748:PRO:HD3   | 1.86                     | 0.40              |
| 2:aB:86:PRO:HB3    | 2:aB:121:TYR:CG    | 2.57                     | 0.40              |
| 11:aB:832:CLA:H3A  | 11:aB:832:CLA:HBA2 | 1.70                     | 0.40              |
| 7:aK:71:GLU:O      | 7:aK:75:THR:OG1    | 2.25                     | 0.40              |
| 11:cA:821:CLA:H3A  | 11:cA:821:CLA:HBA2 | 1.66                     | 0.40              |
| 11:cB:804:CLA:HBA1 | 11:cB:804:CLA:HBD  | 2.04                     | 0.40              |
| 4:cD:43:MET:HE3    | 4:cD:43:MET:HB3    | 2.01                     | 0.40              |
| 11:aA:828:CLA:H41  | 11:aA:828:CLA:H62  | 1.91                     | 0.40              |
| 11:aA:839:CLA:H203 | 11:aA:839:CLA:H162 | 1.91                     | 0.40              |
| 2:aB:501:ASN:OD1   | 2:aB:501:ASN:N     | 2.48                     | 0.40              |
| 11:aB:804:CLA:HBD  | 11:aB:804:CLA:HBA1 | 2.04                     | 0.40              |
| 12:aB:824:F6C:CHB  | 11:aB:838:CLA:HAA2 | 2.51                     | 0.40              |
| 11:bA:819:CLA:H3A  | 11:bA:819:CLA:HBA2 | 1.71                     | 0.40              |
| 11:bA:833:CLA:HBA2 | 8:bL:35:VAL:HG12   | 2.04                     | 0.40              |
| 11:bB:813:CLA:HBA1 | 15:bB:844:BCR:H383 | 2.02                     | 0.40              |
| 5:bE:2:VAL:HG12    | 5:bE:27:VAL:HG21   | 2.02                     | 0.40              |
| 15:bL:207:BCR:H15C | 15:bL:207:BCR:H351 | 1.84                     | 0.40              |
| 1:cA:455:LEU:HB3   | 1:cA:573:PHE:HB2   | 2.03                     | 0.40              |
| 1:cA:569:HIS:CD2   | 17:cA:853:LMT:H123 | 2.56                     | 0.40              |
| 11:cA:802:CLA:H13  | 15:cB:846:BCR:H10C | 2.03                     | 0.40              |
| 11:cA:834:CLA:H122 | 11:cA:834:CLA:H8   | 1.87                     | 0.40              |
| 15:cA:850:BCR:H20C | 15:cA:850:BCR:H361 | 1.85                     | 0.40              |
| 2:cB:280:ILE:HD13  | 2:cB:280:ILE:HA    | 1.95                     | 0.40              |
| 15:cB:844:BCR:H15C | 15:cB:844:BCR:H351 | 1.91                     | 0.40              |
| 4:cD:78:LYS:HD2    | 4:cD:79:PRO:HA     | 2.02                     | 0.40              |
| 5:cE:2:VAL:HG12    | 5:cE:27:VAL:HG21   | 2.02                     | 0.40              |
| 15:cL:208:BCR:H371 | 15:cL:208:BCR:H24C | 1.88                     | 0.40              |
| 1:aA:295:HIS:HB3   | 11:aA:819:CLA:HMB1 | 2.04                     | 0.40              |
| 11:aA:802:CLA:H13  | 15:aB:846:BCR:H10C | 2.03                     | 0.40              |
| 11:aA:813:CLA:H3A  | 11:aA:813:CLA:HBA2 | 1.80                     | 0.40              |
| 2:bB:236:ASN:OD1   | 2:bB:236:ASN:N     | 2.54                     | 0.40              |
| 11:bB:805:CLA:H142 | 11:bB:805:CLA:H111 | 1.88                     | 0.40              |
| 11:bB:808:CLA:O1A  | 11:bB:826:CLA:HBD  | 2.21                     | 0.40              |
| 8:bL:83:ARG:HA     | 8:bL:89:ALA:HB2    | 2.03                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:cA:630:TRP:HE1   | 11:cB:803:CLA:C1D  | 2.34                     | 0.40              |
| 11:cA:803:CLA:H91  | 15:cA:851:BCR:H383 | 2.03                     | 0.40              |
| 12:cB:824:F6C:CHB  | 11:cB:838:CLA:HAA2 | 2.52                     | 0.40              |
| 11:cB:837:CLA:H3A  | 11:cB:837:CLA:HBA2 | 1.91                     | 0.40              |
| 15:cB:842:BCR:H15C | 15:cB:842:BCR:H351 | 1.85                     | 0.40              |
| 2:aB:343:TRP:HE1   | 11:aB:823:CLA:C2B  | 2.35                     | 0.40              |
| 15:aB:845:BCR:H15C | 15:aB:845:BCR:H351 | 1.85                     | 0.40              |
| 8:aL:83:ARG:HA     | 8:aL:89:ALA:HB2    | 2.03                     | 0.40              |
| 11:bA:809:CLA:H3A  | 11:bA:809:CLA:HBA2 | 1.53                     | 0.40              |
| 15:bA:850:BCR:H11C | 15:bA:850:BCR:H341 | 1.98                     | 0.40              |
| 11:bB:801:CLA:H202 | 11:bB:802:CLA:HHB  | 2.03                     | 0.40              |
| 1:cA:295:HIS:HB3   | 11:cA:819:CLA:HMB1 | 2.04                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | aA    | 713/784 (91%) | 696 (98%) | 17 (2%) | 0        | 100         | 100 |
| 1   | bA    | 713/784 (91%) | 696 (98%) | 17 (2%) | 0        | 100         | 100 |
| 1   | cA    | 713/784 (91%) | 696 (98%) | 17 (2%) | 0        | 100         | 100 |
| 2   | aB    | 723/743 (97%) | 696 (96%) | 26 (4%) | 1 (0%)   | 48          | 63  |
| 2   | bB    | 723/743 (97%) | 696 (96%) | 26 (4%) | 1 (0%)   | 48          | 63  |
| 2   | cB    | 723/743 (97%) | 696 (96%) | 26 (4%) | 1 (0%)   | 48          | 63  |
| 3   | aC    | 78/81 (96%)   | 75 (96%)  | 3 (4%)  | 0        | 100         | 100 |
| 3   | bC    | 78/81 (96%)   | 75 (96%)  | 3 (4%)  | 0        | 100         | 100 |
| 3   | cC    | 78/81 (96%)   | 75 (96%)  | 3 (4%)  | 0        | 100         | 100 |
| 4   | aD    | 96/142 (68%)  | 94 (98%)  | 2 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 4   | bD    | 96/142 (68%)    | 94 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 4   | cD    | 96/142 (68%)    | 94 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 5   | aE    | 59/68 (87%)     | 54 (92%)   | 5 (8%)   | 0        | 100         | 100 |
| 5   | bE    | 59/68 (87%)     | 54 (92%)   | 5 (8%)   | 0        | 100         | 100 |
| 5   | cE    | 59/68 (87%)     | 54 (92%)   | 5 (8%)   | 0        | 100         | 100 |
| 6   | aI    | 39/63 (62%)     | 36 (92%)   | 3 (8%)   | 0        | 100         | 100 |
| 6   | bI    | 39/63 (62%)     | 36 (92%)   | 3 (8%)   | 0        | 100         | 100 |
| 6   | cI    | 39/63 (62%)     | 36 (92%)   | 3 (8%)   | 0        | 100         | 100 |
| 7   | aK    | 42/96 (44%)     | 40 (95%)   | 2 (5%)   | 0        | 100         | 100 |
| 7   | bK    | 42/96 (44%)     | 40 (95%)   | 2 (5%)   | 0        | 100         | 100 |
| 7   | cK    | 42/96 (44%)     | 40 (95%)   | 2 (5%)   | 0        | 100         | 100 |
| 8   | aL    | 170/189 (90%)   | 169 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 8   | bL    | 170/189 (90%)   | 169 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 8   | cL    | 170/189 (90%)   | 169 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 9   | aM    | 29/31 (94%)     | 27 (93%)   | 2 (7%)   | 0        | 100         | 100 |
| 9   | bM    | 29/31 (94%)     | 27 (93%)   | 2 (7%)   | 0        | 100         | 100 |
| 9   | cM    | 29/31 (94%)     | 27 (93%)   | 2 (7%)   | 0        | 100         | 100 |
| All | All   | 5847/6591 (89%) | 5661 (97%) | 183 (3%) | 3 (0%)   | 49          | 63  |

All (3) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | aB    | 237 | PRO  |
| 2   | bB    | 237 | PRO  |
| 2   | cB    | 237 | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 1   | aA    | 578/633 (91%)   | 562 (97%)  | 16 (3%)  | 38          | 58  |
| 1   | bA    | 578/633 (91%)   | 562 (97%)  | 16 (3%)  | 38          | 58  |
| 1   | cA    | 578/633 (91%)   | 562 (97%)  | 16 (3%)  | 38          | 58  |
| 2   | aB    | 586/598 (98%)   | 576 (98%)  | 10 (2%)  | 53          | 73  |
| 2   | bB    | 586/598 (98%)   | 576 (98%)  | 10 (2%)  | 53          | 73  |
| 2   | cB    | 586/598 (98%)   | 576 (98%)  | 10 (2%)  | 53          | 73  |
| 3   | aC    | 68/69 (99%)     | 68 (100%)  | 0        | 100         | 100 |
| 3   | bC    | 68/69 (99%)     | 68 (100%)  | 0        | 100         | 100 |
| 3   | cC    | 68/69 (99%)     | 68 (100%)  | 0        | 100         | 100 |
| 4   | aD    | 80/115 (70%)    | 80 (100%)  | 0        | 100         | 100 |
| 4   | bD    | 80/115 (70%)    | 80 (100%)  | 0        | 100         | 100 |
| 4   | cD    | 80/115 (70%)    | 80 (100%)  | 0        | 100         | 100 |
| 5   | aE    | 54/61 (88%)     | 49 (91%)   | 5 (9%)   | 8           | 13  |
| 5   | bE    | 54/61 (88%)     | 49 (91%)   | 5 (9%)   | 8           | 13  |
| 5   | cE    | 54/61 (88%)     | 49 (91%)   | 5 (9%)   | 8           | 13  |
| 6   | aI    | 36/52 (69%)     | 35 (97%)   | 1 (3%)   | 38          | 58  |
| 6   | bI    | 36/52 (69%)     | 35 (97%)   | 1 (3%)   | 38          | 58  |
| 6   | cI    | 36/52 (69%)     | 35 (97%)   | 1 (3%)   | 38          | 58  |
| 7   | aK    | 30/67 (45%)     | 28 (93%)   | 2 (7%)   | 15          | 24  |
| 7   | bK    | 30/67 (45%)     | 28 (93%)   | 2 (7%)   | 15          | 24  |
| 7   | cK    | 30/67 (45%)     | 28 (93%)   | 2 (7%)   | 15          | 24  |
| 8   | aL    | 136/149 (91%)   | 136 (100%) | 0        | 100         | 100 |
| 8   | bL    | 136/149 (91%)   | 136 (100%) | 0        | 100         | 100 |
| 8   | cL    | 136/149 (91%)   | 136 (100%) | 0        | 100         | 100 |
| 9   | aM    | 27/27 (100%)    | 27 (100%)  | 0        | 100         | 100 |
| 9   | bM    | 27/27 (100%)    | 27 (100%)  | 0        | 100         | 100 |
| 9   | cM    | 27/27 (100%)    | 27 (100%)  | 0        | 100         | 100 |
| All | All   | 4785/5313 (90%) | 4683 (98%) | 102 (2%) | 46          | 67  |

All (102) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | aA    | 98  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | aA    | 106 | ASP  |
| 1   | aA    | 116 | VAL  |
| 1   | aA    | 168 | MET  |
| 1   | aA    | 234 | GLU  |
| 1   | aA    | 236 | ILE  |
| 1   | aA    | 247 | SER  |
| 1   | aA    | 251 | ASP  |
| 1   | aA    | 443 | THR  |
| 1   | aA    | 654 | VAL  |
| 1   | aA    | 661 | SER  |
| 1   | aA    | 688 | SER  |
| 1   | aA    | 731 | GLU  |
| 1   | aA    | 733 | ILE  |
| 1   | aA    | 741 | LYS  |
| 1   | aA    | 754 | THR  |
| 2   | aB    | 33  | SER  |
| 2   | aB    | 306 | GLU  |
| 2   | aB    | 376 | SER  |
| 2   | aB    | 408 | GLU  |
| 2   | aB    | 418 | MET  |
| 2   | aB    | 505 | SER  |
| 2   | aB    | 511 | VAL  |
| 2   | aB    | 513 | ASN  |
| 2   | aB    | 555 | LYS  |
| 2   | aB    | 562 | ASP  |
| 5   | aE    | 9   | ARG  |
| 5   | aE    | 29  | GLN  |
| 5   | aE    | 37  | ILE  |
| 5   | aE    | 56  | SER  |
| 5   | aE    | 57  | GLU  |
| 6   | aI    | 21  | ILE  |
| 7   | aK    | 71  | GLU  |
| 7   | aK    | 82  | LEU  |
| 1   | bA    | 98  | SER  |
| 1   | bA    | 106 | ASP  |
| 1   | bA    | 116 | VAL  |
| 1   | bA    | 168 | MET  |
| 1   | bA    | 234 | GLU  |
| 1   | bA    | 236 | ILE  |
| 1   | bA    | 247 | SER  |
| 1   | bA    | 251 | ASP  |
| 1   | bA    | 443 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | bA    | 654 | VAL  |
| 1   | bA    | 661 | SER  |
| 1   | bA    | 688 | SER  |
| 1   | bA    | 731 | GLU  |
| 1   | bA    | 733 | ILE  |
| 1   | bA    | 741 | LYS  |
| 1   | bA    | 754 | THR  |
| 2   | bB    | 33  | SER  |
| 2   | bB    | 306 | GLU  |
| 2   | bB    | 376 | SER  |
| 2   | bB    | 408 | GLU  |
| 2   | bB    | 418 | MET  |
| 2   | bB    | 505 | SER  |
| 2   | bB    | 511 | VAL  |
| 2   | bB    | 513 | ASN  |
| 2   | bB    | 555 | LYS  |
| 2   | bB    | 562 | ASP  |
| 5   | bE    | 9   | ARG  |
| 5   | bE    | 29  | GLN  |
| 5   | bE    | 37  | ILE  |
| 5   | bE    | 56  | SER  |
| 5   | bE    | 57  | GLU  |
| 6   | bI    | 21  | ILE  |
| 7   | bK    | 71  | GLU  |
| 7   | bK    | 82  | LEU  |
| 1   | cA    | 98  | SER  |
| 1   | cA    | 106 | ASP  |
| 1   | cA    | 116 | VAL  |
| 1   | cA    | 168 | MET  |
| 1   | cA    | 234 | GLU  |
| 1   | cA    | 236 | ILE  |
| 1   | cA    | 247 | SER  |
| 1   | cA    | 251 | ASP  |
| 1   | cA    | 443 | THR  |
| 1   | cA    | 654 | VAL  |
| 1   | cA    | 661 | SER  |
| 1   | cA    | 688 | SER  |
| 1   | cA    | 731 | GLU  |
| 1   | cA    | 733 | ILE  |
| 1   | cA    | 741 | LYS  |
| 1   | cA    | 754 | THR  |
| 2   | cB    | 33  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | cB    | 306 | GLU  |
| 2   | cB    | 376 | SER  |
| 2   | cB    | 408 | GLU  |
| 2   | cB    | 418 | MET  |
| 2   | cB    | 505 | SER  |
| 2   | cB    | 511 | VAL  |
| 2   | cB    | 513 | ASN  |
| 2   | cB    | 555 | LYS  |
| 2   | cB    | 562 | ASP  |
| 5   | cE    | 9   | ARG  |
| 5   | cE    | 29  | GLN  |
| 5   | cE    | 37  | ILE  |
| 5   | cE    | 56  | SER  |
| 5   | cE    | 57  | GLU  |
| 6   | cI    | 21  | ILE  |
| 7   | cK    | 71  | GLU  |
| 7   | cK    | 82  | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | aA    | 61  | HIS  |
| 1   | aA    | 138 | GLN  |
| 1   | aA    | 224 | ASN  |
| 1   | aA    | 267 | ASN  |
| 1   | aA    | 338 | ASN  |
| 1   | aA    | 540 | HIS  |
| 1   | aA    | 670 | GLN  |
| 1   | aA    | 755 | GLN  |
| 2   | aB    | 41  | ASN  |
| 2   | aB    | 83  | ASN  |
| 2   | aB    | 111 | ASN  |
| 2   | aB    | 132 | ASN  |
| 2   | aB    | 205 | GLN  |
| 2   | aB    | 211 | ASN  |
| 2   | aB    | 262 | HIS  |
| 2   | aB    | 300 | ASN  |
| 2   | aB    | 309 | GLN  |
| 2   | aB    | 340 | GLN  |
| 2   | aB    | 512 | ASN  |
| 2   | aB    | 620 | ASN  |
| 2   | aB    | 713 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | aC    | 16  | GLN  |
| 4   | aD    | 52  | HIS  |
| 4   | aD    | 56  | ASN  |
| 6   | aI    | 6   | GLN  |
| 7   | aK    | 48  | GLN  |
| 8   | aL    | 25  | ASN  |
| 8   | aL    | 117 | GLN  |
| 8   | aL    | 143 | GLN  |
| 8   | aL    | 178 | ASN  |
| 1   | bA    | 61  | HIS  |
| 1   | bA    | 138 | GLN  |
| 1   | bA    | 224 | ASN  |
| 1   | bA    | 267 | ASN  |
| 1   | bA    | 338 | ASN  |
| 1   | bA    | 540 | HIS  |
| 1   | bA    | 670 | GLN  |
| 1   | bA    | 755 | GLN  |
| 2   | bB    | 41  | ASN  |
| 2   | bB    | 83  | ASN  |
| 2   | bB    | 111 | ASN  |
| 2   | bB    | 133 | ASN  |
| 2   | bB    | 205 | GLN  |
| 2   | bB    | 262 | HIS  |
| 2   | bB    | 300 | ASN  |
| 2   | bB    | 309 | GLN  |
| 2   | bB    | 340 | GLN  |
| 2   | bB    | 512 | ASN  |
| 2   | bB    | 620 | ASN  |
| 2   | bB    | 713 | GLN  |
| 3   | bC    | 16  | GLN  |
| 4   | bD    | 52  | HIS  |
| 4   | bD    | 56  | ASN  |
| 6   | bI    | 6   | GLN  |
| 7   | bK    | 48  | GLN  |
| 8   | bL    | 25  | ASN  |
| 8   | bL    | 117 | GLN  |
| 8   | bL    | 143 | GLN  |
| 1   | cA    | 61  | HIS  |
| 1   | cA    | 138 | GLN  |
| 1   | cA    | 224 | ASN  |
| 1   | cA    | 267 | ASN  |
| 1   | cA    | 338 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | cA    | 540 | HIS  |
| 1   | cA    | 670 | GLN  |
| 1   | cA    | 755 | GLN  |
| 2   | cB    | 41  | ASN  |
| 2   | cB    | 83  | ASN  |
| 2   | cB    | 111 | ASN  |
| 2   | cB    | 205 | GLN  |
| 2   | cB    | 262 | HIS  |
| 2   | cB    | 300 | ASN  |
| 2   | cB    | 309 | GLN  |
| 2   | cB    | 340 | GLN  |
| 2   | cB    | 512 | ASN  |
| 2   | cB    | 620 | ASN  |
| 2   | cB    | 713 | GLN  |
| 3   | cC    | 16  | GLN  |
| 4   | cD    | 52  | HIS  |
| 4   | cD    | 56  | ASN  |
| 5   | cE    | 51  | ASN  |
| 6   | cI    | 6   | GLN  |
| 7   | cK    | 48  | GLN  |
| 8   | cL    | 25  | ASN  |
| 8   | cL    | 117 | GLN  |
| 8   | cL    | 143 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 363 ligands modelled in this entry, 15 are unknown and 3 are monoatomic - leaving 345 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 |
| 11  | CLA  | aA    | 816 | 1    | 49,53,73     | 2.39 | 21 (42%) | 58,89,113   | 2.92 | 26 (44%) |
| 15  | BCR  | aK    | 102 | -    | 41,41,41     | 1.07 | 2 (4%)   | 56,56,56    | 1.30 | 8 (14%)  |
| 11  | CLA  | cA    | 823 | 1    | 49,53,73     | 2.34 | 20 (40%) | 58,89,113   | 3.06 | 24 (41%) |
| 15  | BCR  | aA    | 851 | -    | 41,41,41     | 1.03 | 2 (4%)   | 56,56,56    | 1.25 | 7 (12%)  |
| 11  | CLA  | bB    | 802 | -    | 61,65,73     | 2.11 | 20 (32%) | 72,103,113  | 2.86 | 31 (43%) |
| 15  | BCR  | aB    | 844 | -    | 41,41,41     | 1.03 | 2 (4%)   | 56,56,56    | 1.24 | 5 (8%)   |
| 11  | CLA  | cA    | 817 | -    | 53,57,73     | 2.30 | 20 (37%) | 61,93,113   | 2.86 | 27 (44%) |
| 11  | CLA  | aB    | 825 | 2    | 69,73,73     | 2.01 | 20 (28%) | 82,113,113  | 2.62 | 30 (36%) |
| 10  | CL0  | bA    | 801 | 1    | 58,73,73     | 3.11 | 16 (27%) | 60,113,113  | 2.63 | 18 (30%) |
| 11  | CLA  | cA    | 837 | 1    | 49,53,73     | 2.40 | 21 (42%) | 58,89,113   | 3.03 | 27 (46%) |
| 11  | CLA  | bB    | 828 | 2    | 59,63,73     | 2.17 | 18 (30%) | 70,101,113  | 2.70 | 30 (42%) |
| 13  | PQN  | bA    | 845 | -    | 34,34,34     | 1.63 | 2 (5%)   | 43,45,45    | 1.16 | 4 (9%)   |
| 11  | CLA  | cA    | 834 | 1    | 69,73,73     | 1.98 | 20 (28%) | 82,113,113  | 2.59 | 33 (40%) |
| 15  | BCR  | cM    | 101 | -    | 41,41,41     | 1.01 | 2 (4%)   | 56,56,56    | 1.31 | 8 (14%)  |
| 11  | CLA  | bB    | 814 | 2    | 49,53,73     | 2.38 | 21 (42%) | 58,89,113   | 2.99 | 27 (46%) |
| 11  | CLA  | bA    | 841 | 1    | 54,58,73     | 2.27 | 21 (38%) | 64,95,113   | 2.89 | 30 (46%) |
| 11  | CLA  | aA    | 819 | 1    | 58,62,73     | 2.19 | 20 (34%) | 68,99,113   | 2.83 | 30 (44%) |
| 14  | SF4  | bC    | 102 | 3    | 0,12,12      | -    | -        | -           | -    | -        |
| 12  | F6C  | aA    | 832 | 1    | 57,59,74     | 2.65 | 26 (45%) | 65,96,114   | 4.09 | 35 (53%) |
| 11  | CLA  | bB    | 821 | -    | 59,63,73     | 2.20 | 21 (35%) | 70,101,113  | 2.74 | 28 (40%) |
| 11  | CLA  | bA    | 816 | 1    | 49,53,73     | 2.40 | 21 (42%) | 58,89,113   | 2.92 | 26 (44%) |
| 11  | CLA  | bB    | 812 | 2    | 69,73,73     | 2.02 | 19 (27%) | 82,113,113  | 2.55 | 32 (39%) |
| 11  | CLA  | bB    | 803 | -    | 65,69,73     | 1.99 | 19 (29%) | 77,108,113  | 2.61 | 27 (35%) |
| 11  | CLA  | bB    | 811 | 2    | 49,53,73     | 2.42 | 21 (42%) | 58,89,113   | 2.90 | 25 (43%) |
| 12  | F6C  | aL    | 202 | 2    | 72,74,74     | 2.42 | 27 (37%) | 83,114,114  | 3.42 | 37 (44%) |
| 11  | CLA  | cB    | 809 | 2    | 51,55,73     | 2.26 | 19 (37%) | 60,91,113   | 2.92 | 26 (43%) |
| 17  | LMT  | cA    | 853 | -    | 36,36,36     | 0.40 | 0        | 47,47,47    | 1.36 | 5 (10%)  |
| 11  | CLA  | aL    | 206 | -    | 69,73,73     | 1.99 | 20 (28%) | 82,113,113  | 2.59 | 31 (37%) |
| 11  | CLA  | aA    | 815 | 1    | 49,53,73     | 2.39 | 20 (40%) | 58,89,113   | 2.93 | 25 (43%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 11  | CLA  | aA    | 843 | 1    | 55,59,73     | 2.25 | 20 (36%) | 64,96,113   | 2.85 | 31 (48%) |
| 11  | CLA  | bA    | 814 | 1    | 69,73,73     | 2.01 | 20 (28%) | 82,113,113  | 2.63 | 31 (37%) |
| 11  | CLA  | aA    | 808 | 1    | 55,59,73     | 2.25 | 21 (38%) | 64,96,113   | 2.94 | 28 (43%) |
| 13  | PQN  | aB    | 841 | -    | 29,29,34     | 1.71 | 2 (6%)   | 37,39,45    | 1.25 | 4 (10%)  |
| 11  | CLA  | bA    | 805 | 1    | 49,53,73     | 2.42 | 21 (42%) | 58,89,113   | 2.99 | 26 (44%) |
| 11  | CLA  | cA    | 840 | 1    | 69,73,73     | 2.00 | 20 (28%) | 82,113,113  | 2.78 | 34 (41%) |
| 11  | CLA  | aA    | 811 | 1    | 49,53,73     | 2.41 | 20 (40%) | 58,89,113   | 2.95 | 24 (41%) |
| 11  | CLA  | aA    | 812 | 1    | 69,73,73     | 2.03 | 20 (28%) | 82,113,113  | 2.53 | 29 (35%) |
| 11  | CLA  | cB    | 834 | -    | 49,53,73     | 2.42 | 20 (40%) | 58,89,113   | 2.88 | 26 (44%) |
| 11  | CLA  | aB    | 836 | 2    | 55,59,73     | 2.24 | 20 (36%) | 64,96,113   | 2.90 | 30 (46%) |
| 14  | SF4  | aC    | 101 | 3    | 0,12,12      | -    | -        | -           | -    | -        |
| 11  | CLA  | bB    | 826 | 2    | 65,69,73     | 2.02 | 21 (32%) | 77,108,113  | 2.71 | 31 (40%) |
| 12  | F6C  | cB    | 824 | -    | 64,66,74     | 2.49 | 24 (37%) | 73,104,114  | 3.99 | 36 (49%) |
| 11  | CLA  | cB    | 807 | 2    | 65,69,73     | 2.02 | 19 (29%) | 77,108,113  | 2.69 | 31 (40%) |
| 11  | CLA  | aB    | 820 | 2    | 49,53,73     | 2.37 | 20 (40%) | 58,89,113   | 3.01 | 26 (44%) |
| 11  | CLA  | cA    | 813 | 1    | 58,62,73     | 2.19 | 20 (34%) | 68,99,113   | 2.74 | 28 (41%) |
| 11  | CLA  | bA    | 837 | 1    | 49,53,73     | 2.39 | 21 (42%) | 58,89,113   | 3.02 | 27 (46%) |
| 11  | CLA  | aB    | 805 | 2    | 69,73,73     | 1.99 | 21 (30%) | 82,113,113  | 2.63 | 30 (36%) |
| 11  | CLA  | aB    | 817 | 2    | 64,68,73     | 2.07 | 19 (29%) | 76,107,113  | 2.75 | 31 (40%) |
| 11  | CLA  | bA    | 836 | 1    | 49,53,73     | 2.30 | 18 (36%) | 58,89,113   | 2.84 | 27 (46%) |
| 11  | CLA  | cB    | 813 | 2    | 60,64,73     | 2.14 | 21 (35%) | 71,102,113  | 2.71 | 30 (42%) |
| 11  | CLA  | bK    | 101 | 7    | 42,46,73     | 2.31 | 17 (40%) | 49,79,113   | 3.08 | 25 (51%) |
| 11  | CLA  | aA    | 802 | -    | 69,73,73     | 1.98 | 19 (27%) | 82,113,113  | 2.76 | 36 (43%) |
| 11  | CLA  | cB    | 829 | 2    | 49,53,73     | 2.36 | 18 (36%) | 58,89,113   | 2.99 | 28 (48%) |
| 15  | BCR  | cK    | 102 | -    | 41,41,41     | 1.06 | 3 (7%)   | 56,56,56    | 1.30 | 8 (14%)  |
| 11  | CLA  | bB    | 831 | 2    | 60,64,73     | 2.16 | 21 (35%) | 71,102,113  | 2.94 | 32 (45%) |
| 11  | CLA  | cB    | 801 | 2    | 69,73,73     | 1.93 | 18 (26%) | 82,113,113  | 2.72 | 34 (41%) |
| 15  | BCR  | aL    | 203 | -    | 41,41,41     | 1.11 | 3 (7%)   | 56,56,56    | 1.26 | 7 (12%)  |
| 11  | CLA  | cA    | 811 | 1    | 49,53,73     | 2.41 | 20 (40%) | 58,89,113   | 2.96 | 26 (44%) |
| 11  | CLA  | cB    | 810 | 2    | 49,53,73     | 2.37 | 19 (38%) | 58,89,113   | 2.99 | 28 (48%) |
| 11  | CLA  | bB    | 808 | 2    | 69,73,73     | 1.95 | 19 (27%) | 82,113,113  | 2.58 | 31 (37%) |
| 11  | CLA  | cA    | 821 | 1    | 65,69,73     | 2.05 | 21 (32%) | 77,108,113  | 2.59 | 32 (41%) |
| 11  | CLA  | cA    | 818 | 1    | 58,62,73     | 2.13 | 20 (34%) | 68,99,113   | 2.91 | 28 (41%) |
| 15  | BCR  | bL    | 207 | -    | 41,41,41     | 1.06 | 2 (4%)   | 56,56,56    | 1.43 | 11 (19%) |
| 15  | BCR  | bI    | 101 | -    | 41,41,41     | 1.03 | 3 (7%)   | 56,56,56    | 1.25 | 6 (10%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 11  | CLA  | bA    | 820 | 1    | 69,73,73     | 1.99 | 19 (27%) | 82,113,113  | 2.58 | 32 (39%) |
| 11  | CLA  | cB    | 822 | 2    | 49,53,73     | 2.35 | 18 (36%) | 58,89,113   | 3.11 | 25 (43%) |
| 15  | BCR  | bL    | 203 | -    | 41,41,41     | 1.11 | 3 (7%)   | 56,56,56    | 1.24 | 6 (10%)  |
| 11  | CLA  | aA    | 825 | 1    | 69,73,73     | 1.98 | 20 (28%) | 82,113,113  | 2.53 | 33 (40%) |
| 11  | CLA  | aB    | 815 | 2    | 59,63,73     | 2.16 | 21 (35%) | 70,101,113  | 2.76 | 30 (42%) |
| 14  | SF4  | aC    | 102 | 3    | 0,12,12      | -    | -        | -           |      |          |
| 18  | LMG  | cB    | 847 | -    | 46,46,55     | 0.82 | 1 (2%)   | 54,54,63    | 1.38 | 8 (14%)  |
| 11  | CLA  | aA    | 813 | 1    | 58,62,73     | 2.19 | 20 (34%) | 68,99,113   | 2.74 | 28 (41%) |
| 12  | F6C  | bL    | 202 | 2    | 72,74,74     | 2.43 | 27 (37%) | 83,114,114  | 3.42 | 37 (44%) |
| 15  | BCR  | bA    | 851 | -    | 41,41,41     | 1.03 | 2 (4%)   | 56,56,56    | 1.25 | 7 (12%)  |
| 11  | CLA  | aK    | 103 | -    | 55,59,73     | 2.25 | 21 (38%) | 64,96,113   | 2.90 | 29 (45%) |
| 11  | CLA  | bA    | 817 | -    | 53,57,73     | 2.30 | 20 (37%) | 61,93,113   | 2.86 | 28 (45%) |
| 11  | CLA  | bA    | 834 | 1    | 69,73,73     | 1.98 | 20 (28%) | 82,113,113  | 2.59 | 32 (39%) |
| 11  | CLA  | bB    | 823 | 2    | 58,62,73     | 2.17 | 21 (36%) | 68,99,113   | 2.81 | 31 (45%) |
| 11  | CLA  | aB    | 812 | 2    | 69,73,73     | 2.02 | 19 (27%) | 82,113,113  | 2.56 | 32 (39%) |
| 11  | CLA  | cB    | 821 | -    | 59,63,73     | 2.20 | 21 (35%) | 70,101,113  | 2.73 | 28 (40%) |
| 14  | SF4  | cA    | 846 | 2,1  | 0,12,12      | -    | -        | -           |      |          |
| 11  | CLA  | aB    | 832 | 2    | 49,53,73     | 2.41 | 21 (42%) | 58,89,113   | 2.96 | 27 (46%) |
| 11  | CLA  | cB    | 820 | 2    | 49,53,73     | 2.37 | 20 (40%) | 58,89,113   | 3.01 | 25 (43%) |
| 11  | CLA  | cA    | 802 | -    | 69,73,73     | 1.97 | 19 (27%) | 82,113,113  | 2.77 | 36 (43%) |
| 11  | CLA  | bA    | 822 | -    | 69,73,73     | 2.00 | 19 (27%) | 82,113,113  | 2.47 | 30 (36%) |
| 11  | CLA  | cB    | 828 | 2    | 59,63,73     | 2.17 | 18 (30%) | 70,101,113  | 2.70 | 30 (42%) |
| 11  | CLA  | bA    | 810 | 1    | 49,53,73     | 2.36 | 21 (42%) | 58,89,113   | 2.92 | 29 (50%) |
| 11  | CLA  | aB    | 823 | 2    | 58,62,73     | 2.16 | 21 (36%) | 68,99,113   | 2.81 | 31 (45%) |
| 11  | CLA  | cA    | 814 | 1    | 69,73,73     | 2.01 | 20 (28%) | 82,113,113  | 2.62 | 31 (37%) |
| 11  | CLA  | cB    | 838 | 2    | 51,55,73     | 2.31 | 20 (39%) | 60,91,113   | 3.01 | 28 (46%) |
| 11  | CLA  | aA    | 829 | 1    | 69,73,73     | 2.01 | 21 (30%) | 82,113,113  | 4.38 | 32 (39%) |
| 11  | CLA  | aA    | 841 | 1    | 54,58,73     | 2.27 | 21 (38%) | 64,95,113   | 2.88 | 30 (46%) |
| 11  | CLA  | bA    | 806 | 1    | 69,73,73     | 1.99 | 20 (28%) | 82,113,113  | 2.63 | 32 (39%) |
| 13  | PQN  | aA    | 845 | -    | 34,34,34     | 1.63 | 2 (5%)   | 43,45,45    | 1.16 | 4 (9%)   |
| 12  | F6C  | cA    | 844 | -    | 72,74,74     | 2.38 | 26 (36%) | 83,114,114  | 3.66 | 37 (44%) |
| 12  | F6C  | bA    | 844 | -    | 72,74,74     | 2.37 | 25 (34%) | 83,114,114  | 3.66 | 37 (44%) |
| 10  | CL0  | cA    | 801 | 1    | 58,73,73     | 3.12 | 16 (27%) | 60,113,113  | 2.64 | 18 (30%) |
| 18  | LMG  | bB    | 847 | -    | 46,46,55     | 0.82 | 1 (2%)   | 54,54,63    | 1.37 | 8 (14%)  |
| 11  | CLA  | cB    | 818 | -    | 69,73,73     | 1.99 | 20 (28%) | 82,113,113  | 2.51 | 26 (31%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 11  | CLA  | aA    | 806 | 1    | 69,73,73     | 1.98 | 19 (27%) | 82,113,113  | 2.64 | 32 (39%) |
| 11  | CLA  | bA    | 823 | 1    | 49,53,73     | 2.34 | 20 (40%) | 58,89,113   | 3.06 | 24 (41%) |
| 11  | CLA  | bB    | 819 | 2    | 51,55,73     | 2.33 | 21 (41%) | 60,91,113   | 2.84 | 28 (46%) |
| 11  | CLA  | cL    | 204 | 8    | 69,73,73     | 1.99 | 21 (30%) | 82,113,113  | 2.59 | 27 (32%) |
| 11  | CLA  | bB    | 820 | 2    | 49,53,73     | 2.36 | 20 (40%) | 58,89,113   | 3.00 | 25 (43%) |
| 11  | CLA  | cA    | 804 | 1    | 49,53,73     | 2.41 | 20 (40%) | 58,89,113   | 2.95 | 26 (44%) |
| 13  | PQN  | bB    | 841 | -    | 29,29,34     | 1.72 | 2 (6%)   | 37,39,45    | 1.26 | 5 (13%)  |
| 12  | F6C  | aA    | 827 | -    | 62,64,74     | 2.55 | 25 (40%) | 71,102,114  | 4.02 | 36 (50%) |
| 15  | BCR  | bA    | 850 | -    | 41,41,41     | 1.04 | 2 (4%)   | 56,56,56    | 1.21 | 4 (7%)   |
| 11  | CLA  | cL    | 205 | 8    | 69,73,73     | 1.98 | 20 (28%) | 82,113,113  | 2.54 | 28 (34%) |
| 15  | BCR  | bB    | 845 | -    | 41,41,41     | 1.07 | 2 (4%)   | 56,56,56    | 1.27 | 5 (8%)   |
| 11  | CLA  | aB    | 813 | 2    | 60,64,73     | 2.13 | 20 (33%) | 71,102,113  | 2.71 | 30 (42%) |
| 11  | CLA  | bA    | 819 | 1    | 58,62,73     | 2.19 | 20 (34%) | 68,99,113   | 2.83 | 30 (44%) |
| 11  | CLA  | cA    | 838 | 1    | 55,59,73     | 2.22 | 19 (34%) | 64,96,113   | 2.92 | 32 (50%) |
| 11  | CLA  | bA    | 821 | 1    | 65,69,73     | 2.05 | 21 (32%) | 77,108,113  | 2.59 | 32 (41%) |
| 11  | CLA  | aB    | 829 | 2    | 49,53,73     | 2.36 | 18 (36%) | 58,89,113   | 2.98 | 28 (48%) |
| 11  | CLA  | cB    | 812 | 2    | 69,73,73     | 2.01 | 19 (27%) | 82,113,113  | 2.54 | 32 (39%) |
| 11  | CLA  | cB    | 811 | 2    | 49,53,73     | 2.41 | 21 (42%) | 58,89,113   | 2.90 | 25 (43%) |
| 11  | CLA  | aA    | 840 | 1    | 69,73,73     | 1.99 | 20 (28%) | 82,113,113  | 2.78 | 34 (41%) |
| 11  | CLA  | cB    | 832 | 2    | 49,53,73     | 2.42 | 21 (42%) | 58,89,113   | 2.95 | 27 (46%) |
| 11  | CLA  | cA    | 809 | 1    | 49,53,73     | 2.38 | 21 (42%) | 58,89,113   | 3.01 | 28 (48%) |
| 11  | CLA  | aB    | 834 | -    | 49,53,73     | 2.42 | 20 (40%) | 58,89,113   | 2.88 | 26 (44%) |
| 11  | CLA  | bB    | 815 | 2    | 59,63,73     | 2.16 | 21 (35%) | 70,101,113  | 2.77 | 30 (42%) |
| 11  | CLA  | cB    | 833 | 2    | 49,53,73     | 2.41 | 20 (40%) | 58,89,113   | 3.01 | 28 (48%) |
| 11  | CLA  | cB    | 802 | -    | 61,65,73     | 2.11 | 20 (32%) | 72,103,113  | 2.86 | 31 (43%) |
| 11  | CLA  | aA    | 820 | 1    | 69,73,73     | 1.99 | 19 (27%) | 82,113,113  | 2.58 | 32 (39%) |
| 11  | CLA  | bB    | 805 | 2    | 69,73,73     | 1.99 | 21 (30%) | 82,113,113  | 2.63 | 30 (36%) |
| 12  | F6C  | bA    | 830 | 1    | 72,74,74     | 2.35 | 24 (33%) | 83,114,114  | 3.56 | 36 (43%) |
| 13  | PQN  | cA    | 845 | -    | 34,34,34     | 1.63 | 2 (5%)   | 43,45,45    | 1.17 | 4 (9%)   |
| 11  | CLA  | aA    | 817 | -    | 53,57,73     | 2.30 | 20 (37%) | 61,93,113   | 2.86 | 28 (45%) |
| 18  | LMG  | aB    | 847 | -    | 46,46,55     | 0.82 | 1 (2%)   | 54,54,63    | 1.37 | 8 (14%)  |
| 11  | CLA  | cA    | 842 | -    | 49,53,73     | 2.40 | 21 (42%) | 58,89,113   | 2.98 | 27 (46%) |
| 11  | CLA  | bA    | 818 | 1    | 58,62,73     | 2.13 | 20 (34%) | 68,99,113   | 2.90 | 28 (41%) |
| 11  | CLA  | bA    | 825 | 1    | 69,73,73     | 1.98 | 20 (28%) | 82,113,113  | 2.53 | 34 (41%) |
| 11  | CLA  | cB    | 804 | 2    | 54,58,73     | 2.26 | 21 (38%) | 64,95,113   | 2.97 | 31 (48%) |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 15  | BCR  | bB    | 843 | -    | 41,41,41     | 1.04 | 2 (4%)   | 56,56,56    | 1.17 | 3 (5%)   |
| 11  | CLA  | bK    | 103 | -    | 55,59,73     | 2.25 | 21 (38%) | 64,96,113   | 2.91 | 29 (45%) |
| 11  | CLA  | aA    | 805 | 1    | 49,53,73     | 2.41 | 21 (42%) | 58,89,113   | 2.98 | 26 (44%) |
| 11  | CLA  | aB    | 840 | 2    | 49,53,73     | 2.35 | 18 (36%) | 58,89,113   | 2.93 | 26 (44%) |
| 11  | CLA  | cA    | 807 | 1    | 69,73,73     | 1.98 | 20 (28%) | 82,113,113  | 2.64 | 32 (39%) |
| 15  | BCR  | cB    | 848 | -    | 41,41,41     | 1.00 | 2 (4%)   | 56,56,56    | 1.44 | 8 (14%)  |
| 11  | CLA  | aB    | 810 | 2    | 49,53,73     | 2.37 | 19 (38%) | 58,89,113   | 2.99 | 28 (48%) |
| 11  | CLA  | aB    | 806 | 2    | 69,73,73     | 1.98 | 19 (27%) | 82,113,113  | 2.56 | 29 (35%) |
| 11  | CLA  | cA    | 820 | 1    | 69,73,73     | 2.00 | 19 (27%) | 82,113,113  | 2.57 | 32 (39%) |
| 14  | SF4  | cC    | 101 | 3    | 0,12,12      | -    | -        | -           | -    | -        |
| 11  | CLA  | cA    | 810 | 1    | 49,53,73     | 2.36 | 21 (42%) | 58,89,113   | 2.92 | 28 (48%) |
| 11  | CLA  | aA    | 842 | -    | 49,53,73     | 2.39 | 21 (42%) | 58,89,113   | 2.98 | 27 (46%) |
| 11  | CLA  | aB    | 830 | 2    | 53,57,73     | 2.30 | 21 (39%) | 61,93,113   | 2.86 | 28 (45%) |
| 16  | LHG  | cA    | 852 | -    | 48,48,48     | 0.62 | 2 (4%)   | 51,54,54    | 1.26 | 6 (11%)  |
| 11  | CLA  | aA    | 835 | 1    | 69,73,73     | 1.98 | 19 (27%) | 82,113,113  | 2.59 | 29 (35%) |
| 15  | BCR  | cI    | 103 | -    | 41,41,41     | 1.04 | 3 (7%)   | 56,56,56    | 1.25 | 6 (10%)  |
| 17  | LMT  | aA    | 853 | -    | 36,36,36     | 0.40 | 0        | 47,47,47    | 1.36 | 5 (10%)  |
| 11  | CLA  | cA    | 819 | 1    | 58,62,73     | 2.19 | 20 (34%) | 68,99,113   | 2.83 | 30 (44%) |
| 11  | CLA  | bB    | 832 | 2    | 49,53,73     | 2.42 | 21 (42%) | 58,89,113   | 2.96 | 27 (46%) |
| 12  | F6C  | bA    | 832 | 1    | 57,59,74     | 2.65 | 26 (45%) | 65,96,114   | 4.10 | 36 (55%) |
| 15  | BCR  | aB    | 846 | -    | 41,41,41     | 1.04 | 2 (4%)   | 56,56,56    | 1.21 | 5 (8%)   |
| 12  | F6C  | cL    | 202 | 2    | 72,74,74     | 2.42 | 27 (37%) | 83,114,114  | 3.42 | 37 (44%) |
| 11  | CLA  | aA    | 833 | 1    | 69,73,73     | 2.01 | 20 (28%) | 82,113,113  | 2.56 | 28 (34%) |
| 11  | CLA  | aA    | 807 | 1    | 69,73,73     | 1.98 | 20 (28%) | 82,113,113  | 2.63 | 33 (40%) |
| 15  | BCR  | cB    | 845 | -    | 41,41,41     | 1.07 | 2 (4%)   | 56,56,56    | 1.28 | 5 (8%)   |
| 11  | CLA  | cK    | 101 | 7    | 42,46,73     | 2.31 | 17 (40%) | 49,79,113   | 3.09 | 25 (51%) |
| 11  | CLA  | bA    | 802 | -    | 69,73,73     | 1.97 | 19 (27%) | 82,113,113  | 2.76 | 36 (43%) |
| 11  | CLA  | aA    | 824 | -    | 55,59,73     | 2.24 | 19 (34%) | 64,96,113   | 2.89 | 29 (45%) |
| 11  | CLA  | bA    | 804 | 1    | 49,53,73     | 2.42 | 20 (40%) | 58,89,113   | 2.96 | 26 (44%) |
| 11  | CLA  | cL    | 206 | -    | 69,73,73     | 1.98 | 20 (28%) | 82,113,113  | 2.59 | 30 (36%) |
| 11  | CLA  | bA    | 828 | 1    | 64,68,73     | 2.04 | 19 (29%) | 76,107,113  | 2.77 | 31 (40%) |
| 11  | CLA  | aA    | 810 | 1    | 49,53,73     | 2.36 | 21 (42%) | 58,89,113   | 2.93 | 29 (50%) |
| 15  | BCR  | bA    | 848 | -    | 41,41,41     | 1.09 | 2 (4%)   | 56,56,56    | 1.24 | 4 (7%)   |
| 11  | CLA  | bL    | 205 | 8    | 69,73,73     | 1.99 | 20 (28%) | 82,113,113  | 2.55 | 28 (34%) |
| 11  | CLA  | cB    | 840 | 2    | 49,53,73     | 2.35 | 18 (36%) | 58,89,113   | 2.94 | 26 (44%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 11  | CLA  | aB    | 828 | 2    | 59,63,73     | 2.16 | 18 (30%) | 70,101,113  | 2.69 | 30 (42%) |
| 11  | CLA  | cA    | 816 | 1    | 49,53,73     | 2.40 | 21 (42%) | 58,89,113   | 2.92 | 25 (43%) |
| 14  | SF4  | bA    | 846 | 2,1  | 0,12,12      | -    | -        | -           | -    | -        |
| 11  | CLA  | cA    | 839 | 1    | 69,73,73     | 1.97 | 20 (28%) | 82,113,113  | 2.57 | 30 (36%) |
| 11  | CLA  | aB    | 814 | 2    | 49,53,73     | 2.38 | 20 (40%) | 58,89,113   | 2.99 | 27 (46%) |
| 15  | BCR  | cA    | 849 | -    | 41,41,41     | 1.07 | 2 (4%)   | 56,56,56    | 1.30 | 6 (10%)  |
| 11  | CLA  | aA    | 837 | 1    | 49,53,73     | 2.39 | 21 (42%) | 58,89,113   | 3.02 | 27 (46%) |
| 11  | CLA  | aB    | 827 | 2    | 69,73,73     | 1.97 | 19 (27%) | 82,113,113  | 2.43 | 28 (34%) |
| 15  | BCR  | aB    | 843 | -    | 41,41,41     | 1.05 | 2 (4%)   | 56,56,56    | 1.17 | 3 (5%)   |
| 15  | BCR  | aA    | 848 | -    | 41,41,41     | 1.09 | 2 (4%)   | 56,56,56    | 1.24 | 4 (7%)   |
| 12  | F6C  | aB    | 824 | -    | 64,66,74     | 2.49 | 24 (37%) | 73,104,114  | 3.99 | 36 (49%) |
| 15  | BCR  | aL    | 208 | -    | 41,41,41     | 1.03 | 2 (4%)   | 56,56,56    | 1.29 | 8 (14%)  |
| 15  | BCR  | aL    | 207 | -    | 41,41,41     | 1.05 | 2 (4%)   | 56,56,56    | 1.43 | 11 (19%) |
| 15  | BCR  | aB    | 842 | -    | 41,41,41     | 1.03 | 2 (4%)   | 56,56,56    | 1.26 | 5 (8%)   |
| 15  | BCR  | aM    | 101 | -    | 41,41,41     | 1.02 | 2 (4%)   | 56,56,56    | 1.32 | 8 (14%)  |
| 15  | BCR  | cL    | 207 | -    | 41,41,41     | 1.06 | 2 (4%)   | 56,56,56    | 1.42 | 10 (17%) |
| 11  | CLA  | bB    | 813 | 2    | 60,64,73     | 2.13 | 21 (35%) | 71,102,113  | 2.70 | 30 (42%) |
| 11  | CLA  | bB    | 829 | 2    | 49,53,73     | 2.36 | 18 (36%) | 58,89,113   | 2.98 | 28 (48%) |
| 11  | CLA  | cB    | 825 | 2    | 69,73,73     | 2.01 | 20 (28%) | 82,113,113  | 2.62 | 29 (35%) |
| 15  | BCR  | aB    | 845 | -    | 41,41,41     | 1.07 | 2 (4%)   | 56,56,56    | 1.27 | 5 (8%)   |
| 15  | BCR  | bB    | 844 | -    | 41,41,41     | 1.03 | 2 (4%)   | 56,56,56    | 1.24 | 5 (8%)   |
| 11  | CLA  | aB    | 801 | 2    | 69,73,73     | 1.93 | 18 (26%) | 82,113,113  | 2.72 | 34 (41%) |
| 11  | CLA  | cA    | 841 | 1    | 54,58,73     | 2.27 | 21 (38%) | 64,95,113   | 2.88 | 30 (46%) |
| 11  | CLA  | bA    | 839 | 1    | 69,73,73     | 1.98 | 20 (28%) | 82,113,113  | 2.58 | 30 (36%) |
| 11  | CLA  | aA    | 804 | 1    | 49,53,73     | 2.41 | 20 (40%) | 58,89,113   | 2.95 | 26 (44%) |
| 11  | CLA  | cB    | 831 | 2    | 60,64,73     | 2.16 | 21 (35%) | 71,102,113  | 2.94 | 33 (46%) |
| 11  | CLA  | aB    | 826 | 2    | 65,69,73     | 2.02 | 21 (32%) | 77,108,113  | 2.70 | 31 (40%) |
| 11  | CLA  | aA    | 834 | 1    | 69,73,73     | 1.98 | 20 (28%) | 82,113,113  | 2.59 | 32 (39%) |
| 11  | CLA  | bB    | 834 | -    | 49,53,73     | 2.42 | 20 (40%) | 58,89,113   | 2.89 | 26 (44%) |
| 16  | LHG  | bA    | 852 | -    | 48,48,48     | 0.61 | 1 (2%)   | 51,54,54    | 1.27 | 6 (11%)  |
| 11  | CLA  | cA    | 822 | -    | 69,73,73     | 2.00 | 19 (27%) | 82,113,113  | 2.47 | 30 (36%) |
| 11  | CLA  | aA    | 809 | 1    | 49,53,73     | 2.38 | 21 (42%) | 58,89,113   | 3.02 | 28 (48%) |
| 11  | CLA  | bB    | 806 | 2    | 69,73,73     | 1.98 | 19 (27%) | 82,113,113  | 2.57 | 30 (36%) |
| 11  | CLA  | cA    | 803 | -    | 60,64,73     | 2.11 | 18 (30%) | 71,102,113  | 2.76 | 32 (45%) |
| 15  | BCR  | cA    | 851 | -    | 41,41,41     | 1.03 | 2 (4%)   | 56,56,56    | 1.25 | 7 (12%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 11  | CLA  | aA    | 838 | 1    | 55,59,73     | 2.23 | 19 (34%) | 64,96,113   | 2.92 | 32 (50%) |
| 14  | SF4  | cC    | 102 | 3    | 0,12,12      | -    | -        | -           |      |          |
| 15  | BCR  | aA    | 850 | -    | 41,41,41     | 1.05 | 2 (4%)   | 56,56,56    | 1.22 | 4 (7%)   |
| 15  | BCR  | aI    | 101 | -    | 41,41,41     | 1.03 | 3 (7%)   | 56,56,56    | 1.25 | 6 (10%)  |
| 11  | CLA  | aB    | 807 | 2    | 65,69,73     | 2.02 | 19 (29%) | 77,108,113  | 2.69 | 31 (40%) |
| 11  | CLA  | cB    | 827 | 2    | 69,73,73     | 1.97 | 19 (27%) | 82,113,113  | 2.44 | 28 (34%) |
| 11  | CLA  | aA    | 818 | 1    | 58,62,73     | 2.13 | 20 (34%) | 68,99,113   | 2.90 | 28 (41%) |
| 12  | F6C  | aA    | 830 | 1    | 72,74,74     | 2.35 | 24 (33%) | 83,114,114  | 3.57 | 36 (43%) |
| 11  | CLA  | bB    | 836 | 2    | 55,59,73     | 2.25 | 20 (36%) | 64,96,113   | 2.89 | 29 (45%) |
| 11  | CLA  | bB    | 840 | 2    | 49,53,73     | 2.35 | 19 (38%) | 58,89,113   | 2.94 | 26 (44%) |
| 15  | BCR  | aA    | 847 | -    | 41,41,41     | 1.03 | 2 (4%)   | 56,56,56    | 1.37 | 7 (12%)  |
| 11  | CLA  | cB    | 805 | 2    | 69,73,73     | 1.99 | 20 (28%) | 82,113,113  | 2.62 | 30 (36%) |
| 11  | CLA  | aB    | 804 | 2    | 54,58,73     | 2.26 | 21 (38%) | 64,95,113   | 2.98 | 31 (48%) |
| 11  | CLA  | cA    | 835 | 1    | 69,73,73     | 1.98 | 19 (27%) | 82,113,113  | 2.59 | 29 (35%) |
| 11  | CLA  | aA    | 822 | -    | 69,73,73     | 2.00 | 19 (27%) | 82,113,113  | 2.47 | 29 (35%) |
| 11  | CLA  | aB    | 819 | 2    | 51,55,73     | 2.32 | 21 (41%) | 60,91,113   | 2.84 | 28 (46%) |
| 11  | CLA  | bA    | 840 | 1    | 69,73,73     | 2.00 | 20 (28%) | 82,113,113  | 2.78 | 34 (41%) |
| 11  | CLA  | cB    | 835 | -    | 49,53,73     | 2.41 | 21 (42%) | 58,89,113   | 2.98 | 27 (46%) |
| 11  | CLA  | aB    | 809 | 2    | 51,55,73     | 2.27 | 19 (37%) | 60,91,113   | 2.91 | 26 (43%) |
| 11  | CLA  | aB    | 837 | 2    | 59,63,73     | 2.16 | 20 (33%) | 70,101,113  | 2.73 | 29 (41%) |
| 15  | BCR  | aB    | 848 | -    | 41,41,41     | 0.99 | 2 (4%)   | 56,56,56    | 1.44 | 8 (14%)  |
| 11  | CLA  | cA    | 833 | 1    | 69,73,73     | 2.01 | 20 (28%) | 82,113,113  | 2.56 | 28 (34%) |
| 11  | CLA  | aB    | 838 | 2    | 51,55,73     | 2.30 | 20 (39%) | 60,91,113   | 3.00 | 28 (46%) |
| 11  | CLA  | cB    | 814 | 2    | 49,53,73     | 2.38 | 20 (40%) | 58,89,113   | 2.98 | 27 (46%) |
| 12  | F6C  | cA    | 832 | 1    | 57,59,74     | 2.65 | 26 (45%) | 65,96,114   | 4.09 | 35 (53%) |
| 11  | CLA  | cB    | 803 | -    | 65,69,73     | 2.00 | 19 (29%) | 77,108,113  | 2.61 | 27 (35%) |
| 11  | CLA  | cB    | 826 | 2    | 65,69,73     | 2.02 | 21 (32%) | 77,108,113  | 2.71 | 31 (40%) |
| 15  | BCR  | bB    | 846 | -    | 41,41,41     | 1.04 | 2 (4%)   | 56,56,56    | 1.22 | 5 (8%)   |
| 11  | CLA  | aB    | 818 | -    | 69,73,73     | 1.99 | 21 (30%) | 82,113,113  | 2.51 | 26 (31%) |
| 12  | F6C  | cA    | 830 | 1    | 72,74,74     | 2.35 | 24 (33%) | 83,114,114  | 3.56 | 36 (43%) |
| 11  | CLA  | cA    | 829 | 1    | 69,73,73     | 2.01 | 20 (28%) | 82,113,113  | 4.38 | 32 (39%) |
| 11  | CLA  | bA    | 803 | -    | 60,64,73     | 2.10 | 18 (30%) | 71,102,113  | 2.76 | 32 (45%) |
| 15  | BCR  | cA    | 847 | -    | 41,41,41     | 1.03 | 2 (4%)   | 56,56,56    | 1.37 | 7 (12%)  |
| 11  | CLA  | bB    | 827 | 2    | 69,73,73     | 1.97 | 19 (27%) | 82,113,113  | 2.44 | 28 (34%) |
| 11  | CLA  | bA    | 838 | 1    | 55,59,73     | 2.22 | 19 (34%) | 64,96,113   | 2.93 | 32 (50%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 11  | CLA  | aB    | 839 | -    | 69,73,73     | 1.97 | 20 (28%) | 82,113,113  | 2.49 | 28 (34%) |
| 15  | BCR  | bB    | 842 | -    | 41,41,41     | 1.03 | 2 (4%)   | 56,56,56    | 1.26 | 5 (8%)   |
| 11  | CLA  | bB    | 825 | 2    | 69,73,73     | 2.01 | 20 (28%) | 82,113,113  | 2.62 | 30 (36%) |
| 15  | BCR  | aA    | 849 | -    | 41,41,41     | 1.07 | 2 (4%)   | 56,56,56    | 1.31 | 6 (10%)  |
| 11  | CLA  | cA    | 831 | 1    | 69,73,73     | 1.98 | 19 (27%) | 82,113,113  | 2.56 | 30 (36%) |
| 11  | CLA  | cA    | 815 | 1    | 49,53,73     | 2.39 | 19 (38%) | 58,89,113   | 2.93 | 26 (44%) |
| 11  | CLA  | cK    | 103 | -    | 55,59,73     | 2.24 | 21 (38%) | 64,96,113   | 2.91 | 29 (45%) |
| 13  | PQN  | cB    | 841 | -    | 29,29,34     | 1.73 | 2 (6%)   | 37,39,45    | 1.27 | 5 (13%)  |
| 11  | CLA  | bA    | 809 | 1    | 49,53,73     | 2.38 | 21 (42%) | 58,89,113   | 3.01 | 28 (48%) |
| 11  | CLA  | bA    | 831 | 1    | 69,73,73     | 1.98 | 20 (28%) | 82,113,113  | 2.57 | 30 (36%) |
| 11  | CLA  | cA    | 808 | 1    | 55,59,73     | 2.25 | 21 (38%) | 64,96,113   | 2.94 | 28 (43%) |
| 11  | CLA  | aA    | 828 | 1    | 64,68,73     | 2.04 | 19 (29%) | 76,107,113  | 2.77 | 31 (40%) |
| 11  | CLA  | bB    | 835 | -    | 49,53,73     | 2.41 | 21 (42%) | 58,89,113   | 2.98 | 27 (46%) |
| 15  | BCR  | cB    | 846 | -    | 41,41,41     | 1.04 | 2 (4%)   | 56,56,56    | 1.21 | 5 (8%)   |
| 11  | CLA  | aA    | 814 | 1    | 69,73,73     | 2.01 | 20 (28%) | 82,113,113  | 2.62 | 31 (37%) |
| 15  | BCR  | cA    | 850 | -    | 41,41,41     | 1.05 | 2 (4%)   | 56,56,56    | 1.21 | 3 (5%)   |
| 11  | CLA  | cB    | 836 | 2    | 55,59,73     | 2.24 | 20 (36%) | 64,96,113   | 2.89 | 30 (46%) |
| 11  | CLA  | aA    | 836 | 1    | 49,53,73     | 2.30 | 18 (36%) | 58,89,113   | 2.85 | 26 (44%) |
| 12  | F6C  | bA    | 826 | -    | 72,74,74     | 2.45 | 23 (31%) | 83,114,114  | 3.44 | 34 (40%) |
| 11  | CLA  | bA    | 812 | 1    | 69,73,73     | 2.03 | 20 (28%) | 82,113,113  | 2.54 | 29 (35%) |
| 11  | CLA  | cA    | 812 | 1    | 69,73,73     | 2.03 | 20 (28%) | 82,113,113  | 2.53 | 28 (34%) |
| 12  | F6C  | bA    | 827 | -    | 62,64,74     | 2.54 | 24 (38%) | 71,102,114  | 4.02 | 36 (50%) |
| 11  | CLA  | bL    | 204 | 8    | 69,73,73     | 1.99 | 21 (30%) | 82,113,113  | 2.59 | 27 (32%) |
| 12  | F6C  | bB    | 824 | -    | 64,66,74     | 2.49 | 24 (37%) | 73,104,114  | 3.98 | 36 (49%) |
| 11  | CLA  | bB    | 833 | 2    | 49,53,73     | 2.41 | 20 (40%) | 58,89,113   | 3.01 | 28 (48%) |
| 11  | CLA  | cB    | 837 | 2    | 59,63,73     | 2.17 | 20 (33%) | 70,101,113  | 2.74 | 29 (41%) |
| 11  | CLA  | aB    | 802 | -    | 61,65,73     | 2.11 | 20 (32%) | 72,103,113  | 2.87 | 31 (43%) |
| 15  | BCR  | cB    | 842 | -    | 41,41,41     | 1.03 | 2 (4%)   | 56,56,56    | 1.26 | 5 (8%)   |
| 11  | CLA  | aB    | 816 | 2    | 63,67,73     | 2.12 | 20 (31%) | 74,105,113  | 2.69 | 30 (40%) |
| 11  | CLA  | aA    | 821 | 1    | 65,69,73     | 2.04 | 21 (32%) | 77,108,113  | 2.59 | 32 (41%) |
| 12  | F6C  | aA    | 826 | -    | 72,74,74     | 2.46 | 23 (31%) | 83,114,114  | 3.44 | 34 (40%) |
| 12  | F6C  | cA    | 827 | -    | 62,64,74     | 2.55 | 24 (38%) | 71,102,114  | 4.02 | 36 (50%) |
| 11  | CLA  | bB    | 801 | 2    | 69,73,73     | 1.93 | 19 (27%) | 82,113,113  | 2.72 | 34 (41%) |
| 11  | CLA  | aA    | 803 | -    | 60,64,73     | 2.11 | 18 (30%) | 71,102,113  | 2.76 | 32 (45%) |
| 14  | SF4  | aA    | 846 | 2,1  | 0,12,12      | -    | -        | -           | -    | -        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 11  | CLA  | bB    | 817 | 2    | 64,68,73     | 2.07 | 19 (29%) | 76,107,113  | 2.76 | 31 (40%) |
| 11  | CLA  | cB    | 808 | 2    | 69,73,73     | 1.95 | 20 (28%) | 82,113,113  | 2.58 | 31 (37%) |
| 11  | CLA  | bB    | 810 | 2    | 49,53,73     | 2.37 | 19 (38%) | 58,89,113   | 2.99 | 28 (48%) |
| 12  | F6C  | aA    | 844 | -    | 72,74,74     | 2.37 | 25 (34%) | 83,114,114  | 3.65 | 37 (44%) |
| 11  | CLA  | cA    | 828 | 1    | 64,68,73     | 2.04 | 20 (31%) | 76,107,113  | 2.77 | 31 (40%) |
| 11  | CLA  | aK    | 101 | 7    | 42,46,73     | 2.31 | 17 (40%) | 49,79,113   | 3.08 | 25 (51%) |
| 11  | CLA  | cB    | 815 | 2    | 59,63,73     | 2.16 | 21 (35%) | 70,101,113  | 2.76 | 30 (42%) |
| 15  | BCR  | bM    | 101 | -    | 41,41,41     | 1.02 | 2 (4%)   | 56,56,56    | 1.31 | 8 (14%)  |
| 11  | CLA  | bA    | 842 | -    | 49,53,73     | 2.39 | 21 (42%) | 58,89,113   | 2.97 | 27 (46%) |
| 11  | CLA  | cB    | 839 | -    | 69,73,73     | 1.98 | 20 (28%) | 82,113,113  | 2.49 | 28 (34%) |
| 11  | CLA  | cB    | 817 | 2    | 64,68,73     | 2.06 | 19 (29%) | 76,107,113  | 2.75 | 31 (40%) |
| 15  | BCR  | cB    | 843 | -    | 41,41,41     | 1.05 | 2 (4%)   | 56,56,56    | 1.17 | 3 (5%)   |
| 11  | CLA  | cA    | 825 | 1    | 69,73,73     | 1.98 | 20 (28%) | 82,113,113  | 2.53 | 33 (40%) |
| 11  | CLA  | cA    | 836 | 1    | 49,53,73     | 2.30 | 18 (36%) | 58,89,113   | 2.85 | 27 (46%) |
| 15  | BCR  | bK    | 102 | -    | 41,41,41     | 1.06 | 3 (7%)   | 56,56,56    | 1.30 | 8 (14%)  |
| 15  | BCR  | bA    | 849 | -    | 41,41,41     | 1.06 | 2 (4%)   | 56,56,56    | 1.31 | 6 (10%)  |
| 15  | BCR  | bL    | 208 | -    | 41,41,41     | 1.02 | 2 (4%)   | 56,56,56    | 1.28 | 8 (14%)  |
| 15  | BCR  | cA    | 848 | -    | 41,41,41     | 1.09 | 2 (4%)   | 56,56,56    | 1.24 | 4 (7%)   |
| 11  | CLA  | aB    | 835 | -    | 49,53,73     | 2.40 | 21 (42%) | 58,89,113   | 2.97 | 27 (46%) |
| 11  | CLA  | bB    | 807 | 2    | 65,69,73     | 2.02 | 19 (29%) | 77,108,113  | 2.69 | 31 (40%) |
| 16  | LHG  | aA    | 852 | -    | 48,48,48     | 0.62 | 2 (4%)   | 51,54,54    | 1.26 | 6 (11%)  |
| 10  | CL0  | aA    | 801 | 1    | 58,73,73     | 3.11 | 16 (27%) | 60,113,113  | 2.64 | 18 (30%) |
| 11  | CLA  | aA    | 823 | 1    | 49,53,73     | 2.34 | 20 (40%) | 58,89,113   | 3.06 | 25 (43%) |
| 11  | CLA  | cA    | 843 | 1    | 55,59,73     | 2.25 | 20 (36%) | 64,96,113   | 2.86 | 29 (45%) |
| 11  | CLA  | aB    | 822 | 2    | 49,53,73     | 2.35 | 18 (36%) | 58,89,113   | 3.12 | 25 (43%) |
| 11  | CLA  | aB    | 821 | -    | 59,63,73     | 2.21 | 21 (35%) | 70,101,113  | 2.74 | 28 (40%) |
| 11  | CLA  | bA    | 813 | 1    | 58,62,73     | 2.19 | 20 (34%) | 68,99,113   | 2.74 | 28 (41%) |
| 12  | F6C  | cA    | 826 | -    | 72,74,74     | 2.46 | 23 (31%) | 83,114,114  | 3.44 | 34 (40%) |
| 11  | CLA  | bA    | 843 | 1    | 55,59,73     | 2.25 | 20 (36%) | 64,96,113   | 2.85 | 31 (48%) |
| 11  | CLA  | bA    | 829 | 1    | 69,73,73     | 2.01 | 21 (30%) | 82,113,113  | 4.38 | 32 (39%) |
| 11  | CLA  | aB    | 803 | -    | 65,69,73     | 1.99 | 19 (29%) | 77,108,113  | 2.61 | 27 (35%) |
| 11  | CLA  | bL    | 206 | -    | 69,73,73     | 1.99 | 20 (28%) | 82,113,113  | 2.59 | 30 (36%) |
| 11  | CLA  | bB    | 804 | 2    | 54,58,73     | 2.26 | 21 (38%) | 64,95,113   | 2.97 | 31 (48%) |
| 15  | BCR  | cL    | 208 | -    | 41,41,41     | 1.03 | 2 (4%)   | 56,56,56    | 1.29 | 8 (14%)  |
| 11  | CLA  | bA    | 835 | 1    | 69,73,73     | 1.99 | 19 (27%) | 82,113,113  | 2.59 | 29 (35%) |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 11  | CLA  | bA    | 815 | 1    | 49,53,73     | 2.39 | 19 (38%) | 58,89,113   | 2.93 | 26 (44%) |
| 11  | CLA  | bB    | 809 | 2    | 51,55,73     | 2.27 | 19 (37%) | 60,91,113   | 2.92 | 27 (45%) |
| 11  | CLA  | bB    | 837 | 2    | 59,63,73     | 2.17 | 20 (33%) | 70,101,113  | 2.74 | 29 (41%) |
| 11  | CLA  | cB    | 830 | 2    | 53,57,73     | 2.30 | 21 (39%) | 61,93,113   | 2.86 | 27 (44%) |
| 15  | BCR  | bB    | 848 | -    | 41,41,41     | 1.00 | 2 (4%)   | 56,56,56    | 1.43 | 8 (14%)  |
| 11  | CLA  | bA    | 808 | 1    | 55,59,73     | 2.24 | 21 (38%) | 64,96,113   | 2.94 | 28 (43%) |
| 11  | CLA  | cB    | 806 | 2    | 69,73,73     | 1.98 | 19 (27%) | 82,113,113  | 2.56 | 30 (36%) |
| 11  | CLA  | bB    | 838 | 2    | 51,55,73     | 2.31 | 20 (39%) | 60,91,113   | 3.00 | 28 (46%) |
| 11  | CLA  | aB    | 833 | 2    | 49,53,73     | 2.41 | 20 (40%) | 58,89,113   | 3.01 | 28 (48%) |
| 11  | CLA  | bA    | 811 | 1    | 49,53,73     | 2.41 | 20 (40%) | 58,89,113   | 2.95 | 25 (43%) |
| 11  | CLA  | cB    | 823 | 2    | 58,62,73     | 2.16 | 21 (36%) | 68,99,113   | 2.80 | 31 (45%) |
| 11  | CLA  | aA    | 831 | 1    | 69,73,73     | 1.98 | 18 (26%) | 82,113,113  | 2.56 | 30 (36%) |
| 11  | CLA  | bA    | 807 | 1    | 69,73,73     | 1.98 | 20 (28%) | 82,113,113  | 2.64 | 32 (39%) |
| 11  | CLA  | aB    | 808 | 2    | 69,73,73     | 1.96 | 19 (27%) | 82,113,113  | 2.59 | 31 (37%) |
| 11  | CLA  | bB    | 818 | -    | 69,73,73     | 1.99 | 19 (27%) | 82,113,113  | 2.51 | 26 (31%) |
| 11  | CLA  | aB    | 811 | 2    | 49,53,73     | 2.41 | 21 (42%) | 58,89,113   | 2.90 | 25 (43%) |
| 15  | BCR  | cL    | 203 | -    | 41,41,41     | 1.11 | 3 (7%)   | 56,56,56    | 1.25 | 7 (12%)  |
| 11  | CLA  | cA    | 805 | 1    | 49,53,73     | 2.41 | 21 (42%) | 58,89,113   | 2.99 | 26 (44%) |
| 11  | CLA  | aL    | 204 | 8    | 69,73,73     | 1.99 | 21 (30%) | 82,113,113  | 2.59 | 26 (31%) |
| 11  | CLA  | bA    | 824 | -    | 55,59,73     | 2.24 | 19 (34%) | 64,96,113   | 2.89 | 29 (45%) |
| 11  | CLA  | cB    | 816 | 2    | 63,67,73     | 2.12 | 21 (33%) | 74,105,113  | 2.68 | 30 (40%) |
| 11  | CLA  | cB    | 819 | 2    | 51,55,73     | 2.32 | 21 (41%) | 60,91,113   | 2.84 | 28 (46%) |
| 11  | CLA  | aA    | 839 | 1    | 69,73,73     | 1.98 | 20 (28%) | 82,113,113  | 2.57 | 30 (36%) |
| 11  | CLA  | bB    | 839 | -    | 69,73,73     | 1.98 | 20 (28%) | 82,113,113  | 2.49 | 28 (34%) |
| 17  | LMT  | bA    | 853 | -    | 36,36,36     | 0.40 | 0        | 47,47,47    | 1.36 | 5 (10%)  |
| 11  | CLA  | bB    | 830 | 2    | 53,57,73     | 2.30 | 21 (39%) | 61,93,113   | 2.86 | 28 (45%) |
| 11  | CLA  | bB    | 822 | 2    | 49,53,73     | 2.36 | 19 (38%) | 58,89,113   | 3.12 | 25 (43%) |
| 14  | SF4  | bC    | 101 | 3    | 0,12,12      | -    | -        | -           | -    | -        |
| 11  | CLA  | bA    | 833 | 1    | 69,73,73     | 2.00 | 20 (28%) | 82,113,113  | 2.56 | 28 (34%) |
| 11  | CLA  | bB    | 816 | 2    | 63,67,73     | 2.12 | 21 (33%) | 74,105,113  | 2.68 | 32 (43%) |
| 11  | CLA  | cA    | 806 | 1    | 69,73,73     | 1.99 | 20 (28%) | 82,113,113  | 2.63 | 32 (39%) |
| 15  | BCR  | bA    | 847 | -    | 41,41,41     | 1.03 | 2 (4%)   | 56,56,56    | 1.37 | 7 (12%)  |
| 11  | CLA  | aL    | 205 | 8    | 69,73,73     | 1.99 | 21 (30%) | 82,113,113  | 2.54 | 28 (34%) |
| 11  | CLA  | cA    | 824 | -    | 55,59,73     | 2.23 | 19 (34%) | 64,96,113   | 2.88 | 29 (45%) |
| 15  | BCR  | cB    | 844 | -    | 41,41,41     | 1.03 | 2 (4%)   | 56,56,56    | 1.24 | 5 (8%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 11  | CLA  | aB    | 831 | 2    | 60,64,73     | 2.16 | 20 (33%) | 71,102,113  | 2.93 | 32 (45%) |

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   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 11  | CLA  | aA    | 816 | 1    | 1/1/11/20 | 4/15/91/115   | -       |
| 15  | BCR  | aK    | 102 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 11  | CLA  | cA    | 823 | 1    | 1/1/11/20 | 9/15/91/115   | -       |
| 15  | BCR  | aA    | 851 | -    | -         | 18/29/63/63   | 0/2/2/2 |
| 11  | CLA  | bB    | 802 | -    | 1/1/13/20 | 9/30/106/115  | -       |
| 15  | BCR  | aB    | 844 | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 11  | CLA  | cA    | 817 | -    | 1/1/11/20 | 7/20/96/115   | -       |
| 11  | CLA  | aB    | 825 | 2    | 1/1/15/20 | 10/39/115/115 | -       |
| 10  | CL0  | bA    | 801 | 1    | 3/3/20/25 | 7/37/135/135  | -       |
| 11  | CLA  | cA    | 837 | 1    | 1/1/11/20 | 3/15/91/115   | -       |
| 11  | CLA  | bB    | 828 | 2    | 1/1/13/20 | 5/27/103/115  | -       |
| 13  | PQN  | bA    | 845 | -    | -         | 2/23/43/43    | 0/2/2/2 |
| 11  | CLA  | cA    | 834 | 1    | 1/1/15/20 | 9/39/115/115  | -       |
| 15  | BCR  | cM    | 101 | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 11  | CLA  | bB    | 814 | 2    | 1/1/11/20 | 7/15/91/115   | -       |
| 11  | CLA  | bA    | 841 | 1    | 1/1/12/20 | 4/21/97/115   | -       |
| 11  | CLA  | aA    | 819 | 1    | 1/1/12/20 | 12/26/102/115 | -       |
| 14  | SF4  | bC    | 102 | 3    | -         | -             | 0/6/5/5 |
| 12  | F6C  | aA    | 832 | 1    | 1/1/7/16  | 12/23/79/97   | -       |
| 11  | CLA  | bB    | 821 | -    | 1/1/13/20 | 10/27/103/115 | -       |
| 11  | CLA  | bA    | 816 | 1    | 1/1/11/20 | 4/15/91/115   | -       |
| 11  | CLA  | bB    | 812 | 2    | 1/1/15/20 | 17/39/115/115 | -       |
| 11  | CLA  | bB    | 803 | -    | 1/1/14/20 | 7/35/111/115  | -       |
| 11  | CLA  | bB    | 811 | 2    | 1/1/11/20 | 5/15/91/115   | -       |
| 12  | F6C  | aL    | 202 | 2    | 1/1/10/16 | 15/41/97/97   | -       |
| 11  | CLA  | cB    | 809 | 2    | 1/1/11/20 | 9/18/94/115   | -       |
| 17  | LMT  | cA    | 853 | -    | -         | 11/21/61/61   | 0/2/2/2 |
| 11  | CLA  | aL    | 206 | -    | 1/1/15/20 | 15/39/115/115 | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 11  | CLA  | aA    | 815 | 1    | 1/1/11/20 | 3/15/91/115   | -       |
| 11  | CLA  | aA    | 843 | 1    | 1/1/12/20 | 9/23/99/115   | -       |
| 11  | CLA  | bA    | 814 | 1    | 1/1/15/20 | 14/39/115/115 | -       |
| 11  | CLA  | aA    | 808 | 1    | 1/1/12/20 | 5/23/99/115   | -       |
| 13  | PQN  | aB    | 841 | -    | -         | 2/17/37/43    | 0/2/2/2 |
| 11  | CLA  | bA    | 805 | 1    | 1/1/11/20 | 6/15/91/115   | -       |
| 11  | CLA  | cA    | 840 | 1    | 1/1/15/20 | 17/39/115/115 | -       |
| 11  | CLA  | aA    | 811 | 1    | 1/1/11/20 | 3/15/91/115   | -       |
| 11  | CLA  | aA    | 812 | 1    | 1/1/15/20 | 13/39/115/115 | -       |
| 11  | CLA  | cB    | 834 | -    | 1/1/11/20 | 6/15/91/115   | -       |
| 11  | CLA  | aB    | 836 | 2    | 1/1/12/20 | 10/23/99/115  | -       |
| 14  | SF4  | aC    | 101 | 3    | -         | -             | 0/6/5/5 |
| 11  | CLA  | bB    | 826 | 2    | 1/1/14/20 | 10/35/111/115 | -       |
| 12  | F6C  | cB    | 824 | -    | 1/1/8/16  | 9/32/88/97    | -       |
| 11  | CLA  | cB    | 807 | 2    | 1/1/14/20 | 2/35/111/115  | -       |
| 11  | CLA  | aB    | 820 | 2    | 1/1/11/20 | 8/15/91/115   | -       |
| 11  | CLA  | cA    | 813 | 1    | 1/1/12/20 | 7/26/102/115  | -       |
| 11  | CLA  | bA    | 837 | 1    | 1/1/11/20 | 3/15/91/115   | -       |
| 11  | CLA  | aB    | 805 | 2    | 1/1/15/20 | 12/39/115/115 | -       |
| 11  | CLA  | aB    | 817 | 2    | 1/1/14/20 | 14/33/109/115 | -       |
| 11  | CLA  | bA    | 836 | 1    | 1/1/11/20 | 6/15/91/115   | -       |
| 11  | CLA  | cB    | 813 | 2    | 1/1/13/20 | 12/29/105/115 | -       |
| 11  | CLA  | bK    | 101 | 7    | 1/1/8/20  | 2/6/78/115    | -       |
| 11  | CLA  | aA    | 802 | -    | 1/1/15/20 | 6/39/115/115  | -       |
| 11  | CLA  | cB    | 829 | 2    | 1/1/11/20 | 6/15/91/115   | -       |
| 15  | BCR  | cK    | 102 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 11  | CLA  | bB    | 831 | 2    | 1/1/13/20 | 6/29/105/115  | -       |
| 11  | CLA  | cB    | 801 | 2    | 1/1/15/20 | 8/39/115/115  | -       |
| 15  | BCR  | aL    | 203 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 11  | CLA  | cA    | 811 | 1    | 1/1/11/20 | 3/15/91/115   | -       |
| 11  | CLA  | cB    | 810 | 2    | 1/1/11/20 | 7/15/91/115   | -       |
| 11  | CLA  | bB    | 808 | 2    | 1/1/15/20 | 10/39/115/115 | -       |
| 11  | CLA  | cA    | 821 | 1    | 1/1/14/20 | 15/35/111/115 | -       |
| 11  | CLA  | cA    | 818 | 1    | 1/1/12/20 | 10/26/102/115 | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 15  | BCR  | bL    | 207 | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 15  | BCR  | bI    | 101 | -    | -         | 11/29/63/63   | 0/2/2/2 |
| 11  | CLA  | bA    | 820 | 1    | 1/1/15/20 | 10/39/115/115 | -       |
| 11  | CLA  | cB    | 822 | 2    | -         | 6/15/91/115   | -       |
| 15  | BCR  | bL    | 203 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 11  | CLA  | aA    | 825 | 1    | 1/1/15/20 | 12/39/115/115 | -       |
| 11  | CLA  | aB    | 815 | 2    | 1/1/13/20 | 13/27/103/115 | -       |
| 14  | SF4  | aC    | 102 | 3    | -         | -             | 0/6/5/5 |
| 18  | LMG  | cB    | 847 | -    | -         | 18/41/61/70   | 0/1/1/1 |
| 11  | CLA  | aA    | 813 | 1    | 1/1/12/20 | 7/26/102/115  | -       |
| 12  | F6C  | bL    | 202 | 2    | 1/1/10/16 | 15/41/97/97   | -       |
| 15  | BCR  | bA    | 851 | -    | -         | 18/29/63/63   | 0/2/2/2 |
| 11  | CLA  | aK    | 103 | -    | -         | 6/23/99/115   | -       |
| 11  | CLA  | bA    | 817 | -    | 1/1/11/20 | 7/20/96/115   | -       |
| 11  | CLA  | bA    | 834 | 1    | 1/1/15/20 | 9/39/115/115  | -       |
| 11  | CLA  | bB    | 823 | 2    | 1/1/12/20 | 8/26/102/115  | -       |
| 11  | CLA  | aB    | 812 | 2    | 1/1/15/20 | 17/39/115/115 | -       |
| 11  | CLA  | cB    | 821 | -    | 1/1/13/20 | 9/27/103/115  | -       |
| 14  | SF4  | cA    | 846 | 2,1  | -         | -             | 0/6/5/5 |
| 11  | CLA  | aB    | 832 | 2    | 1/1/11/20 | 8/15/91/115   | -       |
| 11  | CLA  | cB    | 820 | 2    | 1/1/11/20 | 8/15/91/115   | -       |
| 11  | CLA  | cA    | 802 | -    | 1/1/15/20 | 6/39/115/115  | -       |
| 11  | CLA  | bA    | 822 | -    | 1/1/15/20 | 19/39/115/115 | -       |
| 11  | CLA  | cB    | 828 | 2    | 1/1/13/20 | 5/27/103/115  | -       |
| 11  | CLA  | bA    | 810 | 1    | 1/1/11/20 | 4/15/91/115   | -       |
| 11  | CLA  | aB    | 823 | 2    | 1/1/12/20 | 8/26/102/115  | -       |
| 11  | CLA  | cA    | 814 | 1    | 1/1/15/20 | 14/39/115/115 | -       |
| 11  | CLA  | cB    | 838 | 2    | 1/1/11/20 | 5/18/94/115   | -       |
| 11  | CLA  | aA    | 829 | 1    | 1/1/15/20 | 12/39/115/115 | -       |
| 11  | CLA  | aA    | 841 | 1    | 1/1/12/20 | 4/21/97/115   | -       |
| 11  | CLA  | bA    | 806 | 1    | 1/1/15/20 | 13/39/115/115 | -       |
| 13  | PQN  | aA    | 845 | -    | -         | 2/23/43/43    | 0/2/2/2 |
| 12  | F6C  | cA    | 844 | -    | 1/1/10/16 | 11/41/97/97   | -       |
| 12  | F6C  | bA    | 844 | -    | 1/1/10/16 | 11/41/97/97   | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 10  | CL0  | cA    | 801 | 1    | 3/3/20/25 | 7/37/135/135  | -       |
| 18  | LMG  | bB    | 847 | -    | -         | 18/41/61/70   | 0/1/1/1 |
| 11  | CLA  | cB    | 818 | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 11  | CLA  | aA    | 806 | 1    | 1/1/15/20 | 13/39/115/115 | -       |
| 11  | CLA  | bA    | 823 | 1    | 1/1/11/20 | 9/15/91/115   | -       |
| 11  | CLA  | bB    | 819 | 2    | 1/1/11/20 | 11/18/94/115  | -       |
| 11  | CLA  | cL    | 204 | 8    | 1/1/15/20 | 5/39/115/115  | -       |
| 11  | CLA  | bB    | 820 | 2    | 1/1/11/20 | 8/15/91/115   | -       |
| 11  | CLA  | cA    | 804 | 1    | 1/1/11/20 | 11/15/91/115  | -       |
| 13  | PQN  | bB    | 841 | -    | -         | 2/17/37/43    | 0/2/2/2 |
| 12  | F6C  | aA    | 827 | -    | 2/2/8/16  | 10/29/85/97   | -       |
| 15  | BCR  | bA    | 850 | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 11  | CLA  | cL    | 205 | 8    | 1/1/15/20 | 15/39/115/115 | -       |
| 15  | BCR  | bB    | 845 | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 11  | CLA  | aB    | 813 | 2    | 1/1/13/20 | 12/29/105/115 | -       |
| 11  | CLA  | bA    | 819 | 1    | 1/1/12/20 | 12/26/102/115 | -       |
| 11  | CLA  | cA    | 838 | 1    | 1/1/12/20 | 7/23/99/115   | -       |
| 11  | CLA  | bA    | 821 | 1    | 1/1/14/20 | 15/35/111/115 | -       |
| 11  | CLA  | aB    | 829 | 2    | 1/1/11/20 | 6/15/91/115   | -       |
| 11  | CLA  | cB    | 812 | 2    | 1/1/15/20 | 17/39/115/115 | -       |
| 11  | CLA  | cB    | 811 | 2    | 1/1/11/20 | 5/15/91/115   | -       |
| 11  | CLA  | aA    | 840 | 1    | 1/1/15/20 | 18/39/115/115 | -       |
| 11  | CLA  | cB    | 832 | 2    | 1/1/11/20 | 8/15/91/115   | -       |
| 11  | CLA  | cA    | 809 | 1    | 1/1/11/20 | 8/15/91/115   | -       |
| 11  | CLA  | aB    | 834 | -    | 1/1/11/20 | 6/15/91/115   | -       |
| 11  | CLA  | bB    | 815 | 2    | 1/1/13/20 | 13/27/103/115 | -       |
| 11  | CLA  | cB    | 833 | 2    | 1/1/11/20 | 4/15/91/115   | -       |
| 11  | CLA  | cB    | 802 | -    | 1/1/13/20 | 9/30/106/115  | -       |
| 11  | CLA  | aA    | 820 | 1    | 1/1/15/20 | 11/39/115/115 | -       |
| 11  | CLA  | bB    | 805 | 2    | 1/1/15/20 | 12/39/115/115 | -       |
| 12  | F6C  | bA    | 830 | 1    | 1/1/10/16 | 6/41/97/97    | -       |
| 13  | PQN  | cA    | 845 | -    | -         | 2/23/43/43    | 0/2/2/2 |
| 11  | CLA  | aA    | 817 | -    | 1/1/11/20 | 7/20/96/115   | -       |
| 18  | LMG  | aB    | 847 | -    | -         | 18/41/61/70   | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 11  | CLA  | cA    | 842 | -    | 1/1/11/20 | 6/15/91/115   | -       |
| 11  | CLA  | bA    | 818 | 1    | 1/1/12/20 | 10/26/102/115 | -       |
| 11  | CLA  | bA    | 825 | 1    | 1/1/15/20 | 12/39/115/115 | -       |
| 11  | CLA  | cB    | 804 | 2    | 1/1/12/20 | 8/21/97/115   | -       |
| 15  | BCR  | bB    | 843 | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 11  | CLA  | bK    | 103 | -    | -         | 6/23/99/115   | -       |
| 11  | CLA  | aA    | 805 | 1    | 1/1/11/20 | 6/15/91/115   | -       |
| 11  | CLA  | aB    | 840 | 2    | 1/1/11/20 | 5/15/91/115   | -       |
| 11  | CLA  | cA    | 807 | 1    | 1/1/15/20 | 17/39/115/115 | -       |
| 15  | BCR  | cB    | 848 | -    | -         | 18/29/63/63   | 0/2/2/2 |
| 11  | CLA  | aB    | 810 | 2    | 1/1/11/20 | 7/15/91/115   | -       |
| 11  | CLA  | aB    | 806 | 2    | 1/1/15/20 | 18/39/115/115 | -       |
| 11  | CLA  | cA    | 820 | 1    | 1/1/15/20 | 11/39/115/115 | -       |
| 14  | SF4  | cC    | 101 | 3    | -         | -             | 0/6/5/5 |
| 11  | CLA  | cA    | 810 | 1    | 1/1/11/20 | 4/15/91/115   | -       |
| 11  | CLA  | aA    | 842 | -    | 1/1/11/20 | 6/15/91/115   | -       |
| 11  | CLA  | aB    | 830 | 2    | 1/1/11/20 | 8/20/96/115   | -       |
| 16  | LHG  | cA    | 852 | -    | -         | 23/53/53/53   | -       |
| 11  | CLA  | aA    | 835 | 1    | 1/1/15/20 | 11/39/115/115 | -       |
| 15  | BCR  | cI    | 103 | -    | -         | 11/29/63/63   | 0/2/2/2 |
| 17  | LMT  | aA    | 853 | -    | -         | 11/21/61/61   | 0/2/2/2 |
| 11  | CLA  | cA    | 819 | 1    | 1/1/12/20 | 12/26/102/115 | -       |
| 11  | CLA  | bB    | 832 | 2    | 1/1/11/20 | 8/15/91/115   | -       |
| 12  | F6C  | bA    | 832 | 1    | 1/1/7/16  | 12/23/79/97   | -       |
| 15  | BCR  | aB    | 846 | -    | -         | 12/29/63/63   | 0/2/2/2 |
| 12  | F6C  | cL    | 202 | 2    | 1/1/10/16 | 15/41/97/97   | -       |
| 11  | CLA  | aA    | 833 | 1    | 1/1/15/20 | 14/39/115/115 | -       |
| 11  | CLA  | aA    | 807 | 1    | 1/1/15/20 | 17/39/115/115 | -       |
| 15  | BCR  | cB    | 845 | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 11  | CLA  | cK    | 101 | 7    | 1/1/8/20  | 2/6/78/115    | -       |
| 11  | CLA  | bA    | 802 | -    | 1/1/15/20 | 6/39/115/115  | -       |
| 11  | CLA  | aA    | 824 | -    | 1/1/12/20 | 11/23/99/115  | -       |
| 11  | CLA  | bA    | 804 | 1    | 1/1/11/20 | 11/15/91/115  | -       |
| 11  | CLA  | cL    | 206 | -    | 1/1/15/20 | 15/39/115/115 | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 11  | CLA  | bA    | 828 | 1    | 1/1/14/20 | 11/33/109/115 | -       |
| 11  | CLA  | aA    | 810 | 1    | 1/1/11/20 | 4/15/91/115   | -       |
| 15  | BCR  | bA    | 848 | -    | -         | 13/29/63/63   | 0/2/2/2 |
| 11  | CLA  | bL    | 205 | 8    | 1/1/15/20 | 15/39/115/115 | -       |
| 11  | CLA  | cB    | 840 | 2    | 1/1/11/20 | 5/15/91/115   | -       |
| 11  | CLA  | aB    | 828 | 2    | 1/1/13/20 | 5/27/103/115  | -       |
| 11  | CLA  | cA    | 816 | 1    | 1/1/11/20 | 4/15/91/115   | -       |
| 14  | SF4  | bA    | 846 | 2,1  | -         | -             | 0/6/5/5 |
| 11  | CLA  | cA    | 839 | 1    | 1/1/15/20 | 7/39/115/115  | -       |
| 11  | CLA  | aB    | 814 | 2    | 1/1/11/20 | 7/15/91/115   | -       |
| 15  | BCR  | cA    | 849 | -    | -         | 12/29/63/63   | 0/2/2/2 |
| 11  | CLA  | aA    | 837 | 1    | 1/1/11/20 | 3/15/91/115   | -       |
| 11  | CLA  | aB    | 827 | 2    | 1/1/15/20 | 10/39/115/115 | -       |
| 15  | BCR  | aB    | 843 | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 15  | BCR  | aA    | 848 | -    | -         | 13/29/63/63   | 0/2/2/2 |
| 12  | F6C  | aB    | 824 | -    | 1/1/8/16  | 9/32/88/97    | -       |
| 15  | BCR  | aL    | 208 | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 15  | BCR  | aL    | 207 | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 15  | BCR  | aB    | 842 | -    | -         | 14/29/63/63   | 0/2/2/2 |
| 15  | BCR  | aM    | 101 | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 15  | BCR  | cL    | 207 | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 11  | CLA  | bB    | 813 | 2    | 1/1/13/20 | 12/29/105/115 | -       |
| 11  | CLA  | bB    | 829 | 2    | 1/1/11/20 | 6/15/91/115   | -       |
| 11  | CLA  | cB    | 825 | 2    | 1/1/15/20 | 10/39/115/115 | -       |
| 15  | BCR  | aB    | 845 | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 15  | BCR  | bB    | 844 | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 11  | CLA  | aB    | 801 | 2    | 1/1/15/20 | 8/39/115/115  | -       |
| 11  | CLA  | cA    | 841 | 1    | 1/1/12/20 | 4/21/97/115   | -       |
| 11  | CLA  | bA    | 839 | 1    | 1/1/15/20 | 7/39/115/115  | -       |
| 11  | CLA  | aA    | 804 | 1    | 1/1/11/20 | 11/15/91/115  | -       |
| 11  | CLA  | cB    | 831 | 2    | 1/1/13/20 | 6/29/105/115  | -       |
| 11  | CLA  | aB    | 826 | 2    | 1/1/14/20 | 10/35/111/115 | -       |
| 11  | CLA  | aA    | 834 | 1    | 1/1/15/20 | 9/39/115/115  | -       |
| 11  | CLA  | bB    | 834 | -    | 1/1/11/20 | 6/15/91/115   | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 16  | LHG  | bA    | 852 | -    | -         | 23/53/53/53   | -       |
| 11  | CLA  | cA    | 822 | -    | 1/1/15/20 | 19/39/115/115 | -       |
| 11  | CLA  | aA    | 809 | 1    | 1/1/11/20 | 8/15/91/115   | -       |
| 11  | CLA  | bB    | 806 | 2    | 1/1/15/20 | 19/39/115/115 | -       |
| 11  | CLA  | cA    | 803 | -    | 1/1/13/20 | 6/29/105/115  | -       |
| 15  | BCR  | cA    | 851 | -    | -         | 18/29/63/63   | 0/2/2/2 |
| 11  | CLA  | aA    | 838 | 1    | 1/1/12/20 | 7/23/99/115   | -       |
| 14  | SF4  | cC    | 102 | 3    | -         | -             | 0/6/5/5 |
| 15  | BCR  | aA    | 850 | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 15  | BCR  | aI    | 101 | -    | -         | 11/29/63/63   | 0/2/2/2 |
| 11  | CLA  | aB    | 807 | 2    | 1/1/14/20 | 2/35/111/115  | -       |
| 11  | CLA  | cB    | 827 | 2    | 1/1/15/20 | 10/39/115/115 | -       |
| 11  | CLA  | aA    | 818 | 1    | 1/1/12/20 | 10/26/102/115 | -       |
| 12  | F6C  | aA    | 830 | 1    | 1/1/10/16 | 6/41/97/97    | -       |
| 11  | CLA  | bB    | 836 | 2    | 1/1/12/20 | 10/23/99/115  | -       |
| 11  | CLA  | bB    | 840 | 2    | 1/1/11/20 | 5/15/91/115   | -       |
| 15  | BCR  | aA    | 847 | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 11  | CLA  | cB    | 805 | 2    | 1/1/15/20 | 12/39/115/115 | -       |
| 11  | CLA  | aB    | 804 | 2    | 1/1/12/20 | 8/21/97/115   | -       |
| 11  | CLA  | cA    | 835 | 1    | 1/1/15/20 | 11/39/115/115 | -       |
| 11  | CLA  | aA    | 822 | -    | 1/1/15/20 | 19/39/115/115 | -       |
| 11  | CLA  | aB    | 819 | 2    | 1/1/11/20 | 11/18/94/115  | -       |
| 11  | CLA  | bA    | 840 | 1    | 1/1/15/20 | 18/39/115/115 | -       |
| 11  | CLA  | cB    | 835 | -    | 1/1/11/20 | 5/15/91/115   | -       |
| 11  | CLA  | aB    | 809 | 2    | 1/1/11/20 | 9/18/94/115   | -       |
| 11  | CLA  | aB    | 837 | 2    | 1/1/13/20 | 8/27/103/115  | -       |
| 15  | BCR  | aB    | 848 | -    | -         | 18/29/63/63   | 0/2/2/2 |
| 11  | CLA  | cA    | 833 | 1    | 1/1/15/20 | 14/39/115/115 | -       |
| 11  | CLA  | aB    | 838 | 2    | 1/1/11/20 | 5/18/94/115   | -       |
| 11  | CLA  | cB    | 814 | 2    | 1/1/11/20 | 7/15/91/115   | -       |
| 12  | F6C  | cA    | 832 | 1    | 1/1/7/16  | 12/23/79/97   | -       |
| 11  | CLA  | cB    | 803 | -    | 1/1/14/20 | 7/35/111/115  | -       |
| 11  | CLA  | cB    | 826 | 2    | 1/1/14/20 | 10/35/111/115 | -       |
| 15  | BCR  | bB    | 846 | -    | -         | 11/29/63/63   | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 11  | CLA  | aB    | 818 | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 12  | F6C  | cA    | 830 | 1    | 1/1/10/16 | 6/41/97/97    | -       |
| 11  | CLA  | cA    | 829 | 1    | 1/1/15/20 | 12/39/115/115 | -       |
| 11  | CLA  | bA    | 803 | -    | 1/1/13/20 | 6/29/105/115  | -       |
| 15  | BCR  | cA    | 847 | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 11  | CLA  | bB    | 827 | 2    | 1/1/15/20 | 10/39/115/115 | -       |
| 11  | CLA  | bA    | 838 | 1    | 1/1/12/20 | 7/23/99/115   | -       |
| 11  | CLA  | aB    | 839 | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 15  | BCR  | bB    | 842 | -    | -         | 14/29/63/63   | 0/2/2/2 |
| 11  | CLA  | bB    | 825 | 2    | 1/1/15/20 | 10/39/115/115 | -       |
| 15  | BCR  | aA    | 849 | -    | -         | 12/29/63/63   | 0/2/2/2 |
| 11  | CLA  | cA    | 831 | 1    | 1/1/15/20 | 12/39/115/115 | -       |
| 11  | CLA  | cA    | 815 | 1    | 1/1/11/20 | 3/15/91/115   | -       |
| 11  | CLA  | cK    | 103 | -    | -         | 6/23/99/115   | -       |
| 13  | PQN  | cB    | 841 | -    | -         | 2/17/37/43    | 0/2/2/2 |
| 11  | CLA  | bA    | 809 | 1    | 1/1/11/20 | 7/15/91/115   | -       |
| 11  | CLA  | bA    | 831 | 1    | 1/1/15/20 | 12/39/115/115 | -       |
| 11  | CLA  | cA    | 808 | 1    | 1/1/12/20 | 5/23/99/115   | -       |
| 11  | CLA  | aA    | 828 | 1    | 1/1/14/20 | 12/33/109/115 | -       |
| 11  | CLA  | bB    | 835 | -    | 1/1/11/20 | 5/15/91/115   | -       |
| 15  | BCR  | cB    | 846 | -    | -         | 12/29/63/63   | 0/2/2/2 |
| 11  | CLA  | aA    | 814 | 1    | 1/1/15/20 | 14/39/115/115 | -       |
| 15  | BCR  | cA    | 850 | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 11  | CLA  | cB    | 836 | 2    | 1/1/12/20 | 10/23/99/115  | -       |
| 11  | CLA  | aA    | 836 | 1    | 1/1/11/20 | 6/15/91/115   | -       |
| 12  | F6C  | bA    | 826 | -    | 1/1/10/16 | 11/41/97/97   | -       |
| 11  | CLA  | bA    | 812 | 1    | 1/1/15/20 | 13/39/115/115 | -       |
| 11  | CLA  | cA    | 812 | 1    | 1/1/15/20 | 13/39/115/115 | -       |
| 12  | F6C  | bA    | 827 | -    | 2/2/8/16  | 10/29/85/97   | -       |
| 11  | CLA  | bL    | 204 | 8    | 1/1/15/20 | 5/39/115/115  | -       |
| 12  | F6C  | bB    | 824 | -    | 1/1/8/16  | 9/32/88/97    | -       |
| 11  | CLA  | bB    | 833 | 2    | 1/1/11/20 | 4/15/91/115   | -       |
| 11  | CLA  | cB    | 837 | 2    | 1/1/13/20 | 8/27/103/115  | -       |
| 11  | CLA  | aB    | 802 | -    | 1/1/13/20 | 9/30/106/115  | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 15  | BCR  | cB    | 842 | -    | -         | 14/29/63/63   | 0/2/2/2 |
| 11  | CLA  | aB    | 816 | 2    | 1/1/13/20 | 12/32/108/115 | -       |
| 11  | CLA  | aA    | 821 | 1    | 1/1/14/20 | 15/35/111/115 | -       |
| 12  | F6C  | aA    | 826 | -    | 1/1/10/16 | 11/41/97/97   | -       |
| 12  | F6C  | cA    | 827 | -    | 2/2/8/16  | 10/29/85/97   | -       |
| 11  | CLA  | bB    | 801 | 2    | 1/1/15/20 | 8/39/115/115  | -       |
| 11  | CLA  | aA    | 803 | -    | 1/1/13/20 | 6/29/105/115  | -       |
| 14  | SF4  | aA    | 846 | 2,1  | -         | -             | 0/6/5/5 |
| 11  | CLA  | bB    | 817 | 2    | 1/1/14/20 | 14/33/109/115 | -       |
| 11  | CLA  | cB    | 808 | 2    | 1/1/15/20 | 10/39/115/115 | -       |
| 11  | CLA  | bB    | 810 | 2    | 1/1/11/20 | 7/15/91/115   | -       |
| 12  | F6C  | aA    | 844 | -    | 1/1/10/16 | 11/41/97/97   | -       |
| 11  | CLA  | cA    | 828 | 1    | 1/1/14/20 | 12/33/109/115 | -       |
| 11  | CLA  | aK    | 101 | 7    | 1/1/8/20  | 2/6/78/115    | -       |
| 11  | CLA  | cB    | 815 | 2    | 1/1/13/20 | 13/27/103/115 | -       |
| 15  | BCR  | bM    | 101 | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 11  | CLA  | bA    | 842 | -    | 1/1/11/20 | 6/15/91/115   | -       |
| 11  | CLA  | cB    | 839 | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 11  | CLA  | cB    | 817 | 2    | 1/1/14/20 | 14/33/109/115 | -       |
| 15  | BCR  | cB    | 843 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 11  | CLA  | cA    | 825 | 1    | 1/1/15/20 | 12/39/115/115 | -       |
| 11  | CLA  | cA    | 836 | 1    | 1/1/11/20 | 6/15/91/115   | -       |
| 15  | BCR  | bK    | 102 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 15  | BCR  | bA    | 849 | -    | -         | 12/29/63/63   | 0/2/2/2 |
| 15  | BCR  | bL    | 208 | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 15  | BCR  | cA    | 848 | -    | -         | 13/29/63/63   | 0/2/2/2 |
| 11  | CLA  | aB    | 835 | -    | 1/1/11/20 | 4/15/91/115   | -       |
| 11  | CLA  | bB    | 807 | 2    | 1/1/14/20 | 2/35/111/115  | -       |
| 16  | LHG  | aA    | 852 | -    | -         | 23/53/53/53   | -       |
| 10  | CL0  | aA    | 801 | 1    | 3/3/20/25 | 7/37/135/135  | -       |
| 11  | CLA  | aA    | 823 | 1    | 1/1/11/20 | 9/15/91/115   | -       |
| 11  | CLA  | cA    | 843 | 1    | 1/1/12/20 | 9/23/99/115   | -       |
| 11  | CLA  | aB    | 822 | 2    | -         | 6/15/91/115   | -       |
| 11  | CLA  | aB    | 821 | -    | 1/1/13/20 | 10/27/103/115 | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 11  | CLA  | bA    | 813 | 1    | 1/1/12/20 | 7/26/102/115  | -       |
| 12  | F6C  | cA    | 826 | -    | 1/1/10/16 | 11/41/97/97   | -       |
| 11  | CLA  | bA    | 843 | 1    | 1/1/12/20 | 9/23/99/115   | -       |
| 11  | CLA  | bA    | 829 | 1    | 1/1/15/20 | 12/39/115/115 | -       |
| 11  | CLA  | aB    | 803 | -    | 1/1/14/20 | 7/35/111/115  | -       |
| 11  | CLA  | bL    | 206 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 11  | CLA  | bB    | 804 | 2    | 1/1/12/20 | 8/21/97/115   | -       |
| 15  | BCR  | cL    | 208 | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 11  | CLA  | bA    | 835 | 1    | 1/1/15/20 | 11/39/115/115 | -       |
| 11  | CLA  | bA    | 815 | 1    | 1/1/11/20 | 3/15/91/115   | -       |
| 11  | CLA  | bB    | 809 | 2    | 1/1/11/20 | 9/18/94/115   | -       |
| 11  | CLA  | bB    | 837 | 2    | 1/1/13/20 | 8/27/103/115  | -       |
| 11  | CLA  | cB    | 830 | 2    | 1/1/11/20 | 8/20/96/115   | -       |
| 15  | BCR  | bB    | 848 | -    | -         | 18/29/63/63   | 0/2/2/2 |
| 11  | CLA  | bA    | 808 | 1    | 1/1/12/20 | 5/23/99/115   | -       |
| 11  | CLA  | cB    | 806 | 2    | 1/1/15/20 | 19/39/115/115 | -       |
| 11  | CLA  | bB    | 838 | 2    | 1/1/11/20 | 5/18/94/115   | -       |
| 11  | CLA  | aB    | 833 | 2    | 1/1/11/20 | 4/15/91/115   | -       |
| 11  | CLA  | bA    | 811 | 1    | 1/1/11/20 | 3/15/91/115   | -       |
| 11  | CLA  | cB    | 823 | 2    | 1/1/12/20 | 8/26/102/115  | -       |
| 11  | CLA  | aA    | 831 | 1    | 1/1/15/20 | 12/39/115/115 | -       |
| 11  | CLA  | bA    | 807 | 1    | 1/1/15/20 | 17/39/115/115 | -       |
| 11  | CLA  | aB    | 808 | 2    | 1/1/15/20 | 10/39/115/115 | -       |
| 11  | CLA  | bB    | 818 | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 11  | CLA  | aB    | 811 | 2    | 1/1/11/20 | 5/15/91/115   | -       |
| 15  | BCR  | cL    | 203 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 11  | CLA  | cA    | 805 | 1    | 1/1/11/20 | 6/15/91/115   | -       |
| 11  | CLA  | aL    | 204 | 8    | 1/1/15/20 | 5/39/115/115  | -       |
| 11  | CLA  | bA    | 824 | -    | 1/1/12/20 | 11/23/99/115  | -       |
| 11  | CLA  | cB    | 816 | 2    | 1/1/13/20 | 12/32/108/115 | -       |
| 11  | CLA  | cB    | 819 | 2    | 1/1/11/20 | 11/18/94/115  | -       |
| 11  | CLA  | aA    | 839 | 1    | 1/1/15/20 | 7/39/115/115  | -       |
| 11  | CLA  | bB    | 839 | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 17  | LMT  | bA    | 853 | -    | -         | 11/21/61/61   | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 11  | CLA  | bB    | 830 | 2    | 1/1/11/20 | 8/20/96/115   | -       |
| 11  | CLA  | bB    | 822 | 2    | -         | 6/15/91/115   | -       |
| 14  | SF4  | bC    | 101 | 3    | -         | -             | 0/6/5/5 |
| 11  | CLA  | bA    | 833 | 1    | 1/1/15/20 | 14/39/115/115 | -       |
| 11  | CLA  | bB    | 816 | 2    | 1/1/13/20 | 12/32/108/115 | -       |
| 11  | CLA  | cA    | 806 | 1    | 1/1/15/20 | 13/39/115/115 | -       |
| 15  | BCR  | bA    | 847 | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 11  | CLA  | aL    | 205 | 8    | 1/1/15/20 | 15/39/115/115 | -       |
| 11  | CLA  | cA    | 824 | -    | 1/1/12/20 | 11/23/99/115  | -       |
| 15  | BCR  | cB    | 844 | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 11  | CLA  | aB    | 831 | 2    | 1/1/13/20 | 6/29/105/115  | -       |

All (5594) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 10  | bA    | 801 | CL0  | C1A-CHA | 9.46 | 1.50        | 1.40     |
| 10  | cA    | 801 | CL0  | C1A-CHA | 9.39 | 1.50        | 1.40     |
| 10  | aA    | 801 | CL0  | C1A-CHA | 9.39 | 1.50        | 1.40     |
| 12  | cA    | 826 | F6C  | C1A-CHA | 9.37 | 1.50        | 1.35     |
| 12  | bA    | 826 | F6C  | C1A-CHA | 9.34 | 1.50        | 1.35     |
| 12  | aA    | 826 | F6C  | C1A-CHA | 9.34 | 1.50        | 1.35     |
| 12  | bL    | 202 | F6C  | C1A-CHA | 9.26 | 1.50        | 1.35     |
| 12  | cL    | 202 | F6C  | C1A-CHA | 9.25 | 1.50        | 1.35     |
| 12  | aL    | 202 | F6C  | C1A-CHA | 9.20 | 1.50        | 1.35     |
| 10  | cA    | 801 | CL0  | C1B-C2B | 9.13 | 1.50        | 1.39     |
| 10  | bA    | 801 | CL0  | C1B-C2B | 9.04 | 1.49        | 1.39     |
| 10  | aA    | 801 | CL0  | C1B-C2B | 9.03 | 1.49        | 1.39     |
| 12  | aA    | 827 | F6C  | C1A-CHA | 8.92 | 1.49        | 1.35     |
| 12  | cA    | 830 | F6C  | C1A-CHA | 8.90 | 1.49        | 1.35     |
| 12  | aA    | 830 | F6C  | C1A-CHA | 8.89 | 1.49        | 1.35     |
| 12  | bA    | 830 | F6C  | C1A-CHA | 8.89 | 1.49        | 1.35     |
| 12  | cA    | 827 | F6C  | C1A-CHA | 8.88 | 1.49        | 1.35     |
| 12  | bA    | 827 | F6C  | C1A-CHA | 8.85 | 1.49        | 1.35     |
| 12  | aB    | 824 | F6C  | C1A-CHA | 8.81 | 1.49        | 1.35     |
| 12  | aA    | 832 | F6C  | C1A-CHA | 8.81 | 1.49        | 1.35     |
| 12  | bB    | 824 | F6C  | C1A-CHA | 8.80 | 1.49        | 1.35     |
| 12  | cB    | 824 | F6C  | C1A-CHA | 8.80 | 1.49        | 1.35     |
| 12  | bA    | 832 | F6C  | C1A-CHA | 8.77 | 1.49        | 1.35     |
| 12  | cA    | 832 | F6C  | C1A-CHA | 8.76 | 1.49        | 1.35     |
| 12  | aA    | 844 | F6C  | C1A-CHA | 8.75 | 1.49        | 1.35     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12  | cA    | 844 | F6C  | C1A-CHA | 8.72  | 1.49        | 1.35     |
| 12  | bA    | 844 | F6C  | C1A-CHA | 8.72  | 1.49        | 1.35     |
| 12  | cA    | 826 | F6C  | C2A-C3A | 7.99  | 1.54        | 1.36     |
| 12  | bA    | 826 | F6C  | C2A-C3A | 7.99  | 1.54        | 1.36     |
| 12  | aA    | 826 | F6C  | C2A-C3A | 7.96  | 1.53        | 1.36     |
| 12  | aL    | 202 | F6C  | C2A-C3A | 7.91  | 1.53        | 1.36     |
| 12  | bL    | 202 | F6C  | C2A-C3A | 7.90  | 1.53        | 1.36     |
| 12  | cL    | 202 | F6C  | C2A-C3A | 7.90  | 1.53        | 1.36     |
| 13  | cA    | 845 | PQN  | C3-C2   | 7.75  | 1.49        | 1.35     |
| 13  | aA    | 845 | PQN  | C3-C2   | 7.73  | 1.49        | 1.35     |
| 13  | bA    | 845 | PQN  | C3-C2   | 7.72  | 1.49        | 1.35     |
| 13  | cB    | 841 | PQN  | C3-C2   | 7.52  | 1.48        | 1.35     |
| 13  | bB    | 841 | PQN  | C3-C2   | 7.49  | 1.48        | 1.35     |
| 13  | aB    | 841 | PQN  | C3-C2   | 7.45  | 1.48        | 1.35     |
| 12  | bA    | 832 | F6C  | C2A-C3A | 7.10  | 1.52        | 1.36     |
| 12  | cA    | 832 | F6C  | C2A-C3A | 7.09  | 1.52        | 1.36     |
| 12  | aA    | 832 | F6C  | C2A-C3A | 7.06  | 1.52        | 1.36     |
| 12  | aA    | 830 | F6C  | C2A-C3A | 7.01  | 1.51        | 1.36     |
| 10  | cA    | 801 | CL0  | C3B-C4B | 7.01  | 1.48        | 1.41     |
| 10  | bA    | 801 | CL0  | C3B-C4B | 7.01  | 1.48        | 1.41     |
| 12  | cA    | 830 | F6C  | C2A-C3A | 6.98  | 1.51        | 1.36     |
| 12  | bA    | 830 | F6C  | C2A-C3A | 6.97  | 1.51        | 1.36     |
| 12  | bA    | 827 | F6C  | C2A-C3A | 6.95  | 1.51        | 1.36     |
| 12  | aA    | 827 | F6C  | C2A-C3A | 6.93  | 1.51        | 1.36     |
| 12  | cA    | 844 | F6C  | C2A-C3A | 6.91  | 1.51        | 1.36     |
| 12  | cA    | 827 | F6C  | C2A-C3A | 6.91  | 1.51        | 1.36     |
| 10  | aA    | 801 | CL0  | C3B-C4B | 6.90  | 1.48        | 1.41     |
| 12  | bA    | 844 | F6C  | C2A-C3A | 6.88  | 1.51        | 1.36     |
| 12  | aA    | 844 | F6C  | C2A-C3A | 6.88  | 1.51        | 1.36     |
| 10  | bA    | 801 | CL0  | C1D-C2D | 6.84  | 1.47        | 1.39     |
| 10  | aA    | 801 | CL0  | C1D-C2D | 6.84  | 1.47        | 1.39     |
| 12  | aB    | 824 | F6C  | C2A-C3A | 6.83  | 1.51        | 1.36     |
| 12  | cB    | 824 | F6C  | C2A-C3A | 6.82  | 1.51        | 1.36     |
| 12  | bB    | 824 | F6C  | C2A-C3A | 6.78  | 1.51        | 1.36     |
| 10  | cA    | 801 | CL0  | C1D-C2D | 6.77  | 1.47        | 1.39     |
| 10  | aA    | 801 | CL0  | C3B-C2B | 6.32  | 1.48        | 1.40     |
| 10  | cA    | 801 | CL0  | C3B-C2B | 6.31  | 1.48        | 1.40     |
| 10  | bA    | 801 | CL0  | C3B-C2B | 6.29  | 1.48        | 1.40     |
| 10  | cA    | 801 | CL0  | C3A-C2A | -5.93 | 1.49        | 1.54     |
| 10  | bA    | 801 | CL0  | C3A-C2A | -5.88 | 1.49        | 1.54     |
| 10  | aA    | 801 | CL0  | C3A-C2A | -5.79 | 1.49        | 1.54     |
| 10  | cA    | 801 | CL0  | C3D-C2D | 5.60  | 1.49        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 10  | aA    | 801 | CL0  | C3D-C2D | 5.60 | 1.49        | 1.39     |
| 10  | bA    | 801 | CL0  | C3D-C2D | 5.51 | 1.49        | 1.39     |
| 11  | bB    | 825 | CLA  | C3C-C2C | 5.41 | 1.48        | 1.36     |
| 11  | cB    | 825 | CLA  | C3C-C2C | 5.40 | 1.48        | 1.36     |
| 11  | aB    | 825 | CLA  | C3C-C2C | 5.39 | 1.48        | 1.36     |
| 11  | bB    | 811 | CLA  | C3C-C2C | 5.37 | 1.48        | 1.36     |
| 11  | aB    | 811 | CLA  | C3C-C2C | 5.37 | 1.48        | 1.36     |
| 11  | cB    | 811 | CLA  | C3C-C2C | 5.37 | 1.48        | 1.36     |
| 11  | bB    | 821 | CLA  | C3C-C2C | 5.33 | 1.48        | 1.36     |
| 11  | aB    | 821 | CLA  | C3C-C2C | 5.32 | 1.48        | 1.36     |
| 11  | cB    | 821 | CLA  | C3C-C2C | 5.31 | 1.48        | 1.36     |
| 11  | cA    | 816 | CLA  | C3C-C2C | 5.29 | 1.48        | 1.36     |
| 11  | aB    | 833 | CLA  | C3C-C2C | 5.29 | 1.48        | 1.36     |
| 11  | cB    | 833 | CLA  | C3C-C2C | 5.29 | 1.48        | 1.36     |
| 11  | aB    | 832 | CLA  | C3C-C2C | 5.28 | 1.48        | 1.36     |
| 11  | bB    | 836 | CLA  | C3C-C2C | 5.28 | 1.48        | 1.36     |
| 11  | cB    | 816 | CLA  | C3C-C2C | 5.27 | 1.48        | 1.36     |
| 11  | bB    | 832 | CLA  | C3C-C2C | 5.27 | 1.48        | 1.36     |
| 11  | bA    | 816 | CLA  | C3C-C2C | 5.27 | 1.48        | 1.36     |
| 11  | bB    | 833 | CLA  | C3C-C2C | 5.27 | 1.48        | 1.36     |
| 11  | aB    | 836 | CLA  | C3C-C2C | 5.26 | 1.48        | 1.36     |
| 11  | cB    | 836 | CLA  | C3C-C2C | 5.26 | 1.48        | 1.36     |
| 11  | aA    | 816 | CLA  | C3C-C2C | 5.26 | 1.48        | 1.36     |
| 11  | cB    | 834 | CLA  | C3C-C2C | 5.26 | 1.48        | 1.36     |
| 11  | aB    | 834 | CLA  | C3C-C2C | 5.25 | 1.48        | 1.36     |
| 11  | bB    | 816 | CLA  | C3C-C2C | 5.24 | 1.48        | 1.36     |
| 11  | cB    | 835 | CLA  | C3C-C2C | 5.24 | 1.48        | 1.36     |
| 11  | bA    | 837 | CLA  | C3C-C2C | 5.24 | 1.48        | 1.36     |
| 11  | aB    | 816 | CLA  | C3C-C2C | 5.23 | 1.48        | 1.36     |
| 11  | cB    | 830 | CLA  | C3C-C2C | 5.23 | 1.48        | 1.36     |
| 11  | bB    | 834 | CLA  | C3C-C2C | 5.23 | 1.48        | 1.36     |
| 11  | bB    | 830 | CLA  | C3C-C2C | 5.23 | 1.48        | 1.36     |
| 11  | aA    | 842 | CLA  | C3C-C2C | 5.22 | 1.48        | 1.36     |
| 11  | bA    | 812 | CLA  | C3C-C2C | 5.22 | 1.48        | 1.36     |
| 11  | bA    | 817 | CLA  | C3C-C2C | 5.22 | 1.48        | 1.36     |
| 11  | cA    | 842 | CLA  | C3C-C2C | 5.22 | 1.48        | 1.36     |
| 11  | aA    | 808 | CLA  | C3C-C2C | 5.22 | 1.48        | 1.36     |
| 11  | bA    | 811 | CLA  | C3C-C2C | 5.22 | 1.48        | 1.36     |
| 11  | aB    | 838 | CLA  | C3C-C2C | 5.22 | 1.48        | 1.36     |
| 11  | bB    | 835 | CLA  | C3C-C2C | 5.22 | 1.48        | 1.36     |
| 11  | aB    | 830 | CLA  | C3C-C2C | 5.22 | 1.48        | 1.36     |
| 11  | bA    | 841 | CLA  | C3C-C2C | 5.22 | 1.48        | 1.36     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 11  | cB    | 832 | CLA  | C3C-C2C | 5.21 | 1.48        | 1.36     |
| 11  | cB    | 838 | CLA  | C3C-C2C | 5.21 | 1.48        | 1.36     |
| 11  | bK    | 103 | CLA  | C3C-C2C | 5.21 | 1.48        | 1.36     |
| 11  | cA    | 812 | CLA  | C3C-C2C | 5.21 | 1.48        | 1.36     |
| 11  | aA    | 817 | CLA  | C3C-C2C | 5.21 | 1.48        | 1.36     |
| 11  | cA    | 811 | CLA  | C3C-C2C | 5.21 | 1.48        | 1.36     |
| 11  | aK    | 103 | CLA  | C3C-C2C | 5.21 | 1.48        | 1.36     |
| 11  | cA    | 804 | CLA  | C3C-C2C | 5.20 | 1.48        | 1.36     |
| 11  | bA    | 824 | CLA  | C3C-C2C | 5.20 | 1.48        | 1.36     |
| 11  | cA    | 808 | CLA  | C3C-C2C | 5.20 | 1.48        | 1.36     |
| 11  | bB    | 814 | CLA  | C3C-C2C | 5.20 | 1.48        | 1.36     |
| 11  | aL    | 206 | CLA  | C3C-C2C | 5.20 | 1.48        | 1.36     |
| 11  | aA    | 841 | CLA  | C3C-C2C | 5.20 | 1.48        | 1.36     |
| 11  | aB    | 835 | CLA  | C3C-C2C | 5.20 | 1.48        | 1.36     |
| 11  | bB    | 831 | CLA  | C3C-C2C | 5.20 | 1.48        | 1.36     |
| 11  | aA    | 811 | CLA  | C3C-C2C | 5.20 | 1.48        | 1.36     |
| 11  | cA    | 837 | CLA  | C3C-C2C | 5.19 | 1.48        | 1.36     |
| 11  | cA    | 841 | CLA  | C3C-C2C | 5.19 | 1.48        | 1.36     |
| 11  | cK    | 103 | CLA  | C3C-C2C | 5.19 | 1.48        | 1.36     |
| 11  | bA    | 842 | CLA  | C3C-C2C | 5.19 | 1.48        | 1.36     |
| 11  | aA    | 837 | CLA  | C3C-C2C | 5.19 | 1.48        | 1.36     |
| 11  | aA    | 831 | CLA  | C3C-C2C | 5.19 | 1.48        | 1.36     |
| 11  | cA    | 817 | CLA  | C3C-C2C | 5.19 | 1.48        | 1.36     |
| 11  | aB    | 831 | CLA  | C3C-C2C | 5.19 | 1.48        | 1.36     |
| 11  | aK    | 101 | CLA  | C3C-C2C | 5.19 | 1.48        | 1.36     |
| 11  | aA    | 812 | CLA  | C3C-C2C | 5.19 | 1.48        | 1.36     |
| 11  | bB    | 838 | CLA  | C3C-C2C | 5.19 | 1.48        | 1.36     |
| 11  | bA    | 831 | CLA  | C3C-C2C | 5.18 | 1.47        | 1.36     |
| 11  | aA    | 842 | CLA  | O2D-CGD | 5.18 | 1.46        | 1.33     |
| 11  | aA    | 815 | CLA  | C3C-C2C | 5.18 | 1.47        | 1.36     |
| 11  | cA    | 815 | CLA  | C3C-C2C | 5.18 | 1.47        | 1.36     |
| 11  | aA    | 804 | CLA  | C3C-C2C | 5.18 | 1.47        | 1.36     |
| 11  | bK    | 101 | CLA  | C3C-C2C | 5.18 | 1.47        | 1.36     |
| 11  | bA    | 808 | CLA  | C3C-C2C | 5.18 | 1.47        | 1.36     |
| 11  | cA    | 842 | CLA  | O2D-CGD | 5.18 | 1.46        | 1.33     |
| 11  | cB    | 814 | CLA  | C3C-C2C | 5.17 | 1.47        | 1.36     |
| 11  | cK    | 101 | CLA  | C3C-C2C | 5.17 | 1.47        | 1.36     |
| 11  | aB    | 814 | CLA  | C3C-C2C | 5.17 | 1.47        | 1.36     |
| 11  | cA    | 824 | CLA  | C3C-C2C | 5.17 | 1.47        | 1.36     |
| 11  | bA    | 842 | CLA  | O2D-CGD | 5.17 | 1.45        | 1.33     |
| 11  | bB    | 819 | CLA  | C3C-C2C | 5.17 | 1.47        | 1.36     |
| 11  | cA    | 839 | CLA  | C3C-C2C | 5.17 | 1.47        | 1.36     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 11  | bA    | 815 | CLA  | C3C-C2C | 5.17 | 1.47        | 1.36     |
| 11  | cB    | 831 | CLA  | C3C-C2C | 5.16 | 1.47        | 1.36     |
| 11  | aB    | 840 | CLA  | C3C-C2C | 5.16 | 1.47        | 1.36     |
| 11  | aB    | 827 | CLA  | C3C-C2C | 5.16 | 1.47        | 1.36     |
| 11  | cA    | 831 | CLA  | C3C-C2C | 5.16 | 1.47        | 1.36     |
| 11  | aA    | 824 | CLA  | C3C-C2C | 5.16 | 1.47        | 1.36     |
| 11  | cB    | 837 | CLA  | C3C-C2C | 5.16 | 1.47        | 1.36     |
| 11  | bB    | 818 | CLA  | C3C-C2C | 5.16 | 1.47        | 1.36     |
| 11  | cB    | 818 | CLA  | C3C-C2C | 5.16 | 1.47        | 1.36     |
| 11  | bL    | 206 | CLA  | C3C-C2C | 5.16 | 1.47        | 1.36     |
| 11  | cB    | 821 | CLA  | O2D-CGD | 5.16 | 1.45        | 1.33     |
| 11  | aB    | 804 | CLA  | C3C-C2C | 5.15 | 1.47        | 1.36     |
| 11  | aB    | 818 | CLA  | C3C-C2C | 5.15 | 1.47        | 1.36     |
| 11  | cB    | 827 | CLA  | C3C-C2C | 5.15 | 1.47        | 1.36     |
| 11  | bA    | 804 | CLA  | C3C-C2C | 5.15 | 1.47        | 1.36     |
| 11  | aA    | 813 | CLA  | C3C-C2C | 5.15 | 1.47        | 1.36     |
| 11  | cB    | 804 | CLA  | C3C-C2C | 5.15 | 1.47        | 1.36     |
| 11  | aA    | 841 | CLA  | O2D-CGD | 5.15 | 1.45        | 1.33     |
| 11  | cL    | 205 | CLA  | C3C-C2C | 5.15 | 1.47        | 1.36     |
| 11  | aB    | 834 | CLA  | O2D-CGD | 5.14 | 1.45        | 1.33     |
| 11  | bB    | 821 | CLA  | O2D-CGD | 5.14 | 1.45        | 1.33     |
| 11  | cA    | 833 | CLA  | C3C-C2C | 5.14 | 1.47        | 1.36     |
| 11  | aA    | 805 | CLA  | C3C-C2C | 5.14 | 1.47        | 1.36     |
| 11  | aL    | 205 | CLA  | C3C-C2C | 5.14 | 1.47        | 1.36     |
| 11  | bB    | 804 | CLA  | C3C-C2C | 5.14 | 1.47        | 1.36     |
| 11  | cA    | 829 | CLA  | C3C-C2C | 5.14 | 1.47        | 1.36     |
| 11  | aB    | 821 | CLA  | O2D-CGD | 5.14 | 1.45        | 1.33     |
| 11  | cA    | 809 | CLA  | C3C-C2C | 5.14 | 1.47        | 1.36     |
| 11  | cB    | 819 | CLA  | C3C-C2C | 5.14 | 1.47        | 1.36     |
| 11  | aA    | 833 | CLA  | C3C-C2C | 5.14 | 1.47        | 1.36     |
| 11  | cA    | 821 | CLA  | C3C-C2C | 5.14 | 1.47        | 1.36     |
| 11  | aB    | 837 | CLA  | C3C-C2C | 5.13 | 1.47        | 1.36     |
| 11  | cA    | 805 | CLA  | C3C-C2C | 5.13 | 1.47        | 1.36     |
| 11  | cB    | 816 | CLA  | O2D-CGD | 5.13 | 1.45        | 1.33     |
| 11  | aA    | 821 | CLA  | C3C-C2C | 5.13 | 1.47        | 1.36     |
| 11  | cB    | 840 | CLA  | C3C-C2C | 5.13 | 1.47        | 1.36     |
| 11  | bA    | 833 | CLA  | C3C-C2C | 5.13 | 1.47        | 1.36     |
| 11  | bB    | 828 | CLA  | C3C-C2C | 5.13 | 1.47        | 1.36     |
| 11  | bA    | 839 | CLA  | C3C-C2C | 5.13 | 1.47        | 1.36     |
| 11  | bA    | 822 | CLA  | C3C-C2C | 5.12 | 1.47        | 1.36     |
| 11  | cL    | 206 | CLA  | C3C-C2C | 5.12 | 1.47        | 1.36     |
| 11  | aL    | 204 | CLA  | C3C-C2C | 5.12 | 1.47        | 1.36     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 11  | cA    | 822 | CLA  | C3C-C2C | 5.12 | 1.47        | 1.36     |
| 11  | aA    | 839 | CLA  | C3C-C2C | 5.12 | 1.47        | 1.36     |
| 11  | aA    | 834 | CLA  | C3C-C2C | 5.12 | 1.47        | 1.36     |
| 11  | aB    | 819 | CLA  | C3C-C2C | 5.12 | 1.47        | 1.36     |
| 11  | bB    | 827 | CLA  | C3C-C2C | 5.12 | 1.47        | 1.36     |
| 11  | bA    | 812 | CLA  | O2D-CGD | 5.12 | 1.45        | 1.33     |
| 11  | aA    | 822 | CLA  | C3C-C2C | 5.12 | 1.47        | 1.36     |
| 11  | cA    | 813 | CLA  | C3C-C2C | 5.12 | 1.47        | 1.36     |
| 11  | bB    | 816 | CLA  | O2D-CGD | 5.12 | 1.45        | 1.33     |
| 11  | cA    | 841 | CLA  | O2D-CGD | 5.12 | 1.45        | 1.33     |
| 11  | aB    | 828 | CLA  | C3C-C2C | 5.12 | 1.47        | 1.36     |
| 11  | bA    | 805 | CLA  | C3C-C2C | 5.12 | 1.47        | 1.36     |
| 11  | bA    | 829 | CLA  | C3C-C2C | 5.12 | 1.47        | 1.36     |
| 11  | bB    | 837 | CLA  | C3C-C2C | 5.12 | 1.47        | 1.36     |
| 11  | aB    | 813 | CLA  | C3C-C2C | 5.11 | 1.47        | 1.36     |
| 11  | bA    | 834 | CLA  | C3C-C2C | 5.11 | 1.47        | 1.36     |
| 11  | bA    | 813 | CLA  | C3C-C2C | 5.11 | 1.47        | 1.36     |
| 11  | cB    | 813 | CLA  | C3C-C2C | 5.11 | 1.47        | 1.36     |
| 11  | bB    | 840 | CLA  | C3C-C2C | 5.11 | 1.47        | 1.36     |
| 11  | cA    | 811 | CLA  | O2D-CGD | 5.11 | 1.45        | 1.33     |
| 11  | cA    | 810 | CLA  | C3C-C2C | 5.11 | 1.47        | 1.36     |
| 11  | bA    | 841 | CLA  | O2D-CGD | 5.11 | 1.45        | 1.33     |
| 11  | bL    | 204 | CLA  | C3C-C2C | 5.11 | 1.47        | 1.36     |
| 11  | cL    | 204 | CLA  | C3C-C2C | 5.11 | 1.47        | 1.36     |
| 11  | cB    | 828 | CLA  | C3C-C2C | 5.11 | 1.47        | 1.36     |
| 11  | bA    | 811 | CLA  | O2D-CGD | 5.10 | 1.45        | 1.33     |
| 11  | bB    | 813 | CLA  | C3C-C2C | 5.10 | 1.47        | 1.36     |
| 11  | aA    | 810 | CLA  | C3C-C2C | 5.10 | 1.47        | 1.36     |
| 11  | cB    | 805 | CLA  | C3C-C2C | 5.10 | 1.47        | 1.36     |
| 11  | aA    | 811 | CLA  | O2D-CGD | 5.10 | 1.45        | 1.33     |
| 11  | bA    | 821 | CLA  | C3C-C2C | 5.10 | 1.47        | 1.36     |
| 11  | aB    | 816 | CLA  | O2D-CGD | 5.10 | 1.45        | 1.33     |
| 11  | aA    | 809 | CLA  | C3C-C2C | 5.10 | 1.47        | 1.36     |
| 11  | aA    | 829 | CLA  | C3C-C2C | 5.10 | 1.47        | 1.36     |
| 11  | bA    | 809 | CLA  | C3C-C2C | 5.10 | 1.47        | 1.36     |
| 11  | cA    | 812 | CLA  | O2D-CGD | 5.10 | 1.45        | 1.33     |
| 11  | bB    | 805 | CLA  | C3C-C2C | 5.10 | 1.47        | 1.36     |
| 11  | bL    | 205 | CLA  | C3C-C2C | 5.10 | 1.47        | 1.36     |
| 11  | cB    | 815 | CLA  | O2D-CGD | 5.09 | 1.45        | 1.33     |
| 11  | bA    | 810 | CLA  | C3C-C2C | 5.09 | 1.47        | 1.36     |
| 11  | cA    | 817 | CLA  | O2D-CGD | 5.09 | 1.45        | 1.33     |
| 11  | cA    | 834 | CLA  | C3C-C2C | 5.09 | 1.47        | 1.36     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 11  | cA    | 840 | CLA  | C3C-C2C | 5.09 | 1.47        | 1.36     |
| 11  | aB    | 835 | CLA  | O2D-CGD | 5.09 | 1.45        | 1.33     |
| 11  | bB    | 834 | CLA  | O2D-CGD | 5.09 | 1.45        | 1.33     |
| 11  | bB    | 810 | CLA  | C3C-C2C | 5.09 | 1.47        | 1.36     |
| 11  | aB    | 810 | CLA  | C3C-C2C | 5.09 | 1.47        | 1.36     |
| 11  | bB    | 839 | CLA  | C3C-C2C | 5.08 | 1.47        | 1.36     |
| 11  | cB    | 834 | CLA  | O2D-CGD | 5.08 | 1.45        | 1.33     |
| 11  | aA    | 840 | CLA  | C3C-C2C | 5.08 | 1.47        | 1.36     |
| 11  | bB    | 835 | CLA  | O2D-CGD | 5.08 | 1.45        | 1.33     |
| 11  | cA    | 823 | CLA  | C3C-C2C | 5.08 | 1.47        | 1.36     |
| 11  | aA    | 814 | CLA  | C3C-C2C | 5.08 | 1.47        | 1.36     |
| 11  | cA    | 843 | CLA  | C3C-C2C | 5.08 | 1.47        | 1.36     |
| 11  | bA    | 843 | CLA  | C3C-C2C | 5.08 | 1.47        | 1.36     |
| 12  | bA    | 844 | F6C  | O2D-CGD | 5.07 | 1.45        | 1.33     |
| 11  | aB    | 815 | CLA  | O2D-CGD | 5.07 | 1.45        | 1.33     |
| 11  | aA    | 823 | CLA  | C3C-C2C | 5.07 | 1.47        | 1.36     |
| 11  | bA    | 814 | CLA  | C3C-C2C | 5.07 | 1.47        | 1.36     |
| 11  | bA    | 808 | CLA  | O2D-CGD | 5.07 | 1.45        | 1.33     |
| 11  | cB    | 820 | CLA  | C3C-C2C | 5.07 | 1.47        | 1.36     |
| 11  | cB    | 839 | CLA  | C3C-C2C | 5.07 | 1.47        | 1.36     |
| 11  | aA    | 838 | CLA  | C3C-C2C | 5.07 | 1.47        | 1.36     |
| 12  | aA    | 844 | F6C  | O2D-CGD | 5.07 | 1.45        | 1.33     |
| 11  | aB    | 839 | CLA  | C3C-C2C | 5.07 | 1.47        | 1.36     |
| 11  | cA    | 814 | CLA  | C3C-C2C | 5.07 | 1.47        | 1.36     |
| 11  | bB    | 815 | CLA  | O2D-CGD | 5.06 | 1.45        | 1.33     |
| 11  | aA    | 843 | CLA  | C3C-C2C | 5.06 | 1.47        | 1.36     |
| 11  | cA    | 836 | CLA  | C3C-C2C | 5.06 | 1.47        | 1.36     |
| 11  | aA    | 808 | CLA  | O2D-CGD | 5.06 | 1.45        | 1.33     |
| 11  | bA    | 823 | CLA  | C3C-C2C | 5.06 | 1.47        | 1.36     |
| 11  | bA    | 817 | CLA  | O2D-CGD | 5.06 | 1.45        | 1.33     |
| 11  | cB    | 835 | CLA  | O2D-CGD | 5.06 | 1.45        | 1.33     |
| 11  | aA    | 804 | CLA  | O2D-CGD | 5.06 | 1.45        | 1.33     |
| 11  | cB    | 810 | CLA  | O2D-CGD | 5.06 | 1.45        | 1.33     |
| 11  | aA    | 836 | CLA  | C3C-C2C | 5.06 | 1.47        | 1.36     |
| 11  | aA    | 812 | CLA  | O2D-CGD | 5.06 | 1.45        | 1.33     |
| 11  | bA    | 840 | CLA  | C3C-C2C | 5.06 | 1.47        | 1.36     |
| 11  | bB    | 806 | CLA  | C3C-C2C | 5.06 | 1.47        | 1.36     |
| 11  | cB    | 810 | CLA  | C3C-C2C | 5.06 | 1.47        | 1.36     |
| 12  | bA    | 830 | F6C  | O2D-CGD | 5.05 | 1.45        | 1.33     |
| 11  | aB    | 836 | CLA  | O2D-CGD | 5.05 | 1.45        | 1.33     |
| 11  | bA    | 803 | CLA  | O2D-CGD | 5.05 | 1.45        | 1.33     |
| 11  | aA    | 819 | CLA  | O2D-CGD | 5.05 | 1.45        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 11  | bB    | 810 | CLA  | O2D-CGD | 5.05 | 1.45        | 1.33     |
| 11  | cB    | 806 | CLA  | C3C-C2C | 5.05 | 1.47        | 1.36     |
| 11  | cB    | 836 | CLA  | O2D-CGD | 5.05 | 1.45        | 1.33     |
| 11  | cA    | 829 | CLA  | O2D-CGD | 5.05 | 1.45        | 1.33     |
| 11  | bB    | 836 | CLA  | O2D-CGD | 5.05 | 1.45        | 1.33     |
| 12  | cA    | 844 | F6C  | O2D-CGD | 5.05 | 1.45        | 1.33     |
| 11  | aB    | 820 | CLA  | O2D-CGD | 5.05 | 1.45        | 1.33     |
| 11  | aB    | 807 | CLA  | C3C-C2C | 5.05 | 1.47        | 1.36     |
| 11  | bA    | 804 | CLA  | O2D-CGD | 5.05 | 1.45        | 1.33     |
| 11  | cA    | 819 | CLA  | O2D-CGD | 5.05 | 1.45        | 1.33     |
| 11  | cA    | 804 | CLA  | O2D-CGD | 5.05 | 1.45        | 1.33     |
| 11  | aA    | 817 | CLA  | O2D-CGD | 5.05 | 1.45        | 1.33     |
| 11  | aB    | 805 | CLA  | C3C-C2C | 5.05 | 1.47        | 1.36     |
| 11  | aB    | 817 | CLA  | C3C-C2C | 5.05 | 1.47        | 1.36     |
| 11  | aA    | 802 | CLA  | C3C-C2C | 5.05 | 1.47        | 1.36     |
| 11  | bB    | 826 | CLA  | C3C-C2C | 5.05 | 1.47        | 1.36     |
| 11  | bA    | 836 | CLA  | C3C-C2C | 5.04 | 1.47        | 1.36     |
| 11  | cB    | 820 | CLA  | O2D-CGD | 5.04 | 1.45        | 1.33     |
| 11  | cA    | 838 | CLA  | C3C-C2C | 5.04 | 1.47        | 1.36     |
| 11  | cA    | 803 | CLA  | O2D-CGD | 5.04 | 1.45        | 1.33     |
| 11  | aA    | 835 | CLA  | C3C-C2C | 5.04 | 1.47        | 1.36     |
| 11  | cA    | 835 | CLA  | C3C-C2C | 5.04 | 1.47        | 1.36     |
| 11  | bA    | 819 | CLA  | O2D-CGD | 5.04 | 1.45        | 1.33     |
| 11  | cA    | 808 | CLA  | O2D-CGD | 5.04 | 1.45        | 1.33     |
| 11  | bA    | 838 | CLA  | C3C-C2C | 5.04 | 1.47        | 1.36     |
| 11  | cB    | 807 | CLA  | C3C-C2C | 5.04 | 1.47        | 1.36     |
| 11  | aB    | 829 | CLA  | O2D-CGD | 5.04 | 1.45        | 1.33     |
| 11  | bA    | 829 | CLA  | O2D-CGD | 5.04 | 1.45        | 1.33     |
| 12  | aA    | 827 | F6C  | O2D-CGD | 5.03 | 1.45        | 1.33     |
| 11  | bB    | 820 | CLA  | C3C-C2C | 5.03 | 1.47        | 1.36     |
| 11  | bB    | 817 | CLA  | C3C-C2C | 5.03 | 1.47        | 1.36     |
| 11  | aB    | 839 | CLA  | O2D-CGD | 5.03 | 1.45        | 1.33     |
| 11  | bB    | 805 | CLA  | O2D-CGD | 5.03 | 1.45        | 1.33     |
| 11  | bB    | 829 | CLA  | O2D-CGD | 5.03 | 1.45        | 1.33     |
| 11  | aA    | 822 | CLA  | O2D-CGD | 5.03 | 1.45        | 1.33     |
| 11  | cB    | 837 | CLA  | O2D-CGD | 5.03 | 1.45        | 1.33     |
| 12  | cA    | 827 | F6C  | O2D-CGD | 5.03 | 1.45        | 1.33     |
| 11  | aB    | 820 | CLA  | C3C-C2C | 5.03 | 1.47        | 1.36     |
| 11  | cA    | 802 | CLA  | C3C-C2C | 5.03 | 1.47        | 1.36     |
| 11  | bB    | 839 | CLA  | O2D-CGD | 5.03 | 1.45        | 1.33     |
| 11  | cB    | 829 | CLA  | O2D-CGD | 5.03 | 1.45        | 1.33     |
| 11  | cA    | 822 | CLA  | O2D-CGD | 5.03 | 1.45        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 11  | bA    | 835 | CLA  | C3C-C2C | 5.03 | 1.47        | 1.36     |
| 11  | aB    | 805 | CLA  | O2D-CGD | 5.03 | 1.45        | 1.33     |
| 11  | cA    | 813 | CLA  | O2D-CGD | 5.03 | 1.45        | 1.33     |
| 11  | aA    | 829 | CLA  | O2D-CGD | 5.03 | 1.45        | 1.33     |
| 12  | cA    | 830 | F6C  | O2D-CGD | 5.03 | 1.45        | 1.33     |
| 11  | aB    | 822 | CLA  | O2D-CGD | 5.02 | 1.45        | 1.33     |
| 11  | aB    | 806 | CLA  | C3C-C2C | 5.02 | 1.47        | 1.36     |
| 11  | bB    | 807 | CLA  | C3C-C2C | 5.02 | 1.47        | 1.36     |
| 11  | aA    | 803 | CLA  | O2D-CGD | 5.02 | 1.45        | 1.33     |
| 12  | aA    | 830 | F6C  | O2D-CGD | 5.02 | 1.45        | 1.33     |
| 11  | cA    | 823 | CLA  | O2D-CGD | 5.02 | 1.45        | 1.33     |
| 11  | cB    | 839 | CLA  | O2D-CGD | 5.02 | 1.45        | 1.33     |
| 11  | bB    | 820 | CLA  | O2D-CGD | 5.02 | 1.45        | 1.33     |
| 11  | aA    | 843 | CLA  | O2D-CGD | 5.02 | 1.45        | 1.33     |
| 11  | bA    | 822 | CLA  | O2D-CGD | 5.02 | 1.45        | 1.33     |
| 11  | cA    | 807 | CLA  | C3C-C2C | 5.02 | 1.47        | 1.36     |
| 11  | bB    | 837 | CLA  | O2D-CGD | 5.02 | 1.45        | 1.33     |
| 11  | aB    | 810 | CLA  | O2D-CGD | 5.02 | 1.45        | 1.33     |
| 11  | aB    | 803 | CLA  | O2D-CGD | 5.02 | 1.45        | 1.33     |
| 11  | aB    | 823 | CLA  | C3C-C2C | 5.02 | 1.47        | 1.36     |
| 11  | aA    | 824 | CLA  | O2D-CGD | 5.02 | 1.45        | 1.33     |
| 11  | cB    | 817 | CLA  | C3C-C2C | 5.02 | 1.47        | 1.36     |
| 11  | aB    | 809 | CLA  | C3C-C2C | 5.01 | 1.47        | 1.36     |
| 11  | cB    | 823 | CLA  | C3C-C2C | 5.01 | 1.47        | 1.36     |
| 11  | bA    | 803 | CLA  | C3C-C2C | 5.01 | 1.47        | 1.36     |
| 13  | cA    | 845 | PQN  | C10-C5  | 5.01 | 1.48        | 1.40     |
| 11  | aB    | 802 | CLA  | C3C-C2C | 5.01 | 1.47        | 1.36     |
| 11  | aA    | 833 | CLA  | O2D-CGD | 5.01 | 1.45        | 1.33     |
| 12  | bA    | 827 | F6C  | O2D-CGD | 5.01 | 1.45        | 1.33     |
| 11  | cB    | 809 | CLA  | C3C-C2C | 5.01 | 1.47        | 1.36     |
| 11  | bB    | 823 | CLA  | O2D-CGD | 5.01 | 1.45        | 1.33     |
| 11  | bB    | 809 | CLA  | C3C-C2C | 5.01 | 1.47        | 1.36     |
| 11  | cB    | 827 | CLA  | O2D-CGD | 5.01 | 1.45        | 1.33     |
| 11  | bL    | 206 | CLA  | O2D-CGD | 5.01 | 1.45        | 1.33     |
| 11  | bB    | 823 | CLA  | C3C-C2C | 5.01 | 1.47        | 1.36     |
| 13  | bA    | 845 | PQN  | C10-C5  | 5.01 | 1.48        | 1.40     |
| 11  | aB    | 811 | CLA  | O2D-CGD | 5.01 | 1.45        | 1.33     |
| 11  | bA    | 802 | CLA  | C3C-C2C | 5.01 | 1.47        | 1.36     |
| 11  | cA    | 843 | CLA  | O2D-CGD | 5.01 | 1.45        | 1.33     |
| 13  | cB    | 841 | PQN  | C10-C5  | 5.00 | 1.48        | 1.40     |
| 11  | aA    | 807 | CLA  | C3C-C2C | 5.00 | 1.47        | 1.36     |
| 11  | cB    | 802 | CLA  | C3C-C2C | 5.00 | 1.47        | 1.36     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 11  | cA    | 824 | CLA  | O2D-CGD | 5.00 | 1.45        | 1.33     |
| 11  | bA    | 824 | CLA  | O2D-CGD | 5.00 | 1.45        | 1.33     |
| 11  | bB    | 802 | CLA  | C3C-C2C | 5.00 | 1.47        | 1.36     |
| 11  | cB    | 803 | CLA  | O2D-CGD | 5.00 | 1.45        | 1.33     |
| 11  | aB    | 837 | CLA  | O2D-CGD | 5.00 | 1.45        | 1.33     |
| 11  | aA    | 813 | CLA  | O2D-CGD | 5.00 | 1.45        | 1.33     |
| 11  | aB    | 818 | CLA  | O2D-CGD | 5.00 | 1.45        | 1.33     |
| 11  | bB    | 822 | CLA  | O2D-CGD | 5.00 | 1.45        | 1.33     |
| 11  | cA    | 816 | CLA  | O2D-CGD | 5.00 | 1.45        | 1.33     |
| 11  | cB    | 805 | CLA  | O2D-CGD | 5.00 | 1.45        | 1.33     |
| 11  | aB    | 826 | CLA  | C3C-C2C | 5.00 | 1.47        | 1.36     |
| 11  | bA    | 807 | CLA  | C3C-C2C | 5.00 | 1.47        | 1.36     |
| 11  | bA    | 823 | CLA  | O2D-CGD | 5.00 | 1.45        | 1.33     |
| 13  | aA    | 845 | PQN  | C10-C5  | 5.00 | 1.48        | 1.40     |
| 11  | bA    | 843 | CLA  | O2D-CGD | 5.00 | 1.45        | 1.33     |
| 11  | cA    | 803 | CLA  | C3C-C2C | 5.00 | 1.47        | 1.36     |
| 11  | bA    | 839 | CLA  | O2D-CGD | 5.00 | 1.45        | 1.33     |
| 11  | cB    | 811 | CLA  | O2D-CGD | 5.00 | 1.45        | 1.33     |
| 11  | aL    | 206 | CLA  | O2D-CGD | 4.99 | 1.45        | 1.33     |
| 11  | cB    | 826 | CLA  | C3C-C2C | 4.99 | 1.47        | 1.36     |
| 11  | aA    | 805 | CLA  | O2D-CGD | 4.99 | 1.45        | 1.33     |
| 11  | bB    | 827 | CLA  | O2D-CGD | 4.99 | 1.45        | 1.33     |
| 11  | cB    | 823 | CLA  | O2D-CGD | 4.99 | 1.45        | 1.33     |
| 11  | bB    | 832 | CLA  | O2D-CGD | 4.99 | 1.45        | 1.33     |
| 11  | bA    | 813 | CLA  | O2D-CGD | 4.99 | 1.45        | 1.33     |
| 11  | aB    | 808 | CLA  | C3C-C2C | 4.99 | 1.47        | 1.36     |
| 11  | bA    | 833 | CLA  | O2D-CGD | 4.99 | 1.45        | 1.33     |
| 11  | aB    | 823 | CLA  | O2D-CGD | 4.99 | 1.45        | 1.33     |
| 11  | bB    | 818 | CLA  | O2D-CGD | 4.99 | 1.45        | 1.33     |
| 11  | cB    | 822 | CLA  | O2D-CGD | 4.99 | 1.45        | 1.33     |
| 11  | aA    | 803 | CLA  | C3C-C2C | 4.98 | 1.47        | 1.36     |
| 11  | bB    | 840 | CLA  | O2D-CGD | 4.98 | 1.45        | 1.33     |
| 11  | aB    | 832 | CLA  | O2D-CGD | 4.98 | 1.45        | 1.33     |
| 11  | cL    | 206 | CLA  | O2D-CGD | 4.98 | 1.45        | 1.33     |
| 11  | bB    | 825 | CLA  | O2D-CGD | 4.98 | 1.45        | 1.33     |
| 13  | bB    | 841 | PQN  | C10-C5  | 4.98 | 1.48        | 1.40     |
| 11  | bA    | 805 | CLA  | CHC-C1C | 4.98 | 1.48        | 1.38     |
| 11  | cA    | 805 | CLA  | CHC-C1C | 4.98 | 1.48        | 1.38     |
| 11  | cA    | 805 | CLA  | O2D-CGD | 4.97 | 1.45        | 1.33     |
| 11  | cA    | 833 | CLA  | O2D-CGD | 4.97 | 1.45        | 1.33     |
| 11  | bA    | 805 | CLA  | O2D-CGD | 4.97 | 1.45        | 1.33     |
| 11  | aB    | 825 | CLA  | O2D-CGD | 4.97 | 1.45        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 11  | aA    | 823 | CLA  | O2D-CGD | 4.97 | 1.45        | 1.33     |
| 11  | cB    | 832 | CLA  | O2D-CGD | 4.97 | 1.45        | 1.33     |
| 11  | aB    | 827 | CLA  | O2D-CGD | 4.97 | 1.45        | 1.33     |
| 11  | cB    | 825 | CLA  | O2D-CGD | 4.97 | 1.45        | 1.33     |
| 11  | bB    | 803 | CLA  | O2D-CGD | 4.97 | 1.45        | 1.33     |
| 11  | bB    | 811 | CLA  | O2D-CGD | 4.97 | 1.45        | 1.33     |
| 12  | cA    | 826 | F6C  | O2D-CGD | 4.97 | 1.45        | 1.33     |
| 11  | cB    | 807 | CLA  | O2D-CGD | 4.96 | 1.45        | 1.33     |
| 11  | bA    | 828 | CLA  | C3C-C2C | 4.96 | 1.47        | 1.36     |
| 11  | cB    | 840 | CLA  | O2D-CGD | 4.96 | 1.45        | 1.33     |
| 12  | aA    | 826 | F6C  | O2D-CGD | 4.96 | 1.45        | 1.33     |
| 11  | bA    | 816 | CLA  | O2D-CGD | 4.96 | 1.45        | 1.33     |
| 11  | aB    | 807 | CLA  | O2D-CGD | 4.96 | 1.45        | 1.33     |
| 11  | bB    | 807 | CLA  | O2D-CGD | 4.96 | 1.45        | 1.33     |
| 11  | bB    | 808 | CLA  | C3C-C2C | 4.96 | 1.47        | 1.36     |
| 11  | bB    | 826 | CLA  | O2D-CGD | 4.96 | 1.45        | 1.33     |
| 11  | cB    | 826 | CLA  | O2D-CGD | 4.95 | 1.45        | 1.33     |
| 11  | bB    | 830 | CLA  | O2D-CGD | 4.95 | 1.45        | 1.33     |
| 12  | bA    | 826 | F6C  | O2D-CGD | 4.95 | 1.45        | 1.33     |
| 11  | cB    | 818 | CLA  | O2D-CGD | 4.95 | 1.45        | 1.33     |
| 11  | cA    | 828 | CLA  | C3C-C2C | 4.95 | 1.47        | 1.36     |
| 11  | aA    | 805 | CLA  | CHC-C1C | 4.95 | 1.48        | 1.38     |
| 13  | aB    | 841 | PQN  | C10-C5  | 4.95 | 1.48        | 1.40     |
| 11  | bA    | 819 | CLA  | C3C-C2C | 4.94 | 1.47        | 1.36     |
| 11  | aA    | 816 | CLA  | O2D-CGD | 4.94 | 1.45        | 1.33     |
| 11  | aB    | 809 | CLA  | O2D-CGD | 4.94 | 1.45        | 1.33     |
| 11  | cB    | 830 | CLA  | O2D-CGD | 4.94 | 1.45        | 1.33     |
| 11  | aA    | 819 | CLA  | C3C-C2C | 4.94 | 1.47        | 1.36     |
| 11  | aA    | 839 | CLA  | O2D-CGD | 4.94 | 1.45        | 1.33     |
| 11  | cA    | 820 | CLA  | C3C-C2C | 4.94 | 1.47        | 1.36     |
| 11  | cB    | 808 | CLA  | C3C-C2C | 4.94 | 1.47        | 1.36     |
| 11  | aB    | 830 | CLA  | O2D-CGD | 4.94 | 1.45        | 1.33     |
| 11  | bB    | 812 | CLA  | C3C-C2C | 4.94 | 1.47        | 1.36     |
| 11  | aB    | 826 | CLA  | O2D-CGD | 4.94 | 1.45        | 1.33     |
| 11  | bB    | 838 | CLA  | O2D-CGD | 4.94 | 1.45        | 1.33     |
| 11  | aA    | 820 | CLA  | C3C-C2C | 4.94 | 1.47        | 1.36     |
| 11  | cB    | 838 | CLA  | O2D-CGD | 4.93 | 1.45        | 1.33     |
| 11  | bA    | 820 | CLA  | C3C-C2C | 4.93 | 1.47        | 1.36     |
| 11  | aA    | 828 | CLA  | C3C-C2C | 4.93 | 1.47        | 1.36     |
| 11  | aB    | 838 | CLA  | O2D-CGD | 4.93 | 1.45        | 1.33     |
| 11  | cA    | 839 | CLA  | O2D-CGD | 4.93 | 1.45        | 1.33     |
| 11  | aB    | 812 | CLA  | C3C-C2C | 4.93 | 1.47        | 1.36     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 11  | aB    | 840 | CLA  | O2D-CGD | 4.93 | 1.45        | 1.33     |
| 11  | bB    | 809 | CLA  | O2D-CGD | 4.93 | 1.45        | 1.33     |
| 11  | cL    | 204 | CLA  | O2D-CGD | 4.93 | 1.45        | 1.33     |
| 11  | cA    | 819 | CLA  | C3C-C2C | 4.92 | 1.47        | 1.36     |
| 11  | aA    | 825 | CLA  | C3C-C2C | 4.92 | 1.47        | 1.36     |
| 11  | bA    | 825 | CLA  | C3C-C2C | 4.92 | 1.47        | 1.36     |
| 11  | cA    | 825 | CLA  | C3C-C2C | 4.92 | 1.47        | 1.36     |
| 11  | cB    | 809 | CLA  | O2D-CGD | 4.92 | 1.45        | 1.33     |
| 11  | bB    | 817 | CLA  | O2D-CGD | 4.92 | 1.45        | 1.33     |
| 11  | bL    | 204 | CLA  | O2D-CGD | 4.92 | 1.45        | 1.33     |
| 11  | cB    | 814 | CLA  | O2D-CGD | 4.91 | 1.45        | 1.33     |
| 11  | bB    | 814 | CLA  | O2D-CGD | 4.91 | 1.45        | 1.33     |
| 11  | aB    | 814 | CLA  | O2D-CGD | 4.90 | 1.45        | 1.33     |
| 11  | bA    | 821 | CLA  | O2D-CGD | 4.90 | 1.45        | 1.33     |
| 11  | aA    | 828 | CLA  | O2D-CGD | 4.90 | 1.45        | 1.33     |
| 11  | bA    | 828 | CLA  | O2D-CGD | 4.90 | 1.45        | 1.33     |
| 11  | cA    | 828 | CLA  | O2D-CGD | 4.90 | 1.45        | 1.33     |
| 11  | aB    | 803 | CLA  | C3C-C2C | 4.90 | 1.47        | 1.36     |
| 11  | cA    | 821 | CLA  | O2D-CGD | 4.90 | 1.45        | 1.33     |
| 11  | aA    | 818 | CLA  | O2D-CGD | 4.90 | 1.45        | 1.33     |
| 11  | aB    | 817 | CLA  | O2D-CGD | 4.90 | 1.45        | 1.33     |
| 11  | cA    | 806 | CLA  | O2D-CGD | 4.90 | 1.45        | 1.33     |
| 11  | cA    | 809 | CLA  | O2D-CGD | 4.90 | 1.45        | 1.33     |
| 11  | aA    | 809 | CLA  | O2D-CGD | 4.89 | 1.45        | 1.33     |
| 11  | cB    | 828 | CLA  | O2D-CGD | 4.89 | 1.45        | 1.33     |
| 11  | bA    | 818 | CLA  | O2D-CGD | 4.89 | 1.45        | 1.33     |
| 11  | aK    | 103 | CLA  | O2D-CGD | 4.89 | 1.45        | 1.33     |
| 11  | aA    | 810 | CLA  | O2D-CGD | 4.89 | 1.45        | 1.33     |
| 11  | aA    | 838 | CLA  | O2D-CGD | 4.89 | 1.45        | 1.33     |
| 11  | aL    | 204 | CLA  | O2D-CGD | 4.89 | 1.45        | 1.33     |
| 11  | cB    | 817 | CLA  | O2D-CGD | 4.89 | 1.45        | 1.33     |
| 11  | aA    | 819 | CLA  | CHC-C1C | 4.89 | 1.48        | 1.38     |
| 11  | bA    | 809 | CLA  | O2D-CGD | 4.89 | 1.45        | 1.33     |
| 11  | cA    | 818 | CLA  | O2D-CGD | 4.89 | 1.45        | 1.33     |
| 11  | cK    | 103 | CLA  | O2D-CGD | 4.88 | 1.45        | 1.33     |
| 11  | aB    | 822 | CLA  | CHC-C1C | 4.88 | 1.48        | 1.38     |
| 11  | bB    | 828 | CLA  | O2D-CGD | 4.88 | 1.45        | 1.33     |
| 11  | cA    | 838 | CLA  | O2D-CGD | 4.88 | 1.45        | 1.33     |
| 11  | bA    | 810 | CLA  | O2D-CGD | 4.88 | 1.45        | 1.33     |
| 11  | cA    | 802 | CLA  | O2D-CGD | 4.88 | 1.45        | 1.33     |
| 11  | cA    | 819 | CLA  | CHC-C1C | 4.88 | 1.48        | 1.38     |
| 11  | aA    | 802 | CLA  | O2D-CGD | 4.88 | 1.45        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 11  | bA    | 802 | CLA  | O2D-CGD | 4.88 | 1.45        | 1.33     |
| 11  | aB    | 819 | CLA  | O2D-CGD | 4.87 | 1.45        | 1.33     |
| 11  | bK    | 103 | CLA  | O2D-CGD | 4.87 | 1.45        | 1.33     |
| 11  | bA    | 806 | CLA  | O2D-CGD | 4.87 | 1.45        | 1.33     |
| 11  | cB    | 812 | CLA  | C3C-C2C | 4.87 | 1.47        | 1.36     |
| 11  | bA    | 807 | CLA  | O2D-CGD | 4.87 | 1.45        | 1.33     |
| 11  | bA    | 838 | CLA  | O2D-CGD | 4.87 | 1.45        | 1.33     |
| 11  | bB    | 816 | CLA  | CHC-C1C | 4.87 | 1.48        | 1.38     |
| 10  | aA    | 801 | CL0  | OBD-CAD | 4.87 | 1.28        | 1.22     |
| 10  | bA    | 801 | CL0  | OBD-CAD | 4.87 | 1.28        | 1.22     |
| 11  | bL    | 205 | CLA  | O2D-CGD | 4.87 | 1.45        | 1.33     |
| 11  | cA    | 810 | CLA  | O2D-CGD | 4.87 | 1.45        | 1.33     |
| 11  | aA    | 821 | CLA  | O2D-CGD | 4.86 | 1.45        | 1.33     |
| 11  | cB    | 803 | CLA  | C3C-C2C | 4.86 | 1.47        | 1.36     |
| 11  | bB    | 803 | CLA  | C3C-C2C | 4.86 | 1.47        | 1.36     |
| 11  | aA    | 806 | CLA  | O2D-CGD | 4.86 | 1.45        | 1.33     |
| 11  | cB    | 822 | CLA  | CHC-C1C | 4.86 | 1.48        | 1.38     |
| 11  | cL    | 205 | CLA  | O2D-CGD | 4.86 | 1.45        | 1.33     |
| 11  | bB    | 822 | CLA  | CHC-C1C | 4.86 | 1.48        | 1.38     |
| 12  | cB    | 824 | F6C  | O2D-CGD | 4.86 | 1.45        | 1.33     |
| 11  | aA    | 807 | CLA  | O2D-CGD | 4.86 | 1.45        | 1.33     |
| 11  | cB    | 819 | CLA  | O2D-CGD | 4.85 | 1.45        | 1.33     |
| 11  | bA    | 819 | CLA  | CHC-C1C | 4.85 | 1.48        | 1.38     |
| 11  | aB    | 815 | CLA  | C3C-C2C | 4.85 | 1.47        | 1.36     |
| 11  | bB    | 819 | CLA  | O2D-CGD | 4.85 | 1.45        | 1.33     |
| 12  | cA    | 832 | F6C  | O2D-CGD | 4.85 | 1.45        | 1.33     |
| 11  | aB    | 828 | CLA  | O2D-CGD | 4.85 | 1.45        | 1.33     |
| 12  | aB    | 824 | F6C  | O2D-CGD | 4.84 | 1.45        | 1.33     |
| 11  | cA    | 807 | CLA  | O2D-CGD | 4.84 | 1.45        | 1.33     |
| 12  | bB    | 824 | F6C  | O2D-CGD | 4.84 | 1.45        | 1.33     |
| 11  | bB    | 833 | CLA  | O2D-CGD | 4.84 | 1.45        | 1.33     |
| 11  | aA    | 834 | CLA  | O2D-CGD | 4.84 | 1.45        | 1.33     |
| 11  | aB    | 821 | CLA  | C1D-ND  | 4.83 | 1.44        | 1.37     |
| 11  | aB    | 816 | CLA  | CHC-C1C | 4.83 | 1.48        | 1.38     |
| 11  | cA    | 834 | CLA  | O2D-CGD | 4.83 | 1.45        | 1.33     |
| 12  | bA    | 832 | F6C  | O2D-CGD | 4.83 | 1.45        | 1.33     |
| 11  | aL    | 205 | CLA  | O2D-CGD | 4.83 | 1.45        | 1.33     |
| 11  | cB    | 832 | CLA  | C1D-ND  | 4.83 | 1.44        | 1.37     |
| 12  | aA    | 832 | F6C  | O2D-CGD | 4.83 | 1.45        | 1.33     |
| 11  | aB    | 834 | CLA  | C1D-ND  | 4.82 | 1.44        | 1.37     |
| 11  | bA    | 840 | CLA  | O2D-CGD | 4.82 | 1.45        | 1.33     |
| 11  | aA    | 820 | CLA  | O2D-CGD | 4.82 | 1.45        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 11  | cB    | 815 | CLA  | C3C-C2C | 4.82 | 1.47        | 1.36     |
| 11  | aB    | 833 | CLA  | O2D-CGD | 4.82 | 1.45        | 1.33     |
| 10  | cA    | 801 | CL0  | OBD-CAD | 4.81 | 1.28        | 1.22     |
| 11  | cA    | 820 | CLA  | O2D-CGD | 4.81 | 1.45        | 1.33     |
| 11  | bB    | 815 | CLA  | C3C-C2C | 4.81 | 1.47        | 1.36     |
| 11  | bA    | 834 | CLA  | O2D-CGD | 4.81 | 1.45        | 1.33     |
| 11  | bA    | 820 | CLA  | O2D-CGD | 4.81 | 1.45        | 1.33     |
| 11  | aA    | 815 | CLA  | O2D-CGD | 4.80 | 1.45        | 1.33     |
| 11  | cB    | 813 | CLA  | O2D-CGD | 4.80 | 1.45        | 1.33     |
| 11  | bB    | 804 | CLA  | O2D-CGD | 4.80 | 1.45        | 1.33     |
| 11  | cB    | 831 | CLA  | C1D-ND  | 4.80 | 1.44        | 1.37     |
| 11  | bA    | 818 | CLA  | CHC-C1C | 4.80 | 1.48        | 1.38     |
| 11  | cB    | 833 | CLA  | O2D-CGD | 4.80 | 1.45        | 1.33     |
| 11  | aA    | 812 | CLA  | C1D-ND  | 4.80 | 1.44        | 1.37     |
| 10  | aA    | 801 | CL0  | CHB-C1B | 4.80 | 1.47        | 1.39     |
| 11  | bA    | 812 | CLA  | C1D-ND  | 4.80 | 1.44        | 1.37     |
| 10  | cA    | 801 | CL0  | O2D-CGD | 4.79 | 1.45        | 1.33     |
| 11  | cB    | 804 | CLA  | CHC-C1C | 4.79 | 1.48        | 1.38     |
| 11  | bB    | 831 | CLA  | C1D-ND  | 4.79 | 1.44        | 1.37     |
| 11  | cB    | 821 | CLA  | C1D-ND  | 4.79 | 1.44        | 1.37     |
| 10  | cA    | 801 | CL0  | CHB-C1B | 4.79 | 1.47        | 1.39     |
| 11  | aB    | 829 | CLA  | C1D-ND  | 4.79 | 1.44        | 1.37     |
| 11  | bB    | 804 | CLA  | CHC-C1C | 4.79 | 1.48        | 1.38     |
| 11  | aB    | 806 | CLA  | O2D-CGD | 4.78 | 1.45        | 1.33     |
| 11  | aA    | 818 | CLA  | C3C-C2C | 4.78 | 1.47        | 1.36     |
| 11  | aB    | 832 | CLA  | C1D-ND  | 4.78 | 1.44        | 1.37     |
| 10  | bA    | 801 | CL0  | O2D-CGD | 4.78 | 1.45        | 1.33     |
| 11  | cA    | 815 | CLA  | O2D-CGD | 4.78 | 1.45        | 1.33     |
| 11  | bB    | 829 | CLA  | C1D-ND  | 4.78 | 1.44        | 1.37     |
| 11  | aB    | 813 | CLA  | O2D-CGD | 4.78 | 1.45        | 1.33     |
| 11  | cA    | 831 | CLA  | O2D-CGD | 4.78 | 1.45        | 1.33     |
| 11  | bA    | 814 | CLA  | O2D-CGD | 4.78 | 1.45        | 1.33     |
| 11  | cA    | 840 | CLA  | O2D-CGD | 4.78 | 1.45        | 1.33     |
| 11  | bB    | 833 | CLA  | CHC-C1C | 4.78 | 1.48        | 1.38     |
| 11  | bB    | 834 | CLA  | C1D-ND  | 4.78 | 1.44        | 1.37     |
| 11  | cB    | 835 | CLA  | C1D-ND  | 4.78 | 1.44        | 1.37     |
| 11  | aA    | 840 | CLA  | O2D-CGD | 4.78 | 1.45        | 1.33     |
| 11  | bA    | 815 | CLA  | O2D-CGD | 4.78 | 1.45        | 1.33     |
| 11  | aB    | 835 | CLA  | C1D-ND  | 4.77 | 1.44        | 1.37     |
| 11  | bB    | 835 | CLA  | C1D-ND  | 4.77 | 1.44        | 1.37     |
| 11  | aB    | 833 | CLA  | CHC-C1C | 4.77 | 1.48        | 1.38     |
| 11  | cB    | 816 | CLA  | CHC-C1C | 4.77 | 1.48        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 11  | cB    | 839 | CLA  | CHC-C1C | 4.77 | 1.48        | 1.38     |
| 11  | aB    | 837 | CLA  | CHC-C1C | 4.77 | 1.48        | 1.38     |
| 10  | bA    | 801 | CL0  | CHB-C1B | 4.77 | 1.47        | 1.39     |
| 11  | cB    | 801 | CLA  | C3C-C2C | 4.77 | 1.47        | 1.36     |
| 11  | bB    | 806 | CLA  | O2D-CGD | 4.77 | 1.44        | 1.33     |
| 10  | aA    | 801 | CL0  | O2D-CGD | 4.76 | 1.44        | 1.33     |
| 11  | cB    | 832 | CLA  | CHC-C1C | 4.76 | 1.48        | 1.38     |
| 11  | aB    | 831 | CLA  | O2D-CGD | 4.76 | 1.44        | 1.33     |
| 11  | cB    | 804 | CLA  | O2D-CGD | 4.76 | 1.44        | 1.33     |
| 11  | cB    | 806 | CLA  | O2D-CGD | 4.76 | 1.44        | 1.33     |
| 11  | aB    | 804 | CLA  | O2D-CGD | 4.76 | 1.44        | 1.33     |
| 11  | aA    | 828 | CLA  | C1D-ND  | 4.76 | 1.44        | 1.37     |
| 11  | bB    | 813 | CLA  | O2D-CGD | 4.76 | 1.44        | 1.33     |
| 11  | cA    | 818 | CLA  | C3C-C2C | 4.76 | 1.47        | 1.36     |
| 11  | cA    | 814 | CLA  | O2D-CGD | 4.76 | 1.44        | 1.33     |
| 11  | bB    | 832 | CLA  | C1D-ND  | 4.75 | 1.44        | 1.37     |
| 11  | cB    | 834 | CLA  | C1D-ND  | 4.75 | 1.44        | 1.37     |
| 11  | aA    | 814 | CLA  | O2D-CGD | 4.75 | 1.44        | 1.33     |
| 11  | aA    | 831 | CLA  | O2D-CGD | 4.75 | 1.44        | 1.33     |
| 11  | bA    | 818 | CLA  | C3C-C2C | 4.75 | 1.47        | 1.36     |
| 11  | bB    | 821 | CLA  | C1D-ND  | 4.75 | 1.44        | 1.37     |
| 11  | bB    | 801 | CLA  | C3C-C2C | 4.75 | 1.47        | 1.36     |
| 11  | cB    | 831 | CLA  | O2D-CGD | 4.74 | 1.44        | 1.33     |
| 11  | cA    | 818 | CLA  | CHC-C1C | 4.74 | 1.48        | 1.38     |
| 11  | bB    | 831 | CLA  | O2D-CGD | 4.74 | 1.44        | 1.33     |
| 11  | bA    | 831 | CLA  | O2D-CGD | 4.74 | 1.44        | 1.33     |
| 11  | aB    | 812 | CLA  | O2D-CGD | 4.73 | 1.44        | 1.33     |
| 11  | aA    | 818 | CLA  | CHC-C1C | 4.73 | 1.48        | 1.38     |
| 11  | bB    | 839 | CLA  | CHC-C1C | 4.73 | 1.48        | 1.38     |
| 11  | cB    | 837 | CLA  | CHC-C1C | 4.73 | 1.48        | 1.38     |
| 11  | aB    | 836 | CLA  | CHC-C1C | 4.73 | 1.48        | 1.38     |
| 11  | bA    | 804 | CLA  | CHC-C1C | 4.73 | 1.48        | 1.38     |
| 11  | cA    | 812 | CLA  | C1D-ND  | 4.73 | 1.44        | 1.37     |
| 11  | aB    | 832 | CLA  | CHC-C1C | 4.73 | 1.48        | 1.38     |
| 11  | bB    | 832 | CLA  | CHC-C1C | 4.73 | 1.48        | 1.38     |
| 11  | bB    | 822 | CLA  | C3C-C2C | 4.73 | 1.47        | 1.36     |
| 11  | cB    | 833 | CLA  | CHC-C1C | 4.73 | 1.48        | 1.38     |
| 11  | aB    | 831 | CLA  | C1D-ND  | 4.73 | 1.44        | 1.37     |
| 11  | aB    | 801 | CLA  | C3C-C2C | 4.72 | 1.47        | 1.36     |
| 11  | bB    | 837 | CLA  | CHC-C1C | 4.72 | 1.47        | 1.38     |
| 11  | aA    | 816 | CLA  | CHC-C1C | 4.72 | 1.47        | 1.38     |
| 11  | cB    | 802 | CLA  | CHC-C1C | 4.72 | 1.47        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 11  | cB    | 829 | CLA  | C1D-ND  | 4.72 | 1.44        | 1.37     |
| 11  | cA    | 804 | CLA  | CHC-C1C | 4.72 | 1.47        | 1.38     |
| 11  | aB    | 804 | CLA  | CHC-C1C | 4.71 | 1.47        | 1.38     |
| 11  | cA    | 816 | CLA  | CHC-C1C | 4.71 | 1.47        | 1.38     |
| 11  | cA    | 828 | CLA  | C1D-ND  | 4.71 | 1.44        | 1.37     |
| 11  | aB    | 822 | CLA  | C3C-C2C | 4.71 | 1.46        | 1.36     |
| 11  | cK    | 103 | CLA  | C1D-ND  | 4.71 | 1.44        | 1.37     |
| 11  | aA    | 836 | CLA  | O2D-CGD | 4.71 | 1.44        | 1.33     |
| 11  | bB    | 836 | CLA  | CHC-C1C | 4.71 | 1.47        | 1.38     |
| 11  | cA    | 836 | CLA  | O2D-CGD | 4.71 | 1.44        | 1.33     |
| 11  | bA    | 828 | CLA  | C1D-ND  | 4.71 | 1.44        | 1.37     |
| 11  | aB    | 802 | CLA  | CHC-C1C | 4.71 | 1.47        | 1.38     |
| 11  | aA    | 804 | CLA  | CHC-C1C | 4.70 | 1.47        | 1.38     |
| 11  | bK    | 103 | CLA  | C1D-ND  | 4.70 | 1.44        | 1.37     |
| 11  | cB    | 822 | CLA  | C3C-C2C | 4.70 | 1.46        | 1.36     |
| 11  | cA    | 803 | CLA  | CHC-C1C | 4.70 | 1.47        | 1.38     |
| 11  | cB    | 812 | CLA  | O2D-CGD | 4.70 | 1.44        | 1.33     |
| 11  | bB    | 818 | CLA  | CHC-C1C | 4.70 | 1.47        | 1.38     |
| 11  | bK    | 101 | CLA  | CHC-C1C | 4.70 | 1.47        | 1.38     |
| 11  | cB    | 822 | CLA  | C1D-ND  | 4.70 | 1.44        | 1.37     |
| 11  | bB    | 819 | CLA  | CHC-C1C | 4.70 | 1.47        | 1.38     |
| 11  | aB    | 830 | CLA  | C1D-ND  | 4.70 | 1.44        | 1.37     |
| 11  | cB    | 818 | CLA  | CHC-C1C | 4.70 | 1.47        | 1.38     |
| 11  | cB    | 836 | CLA  | CHC-C1C | 4.69 | 1.47        | 1.38     |
| 11  | bA    | 804 | CLA  | C1D-ND  | 4.69 | 1.44        | 1.37     |
| 11  | aK    | 103 | CLA  | C1D-ND  | 4.69 | 1.44        | 1.37     |
| 11  | cK    | 101 | CLA  | C1D-ND  | 4.69 | 1.44        | 1.37     |
| 11  | aB    | 839 | CLA  | CHC-C1C | 4.69 | 1.47        | 1.38     |
| 11  | aK    | 101 | CLA  | CHC-C1C | 4.69 | 1.47        | 1.38     |
| 11  | cA    | 842 | CLA  | CHC-C1C | 4.69 | 1.47        | 1.38     |
| 11  | aK    | 101 | CLA  | C1D-ND  | 4.69 | 1.44        | 1.37     |
| 11  | aA    | 803 | CLA  | CHC-C1C | 4.69 | 1.47        | 1.38     |
| 11  | bB    | 822 | CLA  | C1D-ND  | 4.69 | 1.44        | 1.37     |
| 11  | aB    | 819 | CLA  | CHC-C1C | 4.68 | 1.47        | 1.38     |
| 11  | cB    | 801 | CLA  | O2D-CGD | 4.68 | 1.44        | 1.33     |
| 11  | aA    | 837 | CLA  | CHC-C1C | 4.68 | 1.47        | 1.38     |
| 11  | bA    | 816 | CLA  | CHC-C1C | 4.68 | 1.47        | 1.38     |
| 11  | bA    | 836 | CLA  | O2D-CGD | 4.68 | 1.44        | 1.33     |
| 11  | bB    | 802 | CLA  | CHC-C1C | 4.68 | 1.47        | 1.38     |
| 11  | bB    | 812 | CLA  | O2D-CGD | 4.68 | 1.44        | 1.33     |
| 11  | bB    | 812 | CLA  | C1D-ND  | 4.68 | 1.44        | 1.37     |
| 11  | bB    | 814 | CLA  | C1D-ND  | 4.68 | 1.44        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 11  | bB    | 801 | CLA  | O2D-CGD | 4.67 | 1.44        | 1.33     |
| 11  | bA    | 825 | CLA  | O2D-CGD | 4.67 | 1.44        | 1.33     |
| 11  | bB    | 815 | CLA  | CHC-C1C | 4.67 | 1.47        | 1.38     |
| 11  | aA    | 804 | CLA  | C1D-ND  | 4.67 | 1.44        | 1.37     |
| 11  | aB    | 818 | CLA  | CHC-C1C | 4.67 | 1.47        | 1.38     |
| 11  | bA    | 803 | CLA  | CHC-C1C | 4.67 | 1.47        | 1.38     |
| 11  | cB    | 830 | CLA  | C1D-ND  | 4.67 | 1.44        | 1.37     |
| 11  | aA    | 825 | CLA  | O2D-CGD | 4.67 | 1.44        | 1.33     |
| 11  | cA    | 837 | CLA  | CHC-C1C | 4.67 | 1.47        | 1.38     |
| 11  | cA    | 806 | CLA  | C3C-C2C | 4.67 | 1.46        | 1.36     |
| 11  | aB    | 815 | CLA  | CHC-C1C | 4.67 | 1.47        | 1.38     |
| 11  | bA    | 842 | CLA  | CHC-C1C | 4.67 | 1.47        | 1.38     |
| 11  | cK    | 101 | CLA  | CHC-C1C | 4.66 | 1.47        | 1.38     |
| 11  | bA    | 806 | CLA  | C3C-C2C | 4.66 | 1.46        | 1.36     |
| 11  | bB    | 830 | CLA  | C1D-ND  | 4.66 | 1.44        | 1.37     |
| 11  | cB    | 814 | CLA  | C1D-ND  | 4.66 | 1.44        | 1.37     |
| 11  | aB    | 801 | CLA  | O2D-CGD | 4.66 | 1.44        | 1.33     |
| 11  | aB    | 822 | CLA  | C1D-ND  | 4.66 | 1.44        | 1.37     |
| 11  | bA    | 812 | CLA  | CHC-C1C | 4.66 | 1.47        | 1.38     |
| 11  | aB    | 811 | CLA  | C1D-ND  | 4.66 | 1.44        | 1.37     |
| 11  | bB    | 833 | CLA  | C1D-ND  | 4.66 | 1.44        | 1.37     |
| 11  | bA    | 837 | CLA  | CHC-C1C | 4.66 | 1.47        | 1.38     |
| 11  | cB    | 819 | CLA  | CHC-C1C | 4.66 | 1.47        | 1.38     |
| 11  | cA    | 825 | CLA  | O2D-CGD | 4.66 | 1.44        | 1.33     |
| 11  | cB    | 815 | CLA  | CHC-C1C | 4.66 | 1.47        | 1.38     |
| 11  | cA    | 811 | CLA  | CHC-C1C | 4.65 | 1.47        | 1.38     |
| 11  | cA    | 804 | CLA  | C1D-ND  | 4.65 | 1.44        | 1.37     |
| 11  | cA    | 805 | CLA  | C1D-ND  | 4.65 | 1.44        | 1.37     |
| 11  | cB    | 811 | CLA  | C1D-ND  | 4.65 | 1.44        | 1.37     |
| 11  | cA    | 808 | CLA  | CHC-C1C | 4.65 | 1.47        | 1.38     |
| 11  | bK    | 101 | CLA  | C1D-ND  | 4.65 | 1.44        | 1.37     |
| 11  | aB    | 817 | CLA  | O2A-CGA | 4.65 | 1.46        | 1.33     |
| 11  | aB    | 815 | CLA  | C1D-ND  | 4.65 | 1.44        | 1.37     |
| 11  | aB    | 808 | CLA  | O2D-CGD | 4.65 | 1.44        | 1.33     |
| 11  | aA    | 842 | CLA  | CHC-C1C | 4.64 | 1.47        | 1.38     |
| 11  | aB    | 811 | CLA  | CHC-C1C | 4.64 | 1.47        | 1.38     |
| 11  | bB    | 808 | CLA  | O2D-CGD | 4.64 | 1.44        | 1.33     |
| 11  | aA    | 808 | CLA  | CHC-C1C | 4.64 | 1.47        | 1.38     |
| 11  | aB    | 806 | CLA  | CHC-C1C | 4.64 | 1.47        | 1.38     |
| 11  | cB    | 811 | CLA  | CHC-C1C | 4.64 | 1.47        | 1.38     |
| 11  | cB    | 808 | CLA  | O2D-CGD | 4.64 | 1.44        | 1.33     |
| 11  | cA    | 807 | CLA  | C1D-ND  | 4.64 | 1.44        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 11  | cA    | 841 | CLA  | CHC-C1C | 4.63 | 1.47        | 1.38     |
| 11  | bA    | 805 | CLA  | C1D-ND  | 4.63 | 1.43        | 1.37     |
| 11  | bB    | 811 | CLA  | CHC-C1C | 4.63 | 1.47        | 1.38     |
| 11  | cA    | 828 | CLA  | CHC-C1C | 4.63 | 1.47        | 1.38     |
| 11  | bA    | 841 | CLA  | CHC-C1C | 4.63 | 1.47        | 1.38     |
| 11  | bA    | 815 | CLA  | C1D-ND  | 4.63 | 1.43        | 1.37     |
| 11  | bB    | 817 | CLA  | O2A-CGA | 4.63 | 1.46        | 1.33     |
| 11  | bA    | 808 | CLA  | CHC-C1C | 4.63 | 1.47        | 1.38     |
| 11  | aA    | 806 | CLA  | C3C-C2C | 4.63 | 1.46        | 1.36     |
| 11  | bA    | 837 | CLA  | O2D-CGD | 4.62 | 1.44        | 1.33     |
| 11  | cB    | 825 | CLA  | C1D-ND  | 4.62 | 1.43        | 1.37     |
| 11  | cB    | 817 | CLA  | O2A-CGA | 4.62 | 1.46        | 1.33     |
| 11  | aB    | 833 | CLA  | C1D-ND  | 4.62 | 1.43        | 1.37     |
| 11  | bB    | 825 | CLA  | C1D-ND  | 4.62 | 1.43        | 1.37     |
| 11  | cB    | 815 | CLA  | C1D-ND  | 4.62 | 1.43        | 1.37     |
| 11  | aA    | 812 | CLA  | CHC-C1C | 4.62 | 1.47        | 1.38     |
| 11  | aA    | 811 | CLA  | CHC-C1C | 4.62 | 1.47        | 1.38     |
| 11  | bA    | 811 | CLA  | CHC-C1C | 4.62 | 1.47        | 1.38     |
| 11  | bA    | 807 | CLA  | C1D-ND  | 4.62 | 1.43        | 1.37     |
| 11  | aB    | 812 | CLA  | C1D-ND  | 4.62 | 1.43        | 1.37     |
| 11  | aB    | 830 | CLA  | CHC-C1C | 4.62 | 1.47        | 1.38     |
| 11  | cA    | 811 | CLA  | C1D-ND  | 4.62 | 1.43        | 1.37     |
| 11  | aL    | 205 | CLA  | CHC-C1C | 4.62 | 1.47        | 1.38     |
| 11  | bB    | 811 | CLA  | C1D-ND  | 4.62 | 1.43        | 1.37     |
| 11  | aB    | 814 | CLA  | C1D-ND  | 4.62 | 1.43        | 1.37     |
| 11  | cB    | 833 | CLA  | C1D-ND  | 4.61 | 1.43        | 1.37     |
| 11  | bL    | 205 | CLA  | CHC-C1C | 4.61 | 1.47        | 1.38     |
| 11  | cA    | 837 | CLA  | C1D-ND  | 4.61 | 1.43        | 1.37     |
| 11  | aA    | 828 | CLA  | CHC-C1C | 4.61 | 1.47        | 1.38     |
| 11  | cB    | 820 | CLA  | C1D-ND  | 4.61 | 1.43        | 1.37     |
| 11  | cB    | 806 | CLA  | CHC-C1C | 4.61 | 1.47        | 1.38     |
| 11  | bA    | 811 | CLA  | C1D-ND  | 4.61 | 1.43        | 1.37     |
| 11  | cA    | 815 | CLA  | C1D-ND  | 4.61 | 1.43        | 1.37     |
| 11  | aB    | 825 | CLA  | C1D-ND  | 4.60 | 1.43        | 1.37     |
| 11  | cB    | 812 | CLA  | C1D-ND  | 4.60 | 1.43        | 1.37     |
| 11  | aA    | 841 | CLA  | CHC-C1C | 4.60 | 1.47        | 1.38     |
| 11  | cA    | 812 | CLA  | CHC-C1C | 4.60 | 1.47        | 1.38     |
| 11  | cB    | 823 | CLA  | CHC-C1C | 4.60 | 1.47        | 1.38     |
| 11  | aA    | 815 | CLA  | C1D-ND  | 4.60 | 1.43        | 1.37     |
| 11  | cA    | 819 | CLA  | C1D-ND  | 4.60 | 1.43        | 1.37     |
| 11  | bA    | 833 | CLA  | CHC-C1C | 4.60 | 1.47        | 1.38     |
| 11  | bB    | 830 | CLA  | CHC-C1C | 4.60 | 1.47        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 11  | cA    | 837 | CLA  | O2D-CGD | 4.60 | 1.44        | 1.33     |
| 11  | bA    | 814 | CLA  | CHC-C1C | 4.59 | 1.47        | 1.38     |
| 11  | cL    | 205 | CLA  | CHC-C1C | 4.59 | 1.47        | 1.38     |
| 11  | bB    | 815 | CLA  | C1D-ND  | 4.59 | 1.43        | 1.37     |
| 11  | aA    | 837 | CLA  | O2D-CGD | 4.59 | 1.44        | 1.33     |
| 11  | bA    | 828 | CLA  | CHC-C1C | 4.59 | 1.47        | 1.38     |
| 11  | bB    | 823 | CLA  | CHC-C1C | 4.59 | 1.47        | 1.38     |
| 11  | cA    | 814 | CLA  | CHC-C1C | 4.59 | 1.47        | 1.38     |
| 11  | cB    | 820 | CLA  | CHC-C1C | 4.59 | 1.47        | 1.38     |
| 11  | bB    | 806 | CLA  | CHC-C1C | 4.59 | 1.47        | 1.38     |
| 11  | aB    | 810 | CLA  | C1D-ND  | 4.58 | 1.43        | 1.37     |
| 11  | aB    | 823 | CLA  | CHC-C1C | 4.58 | 1.47        | 1.38     |
| 11  | cB    | 829 | CLA  | C3C-C2C | 4.58 | 1.46        | 1.36     |
| 11  | aA    | 817 | CLA  | C1D-ND  | 4.58 | 1.43        | 1.37     |
| 11  | bB    | 832 | CLA  | O2A-CGA | 4.58 | 1.45        | 1.30     |
| 11  | aA    | 807 | CLA  | C1D-ND  | 4.58 | 1.43        | 1.37     |
| 11  | bA    | 822 | CLA  | CHC-C1C | 4.58 | 1.47        | 1.38     |
| 11  | cB    | 832 | CLA  | O2A-CGA | 4.58 | 1.45        | 1.30     |
| 11  | aA    | 814 | CLA  | CHC-C1C | 4.57 | 1.47        | 1.38     |
| 11  | aA    | 816 | CLA  | C1D-ND  | 4.57 | 1.43        | 1.37     |
| 11  | bB    | 829 | CLA  | O2A-CGA | 4.57 | 1.45        | 1.30     |
| 11  | bB    | 825 | CLA  | CHC-C1C | 4.57 | 1.47        | 1.38     |
| 11  | aA    | 840 | CLA  | C1D-ND  | 4.57 | 1.43        | 1.37     |
| 11  | aB    | 802 | CLA  | O2D-CGD | 4.57 | 1.44        | 1.33     |
| 11  | bB    | 829 | CLA  | CHD-C1D | 4.57 | 1.47        | 1.38     |
| 11  | aA    | 837 | CLA  | C1D-ND  | 4.57 | 1.43        | 1.37     |
| 11  | cB    | 829 | CLA  | CHD-C1D | 4.57 | 1.47        | 1.38     |
| 11  | aA    | 822 | CLA  | CHC-C1C | 4.56 | 1.47        | 1.38     |
| 12  | cL    | 202 | F6C  | O2D-CGD | 4.56 | 1.44        | 1.33     |
| 11  | bA    | 816 | CLA  | C1D-ND  | 4.56 | 1.43        | 1.37     |
| 11  | aB    | 820 | CLA  | C1D-ND  | 4.56 | 1.43        | 1.37     |
| 11  | bA    | 840 | CLA  | C1D-ND  | 4.56 | 1.43        | 1.37     |
| 11  | bA    | 804 | CLA  | O2A-CGA | 4.56 | 1.45        | 1.30     |
| 11  | bB    | 820 | CLA  | C1D-ND  | 4.56 | 1.43        | 1.37     |
| 11  | cA    | 809 | CLA  | CHC-C1C | 4.56 | 1.47        | 1.38     |
| 11  | cB    | 840 | CLA  | O2A-CGA | 4.56 | 1.45        | 1.30     |
| 11  | cB    | 830 | CLA  | CHC-C1C | 4.56 | 1.47        | 1.38     |
| 11  | bB    | 802 | CLA  | O2D-CGD | 4.56 | 1.44        | 1.33     |
| 11  | bA    | 811 | CLA  | O2A-CGA | 4.56 | 1.45        | 1.30     |
| 11  | cB    | 820 | CLA  | O2A-CGA | 4.56 | 1.45        | 1.30     |
| 11  | bB    | 831 | CLA  | CHC-C1C | 4.56 | 1.47        | 1.38     |
| 11  | bB    | 829 | CLA  | C3C-C2C | 4.56 | 1.46        | 1.36     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 11  | aB    | 833 | CLA  | O2A-CGA | 4.56 | 1.45        | 1.30     |
| 11  | aB    | 832 | CLA  | O2A-CGA | 4.56 | 1.45        | 1.30     |
| 11  | aA    | 805 | CLA  | C1D-ND  | 4.56 | 1.43        | 1.37     |
| 11  | bB    | 810 | CLA  | C1D-ND  | 4.56 | 1.43        | 1.37     |
| 11  | aA    | 835 | CLA  | CHC-C1C | 4.56 | 1.47        | 1.38     |
| 11  | bB    | 820 | CLA  | CHC-C1C | 4.56 | 1.47        | 1.38     |
| 11  | bA    | 816 | CLA  | O2A-CGA | 4.56 | 1.45        | 1.30     |
| 11  | bA    | 817 | CLA  | C1D-ND  | 4.56 | 1.43        | 1.37     |
| 12  | cA    | 844 | F6C  | CHC-C4B | 4.56 | 1.47        | 1.38     |
| 11  | aB    | 825 | CLA  | CHC-C1C | 4.55 | 1.47        | 1.38     |
| 11  | aA    | 813 | CLA  | CHC-C1C | 4.55 | 1.47        | 1.38     |
| 11  | bB    | 834 | CLA  | O2A-CGA | 4.55 | 1.45        | 1.30     |
| 11  | aA    | 807 | CLA  | CHC-C1C | 4.55 | 1.47        | 1.38     |
| 11  | aA    | 843 | CLA  | C1D-ND  | 4.55 | 1.43        | 1.37     |
| 11  | aA    | 804 | CLA  | O2A-CGA | 4.55 | 1.45        | 1.30     |
| 11  | bA    | 809 | CLA  | CHC-C1C | 4.55 | 1.47        | 1.38     |
| 11  | aA    | 809 | CLA  | CHC-C1C | 4.55 | 1.47        | 1.38     |
| 11  | bB    | 820 | CLA  | O2A-CGA | 4.55 | 1.45        | 1.30     |
| 11  | bA    | 819 | CLA  | C1D-ND  | 4.55 | 1.43        | 1.37     |
| 11  | cA    | 817 | CLA  | C1D-ND  | 4.55 | 1.43        | 1.37     |
| 11  | bA    | 835 | CLA  | CHC-C1C | 4.55 | 1.47        | 1.38     |
| 11  | aA    | 833 | CLA  | CHC-C1C | 4.55 | 1.47        | 1.38     |
| 11  | aA    | 842 | CLA  | O2A-CGA | 4.55 | 1.45        | 1.30     |
| 11  | cA    | 835 | CLA  | O2D-CGD | 4.55 | 1.44        | 1.33     |
| 11  | aB    | 806 | CLA  | C1D-ND  | 4.55 | 1.43        | 1.37     |
| 11  | bA    | 843 | CLA  | C1D-ND  | 4.55 | 1.43        | 1.37     |
| 11  | bB    | 840 | CLA  | O2A-CGA | 4.55 | 1.45        | 1.30     |
| 11  | aA    | 824 | CLA  | CHC-C1C | 4.55 | 1.47        | 1.38     |
| 11  | bA    | 837 | CLA  | C1D-ND  | 4.55 | 1.43        | 1.37     |
| 11  | bB    | 826 | CLA  | CHC-C1C | 4.55 | 1.47        | 1.38     |
| 12  | bA    | 844 | F6C  | CHC-C4B | 4.55 | 1.47        | 1.38     |
| 11  | bL    | 206 | CLA  | CHC-C1C | 4.54 | 1.47        | 1.38     |
| 11  | cA    | 804 | CLA  | O2A-CGA | 4.54 | 1.45        | 1.30     |
| 10  | aA    | 801 | CL0  | CHC-C4B | 4.54 | 1.47        | 1.39     |
| 11  | cA    | 806 | CLA  | C1D-ND  | 4.54 | 1.43        | 1.37     |
| 11  | aA    | 824 | CLA  | C1D-ND  | 4.54 | 1.43        | 1.37     |
| 11  | cB    | 831 | CLA  | CHC-C1C | 4.54 | 1.47        | 1.38     |
| 11  | aB    | 829 | CLA  | O2A-CGA | 4.54 | 1.45        | 1.30     |
| 11  | aB    | 834 | CLA  | O2A-CGA | 4.54 | 1.45        | 1.30     |
| 11  | aA    | 810 | CLA  | CHC-C1C | 4.54 | 1.47        | 1.38     |
| 11  | bA    | 835 | CLA  | O2D-CGD | 4.54 | 1.44        | 1.33     |
| 12  | aL    | 202 | F6C  | O2D-CGD | 4.54 | 1.44        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 11  | aA    | 811 | CLA  | O2A-CGA | 4.54 | 1.45        | 1.30     |
| 11  | cA    | 810 | CLA  | CHC-C1C | 4.54 | 1.47        | 1.38     |
| 11  | bA    | 805 | CLA  | O2A-CGA | 4.54 | 1.45        | 1.30     |
| 12  | bL    | 202 | F6C  | O2D-CGD | 4.54 | 1.44        | 1.33     |
| 10  | cA    | 801 | CL0  | CHC-C4B | 4.54 | 1.47        | 1.39     |
| 11  | aB    | 814 | CLA  | O2A-CGA | 4.54 | 1.45        | 1.30     |
| 11  | bA    | 840 | CLA  | CHC-C1C | 4.54 | 1.47        | 1.38     |
| 11  | cA    | 805 | CLA  | O2A-CGA | 4.54 | 1.45        | 1.30     |
| 11  | aB    | 820 | CLA  | CHC-C1C | 4.54 | 1.47        | 1.38     |
| 11  | cK    | 103 | CLA  | CHC-C1C | 4.54 | 1.47        | 1.38     |
| 11  | aB    | 820 | CLA  | O2A-CGA | 4.54 | 1.45        | 1.30     |
| 11  | aL    | 206 | CLA  | CHC-C1C | 4.54 | 1.47        | 1.38     |
| 11  | bA    | 809 | CLA  | O2A-CGA | 4.54 | 1.45        | 1.30     |
| 11  | aB    | 829 | CLA  | C3C-C2C | 4.54 | 1.46        | 1.36     |
| 11  | cA    | 807 | CLA  | CHC-C1C | 4.54 | 1.47        | 1.38     |
| 11  | cB    | 829 | CLA  | O2A-CGA | 4.54 | 1.45        | 1.30     |
| 11  | aA    | 815 | CLA  | O2A-CGA | 4.54 | 1.45        | 1.30     |
| 11  | aA    | 811 | CLA  | C1D-ND  | 4.54 | 1.43        | 1.37     |
| 11  | cB    | 826 | CLA  | CHC-C1C | 4.54 | 1.47        | 1.38     |
| 11  | bA    | 824 | CLA  | C1D-ND  | 4.54 | 1.43        | 1.37     |
| 11  | bB    | 806 | CLA  | C1D-ND  | 4.54 | 1.43        | 1.37     |
| 11  | aB    | 840 | CLA  | O2A-CGA | 4.53 | 1.45        | 1.30     |
| 11  | aA    | 819 | CLA  | C1D-ND  | 4.53 | 1.43        | 1.37     |
| 11  | cB    | 833 | CLA  | O2A-CGA | 4.53 | 1.45        | 1.30     |
| 11  | aB    | 831 | CLA  | CHC-C1C | 4.53 | 1.47        | 1.38     |
| 11  | bB    | 836 | CLA  | C1D-ND  | 4.53 | 1.43        | 1.37     |
| 11  | cA    | 811 | CLA  | O2A-CGA | 4.53 | 1.45        | 1.30     |
| 11  | bA    | 824 | CLA  | CHC-C1C | 4.53 | 1.47        | 1.38     |
| 11  | cA    | 815 | CLA  | O2A-CGA | 4.53 | 1.45        | 1.30     |
| 11  | bA    | 820 | CLA  | C1D-ND  | 4.53 | 1.43        | 1.37     |
| 11  | cA    | 833 | CLA  | CHC-C1C | 4.53 | 1.47        | 1.38     |
| 11  | cA    | 809 | CLA  | O2A-CGA | 4.53 | 1.45        | 1.30     |
| 11  | bA    | 842 | CLA  | O2A-CGA | 4.53 | 1.45        | 1.30     |
| 11  | bA    | 806 | CLA  | C1D-ND  | 4.53 | 1.43        | 1.37     |
| 11  | aB    | 826 | CLA  | CHC-C1C | 4.53 | 1.47        | 1.38     |
| 11  | bA    | 835 | CLA  | C1D-ND  | 4.53 | 1.43        | 1.37     |
| 11  | aA    | 809 | CLA  | O2A-CGA | 4.53 | 1.45        | 1.30     |
| 11  | cA    | 822 | CLA  | CHC-C1C | 4.53 | 1.47        | 1.38     |
| 11  | cA    | 842 | CLA  | O2A-CGA | 4.53 | 1.45        | 1.30     |
| 11  | aA    | 835 | CLA  | O2D-CGD | 4.53 | 1.44        | 1.33     |
| 11  | cB    | 814 | CLA  | O2A-CGA | 4.53 | 1.45        | 1.30     |
| 11  | cA    | 808 | CLA  | C1D-ND  | 4.53 | 1.43        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 11  | cB    | 806 | CLA  | C1D-ND  | 4.53 | 1.43        | 1.37     |
| 11  | cB    | 810 | CLA  | C1D-ND  | 4.53 | 1.43        | 1.37     |
| 11  | bA    | 813 | CLA  | CHC-C1C | 4.53 | 1.47        | 1.38     |
| 11  | cA    | 843 | CLA  | C1D-ND  | 4.53 | 1.43        | 1.37     |
| 11  | bB    | 814 | CLA  | O2A-CGA | 4.53 | 1.45        | 1.30     |
| 11  | cB    | 802 | CLA  | O2D-CGD | 4.53 | 1.44        | 1.33     |
| 11  | bA    | 829 | CLA  | C1D-ND  | 4.52 | 1.43        | 1.37     |
| 11  | aA    | 816 | CLA  | O2A-CGA | 4.52 | 1.45        | 1.30     |
| 11  | bB    | 811 | CLA  | O2A-CGA | 4.52 | 1.45        | 1.30     |
| 11  | cA    | 813 | CLA  | CHC-C1C | 4.52 | 1.47        | 1.38     |
| 12  | aA    | 844 | F6C  | CHC-C4B | 4.52 | 1.47        | 1.38     |
| 11  | aA    | 806 | CLA  | C1D-ND  | 4.52 | 1.43        | 1.37     |
| 11  | cA    | 816 | CLA  | C1D-ND  | 4.52 | 1.43        | 1.37     |
| 11  | cA    | 833 | CLA  | C1D-ND  | 4.52 | 1.43        | 1.37     |
| 11  | cA    | 824 | CLA  | CHC-C1C | 4.52 | 1.47        | 1.38     |
| 11  | bB    | 821 | CLA  | CHC-C1C | 4.52 | 1.47        | 1.38     |
| 11  | cA    | 814 | CLA  | C1D-ND  | 4.52 | 1.43        | 1.37     |
| 11  | bB    | 833 | CLA  | O2A-CGA | 4.52 | 1.45        | 1.30     |
| 11  | cA    | 820 | CLA  | C1D-ND  | 4.52 | 1.43        | 1.37     |
| 11  | cA    | 840 | CLA  | C1D-ND  | 4.52 | 1.43        | 1.37     |
| 11  | aB    | 835 | CLA  | CHC-C1C | 4.52 | 1.47        | 1.38     |
| 11  | cB    | 834 | CLA  | O2A-CGA | 4.52 | 1.45        | 1.30     |
| 11  | bA    | 829 | CLA  | CHC-C1C | 4.52 | 1.47        | 1.38     |
| 11  | cA    | 835 | CLA  | CHC-C1C | 4.52 | 1.47        | 1.38     |
| 11  | aB    | 835 | CLA  | O2A-CGA | 4.52 | 1.45        | 1.30     |
| 11  | bB    | 810 | CLA  | O2A-CGA | 4.52 | 1.45        | 1.30     |
| 11  | cB    | 825 | CLA  | CHC-C1C | 4.52 | 1.47        | 1.38     |
| 11  | bA    | 815 | CLA  | O2A-CGA | 4.52 | 1.45        | 1.30     |
| 11  | aB    | 829 | CLA  | CHD-C1D | 4.52 | 1.47        | 1.38     |
| 11  | cA    | 816 | CLA  | O2A-CGA | 4.52 | 1.45        | 1.30     |
| 11  | aB    | 821 | CLA  | CHC-C1C | 4.52 | 1.47        | 1.38     |
| 11  | bA    | 808 | CLA  | C1D-ND  | 4.52 | 1.43        | 1.37     |
| 11  | aA    | 805 | CLA  | O2A-CGA | 4.51 | 1.45        | 1.30     |
| 11  | cB    | 816 | CLA  | C1D-ND  | 4.51 | 1.43        | 1.37     |
| 11  | aK    | 103 | CLA  | CHC-C1C | 4.51 | 1.47        | 1.38     |
| 11  | cL    | 206 | CLA  | CHC-C1C | 4.51 | 1.47        | 1.38     |
| 11  | bA    | 810 | CLA  | CHC-C1C | 4.51 | 1.47        | 1.38     |
| 11  | bB    | 835 | CLA  | O2A-CGA | 4.51 | 1.45        | 1.30     |
| 11  | aA    | 808 | CLA  | C1D-ND  | 4.51 | 1.43        | 1.37     |
| 11  | aB    | 804 | CLA  | C1D-ND  | 4.51 | 1.43        | 1.37     |
| 11  | cB    | 810 | CLA  | O2A-CGA | 4.51 | 1.45        | 1.30     |
| 11  | cB    | 804 | CLA  | C1D-ND  | 4.51 | 1.43        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 11  | bB    | 827 | CLA  | CHC-C1C | 4.51 | 1.47        | 1.38     |
| 11  | aA    | 843 | CLA  | CHC-C1C | 4.51 | 1.47        | 1.38     |
| 11  | bB    | 804 | CLA  | C1D-ND  | 4.51 | 1.43        | 1.37     |
| 11  | cA    | 843 | CLA  | CHC-C1C | 4.51 | 1.47        | 1.38     |
| 11  | cA    | 842 | CLA  | C1D-ND  | 4.51 | 1.43        | 1.37     |
| 11  | cA    | 813 | CLA  | C1D-ND  | 4.51 | 1.43        | 1.37     |
| 11  | aB    | 836 | CLA  | C1D-ND  | 4.50 | 1.43        | 1.37     |
| 11  | bA    | 836 | CLA  | O2A-CGA | 4.50 | 1.45        | 1.30     |
| 11  | cA    | 829 | CLA  | CHC-C1C | 4.50 | 1.47        | 1.38     |
| 11  | cA    | 835 | CLA  | C1D-ND  | 4.50 | 1.43        | 1.37     |
| 11  | bA    | 807 | CLA  | CHC-C1C | 4.50 | 1.47        | 1.38     |
| 11  | bK    | 103 | CLA  | CHC-C1C | 4.50 | 1.47        | 1.38     |
| 11  | aB    | 812 | CLA  | CHD-C1D | 4.50 | 1.47        | 1.38     |
| 11  | aB    | 811 | CLA  | O2A-CGA | 4.50 | 1.45        | 1.30     |
| 11  | cA    | 825 | CLA  | C1D-ND  | 4.50 | 1.43        | 1.37     |
| 11  | cA    | 840 | CLA  | CHC-C1C | 4.50 | 1.47        | 1.38     |
| 11  | cB    | 835 | CLA  | CHC-C1C | 4.50 | 1.47        | 1.38     |
| 11  | bA    | 809 | CLA  | C1D-ND  | 4.50 | 1.43        | 1.37     |
| 11  | aA    | 814 | CLA  | C1D-ND  | 4.50 | 1.43        | 1.37     |
| 11  | aA    | 837 | CLA  | O2A-CGA | 4.50 | 1.45        | 1.30     |
| 11  | cB    | 821 | CLA  | CHC-C1C | 4.49 | 1.47        | 1.38     |
| 11  | cA    | 810 | CLA  | O2A-CGA | 4.49 | 1.45        | 1.30     |
| 11  | bL    | 204 | CLA  | CHC-C1C | 4.49 | 1.47        | 1.38     |
| 11  | cB    | 835 | CLA  | O2A-CGA | 4.49 | 1.45        | 1.30     |
| 11  | aA    | 842 | CLA  | C1D-ND  | 4.49 | 1.43        | 1.37     |
| 11  | cA    | 836 | CLA  | O2A-CGA | 4.49 | 1.45        | 1.30     |
| 11  | bA    | 843 | CLA  | CHC-C1C | 4.49 | 1.47        | 1.38     |
| 10  | bA    | 801 | CL0  | CHC-C4B | 4.49 | 1.46        | 1.39     |
| 11  | bA    | 823 | CLA  | CHC-C1C | 4.49 | 1.47        | 1.38     |
| 11  | aB    | 805 | CLA  | C1D-ND  | 4.49 | 1.43        | 1.37     |
| 11  | cB    | 812 | CLA  | CHD-C1D | 4.49 | 1.47        | 1.38     |
| 11  | cB    | 811 | CLA  | O2A-CGA | 4.49 | 1.45        | 1.30     |
| 11  | cA    | 809 | CLA  | C1D-ND  | 4.49 | 1.43        | 1.37     |
| 11  | aA    | 825 | CLA  | C1D-ND  | 4.49 | 1.43        | 1.37     |
| 11  | aA    | 823 | CLA  | CHC-C1C | 4.49 | 1.47        | 1.38     |
| 11  | aA    | 829 | CLA  | C1D-ND  | 4.49 | 1.43        | 1.37     |
| 11  | cA    | 821 | CLA  | CHC-C1C | 4.49 | 1.47        | 1.38     |
| 11  | aA    | 809 | CLA  | C1D-ND  | 4.48 | 1.43        | 1.37     |
| 11  | aB    | 816 | CLA  | C1D-ND  | 4.48 | 1.43        | 1.37     |
| 11  | aL    | 204 | CLA  | CHC-C1C | 4.48 | 1.47        | 1.38     |
| 11  | cA    | 823 | CLA  | CHC-C1C | 4.48 | 1.47        | 1.38     |
| 11  | cB    | 805 | CLA  | CHC-C1C | 4.48 | 1.47        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 11  | aA    | 836 | CLA  | O2A-CGA | 4.48 | 1.45        | 1.30     |
| 11  | aA    | 835 | CLA  | C1D-ND  | 4.48 | 1.43        | 1.37     |
| 11  | bB    | 838 | CLA  | CHC-C1C | 4.48 | 1.47        | 1.38     |
| 11  | aA    | 833 | CLA  | C1D-ND  | 4.48 | 1.43        | 1.37     |
| 11  | aB    | 810 | CLA  | O2A-CGA | 4.48 | 1.45        | 1.30     |
| 11  | cA    | 824 | CLA  | C1D-ND  | 4.48 | 1.43        | 1.37     |
| 11  | bA    | 837 | CLA  | O2A-CGA | 4.48 | 1.45        | 1.30     |
| 11  | aA    | 840 | CLA  | CHC-C1C | 4.48 | 1.47        | 1.38     |
| 11  | aA    | 838 | CLA  | CHC-C1C | 4.48 | 1.47        | 1.38     |
| 11  | aA    | 813 | CLA  | C1D-ND  | 4.48 | 1.43        | 1.37     |
| 11  | bB    | 812 | CLA  | CHD-C1D | 4.48 | 1.47        | 1.38     |
| 11  | cA    | 837 | CLA  | O2A-CGA | 4.48 | 1.45        | 1.30     |
| 11  | aA    | 806 | CLA  | CHC-C1C | 4.47 | 1.47        | 1.38     |
| 11  | bB    | 835 | CLA  | CHC-C1C | 4.47 | 1.47        | 1.38     |
| 11  | aB    | 827 | CLA  | CHC-C1C | 4.47 | 1.47        | 1.38     |
| 11  | bB    | 813 | CLA  | C1D-ND  | 4.47 | 1.43        | 1.37     |
| 11  | cA    | 839 | CLA  | C1D-ND  | 4.47 | 1.43        | 1.37     |
| 11  | cB    | 836 | CLA  | C1D-ND  | 4.47 | 1.43        | 1.37     |
| 11  | aA    | 810 | CLA  | O2A-CGA | 4.47 | 1.45        | 1.30     |
| 11  | cB    | 827 | CLA  | CHC-C1C | 4.47 | 1.47        | 1.38     |
| 11  | cB    | 822 | CLA  | O2A-CGA | 4.47 | 1.45        | 1.30     |
| 11  | aB    | 838 | CLA  | CHC-C1C | 4.47 | 1.47        | 1.38     |
| 11  | aA    | 829 | CLA  | CHC-C1C | 4.47 | 1.47        | 1.38     |
| 11  | cB    | 805 | CLA  | C1D-ND  | 4.47 | 1.43        | 1.37     |
| 11  | bA    | 810 | CLA  | O2A-CGA | 4.47 | 1.45        | 1.30     |
| 11  | aA    | 820 | CLA  | C1D-ND  | 4.47 | 1.43        | 1.37     |
| 11  | bA    | 825 | CLA  | C1D-ND  | 4.47 | 1.43        | 1.37     |
| 11  | bA    | 813 | CLA  | C1D-ND  | 4.46 | 1.43        | 1.37     |
| 11  | bA    | 833 | CLA  | C1D-ND  | 4.46 | 1.43        | 1.37     |
| 11  | bA    | 821 | CLA  | CHC-C1C | 4.46 | 1.47        | 1.38     |
| 11  | bB    | 805 | CLA  | C1D-ND  | 4.46 | 1.43        | 1.37     |
| 11  | cA    | 829 | CLA  | C1D-ND  | 4.46 | 1.43        | 1.37     |
| 11  | aB    | 805 | CLA  | CHC-C1C | 4.46 | 1.47        | 1.38     |
| 11  | bA    | 842 | CLA  | C1D-ND  | 4.46 | 1.43        | 1.37     |
| 11  | bA    | 838 | CLA  | CHC-C1C | 4.46 | 1.47        | 1.38     |
| 11  | bB    | 822 | CLA  | O2A-CGA | 4.46 | 1.45        | 1.30     |
| 11  | aA    | 834 | CLA  | CHC-C1C | 4.46 | 1.47        | 1.38     |
| 11  | cA    | 806 | CLA  | CHC-C1C | 4.45 | 1.47        | 1.38     |
| 11  | bB    | 816 | CLA  | C1D-ND  | 4.45 | 1.43        | 1.37     |
| 11  | bA    | 834 | CLA  | CHC-C1C | 4.45 | 1.47        | 1.38     |
| 11  | aB    | 822 | CLA  | O2A-CGA | 4.45 | 1.45        | 1.30     |
| 11  | cB    | 838 | CLA  | CHC-C1C | 4.45 | 1.47        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | bB    | 805 | CLA  | CHC-C1C | 4.45  | 1.47        | 1.38     |
| 11  | aA    | 821 | CLA  | CHC-C1C | 4.45  | 1.47        | 1.38     |
| 11  | aA    | 839 | CLA  | C1D-ND  | 4.45  | 1.43        | 1.37     |
| 11  | bA    | 814 | CLA  | C1D-ND  | 4.44  | 1.43        | 1.37     |
| 11  | cB    | 801 | CLA  | CHC-C1C | 4.44  | 1.47        | 1.38     |
| 12  | cL    | 202 | F6C  | O2A-CGA | 4.44  | 1.46        | 1.33     |
| 11  | bB    | 834 | CLA  | CHC-C1C | 4.44  | 1.47        | 1.38     |
| 12  | aL    | 202 | F6C  | O2A-CGA | 4.44  | 1.46        | 1.33     |
| 11  | cB    | 813 | CLA  | C1D-ND  | 4.44  | 1.43        | 1.37     |
| 11  | aB    | 808 | CLA  | CHC-C1C | 4.43  | 1.47        | 1.38     |
| 11  | aB    | 813 | CLA  | C1D-ND  | 4.43  | 1.43        | 1.37     |
| 11  | cL    | 204 | CLA  | CHC-C1C | 4.43  | 1.47        | 1.38     |
| 11  | bA    | 839 | CLA  | C1D-ND  | 4.43  | 1.43        | 1.37     |
| 11  | aA    | 839 | CLA  | CHC-C1C | 4.43  | 1.47        | 1.38     |
| 11  | bA    | 806 | CLA  | CHC-C1C | 4.43  | 1.47        | 1.38     |
| 11  | cA    | 838 | CLA  | CHC-C1C | 4.43  | 1.47        | 1.38     |
| 11  | aB    | 840 | CLA  | C1D-ND  | 4.43  | 1.43        | 1.37     |
| 11  | bB    | 840 | CLA  | C1D-ND  | 4.43  | 1.43        | 1.37     |
| 12  | bL    | 202 | F6C  | O2A-CGA | 4.42  | 1.46        | 1.33     |
| 12  | bA    | 827 | F6C  | CHC-C4B | 4.42  | 1.47        | 1.38     |
| 11  | bB    | 834 | CLA  | CHD-C1D | 4.42  | 1.47        | 1.38     |
| 11  | cA    | 817 | CLA  | CHC-C1C | 4.42  | 1.47        | 1.38     |
| 11  | cB    | 813 | CLA  | CHC-C1C | 4.42  | 1.47        | 1.38     |
| 11  | bB    | 812 | CLA  | CHC-C1C | 4.42  | 1.47        | 1.38     |
| 11  | cA    | 834 | CLA  | CHC-C1C | 4.42  | 1.47        | 1.38     |
| 11  | cB    | 810 | CLA  | CHC-C1C | 4.42  | 1.47        | 1.38     |
| 11  | cB    | 834 | CLA  | CHD-C1D | 4.42  | 1.47        | 1.38     |
| 11  | cB    | 834 | CLA  | CHC-C1C | 4.41  | 1.47        | 1.38     |
| 11  | cB    | 840 | CLA  | C1D-ND  | 4.41  | 1.43        | 1.37     |
| 11  | aB    | 810 | CLA  | CHC-C1C | 4.41  | 1.47        | 1.38     |
| 11  | bB    | 814 | CLA  | CHC-C1C | 4.41  | 1.47        | 1.38     |
| 11  | bA    | 839 | CLA  | CHC-C1C | 4.41  | 1.47        | 1.38     |
| 11  | bA    | 817 | CLA  | CHC-C1C | 4.41  | 1.47        | 1.38     |
| 12  | aA    | 827 | F6C  | CHC-C4B | 4.41  | 1.47        | 1.38     |
| 11  | aB    | 801 | CLA  | CHC-C1C | 4.40  | 1.47        | 1.38     |
| 11  | cA    | 825 | CLA  | CHC-C1C | 4.40  | 1.47        | 1.38     |
| 11  | aA    | 817 | CLA  | CHC-C1C | 4.40  | 1.47        | 1.38     |
| 11  | aA    | 825 | CLA  | CHC-C1C | 4.40  | 1.47        | 1.38     |
| 11  | aB    | 812 | CLA  | CHC-C1C | 4.40  | 1.47        | 1.38     |
| 11  | aB    | 814 | CLA  | CHC-C1C | 4.40  | 1.47        | 1.38     |
| 11  | aB    | 834 | CLA  | CHC-C1C | 4.40  | 1.47        | 1.38     |
| 11  | cB    | 828 | CLA  | C1B-NB  | -4.40 | 1.32        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | bA    | 823 | CLA  | O2A-CGA | 4.40  | 1.45        | 1.30     |
| 11  | cA    | 839 | CLA  | CHC-C1C | 4.40  | 1.47        | 1.38     |
| 11  | aB    | 837 | CLA  | C1D-ND  | 4.40  | 1.43        | 1.37     |
| 11  | bB    | 838 | CLA  | C1D-ND  | 4.40  | 1.43        | 1.37     |
| 11  | cA    | 823 | CLA  | O2A-CGA | 4.39  | 1.45        | 1.30     |
| 11  | bB    | 801 | CLA  | CHC-C1C | 4.39  | 1.47        | 1.38     |
| 11  | cB    | 838 | CLA  | C1D-ND  | 4.39  | 1.43        | 1.37     |
| 11  | aA    | 834 | CLA  | C1D-ND  | 4.39  | 1.43        | 1.37     |
| 11  | bB    | 810 | CLA  | CHC-C1C | 4.39  | 1.47        | 1.38     |
| 11  | aB    | 817 | CLA  | CHC-C1C | 4.39  | 1.47        | 1.38     |
| 11  | cB    | 817 | CLA  | CHC-C1C | 4.39  | 1.47        | 1.38     |
| 11  | bB    | 817 | CLA  | CHC-C1C | 4.39  | 1.47        | 1.38     |
| 12  | aL    | 202 | F6C  | CHC-C4B | 4.39  | 1.47        | 1.38     |
| 11  | aB    | 834 | CLA  | CHD-C1D | 4.38  | 1.47        | 1.38     |
| 11  | cB    | 812 | CLA  | CHC-C1C | 4.38  | 1.47        | 1.38     |
| 11  | bB    | 808 | CLA  | CHC-C1C | 4.38  | 1.47        | 1.38     |
| 12  | bL    | 202 | F6C  | CHC-C4B | 4.38  | 1.47        | 1.38     |
| 11  | bB    | 828 | CLA  | CHD-C1D | 4.38  | 1.47        | 1.38     |
| 11  | aL    | 204 | CLA  | C1D-ND  | 4.38  | 1.43        | 1.37     |
| 11  | cB    | 808 | CLA  | CHC-C1C | 4.38  | 1.47        | 1.38     |
| 11  | bB    | 837 | CLA  | C1D-ND  | 4.38  | 1.43        | 1.37     |
| 11  | bB    | 817 | CLA  | C1D-ND  | 4.38  | 1.43        | 1.37     |
| 11  | aB    | 813 | CLA  | CHC-C1C | 4.38  | 1.47        | 1.38     |
| 11  | bA    | 825 | CLA  | CHC-C1C | 4.38  | 1.47        | 1.38     |
| 11  | bB    | 828 | CLA  | C1B-NB  | -4.38 | 1.32        | 1.37     |
| 11  | aB    | 802 | CLA  | O2A-CGA | 4.38  | 1.46        | 1.33     |
| 11  | cA    | 834 | CLA  | C1D-ND  | 4.37  | 1.43        | 1.37     |
| 11  | bB    | 813 | CLA  | CHC-C1C | 4.37  | 1.47        | 1.38     |
| 11  | bB    | 802 | CLA  | O2A-CGA | 4.37  | 1.46        | 1.33     |
| 12  | aA    | 826 | F6C  | CHC-C4B | 4.37  | 1.47        | 1.38     |
| 11  | cB    | 818 | CLA  | C1D-ND  | 4.37  | 1.43        | 1.37     |
| 11  | cB    | 814 | CLA  | CHC-C1C | 4.37  | 1.47        | 1.38     |
| 11  | aA    | 822 | CLA  | C1D-ND  | 4.37  | 1.43        | 1.37     |
| 11  | aA    | 823 | CLA  | O2A-CGA | 4.37  | 1.45        | 1.30     |
| 11  | cB    | 802 | CLA  | O2A-CGA | 4.37  | 1.46        | 1.33     |
| 11  | bA    | 822 | CLA  | C1D-ND  | 4.37  | 1.43        | 1.37     |
| 11  | aA    | 841 | CLA  | C1D-ND  | 4.36  | 1.43        | 1.37     |
| 11  | cL    | 204 | CLA  | C1D-ND  | 4.36  | 1.43        | 1.37     |
| 12  | cL    | 202 | F6C  | CHC-C4B | 4.36  | 1.47        | 1.38     |
| 11  | aB    | 828 | CLA  | CHD-C1D | 4.36  | 1.46        | 1.38     |
| 11  | aB    | 838 | CLA  | C1D-ND  | 4.36  | 1.43        | 1.37     |
| 12  | cA    | 827 | F6C  | CHC-C4B | 4.36  | 1.47        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | bB    | 807 | CLA  | CHC-C1C | 4.35  | 1.47        | 1.38     |
| 11  | bB    | 809 | CLA  | CHC-C1C | 4.35  | 1.47        | 1.38     |
| 11  | aB    | 818 | CLA  | C1D-ND  | 4.35  | 1.43        | 1.37     |
| 11  | bA    | 834 | CLA  | C1D-ND  | 4.35  | 1.43        | 1.37     |
| 11  | cB    | 837 | CLA  | C1D-ND  | 4.35  | 1.43        | 1.37     |
| 11  | aA    | 815 | CLA  | CHC-C1C | 4.35  | 1.47        | 1.38     |
| 11  | bL    | 204 | CLA  | C1D-ND  | 4.34  | 1.43        | 1.37     |
| 11  | cB    | 809 | CLA  | CHC-C1C | 4.34  | 1.47        | 1.38     |
| 11  | aA    | 810 | CLA  | C1D-ND  | 4.34  | 1.43        | 1.37     |
| 11  | cA    | 841 | CLA  | C1D-ND  | 4.34  | 1.43        | 1.37     |
| 11  | aA    | 812 | CLA  | CHD-C1D | 4.34  | 1.46        | 1.38     |
| 11  | aB    | 828 | CLA  | C1B-NB  | -4.34 | 1.32        | 1.37     |
| 11  | cA    | 815 | CLA  | CHC-C1C | 4.34  | 1.47        | 1.38     |
| 11  | cA    | 822 | CLA  | C1D-ND  | 4.33  | 1.43        | 1.37     |
| 12  | cA    | 826 | F6C  | CHC-C4B | 4.33  | 1.47        | 1.38     |
| 11  | cA    | 820 | CLA  | CHC-C1C | 4.33  | 1.47        | 1.38     |
| 11  | aA    | 806 | CLA  | CHD-C1D | 4.33  | 1.46        | 1.38     |
| 11  | bA    | 841 | CLA  | C1D-ND  | 4.32  | 1.43        | 1.37     |
| 11  | cA    | 810 | CLA  | C1D-ND  | 4.32  | 1.43        | 1.37     |
| 11  | cB    | 831 | CLA  | CHD-C1D | 4.32  | 1.46        | 1.38     |
| 11  | bA    | 810 | CLA  | C1D-ND  | 4.32  | 1.43        | 1.37     |
| 11  | aA    | 820 | CLA  | CHC-C1C | 4.32  | 1.47        | 1.38     |
| 11  | bA    | 806 | CLA  | CHD-C1D | 4.32  | 1.46        | 1.38     |
| 11  | bB    | 831 | CLA  | CHD-C1D | 4.32  | 1.46        | 1.38     |
| 12  | bA    | 826 | F6C  | CHC-C4B | 4.31  | 1.47        | 1.38     |
| 11  | bB    | 818 | CLA  | C1D-ND  | 4.31  | 1.43        | 1.37     |
| 11  | cB    | 828 | CLA  | CHD-C1D | 4.31  | 1.46        | 1.38     |
| 11  | aB    | 807 | CLA  | CHC-C1C | 4.31  | 1.47        | 1.38     |
| 11  | aB    | 809 | CLA  | CHC-C1C | 4.31  | 1.47        | 1.38     |
| 11  | bA    | 820 | CLA  | CHC-C1C | 4.31  | 1.47        | 1.38     |
| 11  | cA    | 840 | CLA  | O2A-CGA | 4.31  | 1.45        | 1.33     |
| 11  | aA    | 823 | CLA  | C1D-ND  | 4.31  | 1.43        | 1.37     |
| 11  | aA    | 840 | CLA  | O2A-CGA | 4.30  | 1.45        | 1.33     |
| 11  | cA    | 823 | CLA  | C1D-ND  | 4.30  | 1.43        | 1.37     |
| 11  | bA    | 815 | CLA  | CHD-C1D | 4.30  | 1.46        | 1.38     |
| 11  | aB    | 835 | CLA  | CHD-C1D | 4.30  | 1.46        | 1.38     |
| 11  | cA    | 806 | CLA  | CHD-C1D | 4.30  | 1.46        | 1.38     |
| 11  | cB    | 817 | CLA  | C1D-ND  | 4.30  | 1.43        | 1.37     |
| 11  | bA    | 823 | CLA  | C1D-ND  | 4.30  | 1.43        | 1.37     |
| 11  | bA    | 812 | CLA  | CHD-C1D | 4.30  | 1.46        | 1.38     |
| 11  | bA    | 817 | CLA  | CHD-C1D | 4.30  | 1.46        | 1.38     |
| 11  | bL    | 206 | CLA  | C1D-ND  | 4.29  | 1.43        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | cB    | 835 | CLA  | CHD-C1D | 4.29  | 1.46        | 1.38     |
| 10  | aA    | 801 | CL0  | CHD-C4C | 4.29  | 1.47        | 1.39     |
| 12  | cA    | 832 | F6C  | O2A-CGA | 4.29  | 1.45        | 1.33     |
| 11  | aB    | 831 | CLA  | CHD-C1D | 4.29  | 1.46        | 1.38     |
| 11  | bA    | 815 | CLA  | CHC-C1C | 4.29  | 1.47        | 1.38     |
| 11  | aA    | 838 | CLA  | C1D-ND  | 4.29  | 1.43        | 1.37     |
| 10  | cA    | 801 | CL0  | CHD-C4C | 4.29  | 1.47        | 1.39     |
| 11  | cA    | 821 | CLA  | C1D-ND  | 4.29  | 1.43        | 1.37     |
| 11  | aA    | 802 | CLA  | CHD-C1D | 4.29  | 1.46        | 1.38     |
| 11  | cA    | 817 | CLA  | CHD-C1D | 4.29  | 1.46        | 1.38     |
| 11  | cA    | 802 | CLA  | CHD-C1D | 4.29  | 1.46        | 1.38     |
| 11  | bA    | 840 | CLA  | O2A-CGA | 4.29  | 1.45        | 1.33     |
| 11  | bB    | 832 | CLA  | CHD-C1D | 4.29  | 1.46        | 1.38     |
| 11  | bA    | 838 | CLA  | C1D-ND  | 4.29  | 1.43        | 1.37     |
| 12  | cB    | 824 | F6C  | CHD-C1D | 4.29  | 1.47        | 1.38     |
| 11  | bB    | 835 | CLA  | CHD-C1D | 4.28  | 1.46        | 1.38     |
| 12  | aB    | 824 | F6C  | O2A-CGA | 4.28  | 1.45        | 1.33     |
| 11  | cB    | 807 | CLA  | CHC-C1C | 4.28  | 1.47        | 1.38     |
| 11  | aA    | 835 | CLA  | O2A-CGA | 4.28  | 1.45        | 1.33     |
| 11  | aA    | 803 | CLA  | C1B-NB  | -4.28 | 1.32        | 1.37     |
| 11  | aA    | 815 | CLA  | CHD-C1D | 4.28  | 1.46        | 1.38     |
| 11  | aB    | 814 | CLA  | CHD-C1D | 4.28  | 1.46        | 1.38     |
| 12  | bB    | 824 | F6C  | CHD-C1D | 4.28  | 1.47        | 1.38     |
| 12  | aB    | 824 | F6C  | CHD-C1D | 4.27  | 1.47        | 1.38     |
| 12  | bA    | 832 | F6C  | O2A-CGA | 4.27  | 1.45        | 1.33     |
| 11  | bB    | 801 | CLA  | C1D-ND  | 4.27  | 1.43        | 1.37     |
| 11  | aB    | 817 | CLA  | C1D-ND  | 4.27  | 1.43        | 1.37     |
| 11  | bA    | 814 | CLA  | CHD-C1D | 4.27  | 1.46        | 1.38     |
| 11  | cA    | 812 | CLA  | CHD-C1D | 4.27  | 1.46        | 1.38     |
| 12  | aA    | 832 | F6C  | O2A-CGA | 4.27  | 1.45        | 1.33     |
| 11  | bB    | 813 | CLA  | O2A-CGA | 4.27  | 1.45        | 1.33     |
| 11  | cA    | 838 | CLA  | C1D-ND  | 4.27  | 1.43        | 1.37     |
| 11  | bA    | 835 | CLA  | O2A-CGA | 4.27  | 1.45        | 1.33     |
| 11  | cB    | 813 | CLA  | O2A-CGA | 4.27  | 1.45        | 1.33     |
| 11  | cA    | 815 | CLA  | CHD-C1D | 4.27  | 1.46        | 1.38     |
| 10  | bA    | 801 | CL0  | CHD-C4C | 4.27  | 1.47        | 1.39     |
| 11  | bB    | 828 | CLA  | C1D-ND  | 4.26  | 1.43        | 1.37     |
| 11  | aB    | 832 | CLA  | CHD-C1D | 4.26  | 1.46        | 1.38     |
| 12  | aA    | 830 | F6C  | CHC-C4B | 4.26  | 1.47        | 1.38     |
| 11  | cA    | 811 | CLA  | CHD-C1D | 4.26  | 1.46        | 1.38     |
| 11  | aA    | 817 | CLA  | CHD-C1D | 4.26  | 1.46        | 1.38     |
| 12  | cB    | 824 | F6C  | O2A-CGA | 4.26  | 1.45        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | cB    | 814 | CLA  | CHD-C1D | 4.26  | 1.46        | 1.38     |
| 11  | bA    | 831 | CLA  | C1B-NB  | -4.26 | 1.32        | 1.37     |
| 11  | bB    | 823 | CLA  | O2A-CGA | 4.26  | 1.45        | 1.33     |
| 11  | bB    | 827 | CLA  | O2A-CGA | 4.26  | 1.45        | 1.33     |
| 11  | aB    | 827 | CLA  | O2A-CGA | 4.26  | 1.45        | 1.33     |
| 11  | aB    | 813 | CLA  | O2A-CGA | 4.26  | 1.45        | 1.33     |
| 11  | bA    | 802 | CLA  | CHD-C1D | 4.26  | 1.46        | 1.38     |
| 11  | cB    | 823 | CLA  | O2A-CGA | 4.25  | 1.45        | 1.33     |
| 12  | cA    | 830 | F6C  | CHC-C4B | 4.25  | 1.47        | 1.38     |
| 11  | cA    | 802 | CLA  | CHC-C1C | 4.25  | 1.47        | 1.38     |
| 11  | cB    | 804 | CLA  | O2A-CGA | 4.25  | 1.45        | 1.33     |
| 11  | aA    | 811 | CLA  | CHD-C1D | 4.25  | 1.46        | 1.38     |
| 11  | aA    | 822 | CLA  | O2A-CGA | 4.25  | 1.45        | 1.33     |
| 12  | bB    | 824 | F6C  | O2A-CGA | 4.25  | 1.45        | 1.33     |
| 11  | cB    | 828 | CLA  | C1D-ND  | 4.25  | 1.43        | 1.37     |
| 11  | aB    | 830 | CLA  | CHD-C1D | 4.25  | 1.46        | 1.38     |
| 11  | bB    | 811 | CLA  | CHD-C1D | 4.25  | 1.46        | 1.38     |
| 11  | bB    | 830 | CLA  | CHD-C1D | 4.25  | 1.46        | 1.38     |
| 11  | cB    | 827 | CLA  | O2A-CGA | 4.25  | 1.45        | 1.33     |
| 11  | cB    | 811 | CLA  | CHD-C1D | 4.25  | 1.46        | 1.38     |
| 12  | bA    | 830 | F6C  | CHC-C4B | 4.25  | 1.47        | 1.38     |
| 11  | aA    | 843 | CLA  | O2A-CGA | 4.25  | 1.45        | 1.33     |
| 11  | cA    | 822 | CLA  | O2A-CGA | 4.25  | 1.45        | 1.33     |
| 11  | bA    | 811 | CLA  | CHD-C1D | 4.25  | 1.46        | 1.38     |
| 11  | cA    | 804 | CLA  | CHD-C1D | 4.25  | 1.46        | 1.38     |
| 11  | aL    | 205 | CLA  | C1D-ND  | 4.24  | 1.43        | 1.37     |
| 11  | bA    | 825 | CLA  | CHD-C1D | 4.24  | 1.46        | 1.38     |
| 11  | cA    | 820 | CLA  | CHD-C1D | 4.24  | 1.46        | 1.38     |
| 11  | bB    | 830 | CLA  | O2A-CGA | 4.24  | 1.45        | 1.33     |
| 11  | cA    | 835 | CLA  | O2A-CGA | 4.24  | 1.45        | 1.33     |
| 11  | cA    | 825 | CLA  | CHD-C1D | 4.24  | 1.46        | 1.38     |
| 11  | aA    | 817 | CLA  | O2A-CGA | 4.24  | 1.45        | 1.33     |
| 11  | bB    | 810 | CLA  | CHD-C1D | 4.24  | 1.46        | 1.38     |
| 11  | cB    | 810 | CLA  | CHD-C1D | 4.24  | 1.46        | 1.38     |
| 11  | bB    | 836 | CLA  | O2A-CGA | 4.24  | 1.45        | 1.33     |
| 11  | bA    | 804 | CLA  | CHD-C1D | 4.24  | 1.46        | 1.38     |
| 11  | aA    | 820 | CLA  | O2A-CGA | 4.24  | 1.45        | 1.33     |
| 11  | bA    | 821 | CLA  | C1D-ND  | 4.24  | 1.43        | 1.37     |
| 11  | aA    | 820 | CLA  | CHD-C1D | 4.24  | 1.46        | 1.38     |
| 11  | cB    | 836 | CLA  | O2A-CGA | 4.24  | 1.45        | 1.33     |
| 11  | cA    | 831 | CLA  | CHC-C1C | 4.24  | 1.47        | 1.38     |
| 11  | aB    | 804 | CLA  | O2A-CGA | 4.23  | 1.45        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 11  | cA    | 814 | CLA  | CHD-C1D | 4.23 | 1.46        | 1.38     |
| 11  | bA    | 831 | CLA  | CHC-C1C | 4.23 | 1.47        | 1.38     |
| 11  | aA    | 814 | CLA  | CHD-C1D | 4.23 | 1.46        | 1.38     |
| 11  | aB    | 828 | CLA  | C1D-ND  | 4.23 | 1.43        | 1.37     |
| 11  | bB    | 804 | CLA  | O2A-CGA | 4.23 | 1.45        | 1.33     |
| 11  | cB    | 801 | CLA  | C1D-ND  | 4.23 | 1.43        | 1.37     |
| 11  | cK    | 101 | CLA  | CHD-C1D | 4.23 | 1.46        | 1.38     |
| 11  | cL    | 206 | CLA  | C1D-ND  | 4.23 | 1.43        | 1.37     |
| 11  | bB    | 840 | CLA  | CHC-C1C | 4.23 | 1.47        | 1.38     |
| 11  | cB    | 830 | CLA  | CHD-C1D | 4.23 | 1.46        | 1.38     |
| 11  | cB    | 832 | CLA  | CHD-C1D | 4.23 | 1.46        | 1.38     |
| 11  | aB    | 830 | CLA  | O2A-CGA | 4.23 | 1.45        | 1.33     |
| 11  | cA    | 843 | CLA  | O2A-CGA | 4.23 | 1.45        | 1.33     |
| 11  | aB    | 811 | CLA  | CHD-C1D | 4.23 | 1.46        | 1.38     |
| 11  | bB    | 821 | CLA  | CHD-C1D | 4.23 | 1.46        | 1.38     |
| 11  | bA    | 820 | CLA  | CHD-C1D | 4.22 | 1.46        | 1.38     |
| 11  | aB    | 801 | CLA  | C1D-ND  | 4.22 | 1.43        | 1.37     |
| 11  | aB    | 823 | CLA  | O2A-CGA | 4.22 | 1.45        | 1.33     |
| 11  | bA    | 820 | CLA  | O2A-CGA | 4.22 | 1.45        | 1.33     |
| 11  | cB    | 821 | CLA  | CHD-C1D | 4.22 | 1.46        | 1.38     |
| 11  | aA    | 831 | CLA  | CHC-C1C | 4.22 | 1.46        | 1.38     |
| 11  | aK    | 101 | CLA  | CHD-C1D | 4.22 | 1.46        | 1.38     |
| 11  | bK    | 101 | CLA  | CHD-C1D | 4.22 | 1.46        | 1.38     |
| 11  | aA    | 825 | CLA  | CHD-C1D | 4.22 | 1.46        | 1.38     |
| 11  | cB    | 830 | CLA  | O2A-CGA | 4.22 | 1.45        | 1.33     |
| 11  | bB    | 814 | CLA  | CHD-C1D | 4.22 | 1.46        | 1.38     |
| 11  | aB    | 821 | CLA  | CHD-C1D | 4.22 | 1.46        | 1.38     |
| 11  | bA    | 817 | CLA  | O2A-CGA | 4.22 | 1.45        | 1.33     |
| 11  | aA    | 802 | CLA  | CHC-C1C | 4.22 | 1.46        | 1.38     |
| 11  | cA    | 824 | CLA  | CHD-C1D | 4.22 | 1.46        | 1.38     |
| 11  | bB    | 825 | CLA  | O2A-CGA | 4.22 | 1.45        | 1.33     |
| 11  | aB    | 836 | CLA  | O2A-CGA | 4.21 | 1.45        | 1.33     |
| 11  | cA    | 803 | CLA  | O2A-CGA | 4.21 | 1.45        | 1.33     |
| 11  | bA    | 822 | CLA  | O2A-CGA | 4.21 | 1.45        | 1.33     |
| 11  | bB    | 819 | CLA  | C1D-ND  | 4.21 | 1.43        | 1.37     |
| 12  | cA    | 832 | F6C  | CHC-C4B | 4.21 | 1.46        | 1.38     |
| 11  | bA    | 843 | CLA  | O2A-CGA | 4.21 | 1.45        | 1.33     |
| 11  | cA    | 817 | CLA  | O2A-CGA | 4.21 | 1.45        | 1.33     |
| 11  | aB    | 805 | CLA  | CHD-C1D | 4.21 | 1.46        | 1.38     |
| 11  | aA    | 812 | CLA  | O2A-CGA | 4.21 | 1.45        | 1.33     |
| 11  | cB    | 803 | CLA  | O2A-CGA | 4.21 | 1.45        | 1.33     |
| 11  | aB    | 810 | CLA  | CHD-C1D | 4.21 | 1.46        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | cA    | 820 | CLA  | O2A-CGA | 4.21  | 1.45        | 1.33     |
| 11  | bA    | 803 | CLA  | C1B-NB  | -4.20 | 1.32        | 1.37     |
| 11  | bL    | 205 | CLA  | C1D-ND  | 4.20  | 1.43        | 1.37     |
| 11  | cA    | 803 | CLA  | C1B-NB  | -4.20 | 1.32        | 1.37     |
| 11  | cB    | 819 | CLA  | C1D-ND  | 4.20  | 1.43        | 1.37     |
| 12  | bA    | 832 | F6C  | CHC-C4B | 4.20  | 1.46        | 1.38     |
| 12  | bA    | 826 | F6C  | O2A-CGA | 4.20  | 1.45        | 1.33     |
| 11  | cL    | 205 | CLA  | C1D-ND  | 4.20  | 1.43        | 1.37     |
| 11  | aA    | 804 | CLA  | CHD-C1D | 4.20  | 1.46        | 1.38     |
| 11  | aB    | 819 | CLA  | C1D-ND  | 4.20  | 1.43        | 1.37     |
| 11  | aA    | 821 | CLA  | C1D-ND  | 4.20  | 1.43        | 1.37     |
| 11  | cB    | 828 | CLA  | CHC-C1C | 4.20  | 1.46        | 1.38     |
| 11  | aA    | 831 | CLA  | C1B-NB  | -4.20 | 1.32        | 1.37     |
| 11  | aB    | 825 | CLA  | O2A-CGA | 4.20  | 1.45        | 1.33     |
| 12  | aA    | 826 | F6C  | O2A-CGA | 4.19  | 1.45        | 1.33     |
| 11  | aA    | 803 | CLA  | O2A-CGA | 4.19  | 1.45        | 1.33     |
| 11  | bB    | 803 | CLA  | O2A-CGA | 4.19  | 1.45        | 1.33     |
| 11  | bB    | 821 | CLA  | O2A-CGA | 4.19  | 1.45        | 1.33     |
| 11  | aA    | 836 | CLA  | CHC-C1C | 4.19  | 1.46        | 1.38     |
| 11  | bB    | 816 | CLA  | CHD-C1D | 4.19  | 1.46        | 1.38     |
| 11  | cA    | 819 | CLA  | O2A-CGA | 4.19  | 1.45        | 1.33     |
| 12  | aA    | 830 | F6C  | O2A-CGA | 4.19  | 1.45        | 1.33     |
| 11  | bA    | 824 | CLA  | O2A-CGA | 4.19  | 1.45        | 1.33     |
| 11  | bB    | 828 | CLA  | CHC-C1C | 4.19  | 1.46        | 1.38     |
| 11  | cB    | 825 | CLA  | O2A-CGA | 4.19  | 1.45        | 1.33     |
| 11  | cB    | 821 | CLA  | O2A-CGA | 4.19  | 1.45        | 1.33     |
| 11  | aB    | 833 | CLA  | CHD-C1D | 4.19  | 1.46        | 1.38     |
| 11  | cB    | 833 | CLA  | CHD-C1D | 4.19  | 1.46        | 1.38     |
| 12  | aA    | 832 | F6C  | CHC-C4B | 4.19  | 1.46        | 1.38     |
| 11  | aA    | 824 | CLA  | CHD-C1D | 4.19  | 1.46        | 1.38     |
| 11  | aL    | 206 | CLA  | C1D-ND  | 4.19  | 1.43        | 1.37     |
| 11  | cB    | 823 | CLA  | C1D-ND  | 4.18  | 1.43        | 1.37     |
| 12  | cA    | 826 | F6C  | O2A-CGA | 4.18  | 1.45        | 1.33     |
| 11  | cA    | 831 | CLA  | C1B-NB  | -4.18 | 1.32        | 1.37     |
| 12  | cA    | 830 | F6C  | O2A-CGA | 4.18  | 1.45        | 1.33     |
| 11  | aB    | 816 | CLA  | CHD-C1D | 4.18  | 1.46        | 1.38     |
| 11  | bA    | 803 | CLA  | O2A-CGA | 4.18  | 1.45        | 1.33     |
| 11  | cB    | 815 | CLA  | O2A-CGA | 4.18  | 1.45        | 1.33     |
| 11  | cA    | 816 | CLA  | CHD-C1D | 4.18  | 1.46        | 1.38     |
| 11  | cB    | 806 | CLA  | O2A-CGA | 4.18  | 1.45        | 1.33     |
| 11  | aA    | 824 | CLA  | O2A-CGA | 4.18  | 1.45        | 1.33     |
| 11  | bA    | 802 | CLA  | CHC-C1C | 4.18  | 1.46        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 11  | cA    | 812 | CLA  | O2A-CGA | 4.18 | 1.45        | 1.33     |
| 11  | bA    | 828 | CLA  | O2A-CGA | 4.18 | 1.45        | 1.33     |
| 11  | bA    | 836 | CLA  | CHC-C1C | 4.18 | 1.46        | 1.38     |
| 11  | aA    | 819 | CLA  | O2A-CGA | 4.18 | 1.45        | 1.33     |
| 11  | bA    | 812 | CLA  | O2A-CGA | 4.18 | 1.45        | 1.33     |
| 11  | bB    | 815 | CLA  | O2A-CGA | 4.18 | 1.45        | 1.33     |
| 11  | bA    | 819 | CLA  | O2A-CGA | 4.18 | 1.45        | 1.33     |
| 11  | cA    | 824 | CLA  | O2A-CGA | 4.18 | 1.45        | 1.33     |
| 11  | aB    | 815 | CLA  | O2A-CGA | 4.17 | 1.45        | 1.33     |
| 11  | cB    | 840 | CLA  | CHC-C1C | 4.17 | 1.46        | 1.38     |
| 11  | aB    | 813 | CLA  | CHD-C1D | 4.17 | 1.46        | 1.38     |
| 11  | cB    | 837 | CLA  | O2A-CGA | 4.17 | 1.45        | 1.33     |
| 11  | aB    | 821 | CLA  | O2A-CGA | 4.17 | 1.45        | 1.33     |
| 11  | aA    | 822 | CLA  | CHD-C1D | 4.17 | 1.46        | 1.38     |
| 12  | aA    | 832 | F6C  | CHD-C1D | 4.17 | 1.46        | 1.38     |
| 12  | bA    | 832 | F6C  | CHD-C1D | 4.16 | 1.46        | 1.38     |
| 11  | cA    | 833 | CLA  | CHD-C1D | 4.16 | 1.46        | 1.38     |
| 11  | cB    | 813 | CLA  | CHD-C1D | 4.16 | 1.46        | 1.38     |
| 11  | bK    | 103 | CLA  | O2A-CGA | 4.16 | 1.45        | 1.33     |
| 11  | cA    | 836 | CLA  | CHC-C1C | 4.16 | 1.46        | 1.38     |
| 11  | aB    | 840 | CLA  | CHC-C1C | 4.16 | 1.46        | 1.38     |
| 11  | aB    | 837 | CLA  | O2A-CGA | 4.16 | 1.45        | 1.33     |
| 11  | cB    | 831 | CLA  | O2A-CGA | 4.16 | 1.45        | 1.33     |
| 11  | bA    | 822 | CLA  | CHD-C1D | 4.16 | 1.46        | 1.38     |
| 11  | cA    | 829 | CLA  | CHD-C1D | 4.16 | 1.46        | 1.38     |
| 11  | aA    | 802 | CLA  | C1D-ND  | 4.16 | 1.43        | 1.37     |
| 11  | bA    | 833 | CLA  | CHD-C1D | 4.16 | 1.46        | 1.38     |
| 11  | cA    | 828 | CLA  | O2A-CGA | 4.16 | 1.45        | 1.33     |
| 11  | bB    | 833 | CLA  | CHD-C1D | 4.16 | 1.46        | 1.38     |
| 11  | aA    | 818 | CLA  | C1D-ND  | 4.16 | 1.43        | 1.37     |
| 11  | aB    | 823 | CLA  | C1D-ND  | 4.16 | 1.43        | 1.37     |
| 11  | aB    | 806 | CLA  | O2A-CGA | 4.16 | 1.45        | 1.33     |
| 11  | aB    | 831 | CLA  | O2A-CGA | 4.16 | 1.45        | 1.33     |
| 11  | cK    | 103 | CLA  | O2A-CGA | 4.16 | 1.45        | 1.33     |
| 11  | aB    | 803 | CLA  | O2A-CGA | 4.16 | 1.45        | 1.33     |
| 11  | bB    | 837 | CLA  | O2A-CGA | 4.16 | 1.45        | 1.33     |
| 11  | bA    | 821 | CLA  | O2A-CGA | 4.16 | 1.45        | 1.33     |
| 11  | bA    | 824 | CLA  | CHD-C1D | 4.16 | 1.46        | 1.38     |
| 11  | aA    | 833 | CLA  | O2A-CGA | 4.15 | 1.45        | 1.33     |
| 11  | bB    | 823 | CLA  | C1D-ND  | 4.15 | 1.43        | 1.37     |
| 11  | bB    | 807 | CLA  | O2A-CGA | 4.15 | 1.45        | 1.33     |
| 11  | aA    | 828 | CLA  | O2A-CGA | 4.15 | 1.45        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 11  | bB    | 806 | CLA  | O2A-CGA | 4.15 | 1.45        | 1.33     |
| 11  | cB    | 819 | CLA  | O2A-CGA | 4.15 | 1.45        | 1.33     |
| 11  | bA    | 833 | CLA  | O2A-CGA | 4.15 | 1.45        | 1.33     |
| 11  | cA    | 821 | CLA  | O2A-CGA | 4.15 | 1.45        | 1.33     |
| 11  | cA    | 818 | CLA  | C1D-ND  | 4.15 | 1.43        | 1.37     |
| 11  | aA    | 805 | CLA  | CHD-C1D | 4.15 | 1.46        | 1.38     |
| 11  | aB    | 819 | CLA  | O2A-CGA | 4.15 | 1.45        | 1.33     |
| 12  | cA    | 844 | F6C  | CHD-C1D | 4.15 | 1.46        | 1.38     |
| 11  | bB    | 819 | CLA  | O2A-CGA | 4.15 | 1.45        | 1.33     |
| 11  | aA    | 833 | CLA  | CHD-C1D | 4.15 | 1.46        | 1.38     |
| 12  | cA    | 832 | F6C  | CHD-C1D | 4.15 | 1.46        | 1.38     |
| 11  | bB    | 831 | CLA  | O2A-CGA | 4.14 | 1.45        | 1.33     |
| 11  | cB    | 808 | CLA  | O2A-CGA | 4.14 | 1.45        | 1.33     |
| 11  | aB    | 826 | CLA  | O2A-CGA | 4.14 | 1.45        | 1.33     |
| 11  | cB    | 816 | CLA  | CHD-C1D | 4.14 | 1.46        | 1.38     |
| 11  | bA    | 818 | CLA  | C1D-ND  | 4.14 | 1.43        | 1.37     |
| 11  | cB    | 807 | CLA  | O2A-CGA | 4.14 | 1.45        | 1.33     |
| 11  | cB    | 805 | CLA  | CHD-C1D | 4.14 | 1.46        | 1.38     |
| 11  | cA    | 822 | CLA  | CHD-C1D | 4.14 | 1.46        | 1.38     |
| 11  | aB    | 803 | CLA  | CHC-C1C | 4.14 | 1.46        | 1.38     |
| 11  | bB    | 805 | CLA  | CHD-C1D | 4.14 | 1.46        | 1.38     |
| 11  | bB    | 803 | CLA  | CHC-C1C | 4.14 | 1.46        | 1.38     |
| 11  | cB    | 837 | CLA  | CHD-C1D | 4.14 | 1.46        | 1.38     |
| 12  | bA    | 830 | F6C  | O2A-CGA | 4.14 | 1.45        | 1.33     |
| 11  | aB    | 807 | CLA  | O2A-CGA | 4.14 | 1.45        | 1.33     |
| 10  | cA    | 801 | CL0  | CHC-C1C | 4.14 | 1.47        | 1.39     |
| 11  | aB    | 808 | CLA  | O2A-CGA | 4.14 | 1.45        | 1.33     |
| 11  | bB    | 802 | CLA  | C1D-ND  | 4.13 | 1.43        | 1.37     |
| 11  | aK    | 103 | CLA  | O2A-CGA | 4.13 | 1.45        | 1.33     |
| 11  | aA    | 816 | CLA  | CHD-C1D | 4.13 | 1.46        | 1.38     |
| 11  | aB    | 802 | CLA  | C1D-ND  | 4.13 | 1.43        | 1.37     |
| 11  | bB    | 808 | CLA  | O2A-CGA | 4.13 | 1.45        | 1.33     |
| 11  | bB    | 818 | CLA  | O2A-CGA | 4.13 | 1.45        | 1.33     |
| 12  | cA    | 827 | F6C  | O2A-CGA | 4.13 | 1.45        | 1.33     |
| 11  | cA    | 833 | CLA  | O2A-CGA | 4.13 | 1.45        | 1.33     |
| 11  | bA    | 816 | CLA  | CHD-C1D | 4.13 | 1.46        | 1.38     |
| 11  | cA    | 829 | CLA  | O2A-CGA | 4.13 | 1.45        | 1.33     |
| 11  | cB    | 818 | CLA  | O2A-CGA | 4.13 | 1.45        | 1.33     |
| 12  | aA    | 844 | F6C  | CHD-C1D | 4.13 | 1.46        | 1.38     |
| 11  | cB    | 826 | CLA  | O2A-CGA | 4.13 | 1.45        | 1.33     |
| 12  | aA    | 844 | F6C  | O2A-CGA | 4.13 | 1.45        | 1.33     |
| 11  | aB    | 828 | CLA  | CHC-C1C | 4.13 | 1.46        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | bB    | 813 | CLA  | CHD-C1D | 4.13  | 1.46        | 1.38     |
| 11  | aL    | 205 | CLA  | O2A-CGA | 4.13  | 1.45        | 1.33     |
| 11  | aA    | 825 | CLA  | O2A-CGA | 4.12  | 1.45        | 1.33     |
| 11  | aA    | 835 | CLA  | CHD-C1D | 4.12  | 1.46        | 1.38     |
| 11  | bB    | 838 | CLA  | O2A-CGA | 4.12  | 1.45        | 1.33     |
| 11  | bA    | 805 | CLA  | CHD-C1D | 4.12  | 1.46        | 1.38     |
| 12  | bA    | 844 | F6C  | O2A-CGA | 4.12  | 1.45        | 1.33     |
| 12  | bA    | 844 | F6C  | CHD-C1D | 4.12  | 1.46        | 1.38     |
| 11  | cB    | 803 | CLA  | CHC-C1C | 4.12  | 1.46        | 1.38     |
| 11  | aB    | 808 | CLA  | C1B-NB  | -4.12 | 1.32        | 1.37     |
| 11  | cB    | 807 | CLA  | C1D-ND  | 4.12  | 1.43        | 1.37     |
| 11  | bA    | 835 | CLA  | CHD-C1D | 4.12  | 1.46        | 1.38     |
| 11  | aB    | 807 | CLA  | C1D-ND  | 4.12  | 1.43        | 1.37     |
| 11  | cA    | 805 | CLA  | CHD-C1D | 4.12  | 1.46        | 1.38     |
| 12  | bA    | 827 | F6C  | O2A-CGA | 4.12  | 1.45        | 1.33     |
| 11  | bB    | 816 | CLA  | O2A-CGA | 4.12  | 1.45        | 1.33     |
| 10  | aA    | 801 | CL0  | CHC-C1C | 4.12  | 1.47        | 1.39     |
| 11  | aB    | 818 | CLA  | O2A-CGA | 4.12  | 1.45        | 1.33     |
| 11  | aA    | 829 | CLA  | O2A-CGA | 4.12  | 1.45        | 1.33     |
| 11  | cA    | 813 | CLA  | O2A-CGA | 4.12  | 1.45        | 1.33     |
| 11  | cA    | 825 | CLA  | O2A-CGA | 4.12  | 1.45        | 1.33     |
| 12  | aB    | 824 | F6C  | CHC-C4B | 4.12  | 1.46        | 1.38     |
| 11  | aA    | 821 | CLA  | O2A-CGA | 4.11  | 1.45        | 1.33     |
| 11  | cA    | 809 | CLA  | CHD-C1D | 4.11  | 1.46        | 1.38     |
| 11  | bA    | 825 | CLA  | O2A-CGA | 4.11  | 1.45        | 1.33     |
| 11  | aB    | 816 | CLA  | O2A-CGA | 4.11  | 1.45        | 1.33     |
| 11  | bA    | 837 | CLA  | CHD-C1D | 4.11  | 1.46        | 1.38     |
| 10  | bA    | 801 | CL0  | CHC-C1C | 4.11  | 1.47        | 1.39     |
| 11  | aA    | 829 | CLA  | CHD-C1D | 4.11  | 1.46        | 1.38     |
| 11  | bA    | 829 | CLA  | O2A-CGA | 4.11  | 1.45        | 1.33     |
| 11  | bA    | 809 | CLA  | CHD-C1D | 4.11  | 1.46        | 1.38     |
| 11  | bB    | 826 | CLA  | O2A-CGA | 4.11  | 1.45        | 1.33     |
| 11  | cA    | 831 | CLA  | O2A-CGA | 4.11  | 1.45        | 1.33     |
| 11  | cA    | 837 | CLA  | CHD-C1D | 4.11  | 1.46        | 1.38     |
| 11  | aA    | 813 | CLA  | O2A-CGA | 4.11  | 1.45        | 1.33     |
| 11  | cB    | 802 | CLA  | C1D-ND  | 4.11  | 1.43        | 1.37     |
| 11  | aA    | 839 | CLA  | CHD-C1D | 4.11  | 1.46        | 1.38     |
| 11  | bA    | 829 | CLA  | CHD-C1D | 4.10  | 1.46        | 1.38     |
| 11  | bA    | 813 | CLA  | O2A-CGA | 4.10  | 1.45        | 1.33     |
| 11  | aA    | 809 | CLA  | CHD-C1D | 4.10  | 1.46        | 1.38     |
| 11  | aA    | 807 | CLA  | O2A-CGA | 4.10  | 1.45        | 1.33     |
| 11  | bL    | 205 | CLA  | O2A-CGA | 4.10  | 1.45        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | aA    | 818 | CLA  | O2A-CGA | 4.10  | 1.45        | 1.33     |
| 11  | bA    | 834 | CLA  | CHD-C1D | 4.10  | 1.46        | 1.38     |
| 12  | bA    | 826 | F6C  | C3B-C2B | 4.10  | 1.48        | 1.39     |
| 11  | aA    | 831 | CLA  | O2A-CGA | 4.10  | 1.45        | 1.33     |
| 11  | cB    | 838 | CLA  | O2A-CGA | 4.09  | 1.45        | 1.33     |
| 11  | bB    | 837 | CLA  | CHD-C1D | 4.09  | 1.46        | 1.38     |
| 11  | bA    | 807 | CLA  | O2A-CGA | 4.09  | 1.45        | 1.33     |
| 11  | aB    | 838 | CLA  | O2A-CGA | 4.09  | 1.45        | 1.33     |
| 11  | aB    | 829 | CLA  | CHD-C4C | 4.09  | 1.48        | 1.39     |
| 10  | aA    | 801 | CL0  | O2A-CGA | 4.09  | 1.45        | 1.33     |
| 11  | cL    | 205 | CLA  | O2A-CGA | 4.09  | 1.45        | 1.33     |
| 11  | cA    | 818 | CLA  | O2A-CGA | 4.09  | 1.45        | 1.33     |
| 11  | cB    | 816 | CLA  | O2A-CGA | 4.09  | 1.45        | 1.33     |
| 10  | cA    | 801 | CL0  | O2A-CGA | 4.09  | 1.45        | 1.33     |
| 12  | aA    | 827 | F6C  | O2A-CGA | 4.09  | 1.45        | 1.33     |
| 11  | bA    | 839 | CLA  | CHD-C1D | 4.09  | 1.46        | 1.38     |
| 11  | cA    | 835 | CLA  | CHD-C1D | 4.09  | 1.46        | 1.38     |
| 11  | cB    | 829 | CLA  | CHD-C4C | 4.09  | 1.48        | 1.39     |
| 12  | cA    | 826 | F6C  | C3B-C2B | 4.09  | 1.48        | 1.39     |
| 11  | bA    | 818 | CLA  | O2A-CGA | 4.09  | 1.45        | 1.33     |
| 11  | bA    | 831 | CLA  | O2A-CGA | 4.09  | 1.45        | 1.33     |
| 11  | bA    | 802 | CLA  | C1D-ND  | 4.08  | 1.43        | 1.37     |
| 12  | cA    | 844 | F6C  | O2A-CGA | 4.08  | 1.45        | 1.33     |
| 11  | aA    | 834 | CLA  | CHD-C1D | 4.08  | 1.46        | 1.38     |
| 11  | aB    | 837 | CLA  | CHD-C1D | 4.08  | 1.46        | 1.38     |
| 12  | aA    | 826 | F6C  | C3B-C2B | 4.08  | 1.48        | 1.39     |
| 11  | aA    | 841 | CLA  | O2A-CGA | 4.08  | 1.45        | 1.33     |
| 11  | bB    | 815 | CLA  | CHD-C1D | 4.08  | 1.46        | 1.38     |
| 11  | cA    | 802 | CLA  | C1B-NB  | -4.08 | 1.32        | 1.37     |
| 11  | bA    | 841 | CLA  | O2A-CGA | 4.08  | 1.45        | 1.33     |
| 11  | cA    | 839 | CLA  | CHD-C1D | 4.08  | 1.46        | 1.38     |
| 12  | bB    | 824 | F6C  | CHC-C4B | 4.08  | 1.46        | 1.38     |
| 11  | bA    | 840 | CLA  | CHD-C1D | 4.08  | 1.46        | 1.38     |
| 11  | bB    | 829 | CLA  | CHD-C4C | 4.08  | 1.48        | 1.39     |
| 11  | cA    | 802 | CLA  | C1D-ND  | 4.08  | 1.43        | 1.37     |
| 11  | aA    | 837 | CLA  | CHD-C1D | 4.07  | 1.46        | 1.38     |
| 11  | bB    | 807 | CLA  | C1D-ND  | 4.07  | 1.43        | 1.37     |
| 11  | cA    | 807 | CLA  | O2A-CGA | 4.07  | 1.45        | 1.33     |
| 11  | bA    | 814 | CLA  | O2A-CGA | 4.07  | 1.45        | 1.33     |
| 11  | cA    | 843 | CLA  | CHD-C1D | 4.07  | 1.46        | 1.38     |
| 11  | cK    | 103 | CLA  | CHD-C1D | 4.07  | 1.46        | 1.38     |
| 10  | bA    | 801 | CL0  | O2A-CGA | 4.06  | 1.45        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | cB    | 839 | CLA  | O2A-CGA | 4.06  | 1.45        | 1.33     |
| 11  | cA    | 840 | CLA  | CHD-C1D | 4.06  | 1.46        | 1.38     |
| 12  | cB    | 824 | F6C  | CHC-C4B | 4.06  | 1.46        | 1.38     |
| 11  | cA    | 841 | CLA  | O2A-CGA | 4.06  | 1.45        | 1.33     |
| 11  | cA    | 814 | CLA  | O2A-CGA | 4.06  | 1.45        | 1.33     |
| 11  | bA    | 831 | CLA  | C1D-ND  | 4.06  | 1.43        | 1.37     |
| 11  | bB    | 808 | CLA  | C1B-NB  | -4.06 | 1.32        | 1.37     |
| 11  | aB    | 839 | CLA  | O2A-CGA | 4.06  | 1.45        | 1.33     |
| 11  | bA    | 802 | CLA  | C1B-NB  | -4.06 | 1.32        | 1.37     |
| 11  | bB    | 839 | CLA  | O2A-CGA | 4.06  | 1.45        | 1.33     |
| 11  | aB    | 823 | CLA  | CHD-C1D | 4.06  | 1.46        | 1.38     |
| 11  | cB    | 840 | CLA  | CHD-C1D | 4.06  | 1.46        | 1.38     |
| 11  | aA    | 808 | CLA  | CHD-C1D | 4.06  | 1.46        | 1.38     |
| 11  | aA    | 807 | CLA  | CHD-C1D | 4.06  | 1.46        | 1.38     |
| 11  | cB    | 808 | CLA  | C1B-NB  | -4.06 | 1.32        | 1.37     |
| 11  | aB    | 832 | CLA  | CHD-C4C | 4.06  | 1.48        | 1.39     |
| 11  | bB    | 809 | CLA  | O2A-CGA | 4.05  | 1.45        | 1.33     |
| 11  | aB    | 802 | CLA  | CHD-C1D | 4.05  | 1.46        | 1.38     |
| 11  | cB    | 815 | CLA  | CHD-C1D | 4.05  | 1.46        | 1.38     |
| 11  | aB    | 815 | CLA  | CHD-C1D | 4.05  | 1.46        | 1.38     |
| 11  | bA    | 843 | CLA  | CHD-C1D | 4.05  | 1.46        | 1.38     |
| 11  | cA    | 808 | CLA  | O2A-CGA | 4.05  | 1.45        | 1.33     |
| 11  | cB    | 802 | CLA  | CHD-C1D | 4.05  | 1.46        | 1.38     |
| 11  | cB    | 809 | CLA  | O2A-CGA | 4.05  | 1.45        | 1.33     |
| 11  | aB    | 833 | CLA  | CHD-C4C | 4.05  | 1.48        | 1.39     |
| 11  | aA    | 814 | CLA  | O2A-CGA | 4.05  | 1.45        | 1.33     |
| 11  | cA    | 834 | CLA  | CHD-C1D | 4.05  | 1.46        | 1.38     |
| 11  | aB    | 809 | CLA  | O2A-CGA | 4.05  | 1.45        | 1.33     |
| 11  | cL    | 204 | CLA  | O2A-CGA | 4.05  | 1.45        | 1.33     |
| 11  | bA    | 808 | CLA  | CHD-C1D | 4.05  | 1.46        | 1.38     |
| 11  | cB    | 832 | CLA  | CHD-C4C | 4.05  | 1.48        | 1.39     |
| 11  | aA    | 840 | CLA  | CHD-C1D | 4.04  | 1.46        | 1.38     |
| 11  | bB    | 840 | CLA  | CHD-C1D | 4.04  | 1.46        | 1.38     |
| 11  | cA    | 807 | CLA  | CHD-C1D | 4.04  | 1.46        | 1.38     |
| 11  | aA    | 808 | CLA  | O2A-CGA | 4.04  | 1.45        | 1.33     |
| 11  | aA    | 842 | CLA  | CHD-C1D | 4.04  | 1.46        | 1.38     |
| 11  | cA    | 842 | CLA  | CHD-C1D | 4.04  | 1.46        | 1.38     |
| 11  | aL    | 204 | CLA  | O2A-CGA | 4.04  | 1.45        | 1.33     |
| 12  | bB    | 824 | F6C  | CHD-C4C | 4.04  | 1.48        | 1.39     |
| 11  | bA    | 841 | CLA  | CHD-C1D | 4.04  | 1.46        | 1.38     |
| 12  | cA    | 827 | F6C  | CHD-C1D | 4.04  | 1.46        | 1.38     |
| 11  | aK    | 103 | CLA  | CHD-C1D | 4.04  | 1.46        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | aA    | 841 | CLA  | CHD-C1D | 4.04  | 1.46        | 1.38     |
| 11  | bB    | 833 | CLA  | CHD-C4C | 4.04  | 1.48        | 1.39     |
| 11  | aA    | 802 | CLA  | C1B-NB  | -4.04 | 1.32        | 1.37     |
| 11  | bB    | 819 | CLA  | CHD-C1D | 4.03  | 1.46        | 1.38     |
| 11  | bK    | 103 | CLA  | CHD-C1D | 4.03  | 1.46        | 1.38     |
| 11  | aA    | 812 | CLA  | CHD-C4C | 4.03  | 1.48        | 1.39     |
| 11  | bA    | 808 | CLA  | O2A-CGA | 4.03  | 1.45        | 1.33     |
| 11  | aB    | 816 | CLA  | CHD-C4C | 4.03  | 1.48        | 1.39     |
| 12  | aA    | 827 | F6C  | CHD-C1D | 4.03  | 1.46        | 1.38     |
| 11  | cB    | 833 | CLA  | CHD-C4C | 4.03  | 1.48        | 1.39     |
| 11  | cB    | 819 | CLA  | CHD-C1D | 4.03  | 1.46        | 1.38     |
| 11  | bA    | 806 | CLA  | O2A-CGA | 4.03  | 1.45        | 1.33     |
| 12  | aB    | 824 | F6C  | CHD-C4C | 4.03  | 1.48        | 1.39     |
| 11  | cA    | 806 | CLA  | O2A-CGA | 4.03  | 1.45        | 1.33     |
| 11  | cB    | 839 | CLA  | C1D-ND  | 4.03  | 1.43        | 1.37     |
| 11  | aA    | 843 | CLA  | CHD-C1D | 4.03  | 1.46        | 1.38     |
| 11  | aB    | 840 | CLA  | CHD-C1D | 4.03  | 1.46        | 1.38     |
| 11  | cA    | 808 | CLA  | CHD-C1D | 4.03  | 1.46        | 1.38     |
| 11  | aB    | 819 | CLA  | CHD-C1D | 4.03  | 1.46        | 1.38     |
| 11  | bB    | 839 | CLA  | C1D-ND  | 4.03  | 1.43        | 1.37     |
| 11  | bB    | 823 | CLA  | CHD-C1D | 4.02  | 1.46        | 1.38     |
| 11  | bA    | 813 | CLA  | CHD-C1D | 4.02  | 1.46        | 1.38     |
| 11  | bA    | 807 | CLA  | CHD-C1D | 4.02  | 1.46        | 1.38     |
| 11  | bL    | 204 | CLA  | O2A-CGA | 4.02  | 1.45        | 1.33     |
| 11  | cB    | 816 | CLA  | CHD-C4C | 4.02  | 1.48        | 1.39     |
| 11  | cA    | 813 | CLA  | CHD-C1D | 4.02  | 1.46        | 1.38     |
| 11  | aA    | 802 | CLA  | C3D-C2D | 4.02  | 1.49        | 1.39     |
| 11  | bA    | 842 | CLA  | CHD-C1D | 4.02  | 1.46        | 1.38     |
| 11  | bB    | 832 | CLA  | CHD-C4C | 4.01  | 1.48        | 1.39     |
| 11  | cL    | 205 | CLA  | CHD-C1D | 4.01  | 1.46        | 1.38     |
| 11  | cA    | 806 | CLA  | CHD-C4C | 4.01  | 1.48        | 1.39     |
| 11  | aB    | 834 | CLA  | CHD-C4C | 4.01  | 1.48        | 1.39     |
| 11  | bA    | 834 | CLA  | O2A-CGA | 4.01  | 1.45        | 1.33     |
| 11  | bB    | 817 | CLA  | CHD-C1D | 4.01  | 1.46        | 1.38     |
| 11  | aA    | 811 | CLA  | CHD-C4C | 4.01  | 1.48        | 1.39     |
| 11  | bA    | 806 | CLA  | CHD-C4C | 4.01  | 1.48        | 1.39     |
| 12  | aB    | 824 | F6C  | C3D-C2D | 4.00  | 1.49        | 1.39     |
| 11  | cA    | 812 | CLA  | CHD-C4C | 4.00  | 1.48        | 1.39     |
| 11  | aA    | 834 | CLA  | O2A-CGA | 4.00  | 1.45        | 1.33     |
| 11  | cA    | 841 | CLA  | CHD-C1D | 4.00  | 1.46        | 1.38     |
| 12  | bA    | 827 | F6C  | CHD-C1D | 4.00  | 1.46        | 1.38     |
| 11  | aA    | 823 | CLA  | C3D-C2D | 4.00  | 1.49        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 11  | aA    | 806 | CLA  | CHD-C4C | 4.00 | 1.48        | 1.39     |
| 11  | bL    | 204 | CLA  | CHD-C1D | 4.00 | 1.46        | 1.38     |
| 11  | aL    | 205 | CLA  | CHD-C1D | 4.00 | 1.46        | 1.38     |
| 11  | aA    | 810 | CLA  | CHD-C1D | 4.00 | 1.46        | 1.38     |
| 11  | bB    | 802 | CLA  | CHD-C1D | 4.00 | 1.46        | 1.38     |
| 12  | bB    | 824 | F6C  | C3D-C2D | 4.00 | 1.49        | 1.39     |
| 12  | aA    | 844 | F6C  | C3B-C2B | 4.00 | 1.48        | 1.39     |
| 12  | cA    | 844 | F6C  | C3B-C2B | 4.00 | 1.48        | 1.39     |
| 11  | bL    | 205 | CLA  | CHD-C1D | 4.00 | 1.46        | 1.38     |
| 11  | bA    | 812 | CLA  | CHD-C4C | 4.00 | 1.48        | 1.39     |
| 11  | cA    | 811 | CLA  | CHD-C4C | 4.00 | 1.48        | 1.39     |
| 12  | bA    | 844 | F6C  | C3B-C2B | 4.00 | 1.48        | 1.39     |
| 11  | cA    | 838 | CLA  | O2A-CGA | 4.00 | 1.45        | 1.33     |
| 12  | cB    | 824 | F6C  | C3D-C2D | 4.00 | 1.49        | 1.39     |
| 11  | bB    | 834 | CLA  | CHD-C4C | 3.99 | 1.48        | 1.39     |
| 11  | aA    | 806 | CLA  | O2A-CGA | 3.99 | 1.45        | 1.33     |
| 11  | bA    | 802 | CLA  | C3D-C2D | 3.99 | 1.49        | 1.39     |
| 11  | bB    | 816 | CLA  | CHD-C4C | 3.99 | 1.48        | 1.39     |
| 11  | cA    | 810 | CLA  | CHD-C1D | 3.99 | 1.46        | 1.38     |
| 11  | bA    | 831 | CLA  | CHD-C1D | 3.99 | 1.46        | 1.38     |
| 11  | aA    | 813 | CLA  | CHD-C1D | 3.99 | 1.46        | 1.38     |
| 11  | aA    | 831 | CLA  | C1D-ND  | 3.99 | 1.43        | 1.37     |
| 11  | cB    | 834 | CLA  | CHD-C4C | 3.99 | 1.48        | 1.39     |
| 11  | aB    | 835 | CLA  | CHD-C4C | 3.99 | 1.48        | 1.39     |
| 11  | bB    | 835 | CLA  | CHD-C4C | 3.99 | 1.48        | 1.39     |
| 11  | cA    | 802 | CLA  | C3D-C2D | 3.99 | 1.49        | 1.39     |
| 11  | cB    | 823 | CLA  | CHD-C1D | 3.99 | 1.46        | 1.38     |
| 11  | aB    | 836 | CLA  | CHD-C1D | 3.99 | 1.46        | 1.38     |
| 11  | bA    | 804 | CLA  | CHD-C4C | 3.99 | 1.48        | 1.39     |
| 11  | bA    | 811 | CLA  | CHD-C4C | 3.99 | 1.48        | 1.39     |
| 11  | bA    | 823 | CLA  | C3D-C2D | 3.98 | 1.49        | 1.39     |
| 11  | cA    | 823 | CLA  | C3D-C2D | 3.98 | 1.49        | 1.39     |
| 11  | cL    | 206 | CLA  | CHD-C1D | 3.98 | 1.46        | 1.38     |
| 11  | aA    | 838 | CLA  | O2A-CGA | 3.98 | 1.45        | 1.33     |
| 11  | aB    | 812 | CLA  | O2A-CGA | 3.98 | 1.45        | 1.33     |
| 11  | bA    | 819 | CLA  | CHD-C1D | 3.98 | 1.46        | 1.38     |
| 11  | cB    | 812 | CLA  | O2A-CGA | 3.98 | 1.45        | 1.33     |
| 11  | cB    | 804 | CLA  | CHD-C1D | 3.98 | 1.46        | 1.38     |
| 12  | cB    | 824 | F6C  | CHD-C4C | 3.98 | 1.48        | 1.39     |
| 11  | bA    | 810 | CLA  | CHD-C1D | 3.98 | 1.46        | 1.38     |
| 11  | aB    | 817 | CLA  | CHD-C1D | 3.98 | 1.46        | 1.38     |
| 11  | aL    | 206 | CLA  | CHD-C1D | 3.98 | 1.46        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 11  | aB    | 839 | CLA  | C1D-ND  | 3.98 | 1.43        | 1.37     |
| 12  | bA    | 832 | F6C  | CHD-C4C | 3.98 | 1.48        | 1.39     |
| 11  | cB    | 838 | CLA  | CHD-C1D | 3.97 | 1.46        | 1.38     |
| 11  | aA    | 804 | CLA  | CHD-C4C | 3.97 | 1.48        | 1.39     |
| 11  | cL    | 204 | CLA  | CHD-C1D | 3.97 | 1.46        | 1.38     |
| 11  | aB    | 804 | CLA  | CHD-C1D | 3.97 | 1.46        | 1.38     |
| 11  | cB    | 817 | CLA  | CHD-C1D | 3.97 | 1.46        | 1.38     |
| 11  | cA    | 834 | CLA  | O2A-CGA | 3.97 | 1.44        | 1.33     |
| 11  | cB    | 820 | CLA  | CHD-C1D | 3.97 | 1.46        | 1.38     |
| 11  | cB    | 805 | CLA  | CHD-C4C | 3.97 | 1.48        | 1.39     |
| 11  | cA    | 804 | CLA  | CHD-C4C | 3.97 | 1.48        | 1.39     |
| 11  | bB    | 812 | CLA  | O2A-CGA | 3.97 | 1.44        | 1.33     |
| 11  | cB    | 801 | CLA  | O2A-CGA | 3.97 | 1.44        | 1.33     |
| 11  | aB    | 820 | CLA  | CHD-C1D | 3.97 | 1.46        | 1.38     |
| 11  | bB    | 818 | CLA  | CHD-C1D | 3.97 | 1.46        | 1.38     |
| 11  | cK    | 101 | CLA  | CHD-C4C | 3.96 | 1.48        | 1.39     |
| 12  | bL    | 202 | F6C  | C3B-C2B | 3.96 | 1.48        | 1.39     |
| 11  | aK    | 101 | CLA  | CHD-C4C | 3.96 | 1.48        | 1.39     |
| 11  | cA    | 831 | CLA  | C1D-ND  | 3.96 | 1.43        | 1.37     |
| 11  | aA    | 841 | CLA  | C3D-C2D | 3.96 | 1.49        | 1.39     |
| 11  | bB    | 831 | CLA  | CHD-C4C | 3.96 | 1.48        | 1.39     |
| 11  | aB    | 818 | CLA  | CHD-C1D | 3.96 | 1.46        | 1.38     |
| 11  | bB    | 820 | CLA  | CHD-C1D | 3.96 | 1.46        | 1.38     |
| 11  | bB    | 809 | CLA  | C1D-ND  | 3.96 | 1.43        | 1.37     |
| 11  | aA    | 802 | CLA  | O2A-CGA | 3.96 | 1.44        | 1.33     |
| 11  | bL    | 206 | CLA  | CHD-C1D | 3.96 | 1.46        | 1.38     |
| 11  | cA    | 820 | CLA  | CHD-C4C | 3.96 | 1.48        | 1.39     |
| 12  | cL    | 202 | F6C  | CHD-C1D | 3.96 | 1.46        | 1.38     |
| 11  | bA    | 841 | CLA  | C3D-C2D | 3.96 | 1.49        | 1.39     |
| 11  | bA    | 838 | CLA  | CHD-C1D | 3.96 | 1.46        | 1.38     |
| 11  | bB    | 805 | CLA  | CHD-C4C | 3.96 | 1.48        | 1.39     |
| 11  | bA    | 803 | CLA  | C3D-C2D | 3.96 | 1.49        | 1.39     |
| 11  | bK    | 101 | CLA  | CHD-C4C | 3.96 | 1.48        | 1.39     |
| 11  | aB    | 809 | CLA  | C1D-ND  | 3.95 | 1.43        | 1.37     |
| 11  | cB    | 835 | CLA  | CHD-C4C | 3.95 | 1.48        | 1.39     |
| 12  | aL    | 202 | F6C  | CHD-C1D | 3.95 | 1.46        | 1.38     |
| 11  | bB    | 801 | CLA  | O2A-CGA | 3.95 | 1.44        | 1.33     |
| 11  | aA    | 831 | CLA  | CHD-C1D | 3.95 | 1.46        | 1.38     |
| 11  | aA    | 820 | CLA  | CHD-C4C | 3.95 | 1.48        | 1.39     |
| 12  | cA    | 832 | F6C  | CHD-C4C | 3.95 | 1.48        | 1.39     |
| 11  | aL    | 204 | CLA  | CHD-C1D | 3.95 | 1.46        | 1.38     |
| 11  | cA    | 841 | CLA  | C3D-C2D | 3.95 | 1.49        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | bB    | 830 | CLA  | CHD-C4C | 3.95  | 1.48        | 1.39     |
| 11  | cA    | 819 | CLA  | CHD-C1D | 3.95  | 1.46        | 1.38     |
| 11  | aA    | 803 | CLA  | C3D-C2D | 3.95  | 1.49        | 1.39     |
| 11  | bA    | 838 | CLA  | O2A-CGA | 3.95  | 1.44        | 1.33     |
| 11  | bB    | 836 | CLA  | CHD-C1D | 3.95  | 1.46        | 1.38     |
| 11  | bA    | 802 | CLA  | O2A-CGA | 3.95  | 1.44        | 1.33     |
| 11  | cA    | 831 | CLA  | CHD-C1D | 3.95  | 1.46        | 1.38     |
| 11  | bB    | 809 | CLA  | CHD-C1D | 3.95  | 1.46        | 1.38     |
| 11  | cA    | 821 | CLA  | CHD-C1D | 3.95  | 1.46        | 1.38     |
| 11  | cA    | 817 | CLA  | CHD-C4C | 3.95  | 1.48        | 1.39     |
| 11  | cA    | 802 | CLA  | O2A-CGA | 3.94  | 1.44        | 1.33     |
| 11  | bB    | 838 | CLA  | CHD-C1D | 3.94  | 1.46        | 1.38     |
| 11  | bA    | 820 | CLA  | CHD-C4C | 3.94  | 1.48        | 1.39     |
| 11  | aA    | 831 | CLA  | C3D-C2D | 3.94  | 1.49        | 1.39     |
| 12  | cA    | 830 | F6C  | C3B-C2B | 3.94  | 1.48        | 1.39     |
| 11  | cB    | 836 | CLA  | CHD-C1D | 3.94  | 1.46        | 1.38     |
| 11  | aA    | 817 | CLA  | CHD-C4C | 3.94  | 1.48        | 1.39     |
| 11  | cB    | 830 | CLA  | CHD-C4C | 3.94  | 1.48        | 1.39     |
| 11  | cB    | 828 | CLA  | CHD-C4C | 3.94  | 1.48        | 1.39     |
| 11  | aB    | 801 | CLA  | O2A-CGA | 3.94  | 1.44        | 1.33     |
| 11  | aB    | 831 | CLA  | CHD-C4C | 3.94  | 1.48        | 1.39     |
| 11  | bB    | 804 | CLA  | CHD-C1D | 3.94  | 1.46        | 1.38     |
| 11  | bA    | 817 | CLA  | CHD-C4C | 3.94  | 1.48        | 1.39     |
| 12  | cA    | 826 | F6C  | CHD-C1D | 3.94  | 1.46        | 1.38     |
| 11  | aA    | 838 | CLA  | CHD-C1D | 3.93  | 1.46        | 1.38     |
| 11  | cB    | 818 | CLA  | CHD-C1D | 3.93  | 1.46        | 1.38     |
| 11  | bA    | 805 | CLA  | CHD-C4C | 3.93  | 1.48        | 1.39     |
| 11  | aB    | 810 | CLA  | CHD-C4C | 3.93  | 1.48        | 1.39     |
| 11  | cA    | 803 | CLA  | C3D-C2D | 3.93  | 1.49        | 1.39     |
| 11  | bA    | 814 | CLA  | CHD-C4C | 3.93  | 1.48        | 1.39     |
| 11  | aA    | 819 | CLA  | CHD-C1D | 3.93  | 1.46        | 1.38     |
| 11  | aB    | 838 | CLA  | CHD-C1D | 3.93  | 1.46        | 1.38     |
| 11  | aB    | 803 | CLA  | C3D-C2D | 3.93  | 1.49        | 1.39     |
| 12  | bA    | 830 | F6C  | C3D-C2D | 3.93  | 1.49        | 1.39     |
| 12  | cA    | 830 | F6C  | C3D-C2D | 3.93  | 1.49        | 1.39     |
| 11  | bA    | 821 | CLA  | CHD-C1D | 3.93  | 1.46        | 1.38     |
| 11  | aA    | 805 | CLA  | CHD-C4C | 3.93  | 1.48        | 1.39     |
| 11  | bA    | 831 | CLA  | C3D-C2D | 3.93  | 1.49        | 1.39     |
| 12  | cA    | 827 | F6C  | C3D-C2D | 3.93  | 1.49        | 1.39     |
| 11  | bB    | 809 | CLA  | C1B-NB  | -3.93 | 1.32        | 1.37     |
| 11  | aB    | 820 | CLA  | CHD-C4C | 3.92  | 1.48        | 1.39     |
| 11  | cB    | 826 | CLA  | C1D-ND  | 3.92  | 1.43        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | cB    | 809 | CLA  | CHD-C1D | 3.92  | 1.46        | 1.38     |
| 11  | bB    | 820 | CLA  | CHD-C4C | 3.92  | 1.48        | 1.39     |
| 11  | cB    | 831 | CLA  | CHD-C4C | 3.92  | 1.48        | 1.39     |
| 12  | aA    | 832 | F6C  | CHD-C4C | 3.92  | 1.48        | 1.39     |
| 11  | aB    | 814 | CLA  | CHD-C4C | 3.92  | 1.48        | 1.39     |
| 11  | cA    | 814 | CLA  | CHD-C4C | 3.92  | 1.48        | 1.39     |
| 11  | aB    | 806 | CLA  | CHD-C1D | 3.92  | 1.46        | 1.38     |
| 11  | cA    | 831 | CLA  | C3D-C2D | 3.92  | 1.49        | 1.39     |
| 11  | cA    | 809 | CLA  | CHD-C4C | 3.92  | 1.48        | 1.39     |
| 12  | aA    | 830 | F6C  | C3D-C2D | 3.92  | 1.49        | 1.39     |
| 11  | aA    | 836 | CLA  | C1D-ND  | 3.92  | 1.43        | 1.37     |
| 11  | cB    | 820 | CLA  | CHD-C4C | 3.92  | 1.48        | 1.39     |
| 12  | cA    | 844 | F6C  | CHD-C4C | 3.92  | 1.48        | 1.39     |
| 11  | cB    | 803 | CLA  | C3D-C2D | 3.92  | 1.49        | 1.39     |
| 11  | aL    | 206 | CLA  | O2A-CGA | 3.92  | 1.44        | 1.33     |
| 11  | aA    | 809 | CLA  | CHD-C4C | 3.92  | 1.48        | 1.39     |
| 12  | aA    | 826 | F6C  | CHD-C1D | 3.92  | 1.46        | 1.38     |
| 11  | aA    | 815 | CLA  | CHD-C4C | 3.92  | 1.48        | 1.39     |
| 11  | aB    | 830 | CLA  | CHD-C4C | 3.92  | 1.48        | 1.39     |
| 12  | cL    | 202 | F6C  | C3B-C2B | 3.92  | 1.48        | 1.39     |
| 11  | aA    | 821 | CLA  | CHD-C1D | 3.92  | 1.46        | 1.38     |
| 11  | cB    | 809 | CLA  | C1B-NB  | -3.91 | 1.32        | 1.37     |
| 12  | aL    | 202 | F6C  | C3B-C2B | 3.91  | 1.48        | 1.39     |
| 11  | bA    | 839 | CLA  | CHD-C4C | 3.91  | 1.48        | 1.39     |
| 11  | cB    | 810 | CLA  | CHD-C4C | 3.91  | 1.48        | 1.39     |
| 11  | bA    | 842 | CLA  | CHD-C4C | 3.91  | 1.48        | 1.39     |
| 12  | bA    | 827 | F6C  | C3D-C2D | 3.91  | 1.49        | 1.39     |
| 11  | bB    | 814 | CLA  | CHD-C4C | 3.91  | 1.48        | 1.39     |
| 11  | bB    | 828 | CLA  | CHD-C4C | 3.91  | 1.48        | 1.39     |
| 11  | cA    | 805 | CLA  | CHD-C4C | 3.91  | 1.48        | 1.39     |
| 11  | aB    | 812 | CLA  | CHD-C4C | 3.91  | 1.48        | 1.39     |
| 11  | bB    | 839 | CLA  | CHD-C1D | 3.91  | 1.46        | 1.38     |
| 11  | aA    | 833 | CLA  | CHD-C4C | 3.91  | 1.48        | 1.39     |
| 12  | aA    | 827 | F6C  | C3D-C2D | 3.91  | 1.49        | 1.39     |
| 12  | bA    | 844 | F6C  | CHD-C4C | 3.91  | 1.48        | 1.39     |
| 11  | cB    | 817 | CLA  | CHD-C4C | 3.91  | 1.48        | 1.39     |
| 11  | bA    | 817 | CLA  | C1B-NB  | -3.91 | 1.32        | 1.37     |
| 11  | bA    | 815 | CLA  | CHD-C4C | 3.91  | 1.48        | 1.39     |
| 11  | bL    | 206 | CLA  | O2A-CGA | 3.91  | 1.44        | 1.33     |
| 11  | aB    | 828 | CLA  | CHD-C4C | 3.91  | 1.48        | 1.39     |
| 11  | cA    | 842 | CLA  | CHD-C4C | 3.91  | 1.48        | 1.39     |
| 11  | aA    | 808 | CLA  | CHD-C4C | 3.90  | 1.48        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12  | bL    | 202 | F6C  | CHD-C1D | 3.90  | 1.46        | 1.38     |
| 11  | aB    | 809 | CLA  | CHD-C1D | 3.90  | 1.46        | 1.38     |
| 11  | aB    | 838 | CLA  | CHD-C4C | 3.90  | 1.48        | 1.39     |
| 11  | cL    | 206 | CLA  | O2A-CGA | 3.90  | 1.44        | 1.33     |
| 11  | bA    | 815 | CLA  | C1B-NB  | -3.90 | 1.32        | 1.37     |
| 11  | bB    | 826 | CLA  | C1D-ND  | 3.90  | 1.43        | 1.37     |
| 11  | aA    | 839 | CLA  | CHD-C4C | 3.90  | 1.48        | 1.39     |
| 11  | bA    | 824 | CLA  | CHD-C4C | 3.90  | 1.48        | 1.39     |
| 11  | cA    | 815 | CLA  | CHD-C4C | 3.90  | 1.48        | 1.39     |
| 11  | aB    | 808 | CLA  | CHD-C1D | 3.90  | 1.46        | 1.38     |
| 11  | aB    | 829 | CLA  | CHC-C1C | 3.90  | 1.46        | 1.38     |
| 11  | bA    | 836 | CLA  | C1D-ND  | 3.90  | 1.43        | 1.37     |
| 11  | cB    | 812 | CLA  | CHD-C4C | 3.90  | 1.48        | 1.39     |
| 11  | cB    | 839 | CLA  | CHD-C1D | 3.90  | 1.46        | 1.38     |
| 11  | aA    | 816 | CLA  | CHD-C4C | 3.90  | 1.48        | 1.39     |
| 11  | aA    | 842 | CLA  | CHD-C4C | 3.90  | 1.48        | 1.39     |
| 11  | aB    | 826 | CLA  | C1D-ND  | 3.90  | 1.43        | 1.37     |
| 11  | aA    | 805 | CLA  | C3D-C2D | 3.90  | 1.49        | 1.39     |
| 11  | bA    | 805 | CLA  | C3D-C2D | 3.90  | 1.49        | 1.39     |
| 11  | cA    | 838 | CLA  | CHD-C1D | 3.90  | 1.46        | 1.38     |
| 11  | aB    | 811 | CLA  | CHD-C4C | 3.90  | 1.48        | 1.39     |
| 11  | bL    | 205 | CLA  | C3D-C2D | 3.90  | 1.49        | 1.39     |
| 11  | cA    | 840 | CLA  | CHD-C4C | 3.90  | 1.48        | 1.39     |
| 12  | aA    | 844 | F6C  | C3D-C2D | 3.89  | 1.49        | 1.39     |
| 11  | bA    | 833 | CLA  | CHD-C4C | 3.89  | 1.48        | 1.39     |
| 11  | cB    | 805 | CLA  | O2A-CGA | 3.89  | 1.44        | 1.33     |
| 11  | bA    | 809 | CLA  | CHD-C4C | 3.89  | 1.48        | 1.39     |
| 12  | aA    | 830 | F6C  | CHD-C1D | 3.89  | 1.46        | 1.38     |
| 11  | aB    | 817 | CLA  | CHD-C4C | 3.89  | 1.48        | 1.39     |
| 12  | bA    | 826 | F6C  | CHD-C1D | 3.89  | 1.46        | 1.38     |
| 11  | aB    | 839 | CLA  | CHD-C1D | 3.89  | 1.46        | 1.38     |
| 11  | aA    | 829 | CLA  | CHD-C4C | 3.89  | 1.48        | 1.39     |
| 11  | cB    | 814 | CLA  | CHD-C4C | 3.89  | 1.48        | 1.39     |
| 11  | cB    | 837 | CLA  | CHD-C4C | 3.89  | 1.48        | 1.39     |
| 12  | cA    | 844 | F6C  | C3D-C2D | 3.89  | 1.49        | 1.39     |
| 12  | bA    | 830 | F6C  | C3B-C2B | 3.89  | 1.48        | 1.39     |
| 11  | aB    | 805 | CLA  | CHD-C4C | 3.89  | 1.48        | 1.39     |
| 11  | bB    | 810 | CLA  | CHD-C4C | 3.89  | 1.48        | 1.39     |
| 11  | aA    | 817 | CLA  | C1B-NB  | -3.89 | 1.32        | 1.37     |
| 11  | cA    | 820 | CLA  | C1B-NB  | -3.89 | 1.32        | 1.37     |
| 11  | cA    | 805 | CLA  | C3D-C2D | 3.89  | 1.49        | 1.39     |
| 11  | cB    | 806 | CLA  | CHD-C1D | 3.89  | 1.46        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | aB    | 809 | CLA  | C1B-NB  | -3.89 | 1.32        | 1.37     |
| 11  | bB    | 829 | CLA  | C3D-C2D | 3.89  | 1.49        | 1.39     |
| 12  | bA    | 830 | F6C  | CHD-C1D | 3.89  | 1.46        | 1.38     |
| 11  | cA    | 808 | CLA  | CHD-C4C | 3.89  | 1.48        | 1.39     |
| 11  | cB    | 829 | CLA  | CHC-C1C | 3.89  | 1.46        | 1.38     |
| 12  | aA    | 830 | F6C  | C3B-C2B | 3.89  | 1.48        | 1.39     |
| 11  | bA    | 829 | CLA  | CHD-C4C | 3.88  | 1.48        | 1.39     |
| 11  | aA    | 814 | CLA  | CHD-C4C | 3.88  | 1.48        | 1.39     |
| 11  | aB    | 809 | CLA  | C3D-C2D | 3.88  | 1.49        | 1.39     |
| 11  | bB    | 812 | CLA  | CHD-C4C | 3.88  | 1.48        | 1.39     |
| 11  | bA    | 816 | CLA  | CHD-C4C | 3.88  | 1.48        | 1.39     |
| 11  | aL    | 205 | CLA  | C3D-C2D | 3.88  | 1.49        | 1.39     |
| 11  | bB    | 805 | CLA  | O2A-CGA | 3.88  | 1.44        | 1.33     |
| 11  | bB    | 806 | CLA  | CHD-C1D | 3.88  | 1.46        | 1.38     |
| 11  | bB    | 838 | CLA  | CHD-C4C | 3.88  | 1.48        | 1.39     |
| 11  | cB    | 827 | CLA  | C1B-NB  | -3.88 | 1.32        | 1.37     |
| 11  | cA    | 839 | CLA  | CHD-C4C | 3.88  | 1.48        | 1.39     |
| 12  | aA    | 844 | F6C  | CHD-C4C | 3.88  | 1.48        | 1.39     |
| 12  | cA    | 827 | F6C  | C3B-C2B | 3.88  | 1.48        | 1.39     |
| 11  | aA    | 836 | CLA  | CHD-C1D | 3.88  | 1.46        | 1.38     |
| 12  | cA    | 830 | F6C  | CHD-C1D | 3.88  | 1.46        | 1.38     |
| 11  | bA    | 808 | CLA  | CHD-C4C | 3.88  | 1.48        | 1.39     |
| 11  | cA    | 836 | CLA  | CHD-C1D | 3.88  | 1.46        | 1.38     |
| 11  | bB    | 829 | CLA  | CHC-C1C | 3.88  | 1.46        | 1.38     |
| 11  | bB    | 814 | CLA  | C3D-C2D | 3.87  | 1.49        | 1.39     |
| 11  | bB    | 821 | CLA  | CHD-C4C | 3.87  | 1.48        | 1.39     |
| 11  | cB    | 838 | CLA  | CHD-C4C | 3.87  | 1.48        | 1.39     |
| 11  | aA    | 840 | CLA  | CHD-C4C | 3.87  | 1.48        | 1.39     |
| 11  | bB    | 811 | CLA  | CHD-C4C | 3.87  | 1.48        | 1.39     |
| 11  | cB    | 811 | CLA  | CHD-C4C | 3.87  | 1.48        | 1.39     |
| 11  | cA    | 836 | CLA  | C1D-ND  | 3.87  | 1.42        | 1.37     |
| 11  | bB    | 837 | CLA  | CHD-C4C | 3.87  | 1.48        | 1.39     |
| 11  | bB    | 840 | CLA  | C1B-NB  | -3.87 | 1.32        | 1.37     |
| 11  | aA    | 824 | CLA  | CHD-C4C | 3.87  | 1.48        | 1.39     |
| 11  | bB    | 817 | CLA  | CHD-C4C | 3.87  | 1.48        | 1.39     |
| 11  | aA    | 817 | CLA  | C3D-C2D | 3.87  | 1.49        | 1.39     |
| 11  | bA    | 835 | CLA  | C3D-C2D | 3.87  | 1.49        | 1.39     |
| 11  | aB    | 829 | CLA  | C3D-C2D | 3.87  | 1.49        | 1.39     |
| 11  | bB    | 827 | CLA  | CHD-C1D | 3.87  | 1.46        | 1.38     |
| 11  | cB    | 817 | CLA  | C1B-NB  | -3.87 | 1.32        | 1.37     |
| 11  | aB    | 812 | CLA  | C3D-C2D | 3.87  | 1.49        | 1.39     |
| 11  | bA    | 840 | CLA  | CHD-C4C | 3.87  | 1.48        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | aA    | 835 | CLA  | C3D-C2D | 3.87  | 1.49        | 1.39     |
| 11  | aB    | 814 | CLA  | C3D-C2D | 3.87  | 1.49        | 1.39     |
| 12  | bA    | 844 | F6C  | C3D-C2D | 3.87  | 1.49        | 1.39     |
| 11  | bB    | 808 | CLA  | C1D-ND  | 3.87  | 1.42        | 1.37     |
| 11  | aB    | 802 | CLA  | C3D-C2D | 3.87  | 1.49        | 1.39     |
| 11  | cB    | 829 | CLA  | C3D-C2D | 3.87  | 1.49        | 1.39     |
| 11  | cB    | 840 | CLA  | C1B-NB  | -3.87 | 1.32        | 1.37     |
| 11  | cL    | 205 | CLA  | C3D-C2D | 3.87  | 1.49        | 1.39     |
| 11  | cA    | 815 | CLA  | C1B-NB  | -3.86 | 1.32        | 1.37     |
| 11  | bB    | 803 | CLA  | C3D-C2D | 3.86  | 1.49        | 1.39     |
| 11  | bA    | 839 | CLA  | O2A-CGA | 3.86  | 1.44        | 1.33     |
| 11  | aA    | 838 | CLA  | C1B-NB  | -3.86 | 1.32        | 1.37     |
| 11  | bA    | 815 | CLA  | C3D-C2D | 3.86  | 1.49        | 1.39     |
| 11  | aA    | 815 | CLA  | C1B-NB  | -3.86 | 1.32        | 1.37     |
| 11  | cA    | 839 | CLA  | O2A-CGA | 3.86  | 1.44        | 1.33     |
| 11  | aB    | 805 | CLA  | O2A-CGA | 3.86  | 1.44        | 1.33     |
| 11  | cB    | 827 | CLA  | CHD-C1D | 3.86  | 1.45        | 1.38     |
| 11  | aA    | 841 | CLA  | CHD-C4C | 3.86  | 1.48        | 1.39     |
| 11  | aB    | 805 | CLA  | C3D-C2D | 3.86  | 1.49        | 1.39     |
| 11  | bA    | 820 | CLA  | C1B-NB  | -3.86 | 1.32        | 1.37     |
| 11  | bB    | 829 | CLA  | OBD-CAD | 3.86  | 1.29        | 1.22     |
| 11  | bB    | 809 | CLA  | C3D-C2D | 3.86  | 1.49        | 1.39     |
| 11  | cB    | 809 | CLA  | C1D-ND  | 3.86  | 1.42        | 1.37     |
| 11  | bA    | 836 | CLA  | CHD-C1D | 3.86  | 1.45        | 1.38     |
| 11  | bB    | 808 | CLA  | CHD-C1D | 3.86  | 1.45        | 1.38     |
| 11  | cA    | 833 | CLA  | CHD-C4C | 3.86  | 1.48        | 1.39     |
| 11  | cA    | 807 | CLA  | CHD-C4C | 3.86  | 1.48        | 1.39     |
| 11  | aB    | 817 | CLA  | C1B-NB  | -3.86 | 1.32        | 1.37     |
| 11  | cA    | 824 | CLA  | CHD-C4C | 3.86  | 1.48        | 1.39     |
| 11  | aA    | 839 | CLA  | O2A-CGA | 3.86  | 1.44        | 1.33     |
| 12  | cA    | 827 | F6C  | CHD-C4C | 3.86  | 1.48        | 1.39     |
| 11  | bA    | 825 | CLA  | CHD-C4C | 3.86  | 1.48        | 1.39     |
| 11  | bB    | 812 | CLA  | C3D-C2D | 3.86  | 1.49        | 1.39     |
| 12  | bA    | 830 | F6C  | CHB-C1B | 3.86  | 1.48        | 1.39     |
| 11  | cB    | 825 | CLA  | CHD-C1D | 3.86  | 1.45        | 1.38     |
| 11  | aB    | 830 | CLA  | C3D-C2D | 3.86  | 1.49        | 1.39     |
| 11  | aA    | 820 | CLA  | C1B-NB  | -3.85 | 1.32        | 1.37     |
| 12  | bA    | 827 | F6C  | CHD-C4C | 3.85  | 1.48        | 1.39     |
| 11  | cA    | 817 | CLA  | C3D-C2D | 3.85  | 1.49        | 1.39     |
| 11  | aB    | 837 | CLA  | CHD-C4C | 3.85  | 1.48        | 1.39     |
| 11  | cA    | 835 | CLA  | C3D-C2D | 3.85  | 1.49        | 1.39     |
| 11  | cB    | 812 | CLA  | C3D-C2D | 3.85  | 1.49        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | cA    | 816 | CLA  | CHD-C4C | 3.85  | 1.48        | 1.39     |
| 11  | bB    | 830 | CLA  | C3D-C2D | 3.85  | 1.49        | 1.39     |
| 11  | cA    | 817 | CLA  | C1B-NB  | -3.85 | 1.32        | 1.37     |
| 11  | bB    | 802 | CLA  | C3D-C2D | 3.85  | 1.49        | 1.39     |
| 11  | aA    | 815 | CLA  | C3D-C2D | 3.85  | 1.49        | 1.39     |
| 11  | bB    | 805 | CLA  | C3D-C2D | 3.85  | 1.49        | 1.39     |
| 12  | aA    | 830 | F6C  | CHB-C1B | 3.85  | 1.48        | 1.39     |
| 11  | bA    | 837 | CLA  | CHD-C4C | 3.85  | 1.48        | 1.39     |
| 11  | bK    | 103 | CLA  | CHD-C4C | 3.85  | 1.48        | 1.39     |
| 11  | bB    | 828 | CLA  | O2A-CGA | 3.85  | 1.44        | 1.33     |
| 12  | cA    | 826 | F6C  | C3D-C2D | 3.85  | 1.49        | 1.39     |
| 11  | aB    | 827 | CLA  | C1B-NB  | -3.85 | 1.32        | 1.37     |
| 11  | bA    | 817 | CLA  | C3D-C2D | 3.85  | 1.49        | 1.39     |
| 11  | cB    | 830 | CLA  | C3D-C2D | 3.85  | 1.49        | 1.39     |
| 11  | bB    | 825 | CLA  | CHD-C1D | 3.85  | 1.45        | 1.38     |
| 11  | bA    | 841 | CLA  | CHD-C4C | 3.85  | 1.48        | 1.39     |
| 11  | aA    | 825 | CLA  | CHD-C4C | 3.85  | 1.48        | 1.39     |
| 11  | bB    | 816 | CLA  | C3D-C2D | 3.85  | 1.49        | 1.39     |
| 11  | aB    | 821 | CLA  | CHD-C4C | 3.85  | 1.48        | 1.39     |
| 11  | cA    | 802 | CLA  | CHD-C4C | 3.85  | 1.48        | 1.39     |
| 12  | bA    | 826 | F6C  | C3C-C2C | 3.84  | 1.48        | 1.38     |
| 11  | cA    | 811 | CLA  | C3D-C2D | 3.84  | 1.49        | 1.39     |
| 11  | bB    | 817 | CLA  | C1B-NB  | -3.84 | 1.32        | 1.37     |
| 12  | aA    | 827 | F6C  | C3B-C2B | 3.84  | 1.48        | 1.39     |
| 11  | cA    | 812 | CLA  | C3D-C2D | 3.84  | 1.49        | 1.39     |
| 11  | cB    | 805 | CLA  | C3D-C2D | 3.84  | 1.49        | 1.39     |
| 11  | cB    | 802 | CLA  | C3D-C2D | 3.84  | 1.49        | 1.39     |
| 11  | bA    | 807 | CLA  | CHD-C4C | 3.84  | 1.47        | 1.39     |
| 11  | aB    | 828 | CLA  | O2A-CGA | 3.84  | 1.44        | 1.33     |
| 11  | bA    | 835 | CLA  | CHD-C4C | 3.84  | 1.47        | 1.39     |
| 11  | bA    | 804 | CLA  | C3D-C2D | 3.84  | 1.49        | 1.39     |
| 11  | aB    | 835 | CLA  | C3D-C2D | 3.84  | 1.49        | 1.39     |
| 11  | cB    | 808 | CLA  | CHD-C1D | 3.84  | 1.45        | 1.38     |
| 11  | cA    | 829 | CLA  | CHD-C4C | 3.84  | 1.47        | 1.39     |
| 11  | cA    | 841 | CLA  | CHD-C4C | 3.84  | 1.47        | 1.39     |
| 12  | bA    | 827 | F6C  | C3B-C2B | 3.84  | 1.48        | 1.39     |
| 11  | aA    | 807 | CLA  | CHD-C4C | 3.84  | 1.47        | 1.39     |
| 11  | cA    | 815 | CLA  | C3D-C2D | 3.84  | 1.49        | 1.39     |
| 11  | bA    | 838 | CLA  | C1B-NB  | -3.84 | 1.32        | 1.37     |
| 11  | cB    | 835 | CLA  | C3D-C2D | 3.84  | 1.49        | 1.39     |
| 12  | aA    | 826 | F6C  | C3D-C2D | 3.84  | 1.49        | 1.39     |
| 11  | aA    | 813 | CLA  | CHD-C4C | 3.84  | 1.47        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | cA    | 835 | CLA  | CHD-C4C | 3.84  | 1.47        | 1.39     |
| 11  | cA    | 837 | CLA  | CHD-C4C | 3.84  | 1.47        | 1.39     |
| 12  | bA    | 826 | F6C  | C3D-C2D | 3.84  | 1.49        | 1.39     |
| 11  | cB    | 821 | CLA  | CHD-C4C | 3.84  | 1.47        | 1.39     |
| 11  | cA    | 804 | CLA  | C3D-C2D | 3.84  | 1.49        | 1.39     |
| 11  | aB    | 807 | CLA  | CHD-C1D | 3.84  | 1.45        | 1.38     |
| 11  | bL    | 206 | CLA  | C3D-C2D | 3.83  | 1.49        | 1.39     |
| 11  | cB    | 814 | CLA  | C3D-C2D | 3.83  | 1.49        | 1.39     |
| 11  | bA    | 819 | CLA  | CHC-C4B | 3.83  | 1.48        | 1.39     |
| 11  | aA    | 819 | CLA  | CHC-C4B | 3.83  | 1.48        | 1.39     |
| 11  | bB    | 827 | CLA  | C1B-NB  | -3.83 | 1.32        | 1.37     |
| 12  | cA    | 832 | F6C  | C3D-C2D | 3.83  | 1.49        | 1.39     |
| 11  | cB    | 811 | CLA  | C3D-C2D | 3.83  | 1.49        | 1.39     |
| 11  | cK    | 101 | CLA  | C3D-C2D | 3.83  | 1.49        | 1.39     |
| 11  | aK    | 101 | CLA  | C3D-C2D | 3.83  | 1.49        | 1.39     |
| 11  | cL    | 206 | CLA  | C3D-C2D | 3.83  | 1.49        | 1.39     |
| 11  | cA    | 825 | CLA  | CHD-C4C | 3.83  | 1.47        | 1.39     |
| 11  | bB    | 821 | CLA  | C3D-C2D | 3.83  | 1.49        | 1.39     |
| 11  | aB    | 816 | CLA  | C3D-C2D | 3.83  | 1.49        | 1.39     |
| 11  | bB    | 835 | CLA  | C3D-C2D | 3.83  | 1.49        | 1.39     |
| 11  | aA    | 835 | CLA  | CHD-C4C | 3.83  | 1.47        | 1.39     |
| 11  | cB    | 816 | CLA  | C3D-C2D | 3.83  | 1.49        | 1.39     |
| 11  | bA    | 812 | CLA  | C3D-C2D | 3.83  | 1.49        | 1.39     |
| 11  | cB    | 832 | CLA  | C3D-C2D | 3.83  | 1.49        | 1.39     |
| 11  | cB    | 808 | CLA  | C1D-ND  | 3.82  | 1.42        | 1.37     |
| 11  | aA    | 820 | CLA  | C3D-C2D | 3.82  | 1.49        | 1.39     |
| 11  | bK    | 101 | CLA  | C3D-C2D | 3.82  | 1.49        | 1.39     |
| 11  | aA    | 802 | CLA  | CHD-C4C | 3.82  | 1.47        | 1.39     |
| 11  | aB    | 834 | CLA  | C3D-C2D | 3.82  | 1.49        | 1.39     |
| 11  | cB    | 809 | CLA  | C3D-C2D | 3.82  | 1.49        | 1.39     |
| 11  | cB    | 818 | CLA  | C3D-C2D | 3.82  | 1.49        | 1.39     |
| 11  | bB    | 802 | CLA  | C1B-NB  | -3.82 | 1.32        | 1.37     |
| 11  | cA    | 819 | CLA  | CHC-C4B | 3.82  | 1.48        | 1.39     |
| 11  | aB    | 808 | CLA  | C1D-ND  | 3.82  | 1.42        | 1.37     |
| 11  | aA    | 837 | CLA  | CHD-C4C | 3.82  | 1.47        | 1.39     |
| 11  | cB    | 828 | CLA  | O2A-CGA | 3.82  | 1.44        | 1.33     |
| 11  | bB    | 834 | CLA  | C3D-C2D | 3.82  | 1.49        | 1.39     |
| 12  | aA    | 832 | F6C  | C3D-C2D | 3.82  | 1.49        | 1.39     |
| 11  | aL    | 206 | CLA  | C3D-C2D | 3.82  | 1.49        | 1.39     |
| 11  | cB    | 837 | CLA  | C3D-C2D | 3.82  | 1.49        | 1.39     |
| 11  | aB    | 825 | CLA  | CHD-C1D | 3.82  | 1.45        | 1.38     |
| 12  | aA    | 827 | F6C  | CHD-C4C | 3.82  | 1.48        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | aA    | 833 | CLA  | C3D-C2D | 3.81  | 1.49        | 1.39     |
| 12  | cA    | 830 | F6C  | CHB-C1B | 3.81  | 1.47        | 1.39     |
| 10  | cA    | 801 | CL0  | CHD-C1D | 3.81  | 1.45        | 1.39     |
| 11  | aA    | 804 | CLA  | OBD-CAD | 3.81  | 1.29        | 1.22     |
| 11  | cB    | 834 | CLA  | C1B-NB  | -3.81 | 1.32        | 1.37     |
| 11  | bA    | 811 | CLA  | C3D-C2D | 3.81  | 1.49        | 1.39     |
| 11  | bB    | 807 | CLA  | CHD-C4C | 3.81  | 1.47        | 1.39     |
| 11  | cA    | 833 | CLA  | C3D-C2D | 3.81  | 1.49        | 1.39     |
| 11  | aA    | 811 | CLA  | C3D-C2D | 3.81  | 1.49        | 1.39     |
| 11  | aA    | 812 | CLA  | C3D-C2D | 3.81  | 1.49        | 1.39     |
| 11  | bB    | 832 | CLA  | C3D-C2D | 3.81  | 1.49        | 1.39     |
| 11  | cB    | 834 | CLA  | C3D-C2D | 3.81  | 1.49        | 1.39     |
| 11  | aB    | 827 | CLA  | CHD-C1D | 3.81  | 1.45        | 1.38     |
| 11  | bB    | 811 | CLA  | C3D-C2D | 3.81  | 1.49        | 1.39     |
| 12  | cA    | 826 | F6C  | C3C-C2C | 3.81  | 1.48        | 1.38     |
| 11  | bA    | 824 | CLA  | C1B-NB  | -3.81 | 1.32        | 1.37     |
| 11  | aA    | 836 | CLA  | C1B-NB  | -3.81 | 1.32        | 1.37     |
| 11  | bA    | 820 | CLA  | C3D-C2D | 3.81  | 1.49        | 1.39     |
| 11  | bB    | 818 | CLA  | C3D-C2D | 3.81  | 1.49        | 1.39     |
| 11  | bA    | 802 | CLA  | CHD-C4C | 3.81  | 1.47        | 1.39     |
| 11  | aB    | 832 | CLA  | C3D-C2D | 3.81  | 1.49        | 1.39     |
| 12  | bA    | 832 | F6C  | C3D-C2D | 3.81  | 1.49        | 1.39     |
| 11  | aA    | 804 | CLA  | C3D-C2D | 3.81  | 1.49        | 1.39     |
| 11  | bA    | 806 | CLA  | C3D-C2D | 3.81  | 1.49        | 1.39     |
| 11  | cA    | 822 | CLA  | CHD-C4C | 3.81  | 1.47        | 1.39     |
| 11  | aB    | 811 | CLA  | C3D-C2D | 3.80  | 1.49        | 1.39     |
| 11  | cA    | 820 | CLA  | C3D-C2D | 3.80  | 1.49        | 1.39     |
| 11  | aK    | 103 | CLA  | CHD-C4C | 3.80  | 1.47        | 1.39     |
| 11  | aB    | 829 | CLA  | OBD-CAD | 3.80  | 1.29        | 1.22     |
| 11  | cL    | 205 | CLA  | CHD-C4C | 3.80  | 1.47        | 1.39     |
| 11  | aB    | 807 | CLA  | CHD-C4C | 3.80  | 1.47        | 1.39     |
| 11  | aB    | 802 | CLA  | C1B-NB  | -3.80 | 1.32        | 1.37     |
| 11  | cA    | 834 | CLA  | CHD-C4C | 3.80  | 1.47        | 1.39     |
| 12  | aA    | 826 | F6C  | C3C-C2C | 3.80  | 1.48        | 1.38     |
| 11  | bB    | 819 | CLA  | CHD-C4C | 3.80  | 1.47        | 1.39     |
| 11  | aB    | 827 | CLA  | C3D-C2D | 3.80  | 1.49        | 1.39     |
| 11  | cB    | 821 | CLA  | C3D-C2D | 3.80  | 1.49        | 1.39     |
| 11  | cK    | 103 | CLA  | CHD-C4C | 3.80  | 1.47        | 1.39     |
| 11  | aB    | 833 | CLA  | OBD-CAD | 3.80  | 1.29        | 1.22     |
| 11  | cB    | 833 | CLA  | OBD-CAD | 3.80  | 1.29        | 1.22     |
| 11  | bB    | 827 | CLA  | C3D-C2D | 3.80  | 1.49        | 1.39     |
| 11  | bL    | 204 | CLA  | C3D-C2D | 3.80  | 1.49        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | aB    | 818 | CLA  | CHD-C4C | 3.80  | 1.47        | 1.39     |
| 11  | cL    | 204 | CLA  | C3D-C2D | 3.80  | 1.49        | 1.39     |
| 11  | cB    | 829 | CLA  | OBD-CAD | 3.80  | 1.29        | 1.22     |
| 11  | bA    | 805 | CLA  | CHC-C4B | 3.80  | 1.47        | 1.39     |
| 11  | cB    | 802 | CLA  | C1B-NB  | -3.80 | 1.32        | 1.37     |
| 11  | aB    | 837 | CLA  | C3D-C2D | 3.80  | 1.49        | 1.39     |
| 11  | aA    | 822 | CLA  | CHD-C4C | 3.80  | 1.47        | 1.39     |
| 11  | aB    | 821 | CLA  | C3D-C2D | 3.80  | 1.49        | 1.39     |
| 11  | bA    | 810 | CLA  | CHB-C1B | 3.80  | 1.47        | 1.39     |
| 11  | cB    | 819 | CLA  | CHD-C4C | 3.80  | 1.47        | 1.39     |
| 11  | aL    | 204 | CLA  | C3D-C2D | 3.80  | 1.49        | 1.39     |
| 11  | cB    | 807 | CLA  | CHD-C4C | 3.80  | 1.47        | 1.39     |
| 11  | cB    | 807 | CLA  | CHD-C1D | 3.80  | 1.45        | 1.38     |
| 11  | cA    | 822 | CLA  | C3D-C2D | 3.80  | 1.49        | 1.39     |
| 11  | aB    | 819 | CLA  | CHD-C4C | 3.80  | 1.47        | 1.39     |
| 11  | bA    | 834 | CLA  | CHD-C4C | 3.80  | 1.47        | 1.39     |
| 11  | aB    | 840 | CLA  | C1B-NB  | -3.80 | 1.32        | 1.37     |
| 11  | bA    | 805 | CLA  | OBD-CAD | 3.79  | 1.29        | 1.22     |
| 11  | aA    | 822 | CLA  | C3D-C2D | 3.79  | 1.49        | 1.39     |
| 11  | bA    | 822 | CLA  | C3D-C2D | 3.79  | 1.49        | 1.39     |
| 11  | aA    | 843 | CLA  | CHD-C4C | 3.79  | 1.47        | 1.39     |
| 11  | cA    | 843 | CLA  | CHD-C4C | 3.79  | 1.47        | 1.39     |
| 11  | bA    | 823 | CLA  | OBD-CAD | 3.79  | 1.29        | 1.22     |
| 11  | aB    | 818 | CLA  | C3D-C2D | 3.79  | 1.49        | 1.39     |
| 11  | bA    | 813 | CLA  | CHD-C4C | 3.79  | 1.47        | 1.39     |
| 11  | bB    | 819 | CLA  | OBD-CAD | 3.79  | 1.29        | 1.22     |
| 11  | bB    | 807 | CLA  | CHD-C1D | 3.79  | 1.45        | 1.38     |
| 11  | bA    | 804 | CLA  | OBD-CAD | 3.79  | 1.29        | 1.22     |
| 11  | bL    | 205 | CLA  | CHD-C4C | 3.79  | 1.47        | 1.39     |
| 11  | aA    | 843 | CLA  | C3D-C2D | 3.79  | 1.49        | 1.39     |
| 11  | bB    | 840 | CLA  | CHD-C4C | 3.79  | 1.47        | 1.39     |
| 11  | bB    | 822 | CLA  | CHD-C1D | 3.79  | 1.45        | 1.38     |
| 11  | aB    | 821 | CLA  | OBD-CAD | 3.79  | 1.29        | 1.22     |
| 11  | aB    | 801 | CLA  | CHD-C1D | 3.79  | 1.45        | 1.38     |
| 11  | bB    | 802 | CLA  | CHD-C4C | 3.79  | 1.47        | 1.39     |
| 11  | cB    | 827 | CLA  | C3D-C2D | 3.79  | 1.49        | 1.39     |
| 11  | cB    | 836 | CLA  | CHC-C4B | 3.79  | 1.47        | 1.39     |
| 11  | bB    | 837 | CLA  | C3D-C2D | 3.79  | 1.49        | 1.39     |
| 11  | cA    | 838 | CLA  | CHD-C4C | 3.79  | 1.47        | 1.39     |
| 11  | aB    | 810 | CLA  | C3D-C2D | 3.79  | 1.49        | 1.39     |
| 11  | aL    | 205 | CLA  | CHD-C4C | 3.78  | 1.47        | 1.39     |
| 11  | cB    | 806 | CLA  | CHD-C4C | 3.78  | 1.47        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | bA    | 814 | CLA  | C3D-C2D | 3.78  | 1.49        | 1.39     |
| 11  | bA    | 813 | CLA  | C1B-NB  | -3.78 | 1.32        | 1.37     |
| 11  | cB    | 821 | CLA  | OBD-CAD | 3.78  | 1.29        | 1.22     |
| 11  | cA    | 838 | CLA  | C1B-NB  | -3.78 | 1.32        | 1.37     |
| 11  | bB    | 835 | CLA  | OBD-CAD | 3.78  | 1.29        | 1.22     |
| 11  | bB    | 836 | CLA  | CHC-C4B | 3.78  | 1.47        | 1.39     |
| 11  | aA    | 834 | CLA  | CHD-C4C | 3.78  | 1.47        | 1.39     |
| 11  | aB    | 806 | CLA  | CHD-C4C | 3.78  | 1.47        | 1.39     |
| 11  | bA    | 833 | CLA  | C3D-C2D | 3.78  | 1.49        | 1.39     |
| 11  | aB    | 826 | CLA  | C1B-NB  | -3.78 | 1.32        | 1.37     |
| 11  | cA    | 806 | CLA  | C3D-C2D | 3.78  | 1.49        | 1.39     |
| 11  | aB    | 813 | CLA  | CHD-C4C | 3.78  | 1.47        | 1.39     |
| 12  | cA    | 827 | F6C  | CHB-C1B | 3.78  | 1.47        | 1.39     |
| 11  | cB    | 840 | CLA  | CHD-C4C | 3.78  | 1.47        | 1.39     |
| 11  | aA    | 814 | CLA  | C3D-C2D | 3.78  | 1.49        | 1.39     |
| 11  | aB    | 815 | CLA  | C3D-C2D | 3.78  | 1.49        | 1.39     |
| 12  | cL    | 202 | F6C  | C3D-C2D | 3.78  | 1.49        | 1.39     |
| 11  | bA    | 843 | CLA  | CHD-C4C | 3.78  | 1.47        | 1.39     |
| 11  | cA    | 843 | CLA  | C3D-C2D | 3.78  | 1.49        | 1.39     |
| 11  | bB    | 806 | CLA  | CHD-C4C | 3.78  | 1.47        | 1.39     |
| 11  | aB    | 840 | CLA  | CHD-C4C | 3.78  | 1.47        | 1.39     |
| 10  | bA    | 801 | CL0  | CHD-C1D | 3.78  | 1.45        | 1.39     |
| 11  | bB    | 833 | CLA  | OBD-CAD | 3.78  | 1.29        | 1.22     |
| 11  | bB    | 815 | CLA  | C3D-C2D | 3.77  | 1.49        | 1.39     |
| 11  | bB    | 823 | CLA  | CHD-C4C | 3.77  | 1.47        | 1.39     |
| 11  | aA    | 808 | CLA  | C3D-C2D | 3.77  | 1.49        | 1.39     |
| 11  | cB    | 823 | CLA  | CHD-C4C | 3.77  | 1.47        | 1.39     |
| 11  | bB    | 818 | CLA  | CHD-C4C | 3.77  | 1.47        | 1.39     |
| 11  | cA    | 805 | CLA  | CHC-C4B | 3.77  | 1.47        | 1.39     |
| 11  | bA    | 843 | CLA  | C3D-C2D | 3.77  | 1.49        | 1.39     |
| 11  | cB    | 801 | CLA  | CHD-C1D | 3.77  | 1.45        | 1.38     |
| 11  | aA    | 810 | CLA  | CHB-C1B | 3.77  | 1.47        | 1.39     |
| 11  | bA    | 818 | CLA  | C3D-C2D | 3.77  | 1.49        | 1.39     |
| 11  | cA    | 837 | CLA  | C3D-C2D | 3.77  | 1.49        | 1.39     |
| 11  | aA    | 805 | CLA  | CHC-C4B | 3.77  | 1.47        | 1.39     |
| 12  | bA    | 827 | F6C  | CHB-C1B | 3.77  | 1.47        | 1.39     |
| 11  | aB    | 834 | CLA  | C1B-NB  | -3.77 | 1.32        | 1.37     |
| 11  | aA    | 805 | CLA  | OBD-CAD | 3.77  | 1.29        | 1.22     |
| 11  | bB    | 826 | CLA  | C1B-NB  | -3.77 | 1.32        | 1.37     |
| 11  | bB    | 821 | CLA  | OBD-CAD | 3.77  | 1.29        | 1.22     |
| 11  | cB    | 810 | CLA  | C3D-C2D | 3.77  | 1.49        | 1.39     |
| 11  | cB    | 813 | CLA  | CHD-C4C | 3.77  | 1.47        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | bB    | 820 | CLA  | OBD-CAD | 3.77  | 1.29        | 1.22     |
| 11  | bA    | 836 | CLA  | C1B-NB  | -3.77 | 1.32        | 1.37     |
| 11  | aA    | 818 | CLA  | C3D-C2D | 3.77  | 1.49        | 1.39     |
| 11  | bA    | 836 | CLA  | C3D-C2D | 3.77  | 1.49        | 1.39     |
| 11  | cL    | 206 | CLA  | CHD-C4C | 3.77  | 1.47        | 1.39     |
| 11  | bA    | 838 | CLA  | CHD-C4C | 3.77  | 1.47        | 1.39     |
| 11  | bA    | 825 | CLA  | C3D-C2D | 3.77  | 1.49        | 1.39     |
| 12  | aA    | 832 | F6C  | CHB-C1B | 3.76  | 1.47        | 1.39     |
| 11  | aB    | 819 | CLA  | OBD-CAD | 3.76  | 1.29        | 1.22     |
| 11  | bB    | 832 | CLA  | OBD-CAD | 3.76  | 1.29        | 1.22     |
| 11  | aB    | 822 | CLA  | CHD-C1D | 3.76  | 1.45        | 1.38     |
| 11  | cA    | 836 | CLA  | C1B-NB  | -3.76 | 1.32        | 1.37     |
| 11  | bA    | 822 | CLA  | CHD-C4C | 3.76  | 1.47        | 1.39     |
| 11  | cA    | 816 | CLA  | C3D-C2D | 3.76  | 1.49        | 1.39     |
| 11  | aB    | 836 | CLA  | CHC-C4B | 3.76  | 1.47        | 1.39     |
| 12  | bA    | 832 | F6C  | CHB-C1B | 3.76  | 1.47        | 1.39     |
| 11  | aA    | 806 | CLA  | C3D-C2D | 3.76  | 1.49        | 1.39     |
| 11  | cA    | 823 | CLA  | OBD-CAD | 3.76  | 1.29        | 1.22     |
| 11  | aA    | 823 | CLA  | OBD-CAD | 3.76  | 1.29        | 1.22     |
| 11  | cB    | 820 | CLA  | OBD-CAD | 3.76  | 1.29        | 1.22     |
| 11  | cB    | 818 | CLA  | CHD-C4C | 3.76  | 1.47        | 1.39     |
| 11  | bA    | 808 | CLA  | C3D-C2D | 3.76  | 1.49        | 1.39     |
| 11  | cA    | 809 | CLA  | C3D-C2D | 3.76  | 1.49        | 1.39     |
| 11  | bB    | 801 | CLA  | CHD-C1D | 3.76  | 1.45        | 1.38     |
| 11  | cA    | 813 | CLA  | CHD-C4C | 3.76  | 1.47        | 1.39     |
| 11  | aA    | 839 | CLA  | C3D-C2D | 3.76  | 1.49        | 1.39     |
| 11  | cA    | 814 | CLA  | C3D-C2D | 3.76  | 1.49        | 1.39     |
| 11  | cB    | 815 | CLA  | C3D-C2D | 3.76  | 1.49        | 1.39     |
| 11  | bB    | 810 | CLA  | C3D-C2D | 3.76  | 1.49        | 1.39     |
| 11  | cB    | 817 | CLA  | C3D-C2D | 3.76  | 1.49        | 1.39     |
| 11  | cB    | 819 | CLA  | OBD-CAD | 3.76  | 1.29        | 1.22     |
| 11  | bB    | 813 | CLA  | CHD-C4C | 3.76  | 1.47        | 1.39     |
| 11  | bB    | 820 | CLA  | C3D-C2D | 3.76  | 1.49        | 1.39     |
| 11  | cA    | 813 | CLA  | C3D-C2D | 3.76  | 1.49        | 1.39     |
| 11  | cA    | 836 | CLA  | C3D-C2D | 3.76  | 1.49        | 1.39     |
| 12  | aA    | 826 | F6C  | CHB-C1B | 3.76  | 1.47        | 1.39     |
| 11  | aA    | 809 | CLA  | C3D-C2D | 3.76  | 1.49        | 1.39     |
| 11  | cA    | 831 | CLA  | CHD-C4C | 3.76  | 1.47        | 1.39     |
| 10  | aA    | 801 | CL0  | CHD-C1D | 3.76  | 1.45        | 1.39     |
| 11  | aA    | 825 | CLA  | C3D-C2D | 3.76  | 1.49        | 1.39     |
| 11  | cA    | 818 | CLA  | C3D-C2D | 3.76  | 1.49        | 1.39     |
| 11  | bB    | 831 | CLA  | C3D-C2D | 3.75  | 1.49        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12  | aL    | 202 | F6C  | C1D-ND  | 3.75  | 1.43        | 1.37     |
| 11  | cA    | 808 | CLA  | C3D-C2D | 3.75  | 1.49        | 1.39     |
| 11  | aA    | 842 | CLA  | C3D-C2D | 3.75  | 1.49        | 1.39     |
| 11  | bB    | 817 | CLA  | C3D-C2D | 3.75  | 1.49        | 1.39     |
| 11  | aL    | 206 | CLA  | CHD-C4C | 3.75  | 1.47        | 1.39     |
| 11  | cL    | 204 | CLA  | CHD-C4C | 3.75  | 1.47        | 1.39     |
| 11  | cB    | 820 | CLA  | C3D-C2D | 3.75  | 1.49        | 1.39     |
| 11  | aA    | 813 | CLA  | C3D-C2D | 3.75  | 1.49        | 1.39     |
| 12  | bL    | 202 | F6C  | C3D-C2D | 3.75  | 1.49        | 1.39     |
| 11  | aA    | 838 | CLA  | CHD-C4C | 3.75  | 1.47        | 1.39     |
| 12  | cA    | 832 | F6C  | CHB-C1B | 3.75  | 1.47        | 1.39     |
| 11  | cL    | 204 | CLA  | C1B-NB  | -3.75 | 1.32        | 1.37     |
| 11  | cB    | 835 | CLA  | OBD-CAD | 3.75  | 1.28        | 1.22     |
| 11  | bA    | 816 | CLA  | C3D-C2D | 3.75  | 1.49        | 1.39     |
| 12  | aL    | 202 | F6C  | C3D-C2D | 3.75  | 1.49        | 1.39     |
| 12  | aA    | 827 | F6C  | CHB-C1B | 3.75  | 1.47        | 1.39     |
| 11  | aA    | 843 | CLA  | C1B-NB  | -3.75 | 1.32        | 1.37     |
| 11  | bB    | 825 | CLA  | CHD-C4C | 3.75  | 1.47        | 1.39     |
| 11  | cB    | 822 | CLA  | CHD-C1D | 3.75  | 1.45        | 1.38     |
| 11  | cB    | 826 | CLA  | C1B-NB  | -3.75 | 1.32        | 1.37     |
| 11  | bB    | 838 | CLA  | C3D-C2D | 3.75  | 1.49        | 1.39     |
| 11  | cB    | 838 | CLA  | C3D-C2D | 3.75  | 1.49        | 1.39     |
| 11  | cA    | 804 | CLA  | OBD-CAD | 3.75  | 1.28        | 1.22     |
| 11  | cA    | 839 | CLA  | C3D-C2D | 3.75  | 1.49        | 1.39     |
| 11  | bA    | 839 | CLA  | C3D-C2D | 3.75  | 1.49        | 1.39     |
| 11  | cB    | 802 | CLA  | CHD-C4C | 3.75  | 1.47        | 1.39     |
| 11  | cB    | 803 | CLA  | C1B-NB  | -3.75 | 1.32        | 1.37     |
| 11  | cA    | 842 | CLA  | C3D-C2D | 3.75  | 1.49        | 1.39     |
| 11  | aA    | 824 | CLA  | C1B-NB  | -3.75 | 1.32        | 1.37     |
| 11  | bB    | 803 | CLA  | C1B-NB  | -3.75 | 1.32        | 1.37     |
| 11  | bA    | 837 | CLA  | C3D-C2D | 3.75  | 1.49        | 1.39     |
| 11  | cA    | 840 | CLA  | C3D-C2D | 3.75  | 1.49        | 1.39     |
| 11  | cB    | 831 | CLA  | C3D-C2D | 3.75  | 1.49        | 1.39     |
| 11  | bB    | 836 | CLA  | CHD-C4C | 3.75  | 1.47        | 1.39     |
| 11  | aB    | 838 | CLA  | C3D-C2D | 3.75  | 1.49        | 1.39     |
| 11  | aB    | 825 | CLA  | CHD-C4C | 3.75  | 1.47        | 1.39     |
| 11  | bB    | 815 | CLA  | CHD-C4C | 3.75  | 1.47        | 1.39     |
| 11  | bA    | 808 | CLA  | OBD-CAD | 3.75  | 1.28        | 1.22     |
| 11  | aA    | 813 | CLA  | C1B-NB  | -3.74 | 1.32        | 1.37     |
| 11  | aB    | 839 | CLA  | CHC-C4B | 3.74  | 1.47        | 1.39     |
| 11  | bB    | 839 | CLA  | CHC-C4B | 3.74  | 1.47        | 1.39     |
| 11  | aB    | 832 | CLA  | OBD-CAD | 3.74  | 1.28        | 1.22     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | cB    | 832 | CLA  | OBD-CAD | 3.74  | 1.28        | 1.22     |
| 11  | aB    | 815 | CLA  | CHD-C4C | 3.74  | 1.47        | 1.39     |
| 11  | cB    | 815 | CLA  | CHD-C4C | 3.74  | 1.47        | 1.39     |
| 11  | aB    | 817 | CLA  | C3D-C2D | 3.74  | 1.49        | 1.39     |
| 11  | cA    | 810 | CLA  | CHB-C1B | 3.74  | 1.47        | 1.39     |
| 11  | cB    | 818 | CLA  | C1B-NB  | -3.74 | 1.32        | 1.37     |
| 11  | cA    | 805 | CLA  | OBD-CAD | 3.74  | 1.28        | 1.22     |
| 11  | aB    | 802 | CLA  | CHD-C4C | 3.74  | 1.47        | 1.39     |
| 11  | aA    | 819 | CLA  | C3D-C2D | 3.74  | 1.49        | 1.39     |
| 11  | aB    | 810 | CLA  | C1B-NB  | -3.74 | 1.32        | 1.37     |
| 11  | cB    | 813 | CLA  | C3D-C2D | 3.74  | 1.49        | 1.39     |
| 11  | cA    | 824 | CLA  | C1B-NB  | -3.74 | 1.32        | 1.37     |
| 11  | bL    | 206 | CLA  | CHD-C4C | 3.74  | 1.47        | 1.39     |
| 11  | aA    | 817 | CLA  | OBD-CAD | 3.74  | 1.28        | 1.22     |
| 11  | cA    | 842 | CLA  | OBD-CAD | 3.74  | 1.28        | 1.22     |
| 11  | aA    | 831 | CLA  | CHD-C4C | 3.74  | 1.47        | 1.39     |
| 11  | aL    | 204 | CLA  | CHD-C4C | 3.74  | 1.47        | 1.39     |
| 11  | aA    | 840 | CLA  | C3D-C2D | 3.74  | 1.49        | 1.39     |
| 11  | cB    | 822 | CLA  | C3D-C2D | 3.74  | 1.49        | 1.39     |
| 11  | cB    | 810 | CLA  | C1B-NB  | -3.74 | 1.33        | 1.37     |
| 11  | aA    | 816 | CLA  | C3D-C2D | 3.74  | 1.49        | 1.39     |
| 11  | bB    | 804 | CLA  | CHD-C4C | 3.74  | 1.47        | 1.39     |
| 11  | cA    | 819 | CLA  | CHD-C4C | 3.74  | 1.47        | 1.39     |
| 11  | bB    | 815 | CLA  | OBD-CAD | 3.73  | 1.28        | 1.22     |
| 11  | bB    | 834 | CLA  | OBD-CAD | 3.73  | 1.28        | 1.22     |
| 11  | bB    | 833 | CLA  | C3D-C2D | 3.73  | 1.49        | 1.39     |
| 11  | bA    | 810 | CLA  | CHD-C4C | 3.73  | 1.47        | 1.39     |
| 11  | bB    | 818 | CLA  | OBD-CAD | 3.73  | 1.28        | 1.22     |
| 11  | aB    | 820 | CLA  | C3D-C2D | 3.73  | 1.49        | 1.39     |
| 11  | cB    | 834 | CLA  | OBD-CAD | 3.73  | 1.28        | 1.22     |
| 12  | bA    | 826 | F6C  | CHB-C1B | 3.73  | 1.47        | 1.39     |
| 11  | aA    | 836 | CLA  | C3D-C2D | 3.73  | 1.49        | 1.39     |
| 11  | cB    | 836 | CLA  | CHD-C4C | 3.73  | 1.47        | 1.39     |
| 11  | bK    | 103 | CLA  | C3D-C2D | 3.73  | 1.49        | 1.39     |
| 11  | cA    | 825 | CLA  | C3D-C2D | 3.73  | 1.49        | 1.39     |
| 11  | bA    | 817 | CLA  | OBD-CAD | 3.73  | 1.28        | 1.22     |
| 11  | aB    | 819 | CLA  | C3D-C2D | 3.73  | 1.49        | 1.39     |
| 11  | bA    | 840 | CLA  | C3D-C2D | 3.73  | 1.49        | 1.39     |
| 12  | cA    | 826 | F6C  | CHB-C1B | 3.73  | 1.47        | 1.39     |
| 11  | aB    | 822 | CLA  | C3D-C2D | 3.73  | 1.49        | 1.39     |
| 12  | bB    | 824 | F6C  | C3B-C2B | 3.73  | 1.48        | 1.39     |
| 11  | cB    | 833 | CLA  | C3D-C2D | 3.73  | 1.49        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | aB    | 823 | CLA  | CHD-C4C | 3.73  | 1.47        | 1.39     |
| 11  | bA    | 813 | CLA  | C3D-C2D | 3.73  | 1.49        | 1.39     |
| 11  | aA    | 814 | CLA  | OBD-CAD | 3.73  | 1.28        | 1.22     |
| 11  | aB    | 835 | CLA  | OBD-CAD | 3.73  | 1.28        | 1.22     |
| 11  | bB    | 811 | CLA  | OBD-CAD | 3.73  | 1.28        | 1.22     |
| 11  | cA    | 841 | CLA  | OBD-CAD | 3.73  | 1.28        | 1.22     |
| 11  | aB    | 836 | CLA  | CHD-C4C | 3.73  | 1.47        | 1.39     |
| 11  | aB    | 833 | CLA  | C3D-C2D | 3.72  | 1.49        | 1.39     |
| 11  | bA    | 829 | CLA  | C3D-C2D | 3.72  | 1.49        | 1.39     |
| 11  | aB    | 815 | CLA  | OBD-CAD | 3.72  | 1.28        | 1.22     |
| 11  | aB    | 831 | CLA  | C3D-C2D | 3.72  | 1.49        | 1.39     |
| 11  | cA    | 817 | CLA  | OBD-CAD | 3.72  | 1.28        | 1.22     |
| 11  | cA    | 818 | CLA  | CHC-C4B | 3.72  | 1.47        | 1.39     |
| 11  | aB    | 813 | CLA  | C3D-C2D | 3.72  | 1.49        | 1.39     |
| 11  | aB    | 820 | CLA  | OBD-CAD | 3.72  | 1.28        | 1.22     |
| 11  | aA    | 837 | CLA  | C3D-C2D | 3.72  | 1.49        | 1.39     |
| 11  | cB    | 819 | CLA  | C3D-C2D | 3.72  | 1.49        | 1.39     |
| 11  | aB    | 839 | CLA  | C1B-NB  | -3.72 | 1.33        | 1.37     |
| 11  | bB    | 822 | CLA  | C3D-C2D | 3.72  | 1.49        | 1.39     |
| 11  | bB    | 834 | CLA  | C1B-NB  | -3.72 | 1.33        | 1.37     |
| 11  | bA    | 821 | CLA  | CHD-C4C | 3.72  | 1.47        | 1.39     |
| 11  | aA    | 813 | CLA  | CHC-C4B | 3.72  | 1.47        | 1.39     |
| 12  | cL    | 202 | F6C  | C1D-ND  | 3.72  | 1.43        | 1.37     |
| 11  | bA    | 842 | CLA  | OBD-CAD | 3.72  | 1.28        | 1.22     |
| 11  | aA    | 829 | CLA  | C3D-C2D | 3.72  | 1.49        | 1.39     |
| 11  | bA    | 842 | CLA  | C3D-C2D | 3.72  | 1.49        | 1.39     |
| 11  | aK    | 103 | CLA  | C3D-C2D | 3.72  | 1.49        | 1.39     |
| 12  | bL    | 202 | F6C  | C1D-ND  | 3.72  | 1.43        | 1.37     |
| 11  | cA    | 808 | CLA  | OBD-CAD | 3.72  | 1.28        | 1.22     |
| 11  | bB    | 810 | CLA  | C1B-NB  | -3.72 | 1.33        | 1.37     |
| 11  | aA    | 810 | CLA  | OBD-CAD | 3.72  | 1.28        | 1.22     |
| 12  | aB    | 824 | F6C  | C3B-C2B | 3.72  | 1.48        | 1.39     |
| 11  | bA    | 831 | CLA  | CHD-C4C | 3.72  | 1.47        | 1.39     |
| 11  | aA    | 819 | CLA  | CHD-C4C | 3.72  | 1.47        | 1.39     |
| 11  | bA    | 809 | CLA  | C3D-C2D | 3.71  | 1.49        | 1.39     |
| 11  | bB    | 819 | CLA  | C3D-C2D | 3.71  | 1.49        | 1.39     |
| 11  | aB    | 801 | CLA  | CHB-C1B | 3.71  | 1.47        | 1.39     |
| 11  | cB    | 833 | CLA  | CHC-C4B | 3.71  | 1.47        | 1.39     |
| 11  | bA    | 813 | CLA  | CHC-C4B | 3.71  | 1.47        | 1.39     |
| 11  | cB    | 801 | CLA  | CHB-C1B | 3.71  | 1.47        | 1.39     |
| 11  | cB    | 840 | CLA  | C3D-C2D | 3.71  | 1.49        | 1.39     |
| 11  | cA    | 807 | CLA  | C3D-C2D | 3.71  | 1.49        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | cB    | 804 | CLA  | CHD-C4C | 3.71  | 1.47        | 1.39     |
| 11  | cA    | 829 | CLA  | C3D-C2D | 3.71  | 1.49        | 1.39     |
| 11  | aA    | 842 | CLA  | OBD-CAD | 3.71  | 1.28        | 1.22     |
| 11  | cA    | 810 | CLA  | OBD-CAD | 3.71  | 1.28        | 1.22     |
| 11  | cB    | 825 | CLA  | CHD-C4C | 3.71  | 1.47        | 1.39     |
| 11  | cK    | 103 | CLA  | C3D-C2D | 3.71  | 1.49        | 1.39     |
| 11  | aB    | 840 | CLA  | C3D-C2D | 3.71  | 1.49        | 1.39     |
| 11  | bB    | 831 | CLA  | OBD-CAD | 3.71  | 1.28        | 1.22     |
| 12  | aA    | 844 | F6C  | CHC-C1C | 3.71  | 1.47        | 1.39     |
| 11  | aB    | 823 | CLA  | C3D-C2D | 3.71  | 1.49        | 1.39     |
| 11  | bA    | 819 | CLA  | C3D-C2D | 3.71  | 1.49        | 1.39     |
| 11  | bA    | 813 | CLA  | OBD-CAD | 3.71  | 1.28        | 1.22     |
| 11  | aA    | 808 | CLA  | OBD-CAD | 3.71  | 1.28        | 1.22     |
| 11  | cB    | 815 | CLA  | OBD-CAD | 3.71  | 1.28        | 1.22     |
| 11  | aB    | 804 | CLA  | CHD-C4C | 3.71  | 1.47        | 1.39     |
| 12  | cB    | 824 | F6C  | C3B-C2B | 3.71  | 1.47        | 1.39     |
| 11  | bB    | 807 | CLA  | C3D-C2D | 3.70  | 1.49        | 1.39     |
| 11  | cA    | 810 | CLA  | CHD-C4C | 3.70  | 1.47        | 1.39     |
| 11  | bB    | 840 | CLA  | C3D-C2D | 3.70  | 1.49        | 1.39     |
| 11  | bA    | 819 | CLA  | CHD-C4C | 3.70  | 1.47        | 1.39     |
| 11  | cB    | 811 | CLA  | OBD-CAD | 3.70  | 1.28        | 1.22     |
| 11  | bA    | 810 | CLA  | OBD-CAD | 3.70  | 1.28        | 1.22     |
| 11  | cA    | 821 | CLA  | CHD-C4C | 3.70  | 1.47        | 1.39     |
| 11  | cB    | 839 | CLA  | CHC-C4B | 3.70  | 1.47        | 1.39     |
| 11  | aB    | 831 | CLA  | OBD-CAD | 3.70  | 1.28        | 1.22     |
| 11  | bA    | 821 | CLA  | OBD-CAD | 3.70  | 1.28        | 1.22     |
| 11  | bL    | 204 | CLA  | CHD-C4C | 3.70  | 1.47        | 1.39     |
| 11  | aA    | 836 | CLA  | OBD-CAD | 3.70  | 1.28        | 1.22     |
| 11  | bA    | 811 | CLA  | OBD-CAD | 3.70  | 1.28        | 1.22     |
| 11  | aB    | 818 | CLA  | OBD-CAD | 3.70  | 1.28        | 1.22     |
| 11  | bB    | 813 | CLA  | C3D-C2D | 3.70  | 1.49        | 1.39     |
| 11  | bB    | 804 | CLA  | C3D-C2D | 3.70  | 1.49        | 1.39     |
| 11  | aA    | 818 | CLA  | CHC-C4B | 3.70  | 1.47        | 1.39     |
| 11  | cA    | 813 | CLA  | OBD-CAD | 3.70  | 1.28        | 1.22     |
| 11  | bB    | 823 | CLA  | C3D-C2D | 3.70  | 1.49        | 1.39     |
| 11  | cA    | 823 | CLA  | CHD-C1D | 3.70  | 1.45        | 1.38     |
| 11  | bA    | 833 | CLA  | C1B-NB  | -3.70 | 1.33        | 1.37     |
| 11  | aA    | 842 | CLA  | CHC-C4B | 3.70  | 1.47        | 1.39     |
| 11  | cB    | 831 | CLA  | OBD-CAD | 3.70  | 1.28        | 1.22     |
| 11  | aB    | 804 | CLA  | OBD-CAD | 3.70  | 1.28        | 1.22     |
| 12  | bA    | 844 | F6C  | CHB-C1B | 3.70  | 1.47        | 1.39     |
| 11  | aA    | 823 | CLA  | CHD-C4C | 3.70  | 1.47        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | bL    | 204 | CLA  | C1B-NB  | -3.69 | 1.33        | 1.37     |
| 11  | aA    | 810 | CLA  | CHD-C4C | 3.69  | 1.47        | 1.39     |
| 12  | cA    | 827 | F6C  | CHC-C1C | 3.69  | 1.47        | 1.39     |
| 11  | bA    | 807 | CLA  | C3D-C2D | 3.69  | 1.49        | 1.39     |
| 11  | aA    | 812 | CLA  | OBD-CAD | 3.69  | 1.28        | 1.22     |
| 11  | aB    | 834 | CLA  | OBD-CAD | 3.69  | 1.28        | 1.22     |
| 11  | aB    | 807 | CLA  | C3D-C2D | 3.69  | 1.49        | 1.39     |
| 11  | bA    | 835 | CLA  | OBD-CAD | 3.69  | 1.28        | 1.22     |
| 11  | bA    | 823 | CLA  | CHD-C1D | 3.69  | 1.45        | 1.38     |
| 11  | aB    | 818 | CLA  | C1B-NB  | -3.69 | 1.33        | 1.37     |
| 11  | bA    | 828 | CLA  | CHD-C1D | 3.69  | 1.45        | 1.38     |
| 11  | cB    | 825 | CLA  | C3D-C2D | 3.69  | 1.49        | 1.39     |
| 11  | cA    | 813 | CLA  | CHC-C4B | 3.69  | 1.47        | 1.39     |
| 11  | cB    | 823 | CLA  | C3D-C2D | 3.69  | 1.49        | 1.39     |
| 11  | bA    | 825 | CLA  | C1B-NB  | -3.69 | 1.33        | 1.37     |
| 11  | cA    | 813 | CLA  | C1B-NB  | -3.69 | 1.33        | 1.37     |
| 11  | aA    | 821 | CLA  | CHD-C4C | 3.69  | 1.47        | 1.39     |
| 11  | aA    | 837 | CLA  | OBD-CAD | 3.69  | 1.28        | 1.22     |
| 11  | aB    | 804 | CLA  | C3D-C2D | 3.69  | 1.49        | 1.39     |
| 11  | cA    | 828 | CLA  | CHD-C1D | 3.69  | 1.45        | 1.38     |
| 12  | bA    | 830 | F6C  | OBD-CAD | 3.69  | 1.28        | 1.22     |
| 12  | bA    | 826 | F6C  | CHD-C4C | 3.69  | 1.47        | 1.39     |
| 11  | aA    | 841 | CLA  | OBD-CAD | 3.69  | 1.28        | 1.22     |
| 11  | aB    | 816 | CLA  | OBD-CAD | 3.68  | 1.28        | 1.22     |
| 11  | aA    | 823 | CLA  | CHD-C1D | 3.68  | 1.45        | 1.38     |
| 11  | bA    | 806 | CLA  | C1B-NB  | -3.68 | 1.33        | 1.37     |
| 11  | cA    | 819 | CLA  | C3D-C2D | 3.68  | 1.49        | 1.39     |
| 11  | cB    | 828 | CLA  | OBD-CAD | 3.68  | 1.28        | 1.22     |
| 11  | aA    | 807 | CLA  | C3D-C2D | 3.68  | 1.49        | 1.39     |
| 11  | aB    | 811 | CLA  | OBD-CAD | 3.68  | 1.28        | 1.22     |
| 11  | cA    | 806 | CLA  | OBD-CAD | 3.68  | 1.28        | 1.22     |
| 11  | aA    | 833 | CLA  | C1B-NB  | -3.68 | 1.33        | 1.37     |
| 11  | bA    | 841 | CLA  | OBD-CAD | 3.68  | 1.28        | 1.22     |
| 12  | aA    | 827 | F6C  | CHC-C1C | 3.68  | 1.47        | 1.39     |
| 11  | cA    | 814 | CLA  | OBD-CAD | 3.68  | 1.28        | 1.22     |
| 11  | cA    | 837 | CLA  | OBD-CAD | 3.68  | 1.28        | 1.22     |
| 11  | aB    | 825 | CLA  | C3D-C2D | 3.68  | 1.49        | 1.39     |
| 11  | aB    | 833 | CLA  | CHC-C4B | 3.68  | 1.47        | 1.39     |
| 11  | bB    | 809 | CLA  | CHD-C4C | 3.68  | 1.47        | 1.39     |
| 11  | cA    | 843 | CLA  | C1B-NB  | -3.68 | 1.33        | 1.37     |
| 11  | cB    | 836 | CLA  | C3D-C2D | 3.68  | 1.49        | 1.39     |
| 11  | bB    | 801 | CLA  | CHB-C1B | 3.68  | 1.47        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | bB    | 833 | CLA  | CHC-C4B | 3.68  | 1.47        | 1.39     |
| 12  | cA    | 844 | F6C  | CHB-C1B | 3.68  | 1.47        | 1.39     |
| 11  | aA    | 821 | CLA  | OBD-CAD | 3.68  | 1.28        | 1.22     |
| 11  | cB    | 809 | CLA  | CHD-C4C | 3.68  | 1.47        | 1.39     |
| 11  | bB    | 839 | CLA  | C1B-NB  | -3.68 | 1.33        | 1.37     |
| 11  | bB    | 804 | CLA  | OBD-CAD | 3.68  | 1.28        | 1.22     |
| 12  | cA    | 844 | F6C  | OBD-CAD | 3.68  | 1.28        | 1.22     |
| 11  | aA    | 828 | CLA  | CHD-C1D | 3.68  | 1.45        | 1.38     |
| 11  | bA    | 812 | CLA  | OBD-CAD | 3.67  | 1.28        | 1.22     |
| 11  | cA    | 821 | CLA  | OBD-CAD | 3.67  | 1.28        | 1.22     |
| 11  | bA    | 842 | CLA  | CHC-C4B | 3.67  | 1.47        | 1.39     |
| 11  | bA    | 806 | CLA  | OBD-CAD | 3.67  | 1.28        | 1.22     |
| 11  | aA    | 816 | CLA  | CHC-C4B | 3.67  | 1.47        | 1.39     |
| 11  | cB    | 816 | CLA  | OBD-CAD | 3.67  | 1.28        | 1.22     |
| 11  | aB    | 836 | CLA  | C3D-C2D | 3.67  | 1.49        | 1.39     |
| 11  | bA    | 818 | CLA  | CHC-C4B | 3.67  | 1.47        | 1.39     |
| 11  | bA    | 836 | CLA  | OBD-CAD | 3.67  | 1.28        | 1.22     |
| 12  | aA    | 826 | F6C  | OBD-CAD | 3.67  | 1.28        | 1.22     |
| 12  | cA    | 826 | F6C  | OBD-CAD | 3.67  | 1.28        | 1.22     |
| 12  | aA    | 832 | F6C  | C1D-ND  | 3.67  | 1.43        | 1.37     |
| 11  | cA    | 825 | CLA  | C1B-NB  | -3.67 | 1.33        | 1.37     |
| 11  | cK    | 101 | CLA  | CHC-C4B | 3.67  | 1.47        | 1.39     |
| 12  | cA    | 844 | F6C  | CHC-C1C | 3.67  | 1.47        | 1.39     |
| 11  | cA    | 833 | CLA  | C1B-NB  | -3.67 | 1.33        | 1.37     |
| 11  | aA    | 806 | CLA  | OBD-CAD | 3.67  | 1.28        | 1.22     |
| 11  | bA    | 814 | CLA  | OBD-CAD | 3.67  | 1.28        | 1.22     |
| 11  | cL    | 206 | CLA  | OBD-CAD | 3.67  | 1.28        | 1.22     |
| 12  | aL    | 202 | F6C  | CHD-C4C | 3.67  | 1.47        | 1.39     |
| 11  | cA    | 842 | CLA  | CHC-C4B | 3.67  | 1.47        | 1.39     |
| 11  | cA    | 821 | CLA  | C3D-C2D | 3.67  | 1.49        | 1.39     |
| 11  | cB    | 839 | CLA  | C1B-NB  | -3.67 | 1.33        | 1.37     |
| 11  | aB    | 803 | CLA  | C1B-NB  | -3.67 | 1.33        | 1.37     |
| 11  | bA    | 823 | CLA  | CHD-C4C | 3.67  | 1.47        | 1.39     |
| 11  | bB    | 818 | CLA  | C1B-NB  | -3.66 | 1.33        | 1.37     |
| 11  | bB    | 836 | CLA  | C3D-C2D | 3.66  | 1.49        | 1.39     |
| 11  | aB    | 809 | CLA  | CHD-C4C | 3.66  | 1.47        | 1.39     |
| 11  | aA    | 813 | CLA  | OBD-CAD | 3.66  | 1.28        | 1.22     |
| 11  | bB    | 816 | CLA  | OBD-CAD | 3.66  | 1.28        | 1.22     |
| 12  | aA    | 826 | F6C  | CHD-C4C | 3.66  | 1.47        | 1.39     |
| 11  | bA    | 837 | CLA  | OBD-CAD | 3.66  | 1.28        | 1.22     |
| 11  | bB    | 828 | CLA  | OBD-CAD | 3.66  | 1.28        | 1.22     |
| 11  | cA    | 812 | CLA  | OBD-CAD | 3.66  | 1.28        | 1.22     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12  | bL    | 202 | F6C  | CHD-C4C | 3.66  | 1.47        | 1.39     |
| 11  | bB    | 825 | CLA  | C3D-C2D | 3.66  | 1.49        | 1.39     |
| 11  | cB    | 804 | CLA  | C3D-C2D | 3.66  | 1.49        | 1.39     |
| 11  | cB    | 807 | CLA  | C1B-NB  | -3.66 | 1.33        | 1.37     |
| 11  | bA    | 816 | CLA  | CHC-C4B | 3.66  | 1.47        | 1.39     |
| 12  | aA    | 830 | F6C  | CHD-C4C | 3.66  | 1.47        | 1.39     |
| 12  | aA    | 844 | F6C  | OBD-CAD | 3.66  | 1.28        | 1.22     |
| 11  | aA    | 811 | CLA  | OBD-CAD | 3.66  | 1.28        | 1.22     |
| 11  | bB    | 807 | CLA  | C1B-NB  | -3.66 | 1.33        | 1.37     |
| 11  | cA    | 840 | CLA  | CHC-C4B | 3.66  | 1.47        | 1.39     |
| 11  | cB    | 807 | CLA  | C3D-C2D | 3.66  | 1.49        | 1.39     |
| 11  | cA    | 822 | CLA  | OBD-CAD | 3.66  | 1.28        | 1.22     |
| 11  | aA    | 825 | CLA  | C1B-NB  | -3.66 | 1.33        | 1.37     |
| 12  | aA    | 827 | F6C  | C1D-ND  | 3.66  | 1.43        | 1.37     |
| 11  | cA    | 803 | CLA  | OBD-CAD | 3.66  | 1.28        | 1.22     |
| 11  | cA    | 811 | CLA  | OBD-CAD | 3.66  | 1.28        | 1.22     |
| 11  | cK    | 103 | CLA  | OBD-CAD | 3.66  | 1.28        | 1.22     |
| 12  | cA    | 826 | F6C  | CHD-C4C | 3.65  | 1.47        | 1.39     |
| 11  | aB    | 801 | CLA  | OBD-CAD | 3.65  | 1.28        | 1.22     |
| 11  | bB    | 825 | CLA  | CHC-C4B | 3.65  | 1.47        | 1.39     |
| 11  | aA    | 822 | CLA  | OBD-CAD | 3.65  | 1.28        | 1.22     |
| 11  | cA    | 811 | CLA  | C1B-NB  | -3.65 | 1.33        | 1.37     |
| 11  | aB    | 804 | CLA  | CHC-C4B | 3.65  | 1.47        | 1.39     |
| 11  | cA    | 829 | CLA  | OBD-CAD | 3.65  | 1.28        | 1.22     |
| 12  | bA    | 832 | F6C  | C3B-C2B | 3.65  | 1.47        | 1.39     |
| 11  | bA    | 843 | CLA  | OBD-CAD | 3.65  | 1.28        | 1.22     |
| 12  | bA    | 844 | F6C  | OBD-CAD | 3.65  | 1.28        | 1.22     |
| 11  | bB    | 806 | CLA  | C3D-C2D | 3.65  | 1.49        | 1.39     |
| 11  | cA    | 821 | CLA  | CHB-C1B | 3.65  | 1.47        | 1.39     |
| 11  | cA    | 803 | CLA  | CHD-C4C | 3.65  | 1.47        | 1.39     |
| 11  | aB    | 806 | CLA  | C3D-C2D | 3.65  | 1.48        | 1.39     |
| 12  | bA    | 826 | F6C  | OBD-CAD | 3.65  | 1.28        | 1.22     |
| 11  | aB    | 825 | CLA  | CHB-C1B | 3.65  | 1.47        | 1.39     |
| 11  | cA    | 829 | CLA  | C1B-NB  | -3.65 | 1.33        | 1.37     |
| 11  | aB    | 839 | CLA  | CHD-C4C | 3.65  | 1.47        | 1.39     |
| 11  | cA    | 809 | CLA  | OBD-CAD | 3.65  | 1.28        | 1.22     |
| 11  | aB    | 840 | CLA  | OBD-CAD | 3.65  | 1.28        | 1.22     |
| 11  | aB    | 818 | CLA  | CHC-C4B | 3.65  | 1.47        | 1.39     |
| 11  | bA    | 804 | CLA  | CHC-C4B | 3.65  | 1.47        | 1.39     |
| 11  | cA    | 816 | CLA  | CHC-C4B | 3.65  | 1.47        | 1.39     |
| 11  | cB    | 815 | CLA  | CHC-C4B | 3.65  | 1.47        | 1.39     |
| 12  | cL    | 202 | F6C  | CHD-C4C | 3.65  | 1.47        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | bA    | 809 | CLA  | OBD-CAD | 3.65  | 1.28        | 1.22     |
| 11  | aB    | 825 | CLA  | CHC-C4B | 3.64  | 1.47        | 1.39     |
| 11  | aA    | 829 | CLA  | OBD-CAD | 3.64  | 1.28        | 1.22     |
| 11  | cB    | 818 | CLA  | OBD-CAD | 3.64  | 1.28        | 1.22     |
| 11  | aA    | 821 | CLA  | C3D-C2D | 3.64  | 1.48        | 1.39     |
| 11  | bA    | 829 | CLA  | C1B-NB  | -3.64 | 1.33        | 1.37     |
| 11  | bA    | 825 | CLA  | OBD-CAD | 3.64  | 1.28        | 1.22     |
| 11  | cA    | 823 | CLA  | CHD-C4C | 3.64  | 1.47        | 1.39     |
| 12  | cA    | 832 | F6C  | C3B-C2B | 3.64  | 1.47        | 1.39     |
| 12  | aA    | 832 | F6C  | C3B-C2B | 3.64  | 1.47        | 1.39     |
| 11  | bB    | 808 | CLA  | C3D-C2D | 3.64  | 1.48        | 1.39     |
| 11  | bB    | 803 | CLA  | OBD-CAD | 3.64  | 1.28        | 1.22     |
| 12  | bA    | 827 | F6C  | CHC-C1C | 3.64  | 1.47        | 1.39     |
| 12  | bA    | 844 | F6C  | CHC-C1C | 3.64  | 1.47        | 1.39     |
| 11  | aA    | 803 | CLA  | OBD-CAD | 3.64  | 1.28        | 1.22     |
| 11  | aA    | 840 | CLA  | CHC-C4B | 3.64  | 1.47        | 1.39     |
| 11  | aA    | 811 | CLA  | C1B-NB  | -3.64 | 1.33        | 1.37     |
| 11  | aK    | 101 | CLA  | CHC-C4B | 3.64  | 1.47        | 1.39     |
| 12  | bA    | 826 | F6C  | CHC-C1C | 3.64  | 1.47        | 1.39     |
| 11  | cB    | 804 | CLA  | CHC-C4B | 3.64  | 1.47        | 1.39     |
| 11  | cB    | 808 | CLA  | C3D-C2D | 3.63  | 1.48        | 1.39     |
| 11  | aA    | 835 | CLA  | OBD-CAD | 3.63  | 1.28        | 1.22     |
| 11  | bA    | 821 | CLA  | CHB-C1B | 3.63  | 1.47        | 1.39     |
| 12  | cA    | 830 | F6C  | CHD-C4C | 3.63  | 1.47        | 1.39     |
| 11  | aL    | 205 | CLA  | OBD-CAD | 3.63  | 1.28        | 1.22     |
| 11  | cB    | 806 | CLA  | C3D-C2D | 3.63  | 1.48        | 1.39     |
| 11  | bB    | 825 | CLA  | CHB-C1B | 3.63  | 1.47        | 1.39     |
| 11  | cB    | 816 | CLA  | CHC-C4B | 3.63  | 1.47        | 1.39     |
| 11  | bA    | 803 | CLA  | CHD-C4C | 3.63  | 1.47        | 1.39     |
| 12  | cA    | 827 | F6C  | OBD-CAD | 3.63  | 1.28        | 1.22     |
| 11  | cB    | 825 | CLA  | CHC-C4B | 3.63  | 1.47        | 1.39     |
| 11  | cL    | 205 | CLA  | OBD-CAD | 3.63  | 1.28        | 1.22     |
| 11  | bA    | 821 | CLA  | C1B-NB  | -3.63 | 1.33        | 1.37     |
| 11  | bB    | 804 | CLA  | CHC-C4B | 3.63  | 1.47        | 1.39     |
| 11  | cB    | 825 | CLA  | CHB-C1B | 3.63  | 1.47        | 1.39     |
| 12  | aA    | 830 | F6C  | OBD-CAD | 3.63  | 1.28        | 1.22     |
| 11  | cA    | 804 | CLA  | CHC-C4B | 3.63  | 1.47        | 1.39     |
| 11  | aB    | 808 | CLA  | C3D-C2D | 3.63  | 1.48        | 1.39     |
| 11  | cA    | 843 | CLA  | OBD-CAD | 3.63  | 1.28        | 1.22     |
| 12  | cA    | 830 | F6C  | OBD-CAD | 3.63  | 1.28        | 1.22     |
| 11  | bA    | 840 | CLA  | CHC-C4B | 3.63  | 1.47        | 1.39     |
| 11  | aA    | 804 | CLA  | CHC-C4B | 3.63  | 1.47        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | bL    | 205 | CLA  | C1B-NB  | -3.63 | 1.33        | 1.37     |
| 11  | cB    | 832 | CLA  | CHC-C4B | 3.63  | 1.47        | 1.39     |
| 11  | aB    | 803 | CLA  | OBD-CAD | 3.63  | 1.28        | 1.22     |
| 11  | cB    | 803 | CLA  | OBD-CAD | 3.63  | 1.28        | 1.22     |
| 11  | bA    | 824 | CLA  | C3D-C2D | 3.63  | 1.48        | 1.39     |
| 11  | aK    | 103 | CLA  | OBD-CAD | 3.63  | 1.28        | 1.22     |
| 11  | bB    | 840 | CLA  | OBD-CAD | 3.63  | 1.28        | 1.22     |
| 11  | bA    | 821 | CLA  | C3D-C2D | 3.63  | 1.48        | 1.39     |
| 11  | bA    | 822 | CLA  | OBD-CAD | 3.63  | 1.28        | 1.22     |
| 11  | aA    | 806 | CLA  | C1B-NB  | -3.63 | 1.33        | 1.37     |
| 11  | aB    | 822 | CLA  | CHD-C4C | 3.63  | 1.47        | 1.39     |
| 11  | cB    | 822 | CLA  | CHD-C4C | 3.63  | 1.47        | 1.39     |
| 11  | cB    | 803 | CLA  | CHD-C4C | 3.63  | 1.47        | 1.39     |
| 11  | aB    | 822 | CLA  | OBD-CAD | 3.63  | 1.28        | 1.22     |
| 11  | aB    | 828 | CLA  | OBD-CAD | 3.63  | 1.28        | 1.22     |
| 11  | bB    | 817 | CLA  | OBD-CAD | 3.62  | 1.28        | 1.22     |
| 11  | cA    | 836 | CLA  | OBD-CAD | 3.62  | 1.28        | 1.22     |
| 11  | aB    | 807 | CLA  | C1B-NB  | -3.62 | 1.33        | 1.37     |
| 11  | cA    | 806 | CLA  | C1B-NB  | -3.62 | 1.33        | 1.37     |
| 11  | bB    | 803 | CLA  | CHD-C1D | 3.62  | 1.45        | 1.38     |
| 12  | bA    | 827 | F6C  | C1D-ND  | 3.62  | 1.43        | 1.37     |
| 11  | bA    | 843 | CLA  | C1B-NB  | -3.62 | 1.33        | 1.37     |
| 11  | aA    | 824 | CLA  | C3D-C2D | 3.62  | 1.48        | 1.39     |
| 11  | aA    | 809 | CLA  | OBD-CAD | 3.62  | 1.28        | 1.22     |
| 11  | bL    | 205 | CLA  | OBD-CAD | 3.62  | 1.28        | 1.22     |
| 11  | cB    | 822 | CLA  | CHC-C4B | 3.62  | 1.47        | 1.39     |
| 11  | bB    | 837 | CLA  | CHC-C4B | 3.62  | 1.47        | 1.39     |
| 11  | aA    | 834 | CLA  | C3D-C2D | 3.62  | 1.48        | 1.39     |
| 11  | bA    | 828 | CLA  | C3D-C2D | 3.62  | 1.48        | 1.39     |
| 12  | aA    | 844 | F6C  | CHB-C1B | 3.62  | 1.47        | 1.39     |
| 11  | aB    | 832 | CLA  | CHC-C4B | 3.62  | 1.47        | 1.39     |
| 11  | bB    | 839 | CLA  | CHD-C4C | 3.62  | 1.47        | 1.39     |
| 11  | bB    | 818 | CLA  | CHC-C4B | 3.62  | 1.47        | 1.39     |
| 12  | bA    | 830 | F6C  | CHD-C4C | 3.62  | 1.47        | 1.39     |
| 11  | bA    | 829 | CLA  | OBD-CAD | 3.62  | 1.28        | 1.22     |
| 11  | aB    | 805 | CLA  | C1B-NB  | -3.62 | 1.33        | 1.37     |
| 11  | cB    | 837 | CLA  | CHC-C4B | 3.62  | 1.47        | 1.39     |
| 11  | cB    | 821 | CLA  | CHB-C1B | 3.62  | 1.47        | 1.39     |
| 12  | cA    | 827 | F6C  | C1D-ND  | 3.62  | 1.43        | 1.37     |
| 11  | aA    | 829 | CLA  | C1B-NB  | -3.62 | 1.33        | 1.37     |
| 11  | aB    | 816 | CLA  | CHC-C4B | 3.62  | 1.47        | 1.39     |
| 11  | bB    | 815 | CLA  | CHC-C4B | 3.62  | 1.47        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | cA    | 834 | CLA  | C3D-C2D | 3.62  | 1.48        | 1.39     |
| 11  | cA    | 815 | CLA  | OBD-CAD | 3.62  | 1.28        | 1.22     |
| 11  | aB    | 815 | CLA  | CHC-C4B | 3.61  | 1.47        | 1.39     |
| 11  | bB    | 822 | CLA  | CHD-C4C | 3.61  | 1.47        | 1.39     |
| 11  | cA    | 820 | CLA  | OBD-CAD | 3.61  | 1.28        | 1.22     |
| 11  | aL    | 204 | CLA  | C1B-NB  | -3.61 | 1.33        | 1.37     |
| 11  | cA    | 822 | CLA  | C1B-NB  | -3.61 | 1.33        | 1.37     |
| 11  | aL    | 206 | CLA  | OBD-CAD | 3.61  | 1.28        | 1.22     |
| 11  | cA    | 835 | CLA  | OBD-CAD | 3.61  | 1.28        | 1.22     |
| 11  | aB    | 803 | CLA  | CHD-C1D | 3.61  | 1.45        | 1.38     |
| 11  | cB    | 839 | CLA  | CHD-C4C | 3.61  | 1.47        | 1.39     |
| 11  | cB    | 817 | CLA  | OBD-CAD | 3.61  | 1.28        | 1.22     |
| 11  | cB    | 804 | CLA  | OBD-CAD | 3.61  | 1.28        | 1.22     |
| 11  | cB    | 816 | CLA  | C1B-NB  | -3.61 | 1.33        | 1.37     |
| 11  | cB    | 830 | CLA  | C1B-NB  | -3.61 | 1.33        | 1.37     |
| 11  | bA    | 810 | CLA  | C3D-C2D | 3.61  | 1.48        | 1.39     |
| 11  | aA    | 825 | CLA  | OBD-CAD | 3.61  | 1.28        | 1.22     |
| 11  | bL    | 204 | CLA  | OBD-CAD | 3.61  | 1.28        | 1.22     |
| 11  | bB    | 821 | CLA  | CHB-C1B | 3.61  | 1.47        | 1.39     |
| 11  | bB    | 816 | CLA  | C1B-NB  | -3.61 | 1.33        | 1.37     |
| 11  | bA    | 834 | CLA  | C3D-C2D | 3.61  | 1.48        | 1.39     |
| 12  | cA    | 844 | F6C  | C1D-ND  | 3.61  | 1.43        | 1.37     |
| 11  | aA    | 843 | CLA  | OBD-CAD | 3.61  | 1.28        | 1.22     |
| 11  | cA    | 816 | CLA  | OBD-CAD | 3.61  | 1.28        | 1.22     |
| 11  | aB    | 819 | CLA  | C1B-NB  | -3.61 | 1.33        | 1.37     |
| 12  | bA    | 832 | F6C  | C1D-ND  | 3.61  | 1.43        | 1.37     |
| 11  | bB    | 835 | CLA  | CHB-C1B | 3.61  | 1.47        | 1.39     |
| 11  | bB    | 822 | CLA  | CHC-C4B | 3.61  | 1.47        | 1.39     |
| 12  | cA    | 826 | F6C  | CHC-C1C | 3.61  | 1.47        | 1.39     |
| 11  | cA    | 825 | CLA  | OBD-CAD | 3.61  | 1.28        | 1.22     |
| 11  | aB    | 823 | CLA  | C1B-NB  | -3.60 | 1.33        | 1.37     |
| 11  | aA    | 803 | CLA  | CHD-C4C | 3.60  | 1.47        | 1.39     |
| 11  | bA    | 804 | CLA  | CHB-C1B | 3.60  | 1.47        | 1.39     |
| 11  | bK    | 101 | CLA  | CHC-C4B | 3.60  | 1.47        | 1.39     |
| 11  | cB    | 805 | CLA  | C1B-NB  | -3.60 | 1.33        | 1.37     |
| 11  | bA    | 807 | CLA  | CHB-C1B | 3.60  | 1.47        | 1.39     |
| 12  | cA    | 832 | F6C  | C1D-ND  | 3.60  | 1.43        | 1.37     |
| 11  | cB    | 823 | CLA  | C1B-NB  | -3.60 | 1.33        | 1.37     |
| 11  | cA    | 824 | CLA  | C3D-C2D | 3.60  | 1.48        | 1.39     |
| 12  | cB    | 824 | F6C  | CHB-C1B | 3.60  | 1.47        | 1.39     |
| 11  | cA    | 828 | CLA  | C3D-C2D | 3.60  | 1.48        | 1.39     |
| 11  | cA    | 841 | CLA  | CHC-C4B | 3.60  | 1.47        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | cB    | 811 | CLA  | CHC-C4B | 3.60  | 1.47        | 1.39     |
| 11  | aA    | 804 | CLA  | CHB-C1B | 3.60  | 1.47        | 1.39     |
| 11  | cA    | 822 | CLA  | CHB-C1B | 3.60  | 1.47        | 1.39     |
| 11  | cL    | 204 | CLA  | OBD-CAD | 3.60  | 1.28        | 1.22     |
| 11  | bB    | 832 | CLA  | CHC-C4B | 3.60  | 1.47        | 1.39     |
| 11  | aB    | 821 | CLA  | CHB-C1B | 3.60  | 1.47        | 1.39     |
| 11  | aA    | 820 | CLA  | OBD-CAD | 3.60  | 1.28        | 1.22     |
| 11  | bL    | 206 | CLA  | OBD-CAD | 3.60  | 1.28        | 1.22     |
| 11  | aB    | 820 | CLA  | CHB-C1B | 3.60  | 1.47        | 1.39     |
| 11  | cB    | 808 | CLA  | OBD-CAD | 3.60  | 1.28        | 1.22     |
| 11  | cB    | 818 | CLA  | CHC-C4B | 3.60  | 1.47        | 1.39     |
| 12  | aB    | 824 | F6C  | CHB-C1B | 3.60  | 1.47        | 1.39     |
| 11  | aA    | 810 | CLA  | C3D-C2D | 3.60  | 1.48        | 1.39     |
| 11  | bB    | 826 | CLA  | OBD-CAD | 3.60  | 1.28        | 1.22     |
| 11  | aL    | 206 | CLA  | CHB-C1B | 3.60  | 1.47        | 1.39     |
| 11  | aA    | 821 | CLA  | CHB-C1B | 3.60  | 1.47        | 1.39     |
| 12  | bA    | 844 | F6C  | C1D-ND  | 3.60  | 1.43        | 1.37     |
| 12  | aA    | 826 | F6C  | CHC-C1C | 3.60  | 1.47        | 1.39     |
| 11  | bA    | 815 | CLA  | OBD-CAD | 3.60  | 1.28        | 1.22     |
| 11  | cB    | 840 | CLA  | OBD-CAD | 3.60  | 1.28        | 1.22     |
| 11  | bK    | 103 | CLA  | OBD-CAD | 3.60  | 1.28        | 1.22     |
| 11  | cA    | 837 | CLA  | CHC-C4B | 3.59  | 1.47        | 1.39     |
| 11  | cB    | 835 | CLA  | CHB-C1B | 3.59  | 1.47        | 1.39     |
| 11  | bB    | 803 | CLA  | CHD-C4C | 3.59  | 1.47        | 1.39     |
| 11  | aB    | 837 | CLA  | CHC-C4B | 3.59  | 1.47        | 1.39     |
| 11  | cA    | 804 | CLA  | CHB-C1B | 3.59  | 1.47        | 1.39     |
| 12  | bA    | 827 | F6C  | OBD-CAD | 3.59  | 1.28        | 1.22     |
| 11  | aA    | 828 | CLA  | CHB-C1B | 3.59  | 1.47        | 1.39     |
| 11  | bA    | 803 | CLA  | OBD-CAD | 3.59  | 1.28        | 1.22     |
| 11  | aA    | 822 | CLA  | C1B-NB  | -3.59 | 1.33        | 1.37     |
| 11  | bA    | 837 | CLA  | CHC-C4B | 3.59  | 1.47        | 1.39     |
| 11  | aA    | 841 | CLA  | CHC-C4B | 3.59  | 1.47        | 1.39     |
| 11  | aA    | 819 | CLA  | C1B-NB  | -3.59 | 1.33        | 1.37     |
| 11  | cA    | 840 | CLA  | C1B-NB  | -3.59 | 1.33        | 1.37     |
| 11  | aB    | 811 | CLA  | CHC-C4B | 3.59  | 1.47        | 1.39     |
| 11  | bB    | 806 | CLA  | CHC-C4B | 3.59  | 1.47        | 1.39     |
| 11  | cA    | 810 | CLA  | C3D-C2D | 3.59  | 1.48        | 1.39     |
| 12  | aA    | 827 | F6C  | OBD-CAD | 3.59  | 1.28        | 1.22     |
| 11  | bB    | 822 | CLA  | OBD-CAD | 3.59  | 1.28        | 1.22     |
| 11  | bA    | 818 | CLA  | CHD-C1D | 3.59  | 1.45        | 1.38     |
| 12  | bB    | 824 | F6C  | CHB-C1B | 3.59  | 1.47        | 1.39     |
| 11  | bA    | 811 | CLA  | C1B-NB  | -3.59 | 1.33        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | aB    | 822 | CLA  | CHC-C4B | 3.59  | 1.47        | 1.39     |
| 11  | bB    | 819 | CLA  | CHB-C1B | 3.59  | 1.47        | 1.39     |
| 11  | aA    | 837 | CLA  | CHC-C4B | 3.59  | 1.47        | 1.39     |
| 11  | cA    | 807 | CLA  | CHB-C1B | 3.59  | 1.47        | 1.39     |
| 11  | cB    | 819 | CLA  | CHC-C4B | 3.59  | 1.47        | 1.39     |
| 11  | aA    | 821 | CLA  | C1B-NB  | -3.59 | 1.33        | 1.37     |
| 11  | cB    | 826 | CLA  | CHD-C4C | 3.59  | 1.47        | 1.39     |
| 11  | bA    | 841 | CLA  | CHC-C4B | 3.59  | 1.47        | 1.39     |
| 11  | bB    | 801 | CLA  | OBD-CAD | 3.59  | 1.28        | 1.22     |
| 11  | aB    | 835 | CLA  | CHB-C1B | 3.59  | 1.47        | 1.39     |
| 11  | aA    | 839 | CLA  | CHB-C1B | 3.59  | 1.47        | 1.39     |
| 11  | cA    | 823 | CLA  | C1B-NB  | -3.58 | 1.33        | 1.37     |
| 11  | bA    | 836 | CLA  | CHD-C4C | 3.58  | 1.47        | 1.39     |
| 11  | bB    | 826 | CLA  | CHD-C1D | 3.58  | 1.45        | 1.38     |
| 11  | bB    | 811 | CLA  | CHC-C4B | 3.58  | 1.47        | 1.39     |
| 11  | bK    | 103 | CLA  | CHC-C4B | 3.58  | 1.47        | 1.39     |
| 11  | aA    | 807 | CLA  | CHB-C1B | 3.58  | 1.47        | 1.39     |
| 11  | bB    | 816 | CLA  | CHC-C4B | 3.58  | 1.47        | 1.39     |
| 11  | bB    | 820 | CLA  | CHB-C1B | 3.58  | 1.47        | 1.39     |
| 11  | cB    | 803 | CLA  | CHD-C1D | 3.58  | 1.45        | 1.38     |
| 11  | cB    | 826 | CLA  | CHD-C1D | 3.58  | 1.45        | 1.38     |
| 11  | cA    | 818 | CLA  | C1B-NB  | -3.58 | 1.33        | 1.37     |
| 11  | aA    | 838 | CLA  | C3D-C2D | 3.58  | 1.48        | 1.39     |
| 11  | bA    | 822 | CLA  | C1B-NB  | -3.58 | 1.33        | 1.37     |
| 11  | aB    | 808 | CLA  | OBD-CAD | 3.58  | 1.28        | 1.22     |
| 11  | aA    | 839 | CLA  | C1B-NB  | -3.58 | 1.33        | 1.37     |
| 11  | cB    | 827 | CLA  | CHD-C4C | 3.58  | 1.47        | 1.39     |
| 11  | bB    | 826 | CLA  | C3D-C2D | 3.58  | 1.48        | 1.39     |
| 11  | aA    | 822 | CLA  | CHB-C1B | 3.58  | 1.47        | 1.39     |
| 11  | cB    | 807 | CLA  | CHB-C1B | 3.58  | 1.47        | 1.39     |
| 11  | bB    | 826 | CLA  | CHD-C4C | 3.58  | 1.47        | 1.39     |
| 11  | aA    | 816 | CLA  | C1B-NB  | -3.58 | 1.33        | 1.37     |
| 11  | bB    | 802 | CLA  | CHC-C4B | 3.58  | 1.47        | 1.39     |
| 11  | bA    | 822 | CLA  | CHB-C1B | 3.58  | 1.47        | 1.39     |
| 11  | aB    | 803 | CLA  | CHD-C4C | 3.58  | 1.47        | 1.39     |
| 12  | cA    | 832 | F6C  | CHC-C1C | 3.57  | 1.47        | 1.39     |
| 11  | aA    | 828 | CLA  | C3D-C2D | 3.57  | 1.48        | 1.39     |
| 11  | cA    | 838 | CLA  | C3D-C2D | 3.57  | 1.48        | 1.39     |
| 11  | aB    | 807 | CLA  | CHB-C1B | 3.57  | 1.47        | 1.39     |
| 11  | aA    | 815 | CLA  | OBD-CAD | 3.57  | 1.28        | 1.22     |
| 11  | cB    | 801 | CLA  | OBD-CAD | 3.57  | 1.28        | 1.22     |
| 11  | bB    | 823 | CLA  | C1B-NB  | -3.57 | 1.33        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | bL    | 206 | CLA  | CHB-C1B | 3.57  | 1.47        | 1.39     |
| 11  | cL    | 204 | CLA  | CHB-C1B | 3.57  | 1.47        | 1.39     |
| 11  | cA    | 828 | CLA  | CHB-C1B | 3.57  | 1.47        | 1.39     |
| 11  | cA    | 831 | CLA  | OBD-CAD | 3.57  | 1.28        | 1.22     |
| 12  | aA    | 844 | F6C  | C1D-ND  | 3.57  | 1.43        | 1.37     |
| 11  | aL    | 204 | CLA  | OBD-CAD | 3.57  | 1.28        | 1.22     |
| 11  | aA    | 821 | CLA  | CHC-C4B | 3.57  | 1.47        | 1.39     |
| 11  | cB    | 829 | CLA  | C1B-NB  | -3.57 | 1.33        | 1.37     |
| 11  | cL    | 205 | CLA  | C1B-NB  | -3.57 | 1.33        | 1.37     |
| 11  | aB    | 821 | CLA  | CHC-C4B | 3.57  | 1.47        | 1.39     |
| 11  | bB    | 821 | CLA  | CHC-C4B | 3.57  | 1.47        | 1.39     |
| 11  | cB    | 806 | CLA  | CHC-C4B | 3.57  | 1.47        | 1.39     |
| 11  | cB    | 820 | CLA  | CHB-C1B | 3.57  | 1.47        | 1.39     |
| 11  | aB    | 826 | CLA  | OBD-CAD | 3.57  | 1.28        | 1.22     |
| 11  | aA    | 818 | CLA  | CHD-C1D | 3.57  | 1.45        | 1.38     |
| 11  | bB    | 805 | CLA  | C1B-NB  | -3.57 | 1.33        | 1.37     |
| 11  | aB    | 817 | CLA  | OBD-CAD | 3.57  | 1.28        | 1.22     |
| 11  | bB    | 838 | CLA  | CHC-C4B | 3.57  | 1.47        | 1.39     |
| 11  | cB    | 821 | CLA  | CHC-C4B | 3.57  | 1.47        | 1.39     |
| 11  | bA    | 834 | CLA  | OBD-CAD | 3.57  | 1.28        | 1.22     |
| 11  | bB    | 840 | CLA  | CHB-C1B | 3.57  | 1.47        | 1.39     |
| 11  | bB    | 827 | CLA  | CHD-C4C | 3.57  | 1.47        | 1.39     |
| 12  | cB    | 824 | F6C  | C1D-ND  | 3.57  | 1.43        | 1.37     |
| 11  | cB    | 828 | CLA  | CHB-C1B | 3.57  | 1.47        | 1.39     |
| 11  | bB    | 808 | CLA  | OBD-CAD | 3.57  | 1.28        | 1.22     |
| 11  | aL    | 205 | CLA  | C1B-NB  | -3.57 | 1.33        | 1.37     |
| 11  | bB    | 823 | CLA  | OBD-CAD | 3.57  | 1.28        | 1.22     |
| 11  | aB    | 826 | CLA  | CHD-C1D | 3.57  | 1.45        | 1.38     |
| 11  | aB    | 838 | CLA  | CHC-C4B | 3.57  | 1.47        | 1.39     |
| 11  | bA    | 819 | CLA  | C1B-NB  | -3.57 | 1.33        | 1.37     |
| 11  | bA    | 828 | CLA  | CHB-C1B | 3.57  | 1.47        | 1.39     |
| 11  | cB    | 826 | CLA  | C3D-C2D | 3.57  | 1.48        | 1.39     |
| 11  | bB    | 819 | CLA  | CHC-C4B | 3.57  | 1.47        | 1.39     |
| 11  | cA    | 816 | CLA  | C1B-NB  | -3.57 | 1.33        | 1.37     |
| 11  | cA    | 818 | CLA  | OBD-CAD | 3.57  | 1.28        | 1.22     |
| 11  | aB    | 840 | CLA  | CHB-C1B | 3.56  | 1.47        | 1.39     |
| 11  | aA    | 823 | CLA  | CHB-C1B | 3.56  | 1.47        | 1.39     |
| 11  | aA    | 818 | CLA  | C1B-NB  | -3.56 | 1.33        | 1.37     |
| 11  | aB    | 819 | CLA  | CHB-C1B | 3.56  | 1.47        | 1.39     |
| 12  | bA    | 832 | F6C  | CHC-C1C | 3.56  | 1.47        | 1.39     |
| 11  | cA    | 839 | CLA  | CHB-C1B | 3.56  | 1.47        | 1.39     |
| 11  | cB    | 819 | CLA  | CHB-C1B | 3.56  | 1.47        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | bB    | 830 | CLA  | CHC-C4B | 3.56  | 1.47        | 1.39     |
| 11  | cA    | 819 | CLA  | C1B-NB  | -3.56 | 1.33        | 1.37     |
| 11  | bA    | 818 | CLA  | OBD-CAD | 3.56  | 1.28        | 1.22     |
| 11  | cA    | 818 | CLA  | CHD-C1D | 3.56  | 1.45        | 1.38     |
| 12  | aA    | 826 | F6C  | C1D-ND  | 3.56  | 1.43        | 1.37     |
| 11  | cB    | 822 | CLA  | OBD-CAD | 3.56  | 1.28        | 1.22     |
| 11  | aK    | 103 | CLA  | CHC-C4B | 3.56  | 1.47        | 1.39     |
| 11  | bA    | 816 | CLA  | C1B-NB  | -3.56 | 1.33        | 1.37     |
| 11  | aA    | 831 | CLA  | OBD-CAD | 3.56  | 1.28        | 1.22     |
| 11  | cA    | 821 | CLA  | CHC-C4B | 3.56  | 1.47        | 1.39     |
| 11  | cB    | 823 | CLA  | OBD-CAD | 3.56  | 1.28        | 1.22     |
| 11  | cB    | 826 | CLA  | OBD-CAD | 3.56  | 1.28        | 1.22     |
| 11  | aA    | 823 | CLA  | C1B-NB  | -3.56 | 1.33        | 1.37     |
| 11  | cA    | 839 | CLA  | C1B-NB  | -3.56 | 1.33        | 1.37     |
| 11  | cA    | 823 | CLA  | CHB-C1B | 3.56  | 1.47        | 1.39     |
| 11  | cL    | 206 | CLA  | CHB-C1B | 3.56  | 1.47        | 1.39     |
| 11  | aB    | 830 | CLA  | C1B-NB  | -3.56 | 1.33        | 1.37     |
| 12  | aA    | 832 | F6C  | CHC-C1C | 3.56  | 1.47        | 1.39     |
| 11  | aA    | 828 | CLA  | CHD-C4C | 3.55  | 1.47        | 1.39     |
| 11  | cA    | 828 | CLA  | CHD-C4C | 3.55  | 1.47        | 1.39     |
| 11  | aA    | 818 | CLA  | CHD-C4C | 3.55  | 1.47        | 1.39     |
| 11  | aB    | 813 | CLA  | OBD-CAD | 3.55  | 1.28        | 1.22     |
| 12  | cA    | 830 | F6C  | CHC-C1C | 3.55  | 1.47        | 1.39     |
| 11  | aB    | 816 | CLA  | C1B-NB  | -3.55 | 1.33        | 1.37     |
| 11  | cB    | 819 | CLA  | C1B-NB  | -3.55 | 1.33        | 1.37     |
| 11  | bA    | 821 | CLA  | CHC-C4B | 3.55  | 1.47        | 1.39     |
| 11  | cB    | 840 | CLA  | CHB-C1B | 3.55  | 1.47        | 1.39     |
| 11  | bB    | 803 | CLA  | C1D-ND  | 3.55  | 1.42        | 1.37     |
| 11  | aA    | 836 | CLA  | CHD-C4C | 3.55  | 1.47        | 1.39     |
| 11  | bA    | 843 | CLA  | CHC-C4B | 3.55  | 1.47        | 1.39     |
| 11  | cA    | 843 | CLA  | CHC-C4B | 3.55  | 1.47        | 1.39     |
| 11  | bA    | 816 | CLA  | OBD-CAD | 3.55  | 1.28        | 1.22     |
| 12  | aB    | 824 | F6C  | OBD-CAD | 3.55  | 1.28        | 1.22     |
| 11  | cB    | 812 | CLA  | CHB-C1B | 3.55  | 1.47        | 1.39     |
| 11  | bK    | 103 | CLA  | CHB-C1B | 3.55  | 1.47        | 1.39     |
| 12  | bA    | 826 | F6C  | C1D-ND  | 3.54  | 1.43        | 1.37     |
| 11  | aB    | 823 | CLA  | OBD-CAD | 3.54  | 1.28        | 1.22     |
| 11  | aB    | 826 | CLA  | CHD-C4C | 3.54  | 1.47        | 1.39     |
| 11  | aB    | 806 | CLA  | CHC-C4B | 3.54  | 1.47        | 1.39     |
| 11  | cA    | 818 | CLA  | CHD-C4C | 3.54  | 1.47        | 1.39     |
| 11  | bA    | 818 | CLA  | C1B-NB  | -3.54 | 1.33        | 1.37     |
| 11  | bA    | 840 | CLA  | OBD-CAD | 3.54  | 1.28        | 1.22     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | aB    | 819 | CLA  | CHC-C4B | 3.54  | 1.47        | 1.39     |
| 11  | aA    | 840 | CLA  | OBD-CAD | 3.54  | 1.28        | 1.22     |
| 11  | cA    | 836 | CLA  | CHD-C4C | 3.54  | 1.47        | 1.39     |
| 11  | aA    | 834 | CLA  | OBD-CAD | 3.54  | 1.28        | 1.22     |
| 11  | bA    | 839 | CLA  | CHB-C1B | 3.54  | 1.47        | 1.39     |
| 11  | aB    | 826 | CLA  | C3D-C2D | 3.54  | 1.48        | 1.39     |
| 11  | bA    | 823 | CLA  | CHB-C1B | 3.54  | 1.47        | 1.39     |
| 12  | bA    | 830 | F6C  | CHC-C1C | 3.54  | 1.47        | 1.39     |
| 11  | bB    | 819 | CLA  | C1B-NB  | -3.54 | 1.33        | 1.37     |
| 11  | cA    | 821 | CLA  | C1B-NB  | -3.54 | 1.33        | 1.37     |
| 11  | cB    | 831 | CLA  | CHC-C4B | 3.54  | 1.47        | 1.39     |
| 12  | aB    | 824 | F6C  | C1D-ND  | 3.54  | 1.43        | 1.37     |
| 11  | cB    | 803 | CLA  | C1D-ND  | 3.54  | 1.42        | 1.37     |
| 11  | bA    | 838 | CLA  | C3D-C2D | 3.54  | 1.48        | 1.39     |
| 11  | aA    | 824 | CLA  | OBD-CAD | 3.54  | 1.28        | 1.22     |
| 11  | bB    | 830 | CLA  | C1B-NB  | -3.54 | 1.33        | 1.37     |
| 11  | aB    | 827 | CLA  | CHD-C4C | 3.54  | 1.47        | 1.39     |
| 11  | aA    | 816 | CLA  | OBD-CAD | 3.54  | 1.28        | 1.22     |
| 11  | bB    | 807 | CLA  | CHB-C1B | 3.54  | 1.47        | 1.39     |
| 11  | bL    | 204 | CLA  | CHB-C1B | 3.54  | 1.47        | 1.39     |
| 11  | cB    | 806 | CLA  | CHB-C1B | 3.54  | 1.47        | 1.39     |
| 11  | cK    | 103 | CLA  | CHC-C4B | 3.53  | 1.47        | 1.39     |
| 11  | cB    | 838 | CLA  | CHC-C4B | 3.53  | 1.47        | 1.39     |
| 11  | cA    | 834 | CLA  | OBD-CAD | 3.53  | 1.28        | 1.22     |
| 11  | aA    | 810 | CLA  | CHC-C4B | 3.53  | 1.47        | 1.39     |
| 11  | cB    | 822 | CLA  | CHB-C1B | 3.53  | 1.47        | 1.39     |
| 11  | bA    | 820 | CLA  | OBD-CAD | 3.53  | 1.28        | 1.22     |
| 11  | cB    | 801 | CLA  | C3D-C2D | 3.53  | 1.48        | 1.39     |
| 11  | aB    | 829 | CLA  | C1B-NB  | -3.53 | 1.33        | 1.37     |
| 11  | bA    | 805 | CLA  | C1B-NB  | -3.53 | 1.33        | 1.37     |
| 11  | aB    | 831 | CLA  | CHC-C4B | 3.53  | 1.47        | 1.39     |
| 11  | aB    | 812 | CLA  | C1B-NB  | -3.53 | 1.33        | 1.37     |
| 11  | aA    | 803 | CLA  | CHC-C4B | 3.53  | 1.47        | 1.39     |
| 11  | aK    | 103 | CLA  | CHB-C1B | 3.53  | 1.47        | 1.39     |
| 11  | aA    | 834 | CLA  | CHB-C1B | 3.53  | 1.47        | 1.39     |
| 11  | bA    | 828 | CLA  | CHD-C4C | 3.53  | 1.47        | 1.39     |
| 12  | cA    | 826 | F6C  | C1D-ND  | 3.53  | 1.43        | 1.37     |
| 11  | aA    | 838 | CLA  | CHB-C1B | 3.53  | 1.47        | 1.39     |
| 11  | aA    | 843 | CLA  | CHC-C4B | 3.53  | 1.47        | 1.39     |
| 11  | aB    | 806 | CLA  | CHB-C1B | 3.53  | 1.47        | 1.39     |
| 11  | aA    | 818 | CLA  | OBD-CAD | 3.53  | 1.28        | 1.22     |
| 11  | bB    | 828 | CLA  | CHB-C1B | 3.53  | 1.47        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | bB    | 829 | CLA  | CHB-C1B | 3.52  | 1.47        | 1.39     |
| 11  | bB    | 830 | CLA  | OBD-CAD | 3.52  | 1.28        | 1.22     |
| 12  | aA    | 830 | F6C  | CHC-C1C | 3.52  | 1.47        | 1.39     |
| 11  | bB    | 829 | CLA  | C1B-NB  | -3.52 | 1.33        | 1.37     |
| 11  | bB    | 822 | CLA  | CHB-C1B | 3.52  | 1.47        | 1.39     |
| 11  | bA    | 818 | CLA  | CHD-C4C | 3.52  | 1.47        | 1.39     |
| 11  | aB    | 822 | CLA  | CHB-C1B | 3.52  | 1.47        | 1.39     |
| 11  | aL    | 204 | CLA  | CHB-C1B | 3.52  | 1.47        | 1.39     |
| 11  | cB    | 838 | CLA  | C1B-NB  | -3.52 | 1.33        | 1.37     |
| 11  | bA    | 810 | CLA  | CHC-C4B | 3.52  | 1.47        | 1.39     |
| 11  | cA    | 810 | CLA  | CHC-C4B | 3.52  | 1.47        | 1.39     |
| 11  | cB    | 830 | CLA  | CHC-C4B | 3.52  | 1.47        | 1.39     |
| 11  | cA    | 838 | CLA  | CHB-C1B | 3.52  | 1.47        | 1.39     |
| 12  | bB    | 824 | F6C  | C1D-ND  | 3.52  | 1.43        | 1.37     |
| 11  | aB    | 810 | CLA  | CHB-C1B | 3.52  | 1.47        | 1.39     |
| 11  | cK    | 103 | CLA  | CHB-C1B | 3.52  | 1.47        | 1.39     |
| 11  | aB    | 812 | CLA  | CHB-C1B | 3.51  | 1.47        | 1.39     |
| 11  | cB    | 830 | CLA  | OBD-CAD | 3.51  | 1.28        | 1.22     |
| 11  | aB    | 829 | CLA  | CHB-C1B | 3.51  | 1.47        | 1.39     |
| 11  | cA    | 834 | CLA  | CHB-C1B | 3.51  | 1.47        | 1.39     |
| 10  | aA    | 801 | CL0  | CHB-C4A | -3.51 | 1.34        | 1.38     |
| 11  | aB    | 804 | CLA  | CHB-C1B | 3.51  | 1.47        | 1.39     |
| 11  | bB    | 831 | CLA  | CHC-C4B | 3.51  | 1.47        | 1.39     |
| 11  | cB    | 810 | CLA  | CHB-C1B | 3.51  | 1.47        | 1.39     |
| 11  | aB    | 828 | CLA  | CHB-C1B | 3.51  | 1.47        | 1.39     |
| 11  | aB    | 809 | CLA  | CHB-C1B | 3.51  | 1.47        | 1.39     |
| 11  | aA    | 840 | CLA  | C1B-NB  | -3.51 | 1.33        | 1.37     |
| 11  | aB    | 810 | CLA  | OBD-CAD | 3.51  | 1.28        | 1.22     |
| 11  | aB    | 830 | CLA  | OBD-CAD | 3.51  | 1.28        | 1.22     |
| 11  | bB    | 813 | CLA  | OBD-CAD | 3.51  | 1.28        | 1.22     |
| 11  | bB    | 823 | CLA  | CHC-C4B | 3.51  | 1.47        | 1.39     |
| 11  | bL    | 205 | CLA  | CHC-C4B | 3.51  | 1.47        | 1.39     |
| 11  | aB    | 803 | CLA  | C1D-ND  | 3.51  | 1.42        | 1.37     |
| 11  | aB    | 802 | CLA  | CHC-C4B | 3.51  | 1.47        | 1.39     |
| 11  | bB    | 812 | CLA  | CHB-C1B | 3.51  | 1.47        | 1.39     |
| 11  | bA    | 831 | CLA  | OBD-CAD | 3.51  | 1.28        | 1.22     |
| 11  | aB    | 820 | CLA  | CHC-C4B | 3.51  | 1.47        | 1.39     |
| 11  | aB    | 830 | CLA  | CHC-C4B | 3.51  | 1.47        | 1.39     |
| 11  | bA    | 823 | CLA  | C1B-NB  | -3.51 | 1.33        | 1.37     |
| 11  | bA    | 839 | CLA  | C1B-NB  | -3.51 | 1.33        | 1.37     |
| 11  | bA    | 838 | CLA  | CHB-C1B | 3.50  | 1.47        | 1.39     |
| 11  | cB    | 829 | CLA  | CHB-C1B | 3.50  | 1.47        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | cB    | 804 | CLA  | CHB-C1B | 3.50  | 1.47        | 1.39     |
| 11  | aB    | 839 | CLA  | CHB-C1B | 3.50  | 1.47        | 1.39     |
| 11  | bB    | 806 | CLA  | CHB-C1B | 3.50  | 1.47        | 1.39     |
| 11  | cA    | 803 | CLA  | CHC-C4B | 3.50  | 1.47        | 1.39     |
| 11  | bB    | 801 | CLA  | C3D-C2D | 3.50  | 1.48        | 1.39     |
| 11  | cA    | 840 | CLA  | OBD-CAD | 3.50  | 1.28        | 1.22     |
| 11  | aB    | 801 | CLA  | C3D-C2D | 3.50  | 1.48        | 1.39     |
| 11  | bA    | 803 | CLA  | CHC-C4B | 3.50  | 1.47        | 1.39     |
| 11  | aB    | 837 | CLA  | C1B-NB  | -3.50 | 1.33        | 1.37     |
| 11  | cA    | 822 | CLA  | CHC-C4B | 3.50  | 1.47        | 1.39     |
| 11  | aA    | 807 | CLA  | C1B-NB  | -3.50 | 1.33        | 1.37     |
| 11  | cL    | 205 | CLA  | CHC-C4B | 3.50  | 1.47        | 1.39     |
| 11  | cB    | 823 | CLA  | CHC-C4B | 3.50  | 1.47        | 1.39     |
| 11  | bA    | 822 | CLA  | CHC-C4B | 3.50  | 1.47        | 1.39     |
| 11  | aA    | 818 | CLA  | CHB-C1B | 3.50  | 1.47        | 1.39     |
| 11  | bA    | 809 | CLA  | CHC-C4B | 3.49  | 1.47        | 1.39     |
| 11  | cA    | 837 | CLA  | C1B-NB  | -3.49 | 1.33        | 1.37     |
| 11  | bB    | 838 | CLA  | CHB-C1B | 3.49  | 1.47        | 1.39     |
| 11  | aA    | 842 | CLA  | C1B-NB  | -3.49 | 1.33        | 1.37     |
| 12  | cB    | 824 | F6C  | OBD-CAD | 3.49  | 1.28        | 1.22     |
| 11  | aA    | 836 | CLA  | CHB-C1B | 3.49  | 1.47        | 1.39     |
| 11  | bB    | 812 | CLA  | OBD-CAD | 3.49  | 1.28        | 1.22     |
| 11  | cB    | 834 | CLA  | CHB-C1B | 3.49  | 1.47        | 1.39     |
| 11  | aA    | 809 | CLA  | CHC-C4B | 3.49  | 1.47        | 1.39     |
| 11  | bA    | 836 | CLA  | CHB-C1B | 3.49  | 1.47        | 1.39     |
| 11  | cK    | 101 | CLA  | CHB-C1B | 3.49  | 1.47        | 1.39     |
| 11  | aA    | 837 | CLA  | C1B-NB  | -3.49 | 1.33        | 1.37     |
| 11  | bB    | 812 | CLA  | C1B-NB  | -3.49 | 1.33        | 1.37     |
| 11  | aA    | 833 | CLA  | CHB-C1B | 3.49  | 1.47        | 1.39     |
| 11  | bB    | 811 | CLA  | CHB-C1B | 3.49  | 1.47        | 1.39     |
| 11  | cB    | 802 | CLA  | CHC-C4B | 3.49  | 1.47        | 1.39     |
| 11  | bK    | 101 | CLA  | CHB-C1B | 3.49  | 1.47        | 1.39     |
| 11  | aB    | 827 | CLA  | C1D-ND  | 3.49  | 1.42        | 1.37     |
| 11  | bB    | 839 | CLA  | CHB-C1B | 3.49  | 1.47        | 1.39     |
| 11  | bA    | 809 | CLA  | C1B-NB  | -3.49 | 1.33        | 1.37     |
| 11  | cA    | 807 | CLA  | C1B-NB  | -3.49 | 1.33        | 1.37     |
| 11  | cB    | 813 | CLA  | OBD-CAD | 3.49  | 1.28        | 1.22     |
| 11  | bB    | 837 | CLA  | C1B-NB  | -3.49 | 1.33        | 1.37     |
| 11  | aK    | 101 | CLA  | CHB-C1B | 3.49  | 1.47        | 1.39     |
| 11  | bA    | 824 | CLA  | OBD-CAD | 3.49  | 1.28        | 1.22     |
| 11  | cB    | 813 | CLA  | C1B-NB  | -3.49 | 1.33        | 1.37     |
| 11  | cA    | 838 | CLA  | CHC-C4B | 3.48  | 1.47        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | bB    | 813 | CLA  | C1B-NB  | -3.48 | 1.33        | 1.37     |
| 11  | bB    | 809 | CLA  | CHB-C1B | 3.48  | 1.47        | 1.39     |
| 11  | bA    | 807 | CLA  | C1B-NB  | -3.48 | 1.33        | 1.37     |
| 11  | cA    | 824 | CLA  | OBD-CAD | 3.48  | 1.28        | 1.22     |
| 11  | cB    | 802 | CLA  | OBD-CAD | 3.48  | 1.28        | 1.22     |
| 11  | bB    | 832 | CLA  | CHB-C1B | 3.48  | 1.47        | 1.39     |
| 11  | aA    | 807 | CLA  | OBD-CAD | 3.48  | 1.28        | 1.22     |
| 12  | bB    | 824 | F6C  | C3C-C2C | 3.48  | 1.48        | 1.38     |
| 11  | bB    | 838 | CLA  | C1B-NB  | -3.48 | 1.33        | 1.37     |
| 11  | cB    | 812 | CLA  | OBD-CAD | 3.48  | 1.28        | 1.22     |
| 12  | bB    | 824 | F6C  | OBD-CAD | 3.48  | 1.28        | 1.22     |
| 11  | aB    | 806 | CLA  | C1B-NB  | -3.48 | 1.33        | 1.37     |
| 11  | aB    | 834 | CLA  | CHB-C1B | 3.48  | 1.47        | 1.39     |
| 12  | cL    | 202 | F6C  | CHB-C1B | 3.48  | 1.47        | 1.39     |
| 11  | cA    | 812 | CLA  | CHC-C4B | 3.48  | 1.47        | 1.39     |
| 11  | aB    | 838 | CLA  | C1B-NB  | -3.48 | 1.33        | 1.37     |
| 11  | bA    | 828 | CLA  | CHC-C4B | 3.48  | 1.47        | 1.39     |
| 11  | cA    | 818 | CLA  | CHB-C1B | 3.48  | 1.47        | 1.39     |
| 11  | bB    | 837 | CLA  | CHB-C1B | 3.48  | 1.47        | 1.39     |
| 12  | aL    | 202 | F6C  | CHB-C1B | 3.48  | 1.47        | 1.39     |
| 11  | bB    | 826 | CLA  | CHB-C1B | 3.48  | 1.47        | 1.39     |
| 11  | cB    | 811 | CLA  | CHB-C1B | 3.48  | 1.47        | 1.39     |
| 11  | cB    | 809 | CLA  | CHB-C1B | 3.48  | 1.47        | 1.39     |
| 11  | bB    | 808 | CLA  | CHD-C4C | 3.48  | 1.47        | 1.39     |
| 12  | bL    | 202 | F6C  | CHB-C1B | 3.48  | 1.47        | 1.39     |
| 11  | aL    | 206 | CLA  | C1B-NB  | -3.47 | 1.33        | 1.37     |
| 11  | aA    | 813 | CLA  | CHB-C1B | 3.47  | 1.47        | 1.39     |
| 11  | cB    | 839 | CLA  | CHB-C1B | 3.47  | 1.47        | 1.39     |
| 11  | bA    | 834 | CLA  | CHB-C1B | 3.47  | 1.47        | 1.39     |
| 11  | cB    | 810 | CLA  | OBD-CAD | 3.47  | 1.28        | 1.22     |
| 11  | aB    | 820 | CLA  | C1B-NB  | -3.47 | 1.33        | 1.37     |
| 11  | aL    | 205 | CLA  | CHC-C4B | 3.47  | 1.47        | 1.39     |
| 11  | cL    | 206 | CLA  | CHC-C4B | 3.47  | 1.47        | 1.39     |
| 11  | cB    | 826 | CLA  | CHC-C4B | 3.47  | 1.47        | 1.39     |
| 11  | cB    | 812 | CLA  | C1B-NB  | -3.47 | 1.33        | 1.37     |
| 11  | aB    | 813 | CLA  | C1B-NB  | -3.47 | 1.33        | 1.37     |
| 11  | bB    | 803 | CLA  | C4B-NB  | -3.47 | 1.33        | 1.37     |
| 11  | bA    | 838 | CLA  | CHC-C4B | 3.47  | 1.47        | 1.39     |
| 11  | cB    | 803 | CLA  | C4B-NB  | -3.47 | 1.33        | 1.37     |
| 11  | bB    | 804 | CLA  | CHB-C1B | 3.47  | 1.47        | 1.39     |
| 11  | cA    | 842 | CLA  | C1B-NB  | -3.47 | 1.33        | 1.37     |
| 11  | cB    | 837 | CLA  | C1B-NB  | -3.47 | 1.33        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | cB    | 820 | CLA  | CHC-C4B | 3.47  | 1.47        | 1.39     |
| 11  | aB    | 814 | CLA  | OBD-CAD | 3.47  | 1.28        | 1.22     |
| 11  | bA    | 842 | CLA  | C1B-NB  | -3.47 | 1.33        | 1.37     |
| 11  | cB    | 808 | CLA  | CHD-C4C | 3.47  | 1.47        | 1.39     |
| 11  | bA    | 807 | CLA  | CHC-C4B | 3.47  | 1.47        | 1.39     |
| 11  | aA    | 822 | CLA  | CHC-C4B | 3.47  | 1.47        | 1.39     |
| 12  | aB    | 824 | F6C  | C3C-C2C | 3.47  | 1.47        | 1.38     |
| 11  | cA    | 833 | CLA  | CHC-C4B | 3.47  | 1.47        | 1.39     |
| 11  | bA    | 818 | CLA  | CHB-C1B | 3.47  | 1.47        | 1.39     |
| 11  | bB    | 810 | CLA  | CHB-C1B | 3.47  | 1.47        | 1.39     |
| 11  | bA    | 808 | CLA  | CHC-C4B | 3.46  | 1.47        | 1.39     |
| 12  | bA    | 832 | F6C  | C3C-C2C | 3.46  | 1.47        | 1.38     |
| 11  | cB    | 827 | CLA  | C1D-ND  | 3.46  | 1.42        | 1.37     |
| 11  | cA    | 809 | CLA  | CHC-C4B | 3.46  | 1.47        | 1.39     |
| 11  | aA    | 811 | CLA  | CHC-C4B | 3.46  | 1.47        | 1.39     |
| 11  | cB    | 814 | CLA  | OBD-CAD | 3.46  | 1.28        | 1.22     |
| 11  | aA    | 838 | CLA  | CHC-C4B | 3.46  | 1.47        | 1.39     |
| 11  | bA    | 833 | CLA  | CHB-C1B | 3.46  | 1.47        | 1.39     |
| 11  | bB    | 834 | CLA  | CHB-C1B | 3.46  | 1.47        | 1.39     |
| 11  | cA    | 833 | CLA  | CHB-C1B | 3.46  | 1.47        | 1.39     |
| 12  | cB    | 824 | F6C  | C3C-C2C | 3.46  | 1.47        | 1.38     |
| 11  | cB    | 837 | CLA  | CHB-C1B | 3.46  | 1.47        | 1.39     |
| 11  | aB    | 826 | CLA  | CHB-C1B | 3.46  | 1.47        | 1.39     |
| 11  | aB    | 837 | CLA  | CHB-C1B | 3.46  | 1.47        | 1.39     |
| 11  | aB    | 823 | CLA  | CHC-C4B | 3.46  | 1.47        | 1.39     |
| 11  | bB    | 810 | CLA  | OBD-CAD | 3.46  | 1.28        | 1.22     |
| 11  | cA    | 836 | CLA  | CHB-C1B | 3.46  | 1.47        | 1.39     |
| 11  | bK    | 103 | CLA  | C1B-NB  | -3.46 | 1.33        | 1.37     |
| 11  | cA    | 835 | CLA  | C1B-NB  | -3.46 | 1.33        | 1.37     |
| 11  | cA    | 834 | CLA  | C1B-NB  | -3.46 | 1.33        | 1.37     |
| 11  | aB    | 812 | CLA  | OBD-CAD | 3.46  | 1.28        | 1.22     |
| 11  | aA    | 843 | CLA  | CHB-C1B | 3.46  | 1.47        | 1.39     |
| 11  | aB    | 808 | CLA  | CHD-C4C | 3.46  | 1.47        | 1.39     |
| 12  | cB    | 824 | F6C  | CHC-C1C | 3.46  | 1.47        | 1.39     |
| 12  | bB    | 824 | F6C  | CHC-C1C | 3.45  | 1.47        | 1.39     |
| 11  | aB    | 831 | CLA  | C1B-NB  | -3.45 | 1.33        | 1.37     |
| 11  | cA    | 814 | CLA  | C1B-NB  | -3.45 | 1.33        | 1.37     |
| 11  | cB    | 813 | CLA  | CHB-C1B | 3.45  | 1.47        | 1.39     |
| 11  | cB    | 801 | CLA  | CHD-C4C | 3.45  | 1.47        | 1.39     |
| 11  | aB    | 827 | CLA  | CHC-C4B | 3.45  | 1.47        | 1.39     |
| 11  | cA    | 843 | CLA  | CHB-C1B | 3.45  | 1.47        | 1.39     |
| 11  | cB    | 827 | CLA  | OBD-CAD | 3.45  | 1.28        | 1.22     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | aB    | 836 | CLA  | CHB-C1B | 3.45  | 1.47        | 1.39     |
| 11  | bA    | 841 | CLA  | CHB-C1B | 3.45  | 1.47        | 1.39     |
| 11  | bA    | 839 | CLA  | CHC-C4B | 3.45  | 1.47        | 1.39     |
| 11  | aB    | 811 | CLA  | CHB-C1B | 3.45  | 1.47        | 1.39     |
| 11  | bA    | 813 | CLA  | CHB-C1B | 3.45  | 1.47        | 1.39     |
| 11  | bA    | 843 | CLA  | CHB-C1B | 3.45  | 1.47        | 1.39     |
| 11  | aL    | 206 | CLA  | CHC-C4B | 3.45  | 1.47        | 1.39     |
| 12  | aB    | 824 | F6C  | CHC-C1C | 3.45  | 1.47        | 1.39     |
| 11  | cB    | 832 | CLA  | CHB-C1B | 3.45  | 1.47        | 1.39     |
| 11  | bB    | 814 | CLA  | C1B-NB  | -3.45 | 1.33        | 1.37     |
| 11  | cB    | 838 | CLA  | CHB-C1B | 3.45  | 1.47        | 1.39     |
| 11  | bA    | 840 | CLA  | C1B-NB  | -3.45 | 1.33        | 1.37     |
| 11  | bB    | 827 | CLA  | C1D-ND  | 3.45  | 1.42        | 1.37     |
| 11  | aA    | 837 | CLA  | CHB-C1B | 3.45  | 1.47        | 1.39     |
| 11  | cA    | 841 | CLA  | CHB-C1B | 3.45  | 1.47        | 1.39     |
| 12  | bA    | 827 | F6C  | C3C-C2C | 3.45  | 1.47        | 1.38     |
| 11  | cA    | 811 | CLA  | CHB-C1B | 3.45  | 1.47        | 1.39     |
| 11  | bB    | 823 | CLA  | CHB-C1B | 3.45  | 1.47        | 1.39     |
| 11  | bA    | 807 | CLA  | OBD-CAD | 3.44  | 1.28        | 1.22     |
| 11  | aA    | 828 | CLA  | CHC-C4B | 3.44  | 1.47        | 1.39     |
| 11  | cA    | 814 | CLA  | CHC-C4B | 3.44  | 1.47        | 1.39     |
| 11  | aK    | 103 | CLA  | C1B-NB  | -3.44 | 1.33        | 1.37     |
| 11  | cA    | 813 | CLA  | CHB-C1B | 3.44  | 1.47        | 1.39     |
| 11  | bB    | 801 | CLA  | CHD-C4C | 3.44  | 1.47        | 1.39     |
| 11  | cB    | 820 | CLA  | C1B-NB  | -3.44 | 1.33        | 1.37     |
| 11  | cA    | 839 | CLA  | CHC-C4B | 3.44  | 1.47        | 1.39     |
| 11  | bA    | 806 | CLA  | CHC-C4B | 3.44  | 1.47        | 1.39     |
| 10  | bA    | 801 | CL0  | CHB-C4A | -3.44 | 1.34        | 1.38     |
| 11  | bB    | 835 | CLA  | CHC-C4B | 3.44  | 1.47        | 1.39     |
| 11  | aA    | 811 | CLA  | CHB-C1B | 3.44  | 1.47        | 1.39     |
| 11  | aB    | 826 | CLA  | CHC-C4B | 3.44  | 1.47        | 1.39     |
| 11  | bL    | 206 | CLA  | CHC-C4B | 3.44  | 1.47        | 1.39     |
| 11  | aA    | 806 | CLA  | CHC-C4B | 3.44  | 1.47        | 1.39     |
| 11  | bB    | 820 | CLA  | CHC-C4B | 3.44  | 1.47        | 1.39     |
| 11  | aA    | 808 | CLA  | CHC-C4B | 3.44  | 1.47        | 1.39     |
| 11  | aA    | 812 | CLA  | CHC-C4B | 3.44  | 1.47        | 1.39     |
| 11  | aA    | 803 | CLA  | C1D-ND  | 3.44  | 1.42        | 1.37     |
| 11  | bA    | 834 | CLA  | C1B-NB  | -3.44 | 1.33        | 1.37     |
| 11  | cA    | 841 | CLA  | C1B-NB  | -3.44 | 1.33        | 1.37     |
| 11  | bA    | 811 | CLA  | CHC-C4B | 3.44  | 1.47        | 1.39     |
| 11  | bA    | 835 | CLA  | CHC-C4B | 3.44  | 1.47        | 1.39     |
| 11  | cA    | 816 | CLA  | CHB-C1B | 3.44  | 1.47        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12  | aA    | 844 | F6C  | C3C-C2C | 3.44  | 1.47        | 1.38     |
| 11  | bL    | 205 | CLA  | CHB-C1B | 3.44  | 1.47        | 1.39     |
| 11  | cA    | 823 | CLA  | CHC-C4B | 3.44  | 1.47        | 1.39     |
| 12  | bA    | 844 | F6C  | C3C-C2C | 3.43  | 1.47        | 1.38     |
| 11  | cA    | 807 | CLA  | CHC-C4B | 3.43  | 1.47        | 1.39     |
| 11  | cB    | 839 | CLA  | OBD-CAD | 3.43  | 1.28        | 1.22     |
| 11  | aA    | 807 | CLA  | CHC-C4B | 3.43  | 1.47        | 1.39     |
| 11  | bB    | 839 | CLA  | OBD-CAD | 3.43  | 1.28        | 1.22     |
| 11  | bB    | 826 | CLA  | CHC-C4B | 3.43  | 1.47        | 1.39     |
| 11  | cB    | 806 | CLA  | C1B-NB  | -3.43 | 1.33        | 1.37     |
| 11  | aB    | 802 | CLA  | OBD-CAD | 3.43  | 1.28        | 1.22     |
| 11  | aA    | 841 | CLA  | CHB-C1B | 3.43  | 1.47        | 1.39     |
| 11  | bA    | 814 | CLA  | C1B-NB  | -3.43 | 1.33        | 1.37     |
| 11  | bB    | 836 | CLA  | CHB-C1B | 3.43  | 1.47        | 1.39     |
| 11  | cB    | 826 | CLA  | CHB-C1B | 3.43  | 1.47        | 1.39     |
| 11  | aB    | 828 | CLA  | C3D-C2D | 3.43  | 1.48        | 1.39     |
| 11  | cA    | 835 | CLA  | CHC-C4B | 3.43  | 1.47        | 1.39     |
| 12  | cA    | 832 | F6C  | C3C-C2C | 3.43  | 1.47        | 1.38     |
| 11  | aA    | 814 | CLA  | CHC-C4B | 3.43  | 1.47        | 1.39     |
| 11  | bA    | 814 | CLA  | CHC-C4B | 3.43  | 1.47        | 1.39     |
| 11  | aB    | 839 | CLA  | OBD-CAD | 3.43  | 1.28        | 1.22     |
| 11  | aB    | 803 | CLA  | C4B-NB  | -3.43 | 1.33        | 1.37     |
| 11  | bB    | 813 | CLA  | CHB-C1B | 3.43  | 1.47        | 1.39     |
| 11  | bA    | 833 | CLA  | CHC-C4B | 3.43  | 1.47        | 1.39     |
| 11  | bB    | 815 | CLA  | CHB-C1B | 3.43  | 1.47        | 1.39     |
| 11  | aA    | 823 | CLA  | CHC-C4B | 3.43  | 1.47        | 1.39     |
| 11  | aA    | 833 | CLA  | CHC-C4B | 3.42  | 1.47        | 1.39     |
| 11  | aB    | 835 | CLA  | CHC-C4B | 3.42  | 1.47        | 1.39     |
| 11  | cA    | 837 | CLA  | CHB-C1B | 3.42  | 1.47        | 1.39     |
| 12  | cA    | 844 | F6C  | C3C-C2C | 3.42  | 1.47        | 1.38     |
| 11  | bB    | 814 | CLA  | OBD-CAD | 3.42  | 1.28        | 1.22     |
| 12  | aA    | 827 | F6C  | C3C-C2C | 3.42  | 1.47        | 1.38     |
| 11  | cA    | 828 | CLA  | CHC-C4B | 3.42  | 1.47        | 1.39     |
| 11  | cL    | 204 | CLA  | CHC-C4B | 3.42  | 1.47        | 1.39     |
| 11  | bA    | 837 | CLA  | C1B-NB  | -3.42 | 1.33        | 1.37     |
| 12  | cA    | 827 | F6C  | C3C-C2C | 3.42  | 1.47        | 1.38     |
| 11  | bA    | 812 | CLA  | CHC-C4B | 3.42  | 1.47        | 1.39     |
| 11  | aB    | 814 | CLA  | C1B-NB  | -3.42 | 1.33        | 1.37     |
| 11  | aB    | 801 | CLA  | CHD-C4C | 3.42  | 1.47        | 1.39     |
| 11  | aB    | 838 | CLA  | CHB-C1B | 3.42  | 1.47        | 1.39     |
| 11  | bB    | 827 | CLA  | CHC-C4B | 3.42  | 1.47        | 1.39     |
| 11  | aA    | 834 | CLA  | C1B-NB  | -3.42 | 1.33        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | aB    | 827 | CLA  | OBD-CAD | 3.42  | 1.28        | 1.22     |
| 11  | bB    | 811 | CLA  | C1B-NB  | -3.42 | 1.33        | 1.37     |
| 11  | cB    | 836 | CLA  | CHB-C1B | 3.42  | 1.47        | 1.39     |
| 11  | cA    | 808 | CLA  | CHC-C4B | 3.42  | 1.47        | 1.39     |
| 11  | cA    | 805 | CLA  | C1B-NB  | -3.42 | 1.33        | 1.37     |
| 11  | aB    | 813 | CLA  | CHB-C1B | 3.42  | 1.47        | 1.39     |
| 11  | bA    | 831 | CLA  | CHB-C1B | 3.42  | 1.47        | 1.39     |
| 11  | aB    | 832 | CLA  | CHB-C1B | 3.42  | 1.47        | 1.39     |
| 11  | cB    | 835 | CLA  | CHC-C4B | 3.42  | 1.47        | 1.39     |
| 11  | cA    | 814 | CLA  | CHB-C1B | 3.41  | 1.47        | 1.39     |
| 12  | aA    | 832 | F6C  | C3C-C2C | 3.41  | 1.47        | 1.38     |
| 11  | cA    | 811 | CLA  | CHC-C4B | 3.41  | 1.47        | 1.39     |
| 11  | bA    | 838 | CLA  | OBD-CAD | 3.41  | 1.28        | 1.22     |
| 11  | bA    | 837 | CLA  | CHB-C1B | 3.41  | 1.47        | 1.39     |
| 11  | bB    | 802 | CLA  | OBD-CAD | 3.41  | 1.28        | 1.22     |
| 10  | cA    | 801 | CL0  | CHB-C4A | -3.41 | 1.34        | 1.38     |
| 11  | bL    | 206 | CLA  | C1B-NB  | -3.41 | 1.33        | 1.37     |
| 11  | bA    | 811 | CLA  | CHB-C1B | 3.41  | 1.47        | 1.39     |
| 11  | cB    | 814 | CLA  | CHC-C4B | 3.41  | 1.47        | 1.39     |
| 11  | cB    | 827 | CLA  | CHC-C4B | 3.41  | 1.47        | 1.39     |
| 11  | cB    | 815 | CLA  | C1B-NB  | -3.41 | 1.33        | 1.37     |
| 11  | aA    | 835 | CLA  | CHC-C4B | 3.41  | 1.47        | 1.39     |
| 11  | aA    | 839 | CLA  | CHC-C4B | 3.41  | 1.47        | 1.39     |
| 11  | cB    | 828 | CLA  | C3D-C2D | 3.41  | 1.48        | 1.39     |
| 11  | bA    | 823 | CLA  | CHC-C4B | 3.41  | 1.47        | 1.39     |
| 11  | aL    | 205 | CLA  | CHB-C1B | 3.41  | 1.47        | 1.39     |
| 11  | cA    | 806 | CLA  | CHC-C4B | 3.41  | 1.47        | 1.39     |
| 11  | cA    | 807 | CLA  | OBD-CAD | 3.41  | 1.28        | 1.22     |
| 11  | cL    | 205 | CLA  | CHB-C1B | 3.41  | 1.47        | 1.39     |
| 11  | aK    | 101 | CLA  | C1B-NB  | -3.41 | 1.33        | 1.37     |
| 11  | cA    | 831 | CLA  | CHB-C1B | 3.41  | 1.47        | 1.39     |
| 11  | cK    | 103 | CLA  | C1B-NB  | -3.41 | 1.33        | 1.37     |
| 11  | cB    | 823 | CLA  | CHB-C1B | 3.41  | 1.47        | 1.39     |
| 12  | bL    | 202 | F6C  | CHC-C1C | 3.41  | 1.47        | 1.39     |
| 11  | bB    | 814 | CLA  | CHC-C4B | 3.41  | 1.47        | 1.39     |
| 11  | bB    | 806 | CLA  | C1B-NB  | -3.41 | 1.33        | 1.37     |
| 11  | cB    | 814 | CLA  | C1B-NB  | -3.41 | 1.33        | 1.37     |
| 11  | cB    | 815 | CLA  | CHB-C1B | 3.41  | 1.47        | 1.39     |
| 11  | cA    | 809 | CLA  | C1B-NB  | -3.41 | 1.33        | 1.37     |
| 11  | aA    | 816 | CLA  | CHB-C1B | 3.40  | 1.47        | 1.39     |
| 11  | cA    | 829 | CLA  | CHC-C4B | 3.40  | 1.47        | 1.39     |
| 11  | aA    | 808 | CLA  | CHB-C1B | 3.40  | 1.47        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | bB    | 838 | CLA  | OBD-CAD | 3.40  | 1.28        | 1.22     |
| 11  | aB    | 817 | CLA  | CHB-C1B | 3.40  | 1.47        | 1.39     |
| 11  | aB    | 815 | CLA  | CHB-C1B | 3.40  | 1.47        | 1.39     |
| 11  | bB    | 820 | CLA  | C1B-NB  | -3.40 | 1.33        | 1.37     |
| 12  | bL    | 202 | F6C  | C3C-C2C | 3.40  | 1.47        | 1.38     |
| 11  | aA    | 805 | CLA  | C1B-NB  | -3.40 | 1.33        | 1.37     |
| 11  | cB    | 838 | CLA  | OBD-CAD | 3.40  | 1.28        | 1.22     |
| 11  | aA    | 814 | CLA  | CHB-C1B | 3.40  | 1.47        | 1.39     |
| 11  | cB    | 804 | CLA  | C1B-NB  | -3.40 | 1.33        | 1.37     |
| 11  | bB    | 817 | CLA  | CHB-C1B | 3.40  | 1.47        | 1.39     |
| 12  | aL    | 202 | F6C  | C3C-C2C | 3.40  | 1.47        | 1.38     |
| 11  | aA    | 814 | CLA  | C1B-NB  | -3.40 | 1.33        | 1.37     |
| 11  | cB    | 817 | CLA  | CHB-C1B | 3.40  | 1.47        | 1.39     |
| 11  | bB    | 830 | CLA  | CHB-C1B | 3.39  | 1.47        | 1.39     |
| 11  | aA    | 829 | CLA  | CHC-C4B | 3.39  | 1.47        | 1.39     |
| 11  | bA    | 816 | CLA  | CHB-C1B | 3.39  | 1.47        | 1.39     |
| 11  | bA    | 841 | CLA  | C1B-NB  | -3.39 | 1.33        | 1.37     |
| 11  | aB    | 823 | CLA  | CHB-C1B | 3.39  | 1.47        | 1.39     |
| 11  | aA    | 808 | CLA  | C1B-NB  | -3.39 | 1.33        | 1.37     |
| 11  | bB    | 805 | CLA  | CHC-C4B | 3.39  | 1.47        | 1.39     |
| 11  | bA    | 814 | CLA  | CHB-C1B | 3.39  | 1.47        | 1.39     |
| 11  | bA    | 817 | CLA  | CHB-C1B | 3.39  | 1.47        | 1.39     |
| 11  | bL    | 204 | CLA  | CHC-C4B | 3.39  | 1.47        | 1.39     |
| 11  | bB    | 815 | CLA  | C1B-NB  | -3.39 | 1.33        | 1.37     |
| 11  | aB    | 838 | CLA  | OBD-CAD | 3.39  | 1.28        | 1.22     |
| 12  | cA    | 830 | F6C  | C3C-C2C | 3.39  | 1.47        | 1.38     |
| 11  | bA    | 829 | CLA  | CHC-C4B | 3.39  | 1.47        | 1.39     |
| 11  | aA    | 835 | CLA  | C1B-NB  | -3.39 | 1.33        | 1.37     |
| 11  | aA    | 819 | CLA  | CHB-C1B | 3.39  | 1.47        | 1.39     |
| 11  | cB    | 830 | CLA  | CHB-C1B | 3.39  | 1.47        | 1.39     |
| 11  | cA    | 828 | CLA  | C1B-NB  | -3.39 | 1.33        | 1.37     |
| 11  | cA    | 808 | CLA  | CHB-C1B | 3.38  | 1.47        | 1.39     |
| 11  | aB    | 825 | CLA  | C1B-NB  | -3.38 | 1.33        | 1.37     |
| 11  | aB    | 836 | CLA  | C1B-NB  | -3.38 | 1.33        | 1.37     |
| 12  | bA    | 830 | F6C  | C3C-C2C | 3.38  | 1.47        | 1.38     |
| 11  | bB    | 827 | CLA  | OBD-CAD | 3.38  | 1.28        | 1.22     |
| 11  | aA    | 831 | CLA  | CHB-C1B | 3.38  | 1.47        | 1.39     |
| 11  | cA    | 803 | CLA  | C1D-ND  | 3.38  | 1.42        | 1.37     |
| 11  | bB    | 801 | CLA  | CHC-C4B | 3.38  | 1.47        | 1.39     |
| 11  | bB    | 828 | CLA  | C3D-C2D | 3.38  | 1.48        | 1.39     |
| 11  | cB    | 811 | CLA  | C1B-NB  | -3.38 | 1.33        | 1.37     |
| 11  | cB    | 833 | CLA  | CHB-C1B | 3.38  | 1.47        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | bA    | 819 | CLA  | CHB-C1B | 3.38  | 1.47        | 1.39     |
| 12  | cL    | 202 | F6C  | CHC-C1C | 3.38  | 1.47        | 1.39     |
| 11  | bK    | 101 | CLA  | C1B-NB  | -3.38 | 1.33        | 1.37     |
| 11  | cA    | 825 | CLA  | CHC-C4B | 3.38  | 1.47        | 1.39     |
| 12  | cL    | 202 | F6C  | C3C-C2C | 3.38  | 1.47        | 1.38     |
| 11  | bA    | 803 | CLA  | C1D-ND  | 3.38  | 1.42        | 1.37     |
| 11  | aA    | 817 | CLA  | CHB-C1B | 3.38  | 1.47        | 1.39     |
| 11  | aB    | 815 | CLA  | C1B-NB  | -3.38 | 1.33        | 1.37     |
| 11  | aA    | 825 | CLA  | CHC-C4B | 3.38  | 1.47        | 1.39     |
| 11  | bB    | 804 | CLA  | C1B-NB  | -3.37 | 1.33        | 1.37     |
| 11  | aB    | 805 | CLA  | CHC-C4B | 3.37  | 1.47        | 1.39     |
| 11  | cK    | 101 | CLA  | C1B-NB  | -3.37 | 1.33        | 1.37     |
| 11  | aA    | 809 | CLA  | C1B-NB  | -3.37 | 1.33        | 1.37     |
| 11  | bA    | 835 | CLA  | C1B-NB  | -3.37 | 1.33        | 1.37     |
| 11  | bA    | 803 | CLA  | CHD-C1D | 3.37  | 1.45        | 1.38     |
| 11  | aB    | 814 | CLA  | CHC-C4B | 3.37  | 1.47        | 1.39     |
| 12  | aA    | 830 | F6C  | C3C-C2C | 3.37  | 1.47        | 1.38     |
| 11  | aB    | 818 | CLA  | CHB-C1B | 3.37  | 1.47        | 1.39     |
| 11  | aA    | 833 | CLA  | OBD-CAD | 3.37  | 1.28        | 1.22     |
| 11  | aL    | 204 | CLA  | CHC-C4B | 3.37  | 1.47        | 1.39     |
| 11  | cB    | 818 | CLA  | CHB-C1B | 3.37  | 1.47        | 1.39     |
| 11  | cB    | 827 | CLA  | CHB-C1B | 3.37  | 1.47        | 1.39     |
| 11  | cA    | 819 | CLA  | OBD-CAD | 3.37  | 1.28        | 1.22     |
| 11  | cB    | 836 | CLA  | C1B-NB  | -3.37 | 1.33        | 1.37     |
| 11  | bB    | 833 | CLA  | CHB-C1B | 3.37  | 1.47        | 1.39     |
| 11  | bB    | 831 | CLA  | C1B-NB  | -3.37 | 1.33        | 1.37     |
| 11  | bB    | 827 | CLA  | CHB-C1B | 3.37  | 1.47        | 1.39     |
| 11  | cL    | 206 | CLA  | C1B-NB  | -3.37 | 1.33        | 1.37     |
| 11  | aA    | 829 | CLA  | CHB-C1B | 3.37  | 1.47        | 1.39     |
| 11  | bB    | 825 | CLA  | C1B-NB  | -3.37 | 1.33        | 1.37     |
| 11  | aA    | 803 | CLA  | CHD-C1D | 3.37  | 1.45        | 1.38     |
| 11  | bA    | 825 | CLA  | CHB-C1B | 3.36  | 1.47        | 1.39     |
| 11  | bA    | 825 | CLA  | CHC-C4B | 3.36  | 1.47        | 1.39     |
| 11  | aA    | 819 | CLA  | OBD-CAD | 3.36  | 1.28        | 1.22     |
| 11  | cB    | 825 | CLA  | C1B-NB  | -3.36 | 1.33        | 1.37     |
| 11  | aB    | 827 | CLA  | CHB-C1B | 3.36  | 1.47        | 1.39     |
| 11  | aA    | 838 | CLA  | OBD-CAD | 3.36  | 1.28        | 1.22     |
| 11  | aA    | 824 | CLA  | CHB-C1B | 3.36  | 1.47        | 1.39     |
| 11  | cA    | 819 | CLA  | CHB-C1B | 3.36  | 1.47        | 1.39     |
| 11  | bA    | 812 | CLA  | C1B-NB  | -3.36 | 1.33        | 1.37     |
| 11  | cA    | 817 | CLA  | CHB-C1B | 3.36  | 1.47        | 1.39     |
| 11  | cB    | 812 | CLA  | CHC-C4B | 3.36  | 1.47        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | bA    | 833 | CLA  | OBD-CAD | 3.36  | 1.28        | 1.22     |
| 11  | cB    | 801 | CLA  | CHC-C4B | 3.36  | 1.46        | 1.39     |
| 11  | aB    | 801 | CLA  | CHC-C4B | 3.36  | 1.46        | 1.39     |
| 11  | cA    | 838 | CLA  | OBD-CAD | 3.36  | 1.28        | 1.22     |
| 11  | cA    | 803 | CLA  | CHD-C1D | 3.36  | 1.45        | 1.38     |
| 11  | bB    | 818 | CLA  | CHB-C1B | 3.36  | 1.46        | 1.39     |
| 11  | cA    | 825 | CLA  | CHB-C1B | 3.36  | 1.46        | 1.39     |
| 11  | bB    | 812 | CLA  | C4B-NB  | -3.36 | 1.33        | 1.37     |
| 11  | cA    | 829 | CLA  | CHB-C1B | 3.35  | 1.46        | 1.39     |
| 11  | aA    | 812 | CLA  | C1B-NB  | -3.35 | 1.33        | 1.37     |
| 11  | aB    | 804 | CLA  | C1B-NB  | -3.35 | 1.33        | 1.37     |
| 11  | bB    | 839 | CLA  | C3D-C2D | 3.35  | 1.48        | 1.39     |
| 11  | bA    | 819 | CLA  | OBD-CAD | 3.35  | 1.28        | 1.22     |
| 11  | aB    | 833 | CLA  | CHB-C1B | 3.35  | 1.46        | 1.39     |
| 11  | bA    | 829 | CLA  | CHB-C1B | 3.35  | 1.46        | 1.39     |
| 11  | bA    | 834 | CLA  | CHC-C4B | 3.35  | 1.46        | 1.39     |
| 12  | aL    | 202 | F6C  | CHC-C1C | 3.35  | 1.46        | 1.39     |
| 11  | cA    | 810 | CLA  | C1B-NB  | -3.35 | 1.33        | 1.37     |
| 11  | cB    | 831 | CLA  | C1B-NB  | -3.35 | 1.33        | 1.37     |
| 15  | bL    | 203 | BCR  | C1-C6   | -3.35 | 1.49        | 1.53     |
| 11  | aB    | 811 | CLA  | C1B-NB  | -3.35 | 1.33        | 1.37     |
| 11  | cA    | 833 | CLA  | OBD-CAD | 3.35  | 1.28        | 1.22     |
| 11  | cA    | 815 | CLA  | CHB-C1B | 3.35  | 1.46        | 1.39     |
| 11  | aB    | 830 | CLA  | CHB-C1B | 3.35  | 1.46        | 1.39     |
| 11  | aA    | 825 | CLA  | CHB-C1B | 3.35  | 1.46        | 1.39     |
| 11  | aA    | 834 | CLA  | CHC-C4B | 3.35  | 1.46        | 1.39     |
| 11  | bA    | 808 | CLA  | CHB-C1B | 3.35  | 1.46        | 1.39     |
| 11  | aB    | 840 | CLA  | CHC-C4B | 3.35  | 1.46        | 1.39     |
| 11  | aA    | 815 | CLA  | CHB-C1B | 3.35  | 1.46        | 1.39     |
| 11  | aB    | 812 | CLA  | CHC-C4B | 3.35  | 1.46        | 1.39     |
| 15  | aL    | 203 | BCR  | C1-C6   | -3.35 | 1.49        | 1.53     |
| 11  | aA    | 841 | CLA  | C1B-NB  | -3.35 | 1.33        | 1.37     |
| 11  | aB    | 813 | CLA  | CHC-C4B | 3.34  | 1.46        | 1.39     |
| 11  | bB    | 812 | CLA  | CHC-C4B | 3.34  | 1.46        | 1.39     |
| 11  | bB    | 835 | CLA  | C1B-NB  | -3.34 | 1.33        | 1.37     |
| 12  | aA    | 832 | F6C  | OBD-CAD | 3.34  | 1.28        | 1.22     |
| 11  | cA    | 834 | CLA  | CHC-C4B | 3.34  | 1.46        | 1.39     |
| 11  | cA    | 808 | CLA  | C1B-NB  | -3.34 | 1.33        | 1.37     |
| 11  | bA    | 828 | CLA  | C1B-NB  | -3.34 | 1.33        | 1.37     |
| 11  | aA    | 824 | CLA  | CHC-C4B | 3.34  | 1.46        | 1.39     |
| 11  | aB    | 812 | CLA  | C4B-NB  | -3.34 | 1.33        | 1.37     |
| 11  | bB    | 833 | CLA  | C1B-NB  | -3.34 | 1.33        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | cA    | 824 | CLA  | CHB-C1B | 3.34  | 1.46        | 1.39     |
| 11  | cA    | 842 | CLA  | CHB-C1B | 3.34  | 1.46        | 1.39     |
| 11  | aB    | 821 | CLA  | C1B-NB  | -3.34 | 1.33        | 1.37     |
| 11  | cB    | 839 | CLA  | C3D-C2D | 3.34  | 1.48        | 1.39     |
| 11  | bA    | 824 | CLA  | CHB-C1B | 3.33  | 1.46        | 1.39     |
| 11  | cB    | 813 | CLA  | CHC-C4B | 3.33  | 1.46        | 1.39     |
| 11  | cB    | 812 | CLA  | C4B-NB  | -3.33 | 1.33        | 1.37     |
| 11  | cB    | 805 | CLA  | CHC-C4B | 3.33  | 1.46        | 1.39     |
| 11  | aA    | 840 | CLA  | CHB-C1B | 3.33  | 1.46        | 1.39     |
| 11  | bA    | 808 | CLA  | C1B-NB  | -3.33 | 1.33        | 1.37     |
| 11  | bB    | 836 | CLA  | C1B-NB  | -3.33 | 1.33        | 1.37     |
| 11  | aB    | 814 | CLA  | CHB-C1B | 3.33  | 1.46        | 1.39     |
| 11  | aA    | 812 | CLA  | CHB-C1B | 3.33  | 1.46        | 1.39     |
| 15  | cL    | 203 | BCR  | C1-C6   | -3.33 | 1.49        | 1.53     |
| 11  | cA    | 838 | CLA  | C4B-NB  | -3.33 | 1.33        | 1.37     |
| 11  | cB    | 807 | CLA  | CHC-C4B | 3.33  | 1.46        | 1.39     |
| 11  | aA    | 810 | CLA  | C1B-NB  | -3.33 | 1.33        | 1.37     |
| 11  | cB    | 833 | CLA  | C1B-NB  | -3.33 | 1.33        | 1.37     |
| 11  | bA    | 840 | CLA  | CHB-C1B | 3.33  | 1.46        | 1.39     |
| 11  | bB    | 814 | CLA  | CHB-C1B | 3.33  | 1.46        | 1.39     |
| 11  | aB    | 833 | CLA  | C1B-NB  | -3.33 | 1.33        | 1.37     |
| 11  | bA    | 824 | CLA  | CHC-C4B | 3.33  | 1.46        | 1.39     |
| 11  | aB    | 831 | CLA  | CHB-C1B | 3.32  | 1.46        | 1.39     |
| 11  | cA    | 805 | CLA  | CHB-C1B | 3.32  | 1.46        | 1.39     |
| 11  | cA    | 824 | CLA  | CHC-C4B | 3.32  | 1.46        | 1.39     |
| 11  | cB    | 814 | CLA  | CHB-C1B | 3.32  | 1.46        | 1.39     |
| 11  | bA    | 812 | CLA  | CHB-C1B | 3.32  | 1.46        | 1.39     |
| 12  | cA    | 832 | F6C  | OBD-CAD | 3.32  | 1.28        | 1.22     |
| 11  | aA    | 828 | CLA  | C1B-NB  | -3.32 | 1.33        | 1.37     |
| 11  | cB    | 807 | CLA  | OBD-CAD | 3.32  | 1.28        | 1.22     |
| 11  | bB    | 807 | CLA  | CHC-C4B | 3.32  | 1.46        | 1.39     |
| 11  | bA    | 842 | CLA  | CHB-C1B | 3.32  | 1.46        | 1.39     |
| 11  | bB    | 821 | CLA  | C1B-NB  | -3.32 | 1.33        | 1.37     |
| 11  | bB    | 807 | CLA  | OBD-CAD | 3.32  | 1.28        | 1.22     |
| 11  | cB    | 835 | CLA  | C1B-NB  | -3.32 | 1.33        | 1.37     |
| 11  | aB    | 839 | CLA  | C3D-C2D | 3.32  | 1.48        | 1.39     |
| 11  | cB    | 837 | CLA  | OBD-CAD | 3.31  | 1.28        | 1.22     |
| 11  | aB    | 835 | CLA  | C1B-NB  | -3.31 | 1.33        | 1.37     |
| 11  | bB    | 822 | CLA  | C1B-NB  | -3.31 | 1.33        | 1.37     |
| 11  | bA    | 815 | CLA  | CHB-C1B | 3.31  | 1.46        | 1.39     |
| 11  | cB    | 840 | CLA  | CHC-C4B | 3.31  | 1.46        | 1.39     |
| 11  | aB    | 807 | CLA  | CHC-C4B | 3.31  | 1.46        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | cA    | 840 | CLA  | CHB-C1B | 3.31  | 1.46        | 1.39     |
| 11  | cA    | 812 | CLA  | CHB-C1B | 3.31  | 1.46        | 1.39     |
| 11  | cB    | 808 | CLA  | CHC-C4B | 3.31  | 1.46        | 1.39     |
| 12  | bA    | 832 | F6C  | OBD-CAD | 3.31  | 1.28        | 1.22     |
| 11  | bA    | 809 | CLA  | CHB-C1B | 3.31  | 1.46        | 1.39     |
| 11  | bB    | 834 | CLA  | CHC-C4B | 3.30  | 1.46        | 1.39     |
| 11  | cB    | 831 | CLA  | CHB-C1B | 3.30  | 1.46        | 1.39     |
| 11  | cB    | 834 | CLA  | CHC-C4B | 3.30  | 1.46        | 1.39     |
| 11  | bA    | 804 | CLA  | C1B-NB  | -3.30 | 1.33        | 1.37     |
| 11  | aB    | 808 | CLA  | CHC-C4B | 3.30  | 1.46        | 1.39     |
| 11  | bB    | 801 | CLA  | C1B-NB  | -3.30 | 1.33        | 1.37     |
| 11  | bA    | 805 | CLA  | CHB-C1B | 3.29  | 1.46        | 1.39     |
| 11  | aA    | 842 | CLA  | CHB-C1B | 3.29  | 1.46        | 1.39     |
| 11  | bB    | 831 | CLA  | CHB-C1B | 3.29  | 1.46        | 1.39     |
| 11  | bA    | 802 | CLA  | C4B-NB  | -3.29 | 1.33        | 1.37     |
| 11  | bA    | 810 | CLA  | C1B-NB  | -3.29 | 1.33        | 1.37     |
| 11  | cA    | 812 | CLA  | C1B-NB  | -3.29 | 1.33        | 1.37     |
| 11  | cB    | 817 | CLA  | CHC-C4B | 3.29  | 1.46        | 1.39     |
| 11  | bB    | 808 | CLA  | CHC-C4B | 3.29  | 1.46        | 1.39     |
| 11  | aB    | 837 | CLA  | OBD-CAD | 3.29  | 1.28        | 1.22     |
| 11  | bB    | 837 | CLA  | OBD-CAD | 3.29  | 1.28        | 1.22     |
| 11  | cA    | 817 | CLA  | CHC-C4B | 3.29  | 1.46        | 1.39     |
| 11  | bB    | 817 | CLA  | CHC-C4B | 3.29  | 1.46        | 1.39     |
| 11  | cB    | 832 | CLA  | C1B-NB  | -3.28 | 1.33        | 1.37     |
| 15  | aB    | 842 | BCR  | C1-C6   | -3.28 | 1.49        | 1.53     |
| 11  | aA    | 828 | CLA  | OBD-CAD | 3.28  | 1.28        | 1.22     |
| 11  | bB    | 832 | CLA  | C1B-NB  | -3.28 | 1.33        | 1.37     |
| 11  | aB    | 834 | CLA  | CHC-C4B | 3.28  | 1.46        | 1.39     |
| 11  | aB    | 817 | CLA  | CHC-C4B | 3.28  | 1.46        | 1.39     |
| 11  | bB    | 840 | CLA  | CHC-C4B | 3.28  | 1.46        | 1.39     |
| 11  | aB    | 807 | CLA  | OBD-CAD | 3.28  | 1.28        | 1.22     |
| 11  | bB    | 813 | CLA  | CHC-C4B | 3.28  | 1.46        | 1.39     |
| 11  | aA    | 809 | CLA  | CHB-C1B | 3.28  | 1.46        | 1.39     |
| 11  | cA    | 809 | CLA  | CHB-C1B | 3.28  | 1.46        | 1.39     |
| 11  | bB    | 810 | CLA  | CHC-C4B | 3.28  | 1.46        | 1.39     |
| 11  | aA    | 802 | CLA  | C4B-NB  | -3.28 | 1.33        | 1.37     |
| 11  | aB    | 801 | CLA  | C1B-NB  | -3.28 | 1.33        | 1.37     |
| 11  | aA    | 835 | CLA  | CHB-C1B | 3.27  | 1.46        | 1.39     |
| 11  | bA    | 835 | CLA  | CHB-C1B | 3.27  | 1.46        | 1.39     |
| 11  | cA    | 820 | CLA  | CHB-C1B | 3.27  | 1.46        | 1.39     |
| 11  | aB    | 808 | CLA  | CHB-C1B | 3.27  | 1.46        | 1.39     |
| 11  | bA    | 817 | CLA  | CHC-C4B | 3.27  | 1.46        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | aA    | 838 | CLA  | C4B-NB  | -3.27 | 1.33        | 1.37     |
| 11  | aA    | 804 | CLA  | C1B-NB  | -3.27 | 1.33        | 1.37     |
| 11  | cA    | 835 | CLA  | CHB-C1B | 3.27  | 1.46        | 1.39     |
| 11  | bA    | 838 | CLA  | C4B-NB  | -3.27 | 1.33        | 1.37     |
| 11  | cA    | 802 | CLA  | C4B-NB  | -3.26 | 1.33        | 1.37     |
| 15  | bA    | 848 | BCR  | C30-C25 | -3.26 | 1.49        | 1.53     |
| 11  | aA    | 820 | CLA  | CHB-C1B | 3.26  | 1.46        | 1.39     |
| 11  | cB    | 825 | CLA  | OBD-CAD | 3.26  | 1.28        | 1.22     |
| 15  | cB    | 842 | BCR  | C1-C6   | -3.26 | 1.49        | 1.53     |
| 11  | aB    | 816 | CLA  | CHB-C1B | 3.26  | 1.46        | 1.39     |
| 11  | aA    | 805 | CLA  | CHB-C1B | 3.25  | 1.46        | 1.39     |
| 11  | aB    | 817 | CLA  | C4B-NB  | -3.25 | 1.33        | 1.37     |
| 11  | aB    | 828 | CLA  | C4B-NB  | -3.25 | 1.33        | 1.37     |
| 11  | cB    | 816 | CLA  | CHB-C1B | 3.25  | 1.46        | 1.39     |
| 11  | aA    | 803 | CLA  | C4B-NB  | -3.25 | 1.33        | 1.37     |
| 15  | cA    | 848 | BCR  | C30-C25 | -3.25 | 1.49        | 1.53     |
| 11  | aB    | 810 | CLA  | CHC-C4B | 3.25  | 1.46        | 1.39     |
| 11  | cB    | 822 | CLA  | C1B-NB  | -3.25 | 1.33        | 1.37     |
| 11  | aA    | 817 | CLA  | CHC-C4B | 3.25  | 1.46        | 1.39     |
| 11  | bA    | 820 | CLA  | CHB-C1B | 3.25  | 1.46        | 1.39     |
| 11  | bB    | 825 | CLA  | OBD-CAD | 3.25  | 1.28        | 1.22     |
| 11  | cB    | 828 | CLA  | C4B-NB  | -3.25 | 1.33        | 1.37     |
| 11  | bA    | 828 | CLA  | OBD-CAD | 3.24  | 1.28        | 1.22     |
| 11  | cB    | 810 | CLA  | CHC-C4B | 3.24  | 1.46        | 1.39     |
| 11  | cA    | 804 | CLA  | C1B-NB  | -3.24 | 1.33        | 1.37     |
| 11  | cB    | 821 | CLA  | C1B-NB  | -3.24 | 1.33        | 1.37     |
| 11  | aB    | 822 | CLA  | C1B-NB  | -3.24 | 1.33        | 1.37     |
| 11  | bB    | 828 | CLA  | C4B-NB  | -3.24 | 1.33        | 1.37     |
| 15  | aA    | 848 | BCR  | C30-C25 | -3.23 | 1.49        | 1.53     |
| 11  | cB    | 808 | CLA  | CHB-C1B | 3.23  | 1.46        | 1.39     |
| 15  | aK    | 102 | BCR  | C1-C6   | -3.23 | 1.49        | 1.53     |
| 11  | bA    | 802 | CLA  | CHB-C1B | 3.22  | 1.46        | 1.39     |
| 11  | bB    | 808 | CLA  | CHB-C1B | 3.22  | 1.46        | 1.39     |
| 11  | aB    | 805 | CLA  | CHB-C1B | 3.22  | 1.46        | 1.39     |
| 11  | bB    | 816 | CLA  | CHB-C1B | 3.22  | 1.46        | 1.39     |
| 11  | cB    | 801 | CLA  | C1B-NB  | -3.22 | 1.33        | 1.37     |
| 11  | cB    | 809 | CLA  | C4B-NB  | -3.22 | 1.33        | 1.37     |
| 11  | aB    | 825 | CLA  | OBD-CAD | 3.22  | 1.28        | 1.22     |
| 11  | aA    | 820 | CLA  | CHC-C4B | 3.22  | 1.46        | 1.39     |
| 12  | cL    | 202 | F6C  | OBD-CAD | 3.21  | 1.28        | 1.22     |
| 15  | bK    | 102 | BCR  | C1-C6   | -3.21 | 1.49        | 1.53     |
| 11  | aB    | 832 | CLA  | C1B-NB  | -3.21 | 1.33        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12  | bL    | 202 | F6C  | OBD-CAD | 3.21  | 1.28        | 1.22     |
| 11  | aA    | 836 | CLA  | CHC-C4B | 3.21  | 1.46        | 1.39     |
| 11  | aB    | 807 | CLA  | C4B-NB  | -3.21 | 1.33        | 1.37     |
| 11  | cA    | 836 | CLA  | CHC-C4B | 3.20  | 1.46        | 1.39     |
| 11  | cB    | 805 | CLA  | CHB-C1B | 3.20  | 1.46        | 1.39     |
| 11  | bA    | 829 | CLA  | C4B-NB  | -3.20 | 1.33        | 1.37     |
| 11  | bB    | 809 | CLA  | C4B-NB  | -3.20 | 1.33        | 1.37     |
| 15  | bB    | 842 | BCR  | C1-C6   | -3.20 | 1.49        | 1.53     |
| 11  | aA    | 809 | CLA  | C4B-NB  | -3.20 | 1.33        | 1.37     |
| 11  | bA    | 820 | CLA  | CHC-C4B | 3.20  | 1.46        | 1.39     |
| 11  | bA    | 803 | CLA  | C4B-NB  | -3.20 | 1.33        | 1.37     |
| 11  | cA    | 803 | CLA  | C4B-NB  | -3.20 | 1.33        | 1.37     |
| 11  | cA    | 831 | CLA  | C4B-NB  | -3.20 | 1.33        | 1.37     |
| 11  | cA    | 828 | CLA  | OBD-CAD | 3.19  | 1.28        | 1.22     |
| 11  | cA    | 802 | CLA  | CHB-C1B | 3.19  | 1.46        | 1.39     |
| 11  | cA    | 815 | CLA  | CHC-C4B | 3.19  | 1.46        | 1.39     |
| 15  | cK    | 102 | BCR  | C1-C6   | -3.19 | 1.49        | 1.53     |
| 11  | aA    | 802 | CLA  | CHB-C1B | 3.19  | 1.46        | 1.39     |
| 11  | aB    | 809 | CLA  | C4B-NB  | -3.19 | 1.33        | 1.37     |
| 11  | bB    | 805 | CLA  | CHB-C1B | 3.19  | 1.46        | 1.39     |
| 11  | cL    | 204 | CLA  | C4B-NB  | -3.19 | 1.33        | 1.37     |
| 11  | bB    | 807 | CLA  | C4B-NB  | -3.18 | 1.33        | 1.37     |
| 11  | cA    | 820 | CLA  | CHC-C4B | 3.18  | 1.46        | 1.39     |
| 11  | bA    | 802 | CLA  | CHC-C4B | 3.18  | 1.46        | 1.39     |
| 11  | bA    | 815 | CLA  | CHC-C4B | 3.18  | 1.46        | 1.39     |
| 11  | cB    | 805 | CLA  | C4B-NB  | -3.18 | 1.33        | 1.37     |
| 11  | bA    | 828 | CLA  | C4B-NB  | -3.18 | 1.33        | 1.37     |
| 11  | aA    | 829 | CLA  | C4B-NB  | -3.18 | 1.33        | 1.37     |
| 11  | cA    | 815 | CLA  | C4B-NB  | -3.18 | 1.33        | 1.37     |
| 11  | cA    | 829 | CLA  | C4B-NB  | -3.18 | 1.33        | 1.37     |
| 11  | bA    | 836 | CLA  | CHC-C4B | 3.18  | 1.46        | 1.39     |
| 11  | bB    | 805 | CLA  | C4B-NB  | -3.18 | 1.33        | 1.37     |
| 11  | bB    | 817 | CLA  | C4B-NB  | -3.18 | 1.33        | 1.37     |
| 11  | cA    | 809 | CLA  | C4B-NB  | -3.17 | 1.33        | 1.37     |
| 11  | cA    | 833 | CLA  | C4B-NB  | -3.17 | 1.33        | 1.37     |
| 11  | aA    | 815 | CLA  | CHC-C4B | 3.17  | 1.46        | 1.39     |
| 11  | cA    | 802 | CLA  | OBD-CAD | 3.17  | 1.27        | 1.22     |
| 11  | aB    | 809 | CLA  | CHC-C4B | 3.17  | 1.46        | 1.39     |
| 11  | aB    | 827 | CLA  | C4B-NB  | -3.17 | 1.33        | 1.37     |
| 11  | bA    | 831 | CLA  | C4B-NB  | -3.17 | 1.33        | 1.37     |
| 11  | bA    | 809 | CLA  | C4B-NB  | -3.17 | 1.33        | 1.37     |
| 12  | aL    | 202 | F6C  | OBD-CAD | 3.17  | 1.27        | 1.22     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | cB    | 807 | CLA  | C4B-NB  | -3.17 | 1.33        | 1.37     |
| 11  | bB    | 827 | CLA  | C4B-NB  | -3.17 | 1.33        | 1.37     |
| 11  | bB    | 809 | CLA  | CHC-C4B | 3.17  | 1.46        | 1.39     |
| 11  | aA    | 815 | CLA  | C4B-NB  | -3.16 | 1.33        | 1.37     |
| 11  | bA    | 831 | CLA  | CHC-C4B | 3.16  | 1.46        | 1.39     |
| 11  | bB    | 806 | CLA  | C4B-NB  | -3.16 | 1.33        | 1.37     |
| 11  | cA    | 831 | CLA  | CHC-C4B | 3.15  | 1.46        | 1.39     |
| 11  | aA    | 802 | CLA  | OBD-CAD | 3.15  | 1.27        | 1.22     |
| 11  | bL    | 204 | CLA  | C4B-NB  | -3.15 | 1.33        | 1.37     |
| 11  | cB    | 817 | CLA  | C4B-NB  | -3.15 | 1.33        | 1.37     |
| 11  | cB    | 809 | CLA  | CHC-C4B | 3.15  | 1.46        | 1.39     |
| 11  | cB    | 806 | CLA  | OBD-CAD | 3.15  | 1.27        | 1.22     |
| 11  | bA    | 802 | CLA  | OBD-CAD | 3.15  | 1.27        | 1.22     |
| 11  | aB    | 828 | CLA  | CHC-C4B | 3.15  | 1.46        | 1.39     |
| 11  | bA    | 815 | CLA  | C4B-NB  | -3.15 | 1.33        | 1.37     |
| 11  | aA    | 831 | CLA  | CHC-C4B | 3.15  | 1.46        | 1.39     |
| 11  | bA    | 833 | CLA  | C4B-NB  | -3.14 | 1.33        | 1.37     |
| 11  | aB    | 805 | CLA  | C4B-NB  | -3.14 | 1.33        | 1.37     |
| 11  | aA    | 831 | CLA  | C4B-NB  | -3.14 | 1.33        | 1.37     |
| 12  | cA    | 830 | F6C  | C1D-ND  | 3.14  | 1.42        | 1.37     |
| 15  | bB    | 846 | BCR  | C30-C25 | -3.13 | 1.49        | 1.53     |
| 15  | cB    | 846 | BCR  | C30-C25 | -3.13 | 1.49        | 1.53     |
| 11  | cB    | 827 | CLA  | C4B-NB  | -3.13 | 1.33        | 1.37     |
| 11  | aL    | 204 | CLA  | C4B-NB  | -3.13 | 1.33        | 1.37     |
| 12  | cA    | 844 | F6C  | C4A-NA  | -3.13 | 1.33        | 1.37     |
| 15  | cB    | 843 | BCR  | C1-C6   | -3.13 | 1.49        | 1.53     |
| 15  | bB    | 845 | BCR  | C30-C25 | -3.13 | 1.49        | 1.53     |
| 11  | aB    | 806 | CLA  | C4B-NB  | -3.13 | 1.33        | 1.37     |
| 11  | bA    | 814 | CLA  | C4B-NB  | -3.13 | 1.33        | 1.37     |
| 11  | cB    | 828 | CLA  | CHC-C4B | 3.12  | 1.46        | 1.39     |
| 11  | aA    | 814 | CLA  | C4B-NB  | -3.12 | 1.33        | 1.37     |
| 11  | cA    | 814 | CLA  | C4B-NB  | -3.12 | 1.33        | 1.37     |
| 11  | aB    | 806 | CLA  | OBD-CAD | 3.12  | 1.27        | 1.22     |
| 12  | aL    | 202 | F6C  | C1A-C2A | 3.12  | 1.52        | 1.45     |
| 11  | aA    | 802 | CLA  | CHC-C4B | 3.12  | 1.46        | 1.39     |
| 12  | bA    | 844 | F6C  | C4A-NA  | -3.12 | 1.33        | 1.37     |
| 11  | cA    | 802 | CLA  | CHC-C4B | 3.12  | 1.46        | 1.39     |
| 12  | aA    | 844 | F6C  | C4A-NA  | -3.11 | 1.33        | 1.37     |
| 15  | cB    | 845 | BCR  | C30-C25 | -3.11 | 1.49        | 1.53     |
| 12  | aA    | 830 | F6C  | C1D-ND  | 3.11  | 1.42        | 1.37     |
| 11  | bA    | 837 | CLA  | C4B-NB  | -3.11 | 1.33        | 1.37     |
| 11  | aA    | 828 | CLA  | C4B-NB  | -3.10 | 1.33        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | aA    | 833 | CLA  | C4B-NB  | -3.10 | 1.33        | 1.37     |
| 12  | bA    | 830 | F6C  | C1D-ND  | 3.10  | 1.42        | 1.37     |
| 12  | aB    | 824 | F6C  | C4A-NA  | -3.10 | 1.33        | 1.37     |
| 11  | cA    | 837 | CLA  | C4B-NB  | -3.10 | 1.33        | 1.37     |
| 11  | bA    | 834 | CLA  | C4B-NB  | -3.10 | 1.33        | 1.37     |
| 11  | cB    | 808 | CLA  | C4B-NB  | -3.10 | 1.33        | 1.37     |
| 15  | aB    | 845 | BCR  | C30-C25 | -3.10 | 1.49        | 1.53     |
| 11  | cB    | 806 | CLA  | C4B-NB  | -3.10 | 1.33        | 1.37     |
| 15  | bB    | 843 | BCR  | C1-C6   | -3.09 | 1.49        | 1.53     |
| 11  | bB    | 828 | CLA  | CHC-C4B | 3.09  | 1.46        | 1.39     |
| 11  | bB    | 808 | CLA  | C4B-NB  | -3.09 | 1.33        | 1.37     |
| 11  | bB    | 806 | CLA  | OBD-CAD | 3.09  | 1.27        | 1.22     |
| 11  | bB    | 802 | CLA  | CHB-C1B | 3.09  | 1.46        | 1.39     |
| 12  | bB    | 824 | F6C  | C4A-NA  | -3.09 | 1.33        | 1.37     |
| 11  | aA    | 837 | CLA  | C4B-NB  | -3.09 | 1.33        | 1.37     |
| 12  | cB    | 824 | F6C  | C4A-NA  | -3.09 | 1.33        | 1.37     |
| 15  | aA    | 850 | BCR  | C1-C6   | -3.09 | 1.49        | 1.53     |
| 11  | bB    | 801 | CLA  | C1B-C2B | 3.09  | 1.50        | 1.43     |
| 15  | aB    | 843 | BCR  | C1-C6   | -3.09 | 1.49        | 1.53     |
| 15  | aA    | 848 | BCR  | C1-C6   | -3.08 | 1.49        | 1.53     |
| 11  | aB    | 813 | CLA  | C4B-NB  | -3.08 | 1.33        | 1.37     |
| 11  | cB    | 801 | CLA  | C1B-C2B | 3.08  | 1.50        | 1.43     |
| 11  | cB    | 803 | CLA  | CHC-C4B | 3.08  | 1.46        | 1.39     |
| 11  | cA    | 828 | CLA  | C4B-NB  | -3.08 | 1.33        | 1.37     |
| 11  | aB    | 808 | CLA  | C4B-NB  | -3.08 | 1.33        | 1.37     |
| 12  | cA    | 832 | F6C  | C4A-NA  | -3.08 | 1.33        | 1.37     |
| 11  | bB    | 803 | CLA  | CHB-C1B | 3.08  | 1.46        | 1.39     |
| 11  | cB    | 802 | CLA  | CHB-C1B | 3.08  | 1.46        | 1.39     |
| 11  | aB    | 803 | CLA  | CHC-C4B | 3.08  | 1.46        | 1.39     |
| 15  | aB    | 846 | BCR  | C30-C25 | -3.08 | 1.49        | 1.53     |
| 11  | cA    | 825 | CLA  | C4B-NB  | -3.08 | 1.33        | 1.37     |
| 11  | cB    | 813 | CLA  | C4B-NB  | -3.08 | 1.33        | 1.37     |
| 12  | bA    | 832 | F6C  | C4A-NA  | -3.07 | 1.33        | 1.37     |
| 11  | cB    | 803 | CLA  | CHB-C1B | 3.07  | 1.46        | 1.39     |
| 11  | aA    | 835 | CLA  | C4B-NB  | -3.07 | 1.33        | 1.37     |
| 11  | cB    | 826 | CLA  | C4B-NB  | -3.07 | 1.33        | 1.37     |
| 12  | bL    | 202 | F6C  | C1A-C2A | 3.07  | 1.52        | 1.45     |
| 11  | aB    | 802 | CLA  | CHB-C1B | 3.06  | 1.46        | 1.39     |
| 11  | bB    | 803 | CLA  | CHC-C4B | 3.06  | 1.46        | 1.39     |
| 11  | aB    | 803 | CLA  | CHB-C1B | 3.06  | 1.46        | 1.39     |
| 11  | bB    | 801 | CLA  | C4B-NB  | -3.06 | 1.33        | 1.37     |
| 11  | aB    | 801 | CLA  | C1B-C2B | 3.06  | 1.50        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 15  | bA    | 848 | BCR  | C1-C6   | -3.05 | 1.49        | 1.53     |
| 15  | cA    | 848 | BCR  | C1-C6   | -3.05 | 1.49        | 1.53     |
| 11  | aA    | 836 | CLA  | C4B-NB  | -3.05 | 1.33        | 1.37     |
| 15  | cA    | 850 | BCR  | C1-C6   | -3.05 | 1.49        | 1.53     |
| 11  | aB    | 826 | CLA  | C4B-NB  | -3.05 | 1.33        | 1.37     |
| 11  | cA    | 834 | CLA  | C4B-NB  | -3.05 | 1.33        | 1.37     |
| 11  | cA    | 817 | CLA  | C4B-NB  | -3.05 | 1.33        | 1.37     |
| 11  | aA    | 825 | CLA  | C4B-NB  | -3.04 | 1.33        | 1.37     |
| 12  | cL    | 202 | F6C  | C1A-C2A | 3.04  | 1.51        | 1.45     |
| 15  | bA    | 850 | BCR  | C1-C6   | -3.04 | 1.49        | 1.53     |
| 11  | cL    | 206 | CLA  | C4B-NB  | -3.04 | 1.33        | 1.37     |
| 11  | aB    | 802 | CLA  | C4B-NB  | -3.04 | 1.33        | 1.37     |
| 11  | bA    | 836 | CLA  | C4B-NB  | -3.04 | 1.33        | 1.37     |
| 15  | cB    | 844 | BCR  | C1-C6   | -3.04 | 1.49        | 1.53     |
| 11  | bB    | 826 | CLA  | C4B-NB  | -3.04 | 1.33        | 1.37     |
| 11  | cA    | 808 | CLA  | C4B-NB  | -3.04 | 1.33        | 1.37     |
| 11  | aB    | 825 | CLA  | C4B-NB  | -3.04 | 1.33        | 1.37     |
| 11  | bA    | 835 | CLA  | C4B-NB  | -3.04 | 1.33        | 1.37     |
| 11  | cB    | 801 | CLA  | C4B-NB  | -3.03 | 1.33        | 1.37     |
| 11  | bB    | 813 | CLA  | C4B-NB  | -3.03 | 1.33        | 1.37     |
| 11  | cA    | 836 | CLA  | C4B-NB  | -3.03 | 1.33        | 1.37     |
| 12  | cA    | 830 | F6C  | C4A-NA  | -3.03 | 1.33        | 1.37     |
| 11  | bA    | 824 | CLA  | C4B-NB  | -3.03 | 1.33        | 1.37     |
| 11  | bB    | 802 | CLA  | C4B-NB  | -3.03 | 1.33        | 1.37     |
| 11  | aA    | 824 | CLA  | C4B-NB  | -3.03 | 1.33        | 1.37     |
| 12  | aA    | 832 | F6C  | C4A-NA  | -3.02 | 1.33        | 1.37     |
| 11  | aL    | 206 | CLA  | C4B-NB  | -3.02 | 1.33        | 1.37     |
| 11  | bA    | 825 | CLA  | C4B-NB  | -3.02 | 1.33        | 1.37     |
| 11  | cA    | 835 | CLA  | C4B-NB  | -3.02 | 1.33        | 1.37     |
| 11  | bB    | 825 | CLA  | C4B-NB  | -3.02 | 1.33        | 1.37     |
| 11  | cB    | 802 | CLA  | C4B-NB  | -3.02 | 1.33        | 1.37     |
| 11  | cB    | 822 | CLA  | C4B-NB  | -3.01 | 1.33        | 1.37     |
| 11  | cB    | 825 | CLA  | C4B-NB  | -3.01 | 1.33        | 1.37     |
| 11  | aA    | 834 | CLA  | C4B-NB  | -3.00 | 1.33        | 1.37     |
| 11  | aB    | 801 | CLA  | C4B-NB  | -3.00 | 1.33        | 1.37     |
| 11  | aA    | 808 | CLA  | C4B-NB  | -3.00 | 1.33        | 1.37     |
| 11  | aA    | 803 | CLA  | CHB-C1B | 3.00  | 1.46        | 1.39     |
| 15  | bB    | 844 | BCR  | C1-C6   | -2.99 | 1.49        | 1.53     |
| 11  | cA    | 803 | CLA  | CHB-C1B | 2.99  | 1.46        | 1.39     |
| 11  | aB    | 822 | CLA  | C4B-NB  | -2.98 | 1.33        | 1.37     |
| 11  | bB    | 819 | CLA  | C4B-NB  | -2.98 | 1.33        | 1.37     |
| 11  | bL    | 205 | CLA  | C4B-NB  | -2.98 | 1.33        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 15  | aB    | 844 | BCR  | C1-C6   | -2.98 | 1.50        | 1.53     |
| 11  | aL    | 205 | CLA  | C4B-NB  | -2.98 | 1.33        | 1.37     |
| 11  | bB    | 839 | CLA  | C4B-NB  | -2.98 | 1.33        | 1.37     |
| 11  | cL    | 205 | CLA  | C4B-NB  | -2.97 | 1.34        | 1.37     |
| 11  | bA    | 803 | CLA  | CHB-C1B | 2.97  | 1.46        | 1.39     |
| 15  | aA    | 849 | BCR  | C1-C6   | -2.96 | 1.50        | 1.53     |
| 11  | bL    | 206 | CLA  | C4B-NB  | -2.96 | 1.34        | 1.37     |
| 11  | cA    | 820 | CLA  | C4B-NB  | -2.96 | 1.34        | 1.37     |
| 15  | aL    | 208 | BCR  | C30-C25 | -2.96 | 1.50        | 1.53     |
| 11  | cB    | 829 | CLA  | CHC-C4B | 2.96  | 1.46        | 1.39     |
| 11  | bB    | 822 | CLA  | C4B-NB  | -2.96 | 1.34        | 1.37     |
| 11  | bA    | 808 | CLA  | C4B-NB  | -2.96 | 1.34        | 1.37     |
| 11  | bB    | 804 | CLA  | C4B-NB  | -2.95 | 1.34        | 1.37     |
| 11  | bB    | 836 | CLA  | C4B-NB  | -2.95 | 1.34        | 1.37     |
| 11  | cB    | 804 | CLA  | C4B-NB  | -2.95 | 1.34        | 1.37     |
| 11  | bA    | 817 | CLA  | C4B-NB  | -2.95 | 1.34        | 1.37     |
| 11  | aK    | 103 | CLA  | C4B-NB  | -2.95 | 1.34        | 1.37     |
| 11  | cA    | 824 | CLA  | C4B-NB  | -2.95 | 1.34        | 1.37     |
| 11  | cB    | 831 | CLA  | C4B-NB  | -2.95 | 1.34        | 1.37     |
| 12  | aA    | 830 | F6C  | C4A-NA  | -2.94 | 1.34        | 1.37     |
| 11  | bB    | 811 | CLA  | C4B-NB  | -2.94 | 1.34        | 1.37     |
| 11  | aB    | 804 | CLA  | C4B-NB  | -2.94 | 1.34        | 1.37     |
| 11  | aB    | 839 | CLA  | C4B-NB  | -2.94 | 1.34        | 1.37     |
| 11  | aB    | 829 | CLA  | CHC-C4B | 2.93  | 1.46        | 1.39     |
| 11  | aA    | 823 | CLA  | C4B-NB  | -2.93 | 1.34        | 1.37     |
| 11  | cA    | 812 | CLA  | C4B-NB  | -2.93 | 1.34        | 1.37     |
| 15  | cA    | 849 | BCR  | C1-C6   | -2.93 | 1.50        | 1.53     |
| 11  | bB    | 814 | CLA  | C4B-NB  | -2.93 | 1.34        | 1.37     |
| 11  | cB    | 816 | CLA  | C4B-NB  | -2.93 | 1.34        | 1.37     |
| 11  | aA    | 839 | CLA  | OBD-CAD | 2.93  | 1.27        | 1.22     |
| 11  | aB    | 836 | CLA  | C4B-NB  | -2.93 | 1.34        | 1.37     |
| 15  | bL    | 208 | BCR  | C30-C25 | -2.93 | 1.50        | 1.53     |
| 11  | bB    | 830 | CLA  | C4B-NB  | -2.93 | 1.34        | 1.37     |
| 11  | aB    | 831 | CLA  | C4B-NB  | -2.93 | 1.34        | 1.37     |
| 12  | bA    | 830 | F6C  | C4A-NA  | -2.93 | 1.34        | 1.37     |
| 11  | bA    | 839 | CLA  | OBD-CAD | 2.93  | 1.27        | 1.22     |
| 11  | aA    | 820 | CLA  | C4B-NB  | -2.93 | 1.34        | 1.37     |
| 11  | bA    | 807 | CLA  | C4B-NB  | -2.93 | 1.34        | 1.37     |
| 11  | aA    | 806 | CLA  | CHB-C1B | 2.93  | 1.46        | 1.39     |
| 11  | aB    | 816 | CLA  | C4B-NB  | -2.93 | 1.34        | 1.37     |
| 11  | cB    | 837 | CLA  | C4B-NB  | -2.92 | 1.34        | 1.37     |
| 11  | aB    | 830 | CLA  | C4B-NB  | -2.92 | 1.34        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | cA    | 839 | CLA  | OBD-CAD | 2.92  | 1.27        | 1.22     |
| 11  | bA    | 819 | CLA  | C4B-NB  | -2.92 | 1.34        | 1.37     |
| 11  | cB    | 836 | CLA  | OBD-CAD | 2.92  | 1.27        | 1.22     |
| 11  | cA    | 806 | CLA  | CHB-C1B | 2.92  | 1.46        | 1.39     |
| 11  | cB    | 839 | CLA  | C4B-NB  | -2.92 | 1.34        | 1.37     |
| 11  | cB    | 836 | CLA  | C4B-NB  | -2.92 | 1.34        | 1.37     |
| 11  | cB    | 819 | CLA  | C4B-NB  | -2.92 | 1.34        | 1.37     |
| 11  | aB    | 840 | CLA  | C4B-NB  | -2.92 | 1.34        | 1.37     |
| 11  | aB    | 819 | CLA  | C4B-NB  | -2.91 | 1.34        | 1.37     |
| 11  | aA    | 812 | CLA  | C4B-NB  | -2.91 | 1.34        | 1.37     |
| 11  | aA    | 817 | CLA  | C4B-NB  | -2.91 | 1.34        | 1.37     |
| 11  | bK    | 103 | CLA  | C4B-NB  | -2.91 | 1.34        | 1.37     |
| 11  | bA    | 820 | CLA  | C4B-NB  | -2.91 | 1.34        | 1.37     |
| 11  | cB    | 814 | CLA  | C4B-NB  | -2.91 | 1.34        | 1.37     |
| 11  | aA    | 839 | CLA  | C4B-NB  | -2.91 | 1.34        | 1.37     |
| 11  | bA    | 806 | CLA  | CHB-C1B | 2.91  | 1.45        | 1.39     |
| 11  | cA    | 807 | CLA  | C4B-NB  | -2.91 | 1.34        | 1.37     |
| 11  | bA    | 823 | CLA  | C4B-NB  | -2.91 | 1.34        | 1.37     |
| 11  | bA    | 839 | CLA  | C4B-NB  | -2.91 | 1.34        | 1.37     |
| 11  | cA    | 823 | CLA  | C4B-NB  | -2.91 | 1.34        | 1.37     |
| 11  | bB    | 829 | CLA  | CHC-C4B | 2.91  | 1.45        | 1.39     |
| 15  | bA    | 849 | BCR  | C1-C6   | -2.90 | 1.50        | 1.53     |
| 15  | bI    | 101 | BCR  | C1-C6   | -2.90 | 1.50        | 1.53     |
| 11  | cA    | 839 | CLA  | C4B-NB  | -2.90 | 1.34        | 1.37     |
| 15  | aI    | 101 | BCR  | C1-C6   | -2.90 | 1.50        | 1.53     |
| 11  | bB    | 840 | CLA  | C4B-NB  | -2.90 | 1.34        | 1.37     |
| 11  | aB    | 834 | CLA  | C4D-CHA | 2.90  | 1.48        | 1.38     |
| 12  | aA    | 826 | F6C  | C1A-C2A | 2.89  | 1.51        | 1.45     |
| 11  | bA    | 841 | CLA  | C4B-NB  | -2.89 | 1.34        | 1.37     |
| 11  | bB    | 834 | CLA  | C4D-CHA | 2.89  | 1.48        | 1.38     |
| 11  | bB    | 816 | CLA  | C4B-NB  | -2.89 | 1.34        | 1.37     |
| 15  | cI    | 103 | BCR  | C1-C6   | -2.89 | 1.50        | 1.53     |
| 11  | cA    | 810 | CLA  | C4B-NB  | -2.88 | 1.34        | 1.37     |
| 11  | bA    | 810 | CLA  | C4B-NB  | -2.88 | 1.34        | 1.37     |
| 15  | cL    | 208 | BCR  | C30-C25 | -2.88 | 1.50        | 1.53     |
| 11  | cB    | 811 | CLA  | C4B-NB  | -2.88 | 1.34        | 1.37     |
| 11  | aA    | 841 | CLA  | C4B-NB  | -2.88 | 1.34        | 1.37     |
| 11  | bB    | 836 | CLA  | OBD-CAD | 2.88  | 1.27        | 1.22     |
| 11  | aA    | 807 | CLA  | C4B-NB  | -2.88 | 1.34        | 1.37     |
| 11  | aB    | 821 | CLA  | C4D-CHA | 2.88  | 1.48        | 1.38     |
| 11  | cB    | 834 | CLA  | C4D-CHA | 2.88  | 1.48        | 1.38     |
| 11  | cB    | 829 | CLA  | C4D-CHA | 2.88  | 1.48        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | bB    | 831 | CLA  | C4B-NB  | -2.87 | 1.34        | 1.37     |
| 12  | aA    | 827 | F6C  | C4A-NA  | -2.87 | 1.34        | 1.37     |
| 11  | bB    | 810 | CLA  | C4B-NB  | -2.87 | 1.34        | 1.37     |
| 12  | cA    | 826 | F6C  | C1A-C2A | 2.87  | 1.51        | 1.45     |
| 11  | aB    | 809 | CLA  | OBD-CAD | 2.87  | 1.27        | 1.22     |
| 11  | aB    | 805 | CLA  | OBD-CAD | 2.87  | 1.27        | 1.22     |
| 11  | aA    | 819 | CLA  | C4B-NB  | -2.87 | 1.34        | 1.37     |
| 12  | bA    | 826 | F6C  | C1A-C2A | 2.87  | 1.51        | 1.45     |
| 11  | aB    | 811 | CLA  | C4B-NB  | -2.87 | 1.34        | 1.37     |
| 11  | bB    | 829 | CLA  | C4B-NB  | -2.87 | 1.34        | 1.37     |
| 11  | cB    | 810 | CLA  | C4B-NB  | -2.87 | 1.34        | 1.37     |
| 11  | bB    | 837 | CLA  | C4B-NB  | -2.87 | 1.34        | 1.37     |
| 11  | bA    | 806 | CLA  | C4B-NB  | -2.86 | 1.34        | 1.37     |
| 11  | cB    | 805 | CLA  | OBD-CAD | 2.86  | 1.27        | 1.22     |
| 11  | aB    | 830 | CLA  | C4D-CHA | 2.86  | 1.48        | 1.38     |
| 11  | cB    | 815 | CLA  | C4D-CHA | 2.86  | 1.48        | 1.38     |
| 11  | cA    | 806 | CLA  | C4B-NB  | -2.86 | 1.34        | 1.37     |
| 11  | bA    | 805 | CLA  | C4D-CHA | 2.86  | 1.48        | 1.38     |
| 11  | bA    | 811 | CLA  | C4B-NB  | -2.86 | 1.34        | 1.37     |
| 11  | cA    | 841 | CLA  | C4B-NB  | -2.86 | 1.34        | 1.37     |
| 11  | cB    | 830 | CLA  | C4D-CHA | 2.86  | 1.48        | 1.38     |
| 11  | aB    | 814 | CLA  | C4B-NB  | -2.85 | 1.34        | 1.37     |
| 11  | bB    | 809 | CLA  | OBD-CAD | 2.85  | 1.27        | 1.22     |
| 11  | aA    | 805 | CLA  | C4D-CHA | 2.85  | 1.48        | 1.38     |
| 11  | aB    | 829 | CLA  | C4B-NB  | -2.85 | 1.34        | 1.37     |
| 11  | bB    | 830 | CLA  | C4D-CHA | 2.85  | 1.48        | 1.38     |
| 11  | cB    | 829 | CLA  | C4B-NB  | -2.85 | 1.34        | 1.37     |
| 11  | aB    | 820 | CLA  | C4B-NB  | -2.85 | 1.34        | 1.37     |
| 11  | cK    | 103 | CLA  | C4B-NB  | -2.85 | 1.34        | 1.37     |
| 11  | aA    | 811 | CLA  | C4B-NB  | -2.84 | 1.34        | 1.37     |
| 11  | bA    | 843 | CLA  | C4B-NB  | -2.84 | 1.34        | 1.37     |
| 11  | aB    | 815 | CLA  | C4D-CHA | 2.84  | 1.48        | 1.38     |
| 11  | bB    | 829 | CLA  | C4D-CHA | 2.84  | 1.48        | 1.38     |
| 11  | cB    | 840 | CLA  | C4B-NB  | -2.84 | 1.34        | 1.37     |
| 11  | bB    | 815 | CLA  | C4D-CHA | 2.84  | 1.48        | 1.38     |
| 11  | aK    | 101 | CLA  | OBD-CAD | 2.84  | 1.28        | 1.23     |
| 11  | aB    | 829 | CLA  | C4D-CHA | 2.84  | 1.48        | 1.38     |
| 11  | aA    | 806 | CLA  | C4B-NB  | -2.84 | 1.34        | 1.37     |
| 15  | aM    | 101 | BCR  | C1-C6   | -2.84 | 1.50        | 1.53     |
| 11  | aA    | 810 | CLA  | C4B-NB  | -2.84 | 1.34        | 1.37     |
| 11  | cB    | 830 | CLA  | C4B-NB  | -2.84 | 1.34        | 1.37     |
| 15  | bM    | 101 | BCR  | C1-C6   | -2.84 | 1.50        | 1.53     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | cB    | 821 | CLA  | C4D-CHA | 2.84  | 1.48        | 1.38     |
| 11  | cB    | 809 | CLA  | OBD-CAD | 2.84  | 1.27        | 1.22     |
| 11  | aB    | 810 | CLA  | C4B-NB  | -2.84 | 1.34        | 1.37     |
| 11  | cB    | 820 | CLA  | C4B-NB  | -2.84 | 1.34        | 1.37     |
| 11  | bK    | 101 | CLA  | OBD-CAD | 2.83  | 1.28        | 1.23     |
| 11  | bA    | 812 | CLA  | C4B-NB  | -2.83 | 1.34        | 1.37     |
| 11  | cB    | 829 | CLA  | C1B-C2B | 2.83  | 1.49        | 1.43     |
| 11  | aB    | 837 | CLA  | C4B-NB  | -2.83 | 1.34        | 1.37     |
| 11  | cA    | 819 | CLA  | C4B-NB  | -2.83 | 1.34        | 1.37     |
| 11  | cA    | 809 | CLA  | C4D-CHA | 2.83  | 1.48        | 1.38     |
| 11  | cA    | 805 | CLA  | C4D-CHA | 2.83  | 1.48        | 1.38     |
| 11  | aB    | 836 | CLA  | OBD-CAD | 2.83  | 1.27        | 1.22     |
| 11  | aA    | 822 | CLA  | C4B-NB  | -2.83 | 1.34        | 1.37     |
| 11  | bB    | 821 | CLA  | C4D-CHA | 2.83  | 1.48        | 1.38     |
| 11  | bA    | 822 | CLA  | C4B-NB  | -2.83 | 1.34        | 1.37     |
| 11  | cA    | 822 | CLA  | C4B-NB  | -2.83 | 1.34        | 1.37     |
| 11  | aB    | 829 | CLA  | C1B-C2B | 2.82  | 1.49        | 1.43     |
| 11  | bA    | 815 | CLA  | C4D-CHA | 2.82  | 1.48        | 1.38     |
| 11  | cK    | 101 | CLA  | C4B-NB  | -2.82 | 1.34        | 1.37     |
| 11  | aA    | 817 | CLA  | C4D-CHA | 2.82  | 1.48        | 1.38     |
| 11  | bB    | 805 | CLA  | OBD-CAD | 2.82  | 1.27        | 1.22     |
| 11  | cA    | 818 | CLA  | C4B-NB  | -2.82 | 1.34        | 1.37     |
| 11  | cB    | 815 | CLA  | C4B-NB  | -2.82 | 1.34        | 1.37     |
| 11  | aB    | 814 | CLA  | C4D-CHA | 2.82  | 1.48        | 1.38     |
| 12  | bA    | 827 | F6C  | C4A-NA  | -2.82 | 1.34        | 1.37     |
| 11  | bB    | 820 | CLA  | C4B-NB  | -2.82 | 1.34        | 1.37     |
| 11  | aB    | 815 | CLA  | C4B-NB  | -2.82 | 1.34        | 1.37     |
| 11  | bA    | 809 | CLA  | C4D-CHA | 2.82  | 1.48        | 1.38     |
| 11  | cB    | 814 | CLA  | C4D-CHA | 2.82  | 1.48        | 1.38     |
| 11  | bB    | 832 | CLA  | C4D-CHA | 2.82  | 1.48        | 1.38     |
| 11  | cA    | 811 | CLA  | C4B-NB  | -2.82 | 1.34        | 1.37     |
| 11  | bA    | 823 | CLA  | C4D-CHA | 2.81  | 1.48        | 1.38     |
| 11  | bB    | 829 | CLA  | C1B-C2B | 2.81  | 1.49        | 1.43     |
| 11  | aA    | 818 | CLA  | C4B-NB  | -2.81 | 1.34        | 1.37     |
| 11  | cB    | 838 | CLA  | C4B-NB  | -2.81 | 1.34        | 1.37     |
| 11  | bA    | 816 | CLA  | C4D-CHA | 2.81  | 1.48        | 1.38     |
| 11  | aB    | 832 | CLA  | C4D-CHA | 2.81  | 1.48        | 1.38     |
| 11  | bA    | 821 | CLA  | C4D-CHA | 2.81  | 1.48        | 1.38     |
| 11  | aA    | 821 | CLA  | C4D-CHA | 2.81  | 1.48        | 1.38     |
| 11  | cA    | 823 | CLA  | C4D-CHA | 2.81  | 1.48        | 1.38     |
| 11  | bA    | 812 | CLA  | C4D-CHA | 2.81  | 1.48        | 1.38     |
| 11  | cB    | 832 | CLA  | C4D-CHA | 2.81  | 1.48        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | cB    | 831 | CLA  | C4D-CHA | 2.80  | 1.48        | 1.38     |
| 11  | aA    | 823 | CLA  | C4D-CHA | 2.80  | 1.48        | 1.38     |
| 11  | cK    | 101 | CLA  | OBD-CAD | 2.80  | 1.28        | 1.23     |
| 11  | bA    | 817 | CLA  | C4D-CHA | 2.80  | 1.48        | 1.38     |
| 11  | bB    | 831 | CLA  | C4D-CHA | 2.80  | 1.48        | 1.38     |
| 11  | aA    | 809 | CLA  | C4D-CHA | 2.80  | 1.48        | 1.38     |
| 11  | bB    | 814 | CLA  | C4D-CHA | 2.80  | 1.48        | 1.38     |
| 11  | aA    | 815 | CLA  | C4D-CHA | 2.80  | 1.48        | 1.38     |
| 11  | cA    | 812 | CLA  | C4D-CHA | 2.80  | 1.48        | 1.38     |
| 15  | cB    | 845 | BCR  | C1-C6   | -2.80 | 1.50        | 1.53     |
| 11  | bB    | 823 | CLA  | C4D-CHA | 2.80  | 1.48        | 1.38     |
| 11  | bB    | 835 | CLA  | C4D-CHA | 2.80  | 1.48        | 1.38     |
| 11  | cA    | 821 | CLA  | C4D-CHA | 2.80  | 1.48        | 1.38     |
| 11  | bA    | 818 | CLA  | C4B-NB  | -2.80 | 1.34        | 1.37     |
| 11  | aB    | 823 | CLA  | C4D-CHA | 2.80  | 1.48        | 1.38     |
| 11  | aA    | 812 | CLA  | C4D-CHA | 2.79  | 1.48        | 1.38     |
| 11  | aB    | 831 | CLA  | C4D-CHA | 2.79  | 1.48        | 1.38     |
| 11  | cA    | 817 | CLA  | C4D-CHA | 2.79  | 1.48        | 1.38     |
| 11  | cB    | 811 | CLA  | C4D-CHA | 2.79  | 1.48        | 1.38     |
| 11  | aB    | 811 | CLA  | C4D-CHA | 2.79  | 1.48        | 1.38     |
| 11  | cB    | 823 | CLA  | C4D-CHA | 2.79  | 1.48        | 1.38     |
| 11  | cA    | 815 | CLA  | C4D-CHA | 2.79  | 1.48        | 1.38     |
| 11  | bB    | 811 | CLA  | C4D-CHA | 2.79  | 1.48        | 1.38     |
| 11  | bB    | 812 | CLA  | C4D-CHA | 2.79  | 1.48        | 1.38     |
| 11  | cB    | 825 | CLA  | C4D-CHA | 2.79  | 1.48        | 1.38     |
| 15  | aB    | 845 | BCR  | C1-C6   | -2.79 | 1.50        | 1.53     |
| 11  | cA    | 831 | CLA  | C4D-CHA | 2.78  | 1.47        | 1.38     |
| 11  | aB    | 820 | CLA  | C4D-CHA | 2.78  | 1.47        | 1.38     |
| 15  | bL    | 207 | BCR  | C1-C6   | -2.78 | 1.50        | 1.53     |
| 11  | cA    | 825 | CLA  | C4D-CHA | 2.78  | 1.47        | 1.38     |
| 11  | aA    | 807 | CLA  | C4D-CHA | 2.78  | 1.47        | 1.38     |
| 11  | cB    | 812 | CLA  | C4D-CHA | 2.78  | 1.47        | 1.38     |
| 11  | bA    | 831 | CLA  | C4D-CHA | 2.78  | 1.47        | 1.38     |
| 11  | bA    | 841 | CLA  | C4D-CHA | 2.78  | 1.47        | 1.38     |
| 15  | cM    | 101 | BCR  | C1-C6   | -2.78 | 1.50        | 1.53     |
| 11  | bK    | 103 | CLA  | C4D-CHA | 2.78  | 1.47        | 1.38     |
| 11  | cK    | 103 | CLA  | C4D-CHA | 2.78  | 1.47        | 1.38     |
| 12  | aA    | 826 | F6C  | C4A-C3A | 2.78  | 1.50        | 1.45     |
| 11  | aK    | 103 | CLA  | C4D-CHA | 2.78  | 1.47        | 1.38     |
| 12  | cA    | 827 | F6C  | C4A-NA  | -2.78 | 1.34        | 1.37     |
| 11  | aB    | 812 | CLA  | C4D-CHA | 2.78  | 1.47        | 1.38     |
| 11  | cB    | 819 | CLA  | C4D-CHA | 2.78  | 1.47        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | aA    | 825 | CLA  | C4D-CHA | 2.78  | 1.47        | 1.38     |
| 11  | cB    | 835 | CLA  | C4D-CHA | 2.78  | 1.47        | 1.38     |
| 11  | bL    | 204 | CLA  | C4D-CHA | 2.78  | 1.47        | 1.38     |
| 11  | aK    | 101 | CLA  | C4B-NB  | -2.78 | 1.34        | 1.37     |
| 11  | cA    | 807 | CLA  | C4D-CHA | 2.78  | 1.47        | 1.38     |
| 11  | aA    | 819 | CLA  | C4D-CHA | 2.77  | 1.47        | 1.38     |
| 11  | aB    | 835 | CLA  | C4D-CHA | 2.77  | 1.47        | 1.38     |
| 11  | cA    | 819 | CLA  | C4D-CHA | 2.77  | 1.47        | 1.38     |
| 11  | aA    | 843 | CLA  | C4B-NB  | -2.77 | 1.34        | 1.37     |
| 11  | aA    | 831 | CLA  | C4D-CHA | 2.77  | 1.47        | 1.38     |
| 11  | bA    | 825 | CLA  | C4D-CHA | 2.77  | 1.47        | 1.38     |
| 11  | cA    | 841 | CLA  | C4D-CHA | 2.77  | 1.47        | 1.38     |
| 11  | cB    | 832 | CLA  | C4B-NB  | -2.77 | 1.34        | 1.37     |
| 11  | bA    | 807 | CLA  | C4D-CHA | 2.77  | 1.47        | 1.38     |
| 11  | cA    | 816 | CLA  | C4D-CHA | 2.77  | 1.47        | 1.38     |
| 11  | bB    | 813 | CLA  | C1B-C2B | 2.77  | 1.49        | 1.43     |
| 11  | aA    | 816 | CLA  | C4D-CHA | 2.77  | 1.47        | 1.38     |
| 11  | aB    | 819 | CLA  | C4D-CHA | 2.77  | 1.47        | 1.38     |
| 11  | aB    | 832 | CLA  | C4B-NB  | -2.77 | 1.34        | 1.37     |
| 11  | aA    | 841 | CLA  | C4D-CHA | 2.77  | 1.47        | 1.38     |
| 11  | bB    | 820 | CLA  | C4D-CHA | 2.77  | 1.47        | 1.38     |
| 11  | bA    | 811 | CLA  | C4D-CHA | 2.77  | 1.47        | 1.38     |
| 11  | bB    | 825 | CLA  | C4D-CHA | 2.77  | 1.47        | 1.38     |
| 15  | aA    | 851 | BCR  | C30-C25 | -2.76 | 1.50        | 1.53     |
| 11  | cA    | 843 | CLA  | C4B-NB  | -2.76 | 1.34        | 1.37     |
| 11  | cA    | 842 | CLA  | C4D-CHA | 2.76  | 1.47        | 1.38     |
| 11  | bB    | 819 | CLA  | C4D-CHA | 2.76  | 1.47        | 1.38     |
| 11  | cL    | 204 | CLA  | C4D-CHA | 2.76  | 1.47        | 1.38     |
| 11  | aA    | 811 | CLA  | C4D-CHA | 2.76  | 1.47        | 1.38     |
| 15  | bB    | 845 | BCR  | C1-C6   | -2.76 | 1.50        | 1.53     |
| 11  | bA    | 819 | CLA  | C4D-CHA | 2.76  | 1.47        | 1.38     |
| 11  | bB    | 823 | CLA  | C4B-NB  | -2.76 | 1.34        | 1.37     |
| 11  | aB    | 825 | CLA  | C4D-CHA | 2.76  | 1.47        | 1.38     |
| 11  | aL    | 204 | CLA  | C4D-CHA | 2.76  | 1.47        | 1.38     |
| 11  | bK    | 101 | CLA  | C4B-NB  | -2.76 | 1.34        | 1.37     |
| 11  | cB    | 833 | CLA  | C4B-NB  | -2.75 | 1.34        | 1.37     |
| 11  | bA    | 804 | CLA  | C4D-CHA | 2.75  | 1.47        | 1.38     |
| 11  | cA    | 813 | CLA  | C4D-CHA | 2.75  | 1.47        | 1.38     |
| 11  | cB    | 820 | CLA  | C4D-CHA | 2.75  | 1.47        | 1.38     |
| 11  | bA    | 805 | CLA  | C4B-NB  | -2.75 | 1.34        | 1.37     |
| 11  | cB    | 813 | CLA  | C1B-C2B | 2.75  | 1.49        | 1.43     |
| 15  | aL    | 207 | BCR  | C1-C6   | -2.75 | 1.50        | 1.53     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | aA    | 804 | CLA  | C4D-CHA | 2.75  | 1.47        | 1.38     |
| 12  | bA    | 826 | F6C  | C4A-C3A | 2.75  | 1.50        | 1.45     |
| 11  | cA    | 820 | CLA  | C4D-CHA | 2.75  | 1.47        | 1.38     |
| 11  | cB    | 835 | CLA  | C4B-NB  | -2.75 | 1.34        | 1.37     |
| 15  | cL    | 207 | BCR  | C1-C6   | -2.75 | 1.50        | 1.53     |
| 11  | aB    | 816 | CLA  | C4D-CHA | 2.75  | 1.47        | 1.38     |
| 11  | aB    | 833 | CLA  | C4B-NB  | -2.75 | 1.34        | 1.37     |
| 11  | bB    | 833 | CLA  | C4B-NB  | -2.75 | 1.34        | 1.37     |
| 15  | cA    | 847 | BCR  | C1-C6   | -2.75 | 1.50        | 1.53     |
| 11  | aB    | 813 | CLA  | C1B-C2B | 2.75  | 1.49        | 1.43     |
| 11  | bB    | 816 | CLA  | C4D-CHA | 2.75  | 1.47        | 1.38     |
| 11  | cA    | 806 | CLA  | C4D-CHA | 2.75  | 1.47        | 1.38     |
| 15  | cA    | 851 | BCR  | C30-C25 | -2.75 | 1.50        | 1.53     |
| 11  | aA    | 828 | CLA  | C4D-CHA | 2.75  | 1.47        | 1.38     |
| 11  | aB    | 821 | CLA  | C4B-NB  | -2.75 | 1.34        | 1.37     |
| 11  | aB    | 823 | CLA  | C4B-NB  | -2.75 | 1.34        | 1.37     |
| 11  | bB    | 838 | CLA  | C4B-NB  | -2.75 | 1.34        | 1.37     |
| 11  | aA    | 813 | CLA  | C4D-CHA | 2.75  | 1.47        | 1.38     |
| 11  | bB    | 836 | CLA  | C4D-CHA | 2.75  | 1.47        | 1.38     |
| 11  | aA    | 805 | CLA  | C4B-NB  | -2.74 | 1.34        | 1.37     |
| 11  | cA    | 804 | CLA  | C4D-CHA | 2.74  | 1.47        | 1.38     |
| 11  | bA    | 828 | CLA  | C4D-CHA | 2.74  | 1.47        | 1.38     |
| 15  | bA    | 851 | BCR  | C30-C25 | -2.74 | 1.50        | 1.53     |
| 11  | aA    | 806 | CLA  | C4D-CHA | 2.74  | 1.47        | 1.38     |
| 11  | bA    | 820 | CLA  | C4D-CHA | 2.74  | 1.47        | 1.38     |
| 11  | cB    | 836 | CLA  | C4D-CHA | 2.74  | 1.47        | 1.38     |
| 11  | cB    | 816 | CLA  | C4D-CHA | 2.74  | 1.47        | 1.38     |
| 11  | bA    | 804 | CLA  | C4B-NB  | -2.74 | 1.34        | 1.37     |
| 11  | bB    | 815 | CLA  | C4B-NB  | -2.74 | 1.34        | 1.37     |
| 11  | bA    | 813 | CLA  | C4D-CHA | 2.74  | 1.47        | 1.38     |
| 11  | cA    | 811 | CLA  | C4D-CHA | 2.74  | 1.47        | 1.38     |
| 11  | aA    | 820 | CLA  | C4D-CHA | 2.74  | 1.47        | 1.38     |
| 11  | bA    | 822 | CLA  | C4D-CHA | 2.74  | 1.47        | 1.38     |
| 11  | aA    | 842 | CLA  | C4D-CHA | 2.74  | 1.47        | 1.38     |
| 15  | aA    | 847 | BCR  | C1-C6   | -2.74 | 1.50        | 1.53     |
| 11  | cA    | 804 | CLA  | C4B-NB  | -2.74 | 1.34        | 1.37     |
| 11  | cA    | 834 | CLA  | C1B-C2B | 2.73  | 1.49        | 1.43     |
| 11  | cA    | 835 | CLA  | C4D-CHA | 2.73  | 1.47        | 1.38     |
| 11  | bB    | 812 | CLA  | C4C-C3C | 2.73  | 1.49        | 1.45     |
| 11  | cA    | 822 | CLA  | C4D-CHA | 2.73  | 1.47        | 1.38     |
| 11  | aB    | 813 | CLA  | C4D-CHA | 2.73  | 1.47        | 1.38     |
| 11  | bB    | 832 | CLA  | C4B-NB  | -2.73 | 1.34        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | bB    | 835 | CLA  | C4B-NB  | -2.73 | 1.34        | 1.37     |
| 15  | bA    | 847 | BCR  | C1-C6   | -2.73 | 1.50        | 1.53     |
| 11  | cB    | 813 | CLA  | C4D-CHA | 2.73  | 1.47        | 1.38     |
| 11  | cA    | 828 | CLA  | C4D-CHA | 2.73  | 1.47        | 1.38     |
| 11  | bB    | 806 | CLA  | C4D-CHA | 2.73  | 1.47        | 1.38     |
| 11  | bB    | 813 | CLA  | C4D-CHA | 2.73  | 1.47        | 1.38     |
| 11  | bB    | 840 | CLA  | C4D-CHA | 2.73  | 1.47        | 1.38     |
| 11  | cB    | 835 | CLA  | C1B-C2B | 2.73  | 1.49        | 1.43     |
| 11  | bB    | 821 | CLA  | C4B-NB  | -2.73 | 1.34        | 1.37     |
| 11  | cA    | 842 | CLA  | C4B-NB  | -2.73 | 1.34        | 1.37     |
| 11  | bA    | 806 | CLA  | C4D-CHA | 2.73  | 1.47        | 1.38     |
| 11  | aA    | 822 | CLA  | C4D-CHA | 2.73  | 1.47        | 1.38     |
| 11  | aA    | 813 | CLA  | C3B-C4B | 2.73  | 1.50        | 1.42     |
| 12  | cA    | 826 | F6C  | C4A-C3A | 2.73  | 1.50        | 1.45     |
| 11  | bA    | 835 | CLA  | C4D-CHA | 2.72  | 1.47        | 1.38     |
| 11  | cB    | 840 | CLA  | C4D-CHA | 2.72  | 1.47        | 1.38     |
| 11  | bA    | 842 | CLA  | C4D-CHA | 2.72  | 1.47        | 1.38     |
| 11  | aA    | 843 | CLA  | C4D-CHA | 2.72  | 1.47        | 1.38     |
| 11  | aB    | 838 | CLA  | C4B-NB  | -2.72 | 1.34        | 1.37     |
| 11  | bA    | 818 | CLA  | C4D-CHA | 2.72  | 1.47        | 1.38     |
| 11  | cA    | 813 | CLA  | C3B-C4B | 2.72  | 1.50        | 1.42     |
| 11  | bB    | 805 | CLA  | C4D-CHA | 2.72  | 1.47        | 1.38     |
| 11  | aB    | 812 | CLA  | C4C-C3C | 2.72  | 1.49        | 1.45     |
| 11  | aB    | 836 | CLA  | C4D-CHA | 2.72  | 1.47        | 1.38     |
| 11  | cB    | 823 | CLA  | C4B-NB  | -2.72 | 1.34        | 1.37     |
| 11  | bA    | 810 | CLA  | C4D-CHA | 2.72  | 1.47        | 1.38     |
| 11  | cB    | 805 | CLA  | C4D-CHA | 2.72  | 1.47        | 1.38     |
| 12  | aA    | 826 | F6C  | C4A-NA  | -2.72 | 1.34        | 1.37     |
| 11  | cA    | 843 | CLA  | C4D-CHA | 2.71  | 1.47        | 1.38     |
| 11  | bA    | 842 | CLA  | C4B-NB  | -2.71 | 1.34        | 1.37     |
| 11  | bA    | 843 | CLA  | C4D-CHA | 2.71  | 1.47        | 1.38     |
| 11  | cL    | 205 | CLA  | C4D-CHA | 2.71  | 1.47        | 1.38     |
| 11  | aB    | 804 | CLA  | C4D-CHA | 2.71  | 1.47        | 1.38     |
| 11  | cA    | 805 | CLA  | C4B-NB  | -2.71 | 1.34        | 1.37     |
| 11  | cB    | 804 | CLA  | C4D-CHA | 2.71  | 1.47        | 1.38     |
| 11  | bA    | 834 | CLA  | C1B-C2B | 2.71  | 1.49        | 1.43     |
| 11  | aB    | 837 | CLA  | C4D-CHA | 2.71  | 1.47        | 1.38     |
| 11  | cA    | 810 | CLA  | C4D-CHA | 2.71  | 1.47        | 1.38     |
| 11  | bA    | 813 | CLA  | C3B-C4B | 2.71  | 1.50        | 1.42     |
| 11  | aB    | 840 | CLA  | C4D-CHA | 2.71  | 1.47        | 1.38     |
| 11  | aB    | 805 | CLA  | C4D-CHA | 2.71  | 1.47        | 1.38     |
| 11  | cB    | 806 | CLA  | C4D-CHA | 2.71  | 1.47        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | aA    | 810 | CLA  | C4D-CHA | 2.71  | 1.47        | 1.38     |
| 12  | aL    | 202 | F6C  | C4A-C3A | 2.71  | 1.50        | 1.45     |
| 11  | aB    | 822 | CLA  | C4D-CHA | 2.71  | 1.47        | 1.38     |
| 11  | aB    | 806 | CLA  | C4D-CHA | 2.71  | 1.47        | 1.38     |
| 11  | aB    | 835 | CLA  | C1B-C2B | 2.70  | 1.49        | 1.43     |
| 11  | bB    | 834 | CLA  | C4B-NB  | -2.70 | 1.34        | 1.37     |
| 11  | cA    | 818 | CLA  | C4D-CHA | 2.70  | 1.47        | 1.38     |
| 11  | bB    | 804 | CLA  | C4D-CHA | 2.70  | 1.47        | 1.38     |
| 11  | aA    | 835 | CLA  | C4D-CHA | 2.70  | 1.47        | 1.38     |
| 11  | bB    | 837 | CLA  | C4D-CHA | 2.70  | 1.47        | 1.38     |
| 15  | cL    | 207 | BCR  | C30-C25 | -2.70 | 1.50        | 1.53     |
| 11  | bB    | 828 | CLA  | C4D-CHA | 2.70  | 1.47        | 1.38     |
| 11  | aL    | 205 | CLA  | C4D-CHA | 2.70  | 1.47        | 1.38     |
| 11  | aB    | 829 | CLA  | C4C-C3C | 2.70  | 1.49        | 1.45     |
| 11  | aB    | 834 | CLA  | C4B-NB  | -2.69 | 1.34        | 1.37     |
| 11  | cB    | 837 | CLA  | C4D-CHA | 2.69  | 1.47        | 1.38     |
| 11  | aA    | 842 | CLA  | C4B-NB  | -2.69 | 1.34        | 1.37     |
| 11  | bL    | 205 | CLA  | C4D-CHA | 2.69  | 1.47        | 1.38     |
| 11  | cB    | 810 | CLA  | C4D-CHA | 2.69  | 1.47        | 1.38     |
| 11  | bA    | 836 | CLA  | C4D-CHA | 2.69  | 1.47        | 1.38     |
| 11  | aB    | 825 | CLA  | C1B-C2B | 2.69  | 1.49        | 1.43     |
| 11  | bB    | 822 | CLA  | C4D-CHA | 2.69  | 1.47        | 1.38     |
| 11  | aB    | 828 | CLA  | C4D-CHA | 2.69  | 1.47        | 1.38     |
| 11  | cB    | 828 | CLA  | C4D-CHA | 2.69  | 1.47        | 1.38     |
| 11  | aB    | 810 | CLA  | C4D-CHA | 2.69  | 1.47        | 1.38     |
| 11  | bA    | 821 | CLA  | C4B-NB  | -2.69 | 1.34        | 1.37     |
| 11  | bA    | 824 | CLA  | C4D-CHA | 2.68  | 1.47        | 1.38     |
| 11  | aA    | 804 | CLA  | C4B-NB  | -2.68 | 1.34        | 1.37     |
| 11  | aA    | 829 | CLA  | C4D-CHA | 2.68  | 1.47        | 1.38     |
| 11  | cB    | 823 | CLA  | C1B-C2B | 2.68  | 1.49        | 1.43     |
| 11  | cA    | 821 | CLA  | C4B-NB  | -2.68 | 1.34        | 1.37     |
| 11  | bB    | 825 | CLA  | C1B-C2B | 2.68  | 1.49        | 1.43     |
| 11  | aA    | 824 | CLA  | C4D-CHA | 2.68  | 1.47        | 1.38     |
| 11  | cA    | 810 | CLA  | C1B-C2B | 2.68  | 1.49        | 1.43     |
| 11  | cB    | 821 | CLA  | C4B-NB  | -2.68 | 1.34        | 1.37     |
| 11  | cA    | 828 | CLA  | C1B-C2B | 2.68  | 1.49        | 1.43     |
| 11  | cB    | 822 | CLA  | C4D-CHA | 2.68  | 1.47        | 1.38     |
| 11  | cA    | 836 | CLA  | C4D-CHA | 2.68  | 1.47        | 1.38     |
| 11  | bA    | 828 | CLA  | C1B-C2B | 2.68  | 1.49        | 1.43     |
| 11  | aA    | 818 | CLA  | C4D-CHA | 2.68  | 1.47        | 1.38     |
| 11  | bA    | 829 | CLA  | C4D-CHA | 2.68  | 1.47        | 1.38     |
| 11  | aA    | 834 | CLA  | C1B-C2B | 2.68  | 1.49        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | aA    | 838 | CLA  | C4D-CHA | 2.67  | 1.47        | 1.38     |
| 11  | aA    | 810 | CLA  | C1B-C2B | 2.67  | 1.49        | 1.43     |
| 11  | cB    | 812 | CLA  | C4C-C3C | 2.67  | 1.49        | 1.45     |
| 11  | aB    | 835 | CLA  | C4B-NB  | -2.67 | 1.34        | 1.37     |
| 12  | cA    | 826 | F6C  | C4A-NA  | -2.67 | 1.34        | 1.37     |
| 11  | cB    | 825 | CLA  | C1B-C2B | 2.67  | 1.49        | 1.43     |
| 11  | cB    | 818 | CLA  | C4B-NB  | -2.67 | 1.34        | 1.37     |
| 11  | bB    | 810 | CLA  | C4D-CHA | 2.67  | 1.47        | 1.38     |
| 11  | cA    | 840 | CLA  | C4B-NB  | -2.67 | 1.34        | 1.37     |
| 11  | cB    | 833 | CLA  | C4D-CHA | 2.67  | 1.47        | 1.38     |
| 11  | aB    | 808 | CLA  | C4D-CHA | 2.67  | 1.47        | 1.38     |
| 11  | cA    | 829 | CLA  | C4D-CHA | 2.67  | 1.47        | 1.38     |
| 11  | aA    | 836 | CLA  | C4D-CHA | 2.67  | 1.47        | 1.38     |
| 11  | bB    | 834 | CLA  | C4C-C3C | 2.67  | 1.49        | 1.45     |
| 11  | bA    | 840 | CLA  | C4B-NB  | -2.67 | 1.34        | 1.37     |
| 11  | bB    | 823 | CLA  | C1B-C2B | 2.67  | 1.49        | 1.43     |
| 11  | aB    | 818 | CLA  | C4B-NB  | -2.67 | 1.34        | 1.37     |
| 11  | bA    | 838 | CLA  | C4D-CHA | 2.67  | 1.47        | 1.38     |
| 11  | cA    | 824 | CLA  | C4D-CHA | 2.67  | 1.47        | 1.38     |
| 11  | cA    | 839 | CLA  | C4D-CHA | 2.67  | 1.47        | 1.38     |
| 11  | cB    | 808 | CLA  | C4D-CHA | 2.66  | 1.47        | 1.38     |
| 11  | aB    | 833 | CLA  | C4D-CHA | 2.66  | 1.47        | 1.38     |
| 11  | bA    | 839 | CLA  | C4D-CHA | 2.66  | 1.47        | 1.38     |
| 12  | bL    | 202 | F6C  | C4A-C3A | 2.66  | 1.50        | 1.45     |
| 11  | cA    | 837 | CLA  | C4D-CHA | 2.66  | 1.47        | 1.38     |
| 11  | aA    | 821 | CLA  | C4B-NB  | -2.66 | 1.34        | 1.37     |
| 15  | aL    | 207 | BCR  | C30-C25 | -2.66 | 1.50        | 1.53     |
| 11  | aA    | 837 | CLA  | C4D-CHA | 2.66  | 1.47        | 1.38     |
| 11  | bB    | 833 | CLA  | C4D-CHA | 2.66  | 1.47        | 1.38     |
| 11  | aB    | 823 | CLA  | C1B-C2B | 2.66  | 1.49        | 1.43     |
| 11  | bB    | 808 | CLA  | C4D-CHA | 2.66  | 1.47        | 1.38     |
| 11  | cA    | 838 | CLA  | C4D-CHA | 2.66  | 1.47        | 1.38     |
| 11  | aA    | 828 | CLA  | C1B-C2B | 2.66  | 1.49        | 1.43     |
| 15  | bL    | 207 | BCR  | C30-C25 | -2.66 | 1.50        | 1.53     |
| 11  | aA    | 840 | CLA  | C4D-CHA | 2.66  | 1.47        | 1.38     |
| 12  | bA    | 827 | F6C  | C4B-NB  | -2.66 | 1.33        | 1.37     |
| 11  | aB    | 804 | CLA  | C1B-C2B | 2.66  | 1.49        | 1.43     |
| 11  | cB    | 820 | CLA  | C1B-C2B | 2.66  | 1.49        | 1.43     |
| 11  | aA    | 808 | CLA  | C4D-CHA | 2.66  | 1.47        | 1.38     |
| 11  | bB    | 826 | CLA  | C4D-CHA | 2.65  | 1.47        | 1.38     |
| 11  | bB    | 835 | CLA  | C1B-C2B | 2.65  | 1.49        | 1.43     |
| 11  | aB    | 826 | CLA  | C4D-CHA | 2.65  | 1.47        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | bA    | 840 | CLA  | C4D-CHA | 2.65  | 1.47        | 1.38     |
| 15  | aA    | 849 | BCR  | C30-C25 | -2.65 | 1.50        | 1.53     |
| 11  | aA    | 821 | CLA  | C1B-C2B | 2.65  | 1.49        | 1.43     |
| 11  | bB    | 829 | CLA  | C4C-C3C | 2.65  | 1.49        | 1.45     |
| 11  | bB    | 818 | CLA  | C4B-NB  | -2.65 | 1.34        | 1.37     |
| 11  | aL    | 206 | CLA  | C4D-CHA | 2.65  | 1.47        | 1.38     |
| 11  | bA    | 837 | CLA  | C4D-CHA | 2.65  | 1.47        | 1.38     |
| 11  | bB    | 821 | CLA  | C1B-C2B | 2.65  | 1.49        | 1.43     |
| 11  | aA    | 833 | CLA  | C4D-CHA | 2.65  | 1.47        | 1.38     |
| 11  | cL    | 206 | CLA  | C4D-CHA | 2.65  | 1.47        | 1.38     |
| 11  | cB    | 834 | CLA  | C4B-NB  | -2.65 | 1.34        | 1.37     |
| 11  | aB    | 818 | CLA  | C4D-CHA | 2.65  | 1.47        | 1.38     |
| 11  | cA    | 808 | CLA  | C4D-CHA | 2.65  | 1.47        | 1.38     |
| 11  | bB    | 820 | CLA  | C1B-C2B | 2.65  | 1.49        | 1.43     |
| 12  | cL    | 202 | F6C  | C4A-C3A | 2.65  | 1.50        | 1.45     |
| 11  | bA    | 829 | CLA  | C1B-C2B | 2.64  | 1.49        | 1.43     |
| 11  | cB    | 826 | CLA  | C4D-CHA | 2.64  | 1.47        | 1.38     |
| 11  | bA    | 804 | CLA  | C1B-C2B | 2.64  | 1.49        | 1.43     |
| 11  | cA    | 823 | CLA  | C1B-C2B | 2.64  | 1.49        | 1.43     |
| 11  | bA    | 816 | CLA  | C4B-NB  | -2.64 | 1.34        | 1.37     |
| 11  | bA    | 834 | CLA  | C4D-CHA | 2.64  | 1.47        | 1.38     |
| 11  | bB    | 827 | CLA  | C4D-CHA | 2.64  | 1.47        | 1.38     |
| 12  | cA    | 827 | F6C  | C4B-NB  | -2.64 | 1.33        | 1.37     |
| 11  | aA    | 834 | CLA  | C4D-CHA | 2.64  | 1.47        | 1.38     |
| 11  | aA    | 839 | CLA  | C4D-CHA | 2.64  | 1.47        | 1.38     |
| 11  | cA    | 833 | CLA  | C4D-CHA | 2.64  | 1.47        | 1.38     |
| 11  | bA    | 821 | CLA  | C1B-C2B | 2.64  | 1.49        | 1.43     |
| 11  | bB    | 818 | CLA  | C4D-CHA | 2.64  | 1.47        | 1.38     |
| 11  | bL    | 206 | CLA  | C4D-CHA | 2.64  | 1.47        | 1.38     |
| 11  | cB    | 804 | CLA  | C1B-C2B | 2.64  | 1.49        | 1.43     |
| 11  | aA    | 816 | CLA  | C4B-NB  | -2.64 | 1.34        | 1.37     |
| 11  | cA    | 834 | CLA  | C4D-CHA | 2.64  | 1.47        | 1.38     |
| 11  | bB    | 804 | CLA  | C1B-C2B | 2.64  | 1.49        | 1.43     |
| 12  | bA    | 844 | F6C  | C3B-C4B | 2.64  | 1.50        | 1.44     |
| 12  | aA    | 827 | F6C  | C4B-NB  | -2.63 | 1.33        | 1.37     |
| 11  | cB    | 834 | CLA  | C4C-C3C | 2.63  | 1.49        | 1.45     |
| 11  | bA    | 833 | CLA  | C4D-CHA | 2.63  | 1.47        | 1.38     |
| 11  | aA    | 823 | CLA  | C1B-C2B | 2.63  | 1.49        | 1.43     |
| 11  | aB    | 838 | CLA  | C4D-CHA | 2.63  | 1.47        | 1.38     |
| 15  | cA    | 849 | BCR  | C30-C25 | -2.63 | 1.50        | 1.53     |
| 11  | aA    | 804 | CLA  | C1B-C2B | 2.63  | 1.49        | 1.43     |
| 15  | bA    | 849 | BCR  | C30-C25 | -2.63 | 1.50        | 1.53     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | aA    | 807 | CLA  | C1B-C2B | 2.63  | 1.49        | 1.43     |
| 11  | aA    | 829 | CLA  | C1B-C2B | 2.63  | 1.49        | 1.43     |
| 11  | bA    | 807 | CLA  | C1B-C2B | 2.63  | 1.49        | 1.43     |
| 11  | cA    | 829 | CLA  | C1B-C2B | 2.63  | 1.49        | 1.43     |
| 11  | aB    | 821 | CLA  | C1B-C2B | 2.63  | 1.49        | 1.43     |
| 11  | cB    | 838 | CLA  | C4D-CHA | 2.63  | 1.47        | 1.38     |
| 11  | cA    | 804 | CLA  | C1B-C2B | 2.63  | 1.49        | 1.43     |
| 11  | bA    | 808 | CLA  | C4D-CHA | 2.63  | 1.47        | 1.38     |
| 11  | cA    | 821 | CLA  | C1B-C2B | 2.63  | 1.49        | 1.43     |
| 11  | cA    | 840 | CLA  | C4D-CHA | 2.63  | 1.47        | 1.38     |
| 11  | aB    | 827 | CLA  | C4D-CHA | 2.62  | 1.47        | 1.38     |
| 12  | aA    | 844 | F6C  | C3B-C4B | 2.62  | 1.50        | 1.44     |
| 11  | aB    | 803 | CLA  | C4D-CHA | 2.62  | 1.47        | 1.38     |
| 11  | aA    | 808 | CLA  | C1B-C2B | 2.62  | 1.49        | 1.43     |
| 11  | cB    | 821 | CLA  | C1B-C2B | 2.62  | 1.49        | 1.43     |
| 11  | cB    | 802 | CLA  | C4D-CHA | 2.62  | 1.47        | 1.38     |
| 11  | aB    | 820 | CLA  | C1B-C2B | 2.62  | 1.49        | 1.43     |
| 11  | bB    | 838 | CLA  | C4D-CHA | 2.62  | 1.47        | 1.38     |
| 11  | cB    | 818 | CLA  | C4D-CHA | 2.62  | 1.47        | 1.38     |
| 15  | cB    | 848 | BCR  | C1-C6   | -2.62 | 1.50        | 1.53     |
| 15  | bB    | 848 | BCR  | C1-C6   | -2.62 | 1.50        | 1.53     |
| 11  | bA    | 823 | CLA  | C1B-C2B | 2.62  | 1.49        | 1.43     |
| 11  | cB    | 829 | CLA  | C4C-C3C | 2.62  | 1.49        | 1.45     |
| 11  | bB    | 803 | CLA  | C4D-CHA | 2.62  | 1.47        | 1.38     |
| 11  | cB    | 827 | CLA  | C4D-CHA | 2.62  | 1.47        | 1.38     |
| 11  | cB    | 803 | CLA  | C4D-CHA | 2.62  | 1.47        | 1.38     |
| 12  | bL    | 202 | F6C  | C1C-NC  | -2.61 | 1.34        | 1.37     |
| 12  | cA    | 844 | F6C  | C3B-C4B | 2.61  | 1.50        | 1.44     |
| 11  | aA    | 803 | CLA  | C4D-CHA | 2.61  | 1.47        | 1.38     |
| 11  | bA    | 810 | CLA  | C1B-C2B | 2.61  | 1.49        | 1.43     |
| 11  | aB    | 834 | CLA  | C4C-C3C | 2.61  | 1.49        | 1.45     |
| 11  | cB    | 817 | CLA  | C4D-CHA | 2.61  | 1.47        | 1.38     |
| 12  | aA    | 826 | F6C  | C4B-NB  | -2.61 | 1.33        | 1.37     |
| 12  | aL    | 202 | F6C  | C1C-NC  | -2.61 | 1.34        | 1.37     |
| 11  | bB    | 802 | CLA  | C4D-CHA | 2.61  | 1.47        | 1.38     |
| 12  | bA    | 830 | F6C  | C4B-NB  | -2.61 | 1.33        | 1.37     |
| 11  | cA    | 816 | CLA  | C4B-NB  | -2.61 | 1.34        | 1.37     |
| 11  | bA    | 803 | CLA  | C4D-CHA | 2.61  | 1.47        | 1.38     |
| 11  | bA    | 808 | CLA  | C1B-C2B | 2.61  | 1.49        | 1.43     |
| 11  | cA    | 807 | CLA  | C1B-C2B | 2.61  | 1.49        | 1.43     |
| 15  | aB    | 848 | BCR  | C1-C6   | -2.61 | 1.50        | 1.53     |
| 12  | cL    | 202 | F6C  | C1C-NC  | -2.61 | 1.34        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | bB    | 828 | CLA  | C4C-C3C | 2.61  | 1.49        | 1.45     |
| 11  | cB    | 832 | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 12  | aL    | 202 | F6C  | C4B-NB  | -2.60 | 1.33        | 1.37     |
| 11  | cA    | 803 | CLA  | C4D-CHA | 2.60  | 1.47        | 1.38     |
| 12  | bA    | 826 | F6C  | C4A-NA  | -2.60 | 1.34        | 1.37     |
| 11  | aB    | 802 | CLA  | C4D-CHA | 2.60  | 1.47        | 1.38     |
| 11  | cA    | 808 | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 12  | bL    | 202 | F6C  | C4B-NB  | -2.60 | 1.33        | 1.37     |
| 11  | bB    | 807 | CLA  | C4D-CHA | 2.60  | 1.47        | 1.38     |
| 11  | aL    | 206 | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 11  | aK    | 103 | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 12  | cA    | 827 | F6C  | C4A-C3A | 2.60  | 1.50        | 1.45     |
| 11  | cB    | 807 | CLA  | C4D-CHA | 2.60  | 1.47        | 1.38     |
| 11  | cA    | 802 | CLA  | C4D-CHA | 2.60  | 1.47        | 1.38     |
| 15  | cA    | 850 | BCR  | C30-C25 | -2.60 | 1.50        | 1.53     |
| 11  | aA    | 840 | CLA  | C4B-NB  | -2.60 | 1.34        | 1.37     |
| 12  | aA    | 827 | F6C  | C4A-C3A | 2.60  | 1.50        | 1.45     |
| 12  | cA    | 826 | F6C  | C4B-NB  | -2.60 | 1.33        | 1.37     |
| 11  | aB    | 807 | CLA  | C4D-CHA | 2.59  | 1.47        | 1.38     |
| 11  | bL    | 206 | CLA  | C1B-C2B | 2.59  | 1.49        | 1.43     |
| 11  | aB    | 817 | CLA  | C4D-CHA | 2.59  | 1.47        | 1.38     |
| 11  | aB    | 832 | CLA  | C1B-C2B | 2.59  | 1.49        | 1.43     |
| 12  | aA    | 826 | F6C  | C1C-C2C | 2.59  | 1.49        | 1.43     |
| 15  | bL    | 203 | BCR  | C30-C25 | -2.59 | 1.50        | 1.53     |
| 11  | aA    | 841 | CLA  | C1B-C2B | 2.59  | 1.49        | 1.43     |
| 15  | cL    | 203 | BCR  | C30-C25 | -2.59 | 1.50        | 1.53     |
| 15  | cB    | 843 | BCR  | C30-C25 | -2.59 | 1.50        | 1.53     |
| 11  | aB    | 839 | CLA  | C3D-C4D | -2.58 | 1.38        | 1.44     |
| 12  | cB    | 824 | F6C  | C4B-NB  | -2.58 | 1.33        | 1.37     |
| 11  | bL    | 204 | CLA  | C1B-C2B | 2.58  | 1.49        | 1.43     |
| 11  | aB    | 819 | CLA  | C1B-C2B | 2.58  | 1.49        | 1.43     |
| 11  | bB    | 839 | CLA  | C3D-C4D | -2.58 | 1.38        | 1.44     |
| 11  | aA    | 840 | CLA  | C3B-C4B | 2.58  | 1.50        | 1.42     |
| 11  | bB    | 836 | CLA  | C4C-C3C | 2.58  | 1.49        | 1.45     |
| 11  | cA    | 837 | CLA  | C1B-C2B | 2.58  | 1.49        | 1.43     |
| 11  | cB    | 822 | CLA  | C1B-C2B | 2.58  | 1.49        | 1.43     |
| 11  | aB    | 803 | CLA  | C1C-NC  | -2.58 | 1.33        | 1.37     |
| 11  | cA    | 841 | CLA  | C1B-C2B | 2.58  | 1.49        | 1.43     |
| 11  | aB    | 839 | CLA  | C4D-CHA | 2.58  | 1.47        | 1.38     |
| 11  | aA    | 814 | CLA  | C4D-CHA | 2.58  | 1.47        | 1.38     |
| 11  | cA    | 814 | CLA  | C4D-CHA | 2.58  | 1.47        | 1.38     |
| 11  | bA    | 840 | CLA  | C3B-C4B | 2.58  | 1.50        | 1.42     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | bB    | 817 | CLA  | C4D-CHA | 2.58  | 1.47        | 1.38     |
| 11  | cB    | 803 | CLA  | C1C-NC  | -2.58 | 1.33        | 1.37     |
| 11  | bK    | 103 | CLA  | C1B-C2B | 2.58  | 1.49        | 1.43     |
| 11  | bA    | 812 | CLA  | C1B-C2B | 2.58  | 1.49        | 1.43     |
| 12  | bA    | 832 | F6C  | C4B-NB  | -2.57 | 1.33        | 1.37     |
| 11  | bB    | 832 | CLA  | C1B-C2B | 2.57  | 1.49        | 1.43     |
| 11  | bA    | 814 | CLA  | C4D-CHA | 2.57  | 1.47        | 1.38     |
| 15  | aB    | 843 | BCR  | C30-C25 | -2.57 | 1.50        | 1.53     |
| 11  | aA    | 802 | CLA  | C4D-CHA | 2.57  | 1.47        | 1.38     |
| 12  | bA    | 827 | F6C  | C4A-C3A | 2.57  | 1.50        | 1.45     |
| 11  | aL    | 204 | CLA  | C1B-C2B | 2.57  | 1.49        | 1.43     |
| 11  | cL    | 206 | CLA  | C1B-C2B | 2.57  | 1.49        | 1.43     |
| 15  | bA    | 851 | BCR  | C1-C6   | -2.57 | 1.50        | 1.53     |
| 11  | cK    | 103 | CLA  | C1B-C2B | 2.57  | 1.49        | 1.43     |
| 11  | bA    | 802 | CLA  | C4D-CHA | 2.57  | 1.47        | 1.38     |
| 11  | bB    | 822 | CLA  | C1B-C2B | 2.57  | 1.49        | 1.43     |
| 11  | cB    | 836 | CLA  | C4C-C3C | 2.57  | 1.49        | 1.45     |
| 11  | bB    | 819 | CLA  | C1B-C2B | 2.56  | 1.49        | 1.43     |
| 11  | bB    | 839 | CLA  | C4D-CHA | 2.56  | 1.47        | 1.38     |
| 15  | aA    | 850 | BCR  | C30-C25 | -2.56 | 1.50        | 1.53     |
| 11  | cL    | 204 | CLA  | C1B-C2B | 2.56  | 1.49        | 1.43     |
| 12  | cA    | 830 | F6C  | C4B-NB  | -2.56 | 1.33        | 1.37     |
| 15  | aL    | 203 | BCR  | C30-C25 | -2.56 | 1.50        | 1.53     |
| 11  | bA    | 837 | CLA  | C1B-C2B | 2.56  | 1.49        | 1.43     |
| 11  | cA    | 809 | CLA  | C1B-C2B | 2.56  | 1.49        | 1.43     |
| 12  | aB    | 824 | F6C  | C4B-NB  | -2.56 | 1.33        | 1.37     |
| 11  | cB    | 819 | CLA  | C1B-C2B | 2.56  | 1.49        | 1.43     |
| 15  | bA    | 850 | BCR  | C30-C25 | -2.56 | 1.50        | 1.53     |
| 11  | aA    | 818 | CLA  | C1B-C2B | 2.56  | 1.49        | 1.43     |
| 11  | bA    | 809 | CLA  | C1B-C2B | 2.56  | 1.49        | 1.43     |
| 15  | cA    | 851 | BCR  | C1-C6   | -2.56 | 1.50        | 1.53     |
| 11  | cA    | 840 | CLA  | C3B-C4B | 2.56  | 1.50        | 1.42     |
| 15  | aA    | 851 | BCR  | C1-C6   | -2.56 | 1.50        | 1.53     |
| 12  | bB    | 824 | F6C  | C4B-NB  | -2.56 | 1.33        | 1.37     |
| 11  | aB    | 828 | CLA  | C4C-C3C | 2.56  | 1.49        | 1.45     |
| 11  | aB    | 836 | CLA  | C4C-C3C | 2.56  | 1.49        | 1.45     |
| 11  | cB    | 839 | CLA  | C4D-CHA | 2.56  | 1.47        | 1.38     |
| 11  | aA    | 837 | CLA  | C1B-C2B | 2.56  | 1.49        | 1.43     |
| 12  | cA    | 826 | F6C  | C1C-C2C | 2.56  | 1.49        | 1.43     |
| 11  | cB    | 839 | CLA  | C3D-C4D | -2.56 | 1.38        | 1.44     |
| 11  | bK    | 101 | CLA  | C1B-C2B | 2.55  | 1.49        | 1.43     |
| 12  | bA    | 826 | F6C  | C1C-C2C | 2.55  | 1.49        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | aB    | 828 | CLA  | C3D-C4D | -2.55 | 1.38        | 1.44     |
| 11  | aA    | 809 | CLA  | C1B-C2B | 2.55  | 1.49        | 1.43     |
| 11  | cB    | 803 | CLA  | C1B-C2B | 2.55  | 1.49        | 1.43     |
| 12  | cA    | 832 | F6C  | C4B-NB  | -2.55 | 1.33        | 1.37     |
| 11  | cB    | 828 | CLA  | C3D-C4D | -2.55 | 1.38        | 1.44     |
| 11  | bB    | 803 | CLA  | C1B-C2B | 2.55  | 1.49        | 1.43     |
| 11  | cB    | 812 | CLA  | C1B-C2B | 2.55  | 1.49        | 1.43     |
| 11  | aK    | 101 | CLA  | C1B-C2B | 2.55  | 1.49        | 1.43     |
| 11  | bA    | 812 | CLA  | C4C-C3C | 2.55  | 1.49        | 1.45     |
| 12  | bA    | 830 | F6C  | C4A-C3A | 2.54  | 1.50        | 1.45     |
| 12  | cA    | 830 | F6C  | C4A-C3A | 2.54  | 1.50        | 1.45     |
| 11  | cA    | 812 | CLA  | C4C-C3C | 2.54  | 1.49        | 1.45     |
| 11  | bA    | 841 | CLA  | C1B-C2B | 2.54  | 1.49        | 1.43     |
| 11  | cK    | 101 | CLA  | C1B-C2B | 2.54  | 1.49        | 1.43     |
| 12  | aA    | 832 | F6C  | C4B-NB  | -2.54 | 1.33        | 1.37     |
| 11  | aB    | 822 | CLA  | C1B-C2B | 2.54  | 1.49        | 1.43     |
| 12  | aA    | 830 | F6C  | C4B-NB  | -2.54 | 1.33        | 1.37     |
| 11  | cB    | 828 | CLA  | C4C-C3C | 2.54  | 1.49        | 1.45     |
| 11  | bB    | 828 | CLA  | C3D-C4D | -2.54 | 1.38        | 1.44     |
| 11  | aB    | 803 | CLA  | C1B-C2B | 2.54  | 1.49        | 1.43     |
| 11  | bA    | 818 | CLA  | C1B-C2B | 2.53  | 1.49        | 1.43     |
| 11  | cB    | 811 | CLA  | C1B-C2B | 2.53  | 1.49        | 1.43     |
| 11  | bB    | 812 | CLA  | C1B-C2B | 2.53  | 1.49        | 1.43     |
| 12  | bA    | 826 | F6C  | C4B-NB  | -2.53 | 1.33        | 1.37     |
| 12  | cL    | 202 | F6C  | C4B-NB  | -2.53 | 1.33        | 1.37     |
| 11  | aA    | 813 | CLA  | C4B-NB  | -2.53 | 1.34        | 1.37     |
| 11  | aB    | 811 | CLA  | C1B-C2B | 2.53  | 1.49        | 1.43     |
| 15  | bB    | 843 | BCR  | C30-C25 | -2.53 | 1.50        | 1.53     |
| 12  | aA    | 830 | F6C  | C4A-C3A | 2.53  | 1.50        | 1.45     |
| 11  | cB    | 832 | CLA  | C4C-C3C | 2.53  | 1.49        | 1.45     |
| 11  | aB    | 814 | CLA  | C1B-C2B | 2.53  | 1.49        | 1.43     |
| 11  | aB    | 812 | CLA  | C1B-C2B | 2.52  | 1.49        | 1.43     |
| 11  | bB    | 811 | CLA  | C1B-C2B | 2.52  | 1.49        | 1.43     |
| 11  | bB    | 807 | CLA  | C1B-C2B | 2.52  | 1.49        | 1.43     |
| 11  | bB    | 814 | CLA  | C1B-C2B | 2.52  | 1.49        | 1.43     |
| 11  | cB    | 807 | CLA  | C1B-C2B | 2.52  | 1.49        | 1.43     |
| 11  | bB    | 811 | CLA  | C4C-C3C | 2.52  | 1.49        | 1.45     |
| 11  | bA    | 816 | CLA  | C3B-C4B | 2.52  | 1.50        | 1.42     |
| 11  | aA    | 816 | CLA  | C3B-C4B | 2.52  | 1.50        | 1.42     |
| 11  | aB    | 801 | CLA  | C4D-CHA | 2.52  | 1.47        | 1.38     |
| 11  | cB    | 801 | CLA  | C4D-CHA | 2.52  | 1.47        | 1.38     |
| 11  | aB    | 814 | CLA  | C4C-C3C | 2.52  | 1.49        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | cB    | 814 | CLA  | C1B-C2B | 2.52  | 1.49        | 1.43     |
| 11  | bB    | 814 | CLA  | C4C-C3C | 2.52  | 1.49        | 1.45     |
| 11  | bA    | 814 | CLA  | C1B-C2B | 2.52  | 1.49        | 1.43     |
| 11  | aA    | 812 | CLA  | C1B-C2B | 2.52  | 1.49        | 1.43     |
| 11  | cA    | 818 | CLA  | C1B-C2B | 2.52  | 1.49        | 1.43     |
| 11  | aA    | 812 | CLA  | C4C-C3C | 2.51  | 1.49        | 1.45     |
| 11  | bB    | 803 | CLA  | C1C-NC  | -2.51 | 1.33        | 1.37     |
| 11  | bA    | 815 | CLA  | C1B-C2B | 2.51  | 1.49        | 1.43     |
| 11  | cA    | 813 | CLA  | C4B-NB  | -2.51 | 1.34        | 1.37     |
| 11  | aB    | 821 | CLA  | C4C-C3C | 2.51  | 1.49        | 1.45     |
| 11  | cB    | 814 | CLA  | C4C-C3C | 2.51  | 1.49        | 1.45     |
| 11  | cA    | 812 | CLA  | C1B-C2B | 2.50  | 1.49        | 1.43     |
| 11  | aB    | 838 | CLA  | C1B-C2B | 2.50  | 1.49        | 1.43     |
| 12  | aA    | 826 | F6C  | C2B-C1B | 2.50  | 1.49        | 1.44     |
| 11  | bB    | 801 | CLA  | C4D-CHA | 2.50  | 1.47        | 1.38     |
| 11  | bB    | 809 | CLA  | C4D-CHA | 2.50  | 1.47        | 1.38     |
| 11  | bA    | 813 | CLA  | C4B-NB  | -2.50 | 1.34        | 1.37     |
| 11  | cA    | 816 | CLA  | C3B-C4B | 2.50  | 1.50        | 1.42     |
| 15  | aI    | 101 | BCR  | C30-C25 | -2.50 | 1.50        | 1.53     |
| 11  | bB    | 831 | CLA  | C1B-C2B | 2.50  | 1.49        | 1.43     |
| 11  | cA    | 805 | CLA  | C1C-C2C | 2.50  | 1.49        | 1.44     |
| 11  | aA    | 814 | CLA  | C1B-C2B | 2.50  | 1.49        | 1.43     |
| 11  | aB    | 809 | CLA  | C4D-CHA | 2.50  | 1.47        | 1.38     |
| 11  | aB    | 831 | CLA  | C1B-C2B | 2.49  | 1.49        | 1.43     |
| 11  | cB    | 831 | CLA  | C1B-C2B | 2.49  | 1.49        | 1.43     |
| 11  | aK    | 103 | CLA  | C4C-C3C | 2.49  | 1.49        | 1.45     |
| 11  | aA    | 819 | CLA  | C3B-C4B | 2.49  | 1.50        | 1.42     |
| 11  | bA    | 805 | CLA  | C1C-C2C | 2.49  | 1.49        | 1.44     |
| 12  | cA    | 827 | F6C  | C1C-C2C | 2.49  | 1.49        | 1.43     |
| 11  | bB    | 837 | CLA  | C1B-C2B | 2.49  | 1.49        | 1.43     |
| 11  | cA    | 814 | CLA  | C1B-C2B | 2.49  | 1.49        | 1.43     |
| 11  | cB    | 809 | CLA  | C4D-CHA | 2.48  | 1.46        | 1.38     |
| 11  | aB    | 807 | CLA  | C1B-C2B | 2.48  | 1.49        | 1.43     |
| 11  | bB    | 832 | CLA  | C4C-C3C | 2.48  | 1.49        | 1.45     |
| 11  | cA    | 835 | CLA  | C1B-C2B | 2.48  | 1.49        | 1.43     |
| 11  | aA    | 815 | CLA  | C1B-C2B | 2.48  | 1.49        | 1.43     |
| 11  | cB    | 833 | CLA  | C1B-C2B | 2.48  | 1.48        | 1.43     |
| 11  | aA    | 805 | CLA  | C1C-C2C | 2.48  | 1.49        | 1.44     |
| 12  | bA    | 826 | F6C  | CMB-C2B | 2.48  | 1.50        | 1.45     |
| 11  | bA    | 819 | CLA  | C3B-C4B | 2.48  | 1.49        | 1.42     |
| 11  | bB    | 815 | CLA  | C1B-C2B | 2.47  | 1.48        | 1.43     |
| 12  | aA    | 826 | F6C  | CMB-C2B | 2.47  | 1.50        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12  | cA    | 826 | F6C  | CMB-C2B | 2.47  | 1.50        | 1.45     |
| 11  | cB    | 838 | CLA  | C1B-C2B | 2.47  | 1.48        | 1.43     |
| 11  | cA    | 819 | CLA  | C3B-C4B | 2.47  | 1.49        | 1.42     |
| 11  | aB    | 815 | CLA  | C1B-C2B | 2.47  | 1.48        | 1.43     |
| 12  | aA    | 827 | F6C  | C1C-C2C | 2.47  | 1.48        | 1.43     |
| 11  | cA    | 821 | CLA  | C4C-C3C | 2.47  | 1.49        | 1.45     |
| 11  | cA    | 838 | CLA  | C3B-C2B | 2.47  | 1.49        | 1.41     |
| 12  | bA    | 826 | F6C  | C2B-C1B | 2.47  | 1.49        | 1.44     |
| 11  | bB    | 821 | CLA  | C4C-C3C | 2.47  | 1.49        | 1.45     |
| 11  | bB    | 806 | CLA  | C1B-C2B | 2.47  | 1.48        | 1.43     |
| 11  | aB    | 833 | CLA  | C1B-C2B | 2.47  | 1.48        | 1.43     |
| 11  | bB    | 838 | CLA  | C1B-C2B | 2.47  | 1.48        | 1.43     |
| 11  | aB    | 804 | CLA  | C1C-C2C | 2.47  | 1.49        | 1.44     |
| 12  | cA    | 830 | F6C  | C1A-C2A | 2.47  | 1.50        | 1.45     |
| 11  | cB    | 815 | CLA  | C1B-C2B | 2.47  | 1.48        | 1.43     |
| 11  | cA    | 815 | CLA  | C1B-C2B | 2.47  | 1.48        | 1.43     |
| 11  | bB    | 833 | CLA  | C1B-C2B | 2.46  | 1.48        | 1.43     |
| 11  | cK    | 103 | CLA  | C4C-C3C | 2.46  | 1.49        | 1.45     |
| 11  | aA    | 838 | CLA  | C3B-C2B | 2.46  | 1.49        | 1.41     |
| 12  | aL    | 202 | F6C  | C1C-C2C | 2.46  | 1.48        | 1.43     |
| 11  | bA    | 806 | CLA  | C3B-C4B | 2.46  | 1.49        | 1.42     |
| 12  | bL    | 202 | F6C  | C1C-C2C | 2.46  | 1.48        | 1.43     |
| 11  | aB    | 806 | CLA  | C1B-C2B | 2.46  | 1.48        | 1.43     |
| 11  | cB    | 805 | CLA  | C1B-C2B | 2.46  | 1.48        | 1.43     |
| 11  | bB    | 804 | CLA  | C1C-C2C | 2.46  | 1.49        | 1.44     |
| 12  | bA    | 827 | F6C  | C1C-C2C | 2.46  | 1.48        | 1.43     |
| 11  | bA    | 838 | CLA  | C3B-C2B | 2.46  | 1.49        | 1.41     |
| 11  | bB    | 807 | CLA  | C3D-C4D | -2.46 | 1.38        | 1.44     |
| 11  | aA    | 821 | CLA  | C4C-C3C | 2.46  | 1.49        | 1.45     |
| 11  | cB    | 821 | CLA  | C4C-C3C | 2.46  | 1.49        | 1.45     |
| 12  | aA    | 830 | F6C  | C1C-C2C | 2.46  | 1.48        | 1.43     |
| 11  | cB    | 833 | CLA  | C3B-C4B | 2.46  | 1.49        | 1.42     |
| 12  | aA    | 830 | F6C  | C1A-C2A | 2.46  | 1.50        | 1.45     |
| 11  | aB    | 811 | CLA  | C4C-C3C | 2.45  | 1.49        | 1.45     |
| 11  | bB    | 835 | CLA  | C4C-C3C | 2.45  | 1.49        | 1.45     |
| 11  | cA    | 806 | CLA  | C3B-C4B | 2.45  | 1.49        | 1.42     |
| 11  | aA    | 835 | CLA  | C1B-C2B | 2.45  | 1.48        | 1.43     |
| 11  | aB    | 833 | CLA  | C3B-C4B | 2.45  | 1.49        | 1.42     |
| 12  | cL    | 202 | F6C  | C1C-C2C | 2.45  | 1.48        | 1.43     |
| 11  | aA    | 806 | CLA  | C3B-C4B | 2.45  | 1.49        | 1.42     |
| 12  | cA    | 826 | F6C  | C2B-C1B | 2.45  | 1.49        | 1.44     |
| 11  | bA    | 835 | CLA  | C1B-C2B | 2.45  | 1.48        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 15  | cB    | 844 | BCR  | C30-C25 | -2.45 | 1.50        | 1.53     |
| 11  | aB    | 832 | CLA  | C4C-C3C | 2.45  | 1.49        | 1.45     |
| 11  | aA    | 805 | CLA  | C3B-C4B | 2.45  | 1.49        | 1.42     |
| 12  | cA    | 830 | F6C  | C2B-C1B | 2.45  | 1.49        | 1.44     |
| 11  | bB    | 836 | CLA  | C3D-C4D | -2.45 | 1.38        | 1.44     |
| 15  | aB    | 844 | BCR  | C30-C25 | -2.45 | 1.50        | 1.53     |
| 11  | cB    | 811 | CLA  | C4C-C3C | 2.45  | 1.49        | 1.45     |
| 11  | bA    | 824 | CLA  | C3D-C4D | -2.45 | 1.38        | 1.44     |
| 12  | bA    | 830 | F6C  | C1A-C2A | 2.45  | 1.50        | 1.45     |
| 15  | bB    | 844 | BCR  | C30-C25 | -2.45 | 1.50        | 1.53     |
| 12  | cL    | 202 | F6C  | C4A-NA  | -2.45 | 1.34        | 1.37     |
| 12  | bA    | 830 | F6C  | C1C-C2C | 2.45  | 1.48        | 1.43     |
| 15  | cI    | 103 | BCR  | C30-C25 | -2.44 | 1.50        | 1.53     |
| 11  | bA    | 821 | CLA  | C4C-C3C | 2.44  | 1.49        | 1.45     |
| 11  | bB    | 833 | CLA  | C3B-C4B | 2.44  | 1.49        | 1.42     |
| 12  | aL    | 202 | F6C  | C4A-NA  | -2.44 | 1.34        | 1.37     |
| 11  | cA    | 818 | CLA  | C3B-C2B | 2.44  | 1.49        | 1.41     |
| 11  | cB    | 835 | CLA  | C4C-C3C | 2.44  | 1.49        | 1.45     |
| 15  | bI    | 101 | BCR  | C30-C25 | -2.44 | 1.50        | 1.53     |
| 11  | aA    | 818 | CLA  | C3B-C2B | 2.44  | 1.49        | 1.41     |
| 12  | bA    | 832 | F6C  | C4A-C3A | 2.44  | 1.50        | 1.45     |
| 11  | cB    | 806 | CLA  | C1B-C2B | 2.44  | 1.48        | 1.43     |
| 12  | aL    | 202 | F6C  | CMB-C2B | 2.44  | 1.50        | 1.45     |
| 11  | aA    | 838 | CLA  | C3D-C4D | -2.43 | 1.38        | 1.44     |
| 11  | aB    | 807 | CLA  | C3D-C4D | -2.43 | 1.38        | 1.44     |
| 11  | aB    | 836 | CLA  | C3D-C4D | -2.43 | 1.38        | 1.44     |
| 11  | bA    | 839 | CLA  | C1B-C2B | 2.43  | 1.48        | 1.43     |
| 11  | cB    | 804 | CLA  | C1C-C2C | 2.43  | 1.49        | 1.44     |
| 11  | bK    | 103 | CLA  | C4C-C3C | 2.43  | 1.49        | 1.45     |
| 11  | aB    | 837 | CLA  | C1B-C2B | 2.43  | 1.48        | 1.43     |
| 12  | cA    | 830 | F6C  | C1C-C2C | 2.43  | 1.48        | 1.43     |
| 11  | aL    | 204 | CLA  | C3B-C2B | 2.43  | 1.49        | 1.41     |
| 12  | bL    | 202 | F6C  | CMB-C2B | 2.43  | 1.50        | 1.45     |
| 11  | cB    | 810 | CLA  | C1B-C2B | 2.43  | 1.48        | 1.43     |
| 11  | bA    | 805 | CLA  | C3B-C4B | 2.43  | 1.49        | 1.42     |
| 12  | cA    | 832 | F6C  | C1A-C2A | 2.43  | 1.50        | 1.45     |
| 12  | aA    | 830 | F6C  | C2B-C1B | 2.43  | 1.49        | 1.44     |
| 11  | cB    | 838 | CLA  | C3B-C4B | 2.43  | 1.49        | 1.42     |
| 12  | cA    | 832 | F6C  | C4A-C3A | 2.43  | 1.50        | 1.45     |
| 11  | aB    | 805 | CLA  | C1B-C2B | 2.43  | 1.48        | 1.43     |
| 11  | bB    | 830 | CLA  | C4C-C3C | 2.43  | 1.49        | 1.45     |
| 11  | aB    | 803 | CLA  | C4C-C3C | 2.42  | 1.49        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | bB    | 838 | CLA  | C3B-C4B | 2.42  | 1.49        | 1.42     |
| 11  | cK    | 101 | CLA  | C4C-C3C | 2.42  | 1.49        | 1.45     |
| 11  | aB    | 830 | CLA  | C4C-C3C | 2.42  | 1.49        | 1.45     |
| 12  | cA    | 844 | F6C  | C1C-C2C | 2.42  | 1.48        | 1.43     |
| 11  | cA    | 805 | CLA  | C3B-C4B | 2.42  | 1.49        | 1.42     |
| 11  | aB    | 835 | CLA  | C4C-C3C | 2.42  | 1.49        | 1.45     |
| 12  | aA    | 832 | F6C  | C1A-C2A | 2.42  | 1.50        | 1.45     |
| 11  | aB    | 827 | CLA  | C1B-C2B | 2.42  | 1.48        | 1.43     |
| 11  | cB    | 803 | CLA  | C4C-C3C | 2.42  | 1.49        | 1.45     |
| 11  | bA    | 818 | CLA  | C3B-C2B | 2.42  | 1.49        | 1.41     |
| 11  | bB    | 803 | CLA  | C4C-C3C | 2.42  | 1.49        | 1.45     |
| 11  | cB    | 836 | CLA  | C3D-C4D | -2.42 | 1.38        | 1.44     |
| 11  | bB    | 827 | CLA  | C1B-C2B | 2.42  | 1.48        | 1.43     |
| 11  | bA    | 842 | CLA  | C3B-C4B | 2.42  | 1.49        | 1.42     |
| 12  | aA    | 827 | F6C  | CMB-C2B | 2.42  | 1.50        | 1.45     |
| 11  | aB    | 838 | CLA  | C3B-C4B | 2.42  | 1.49        | 1.42     |
| 11  | bL    | 204 | CLA  | C3B-C2B | 2.42  | 1.49        | 1.41     |
| 11  | cB    | 837 | CLA  | C1B-C2B | 2.41  | 1.48        | 1.43     |
| 15  | aK    | 102 | BCR  | C30-C25 | -2.41 | 1.50        | 1.53     |
| 11  | bB    | 805 | CLA  | C1B-C2B | 2.41  | 1.48        | 1.43     |
| 11  | cL    | 204 | CLA  | C3B-C2B | 2.41  | 1.49        | 1.41     |
| 11  | aA    | 839 | CLA  | C1B-C2B | 2.41  | 1.48        | 1.43     |
| 11  | aA    | 843 | CLA  | C1B-C2B | 2.41  | 1.48        | 1.43     |
| 11  | cB    | 827 | CLA  | C1B-C2B | 2.41  | 1.48        | 1.43     |
| 11  | cA    | 824 | CLA  | C3D-C4D | -2.41 | 1.38        | 1.44     |
| 12  | aA    | 832 | F6C  | C4A-C3A | 2.41  | 1.50        | 1.45     |
| 11  | cA    | 839 | CLA  | C1B-C2B | 2.41  | 1.48        | 1.43     |
| 12  | bA    | 844 | F6C  | C1C-C2C | 2.41  | 1.48        | 1.43     |
| 11  | cB    | 807 | CLA  | C3D-C4D | -2.41 | 1.38        | 1.44     |
| 11  | aB    | 809 | CLA  | C3D-C4D | -2.41 | 1.38        | 1.44     |
| 12  | cL    | 202 | F6C  | CMB-C2B | 2.41  | 1.50        | 1.45     |
| 11  | cA    | 842 | CLA  | C3B-C4B | 2.41  | 1.49        | 1.42     |
| 11  | aA    | 824 | CLA  | C3D-C4D | -2.41 | 1.38        | 1.44     |
| 11  | cL    | 205 | CLA  | C1B-C2B | 2.41  | 1.48        | 1.43     |
| 11  | bA    | 838 | CLA  | C1B-C2B | 2.41  | 1.48        | 1.43     |
| 11  | bA    | 815 | CLA  | C4C-C3C | 2.40  | 1.49        | 1.45     |
| 15  | cK    | 102 | BCR  | C30-C25 | -2.40 | 1.50        | 1.53     |
| 11  | bB    | 809 | CLA  | C3D-C4D | -2.40 | 1.38        | 1.44     |
| 11  | cB    | 807 | CLA  | C4C-C3C | 2.40  | 1.49        | 1.45     |
| 11  | bL    | 205 | CLA  | C1B-C2B | 2.40  | 1.48        | 1.43     |
| 12  | bA    | 830 | F6C  | C2B-C1B | 2.40  | 1.49        | 1.44     |
| 12  | bA    | 832 | F6C  | C1A-C2A | 2.40  | 1.50        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | cB    | 838 | CLA  | C4C-C3C | 2.40  | 1.49        | 1.45     |
| 11  | cA    | 838 | CLA  | C1B-C2B | 2.40  | 1.48        | 1.43     |
| 11  | cA    | 843 | CLA  | C1B-C2B | 2.40  | 1.48        | 1.43     |
| 11  | cA    | 838 | CLA  | C3D-C4D | -2.40 | 1.38        | 1.44     |
| 11  | aA    | 838 | CLA  | C1B-C2B | 2.40  | 1.48        | 1.43     |
| 11  | aB    | 831 | CLA  | C4C-C3C | 2.40  | 1.49        | 1.45     |
| 11  | cA    | 839 | CLA  | C4C-C3C | 2.40  | 1.49        | 1.45     |
| 11  | cB    | 830 | CLA  | C4C-C3C | 2.40  | 1.49        | 1.45     |
| 11  | aA    | 842 | CLA  | C3B-C4B | 2.40  | 1.49        | 1.42     |
| 11  | aB    | 810 | CLA  | C1B-C2B | 2.39  | 1.48        | 1.43     |
| 11  | bA    | 806 | CLA  | C1B-C2B | 2.39  | 1.48        | 1.43     |
| 11  | bB    | 810 | CLA  | C1B-C2B | 2.39  | 1.48        | 1.43     |
| 11  | bA    | 803 | CLA  | C3B-C2B | 2.39  | 1.49        | 1.41     |
| 11  | aL    | 205 | CLA  | C1B-C2B | 2.39  | 1.48        | 1.43     |
| 12  | aA    | 844 | F6C  | C1C-C2C | 2.39  | 1.48        | 1.43     |
| 12  | cA    | 827 | F6C  | CMB-C2B | 2.39  | 1.50        | 1.45     |
| 12  | bA    | 827 | F6C  | CMB-C2B | 2.39  | 1.50        | 1.45     |
| 11  | aA    | 839 | CLA  | C4C-C3C | 2.39  | 1.49        | 1.45     |
| 11  | aK    | 101 | CLA  | C4C-C3C | 2.39  | 1.49        | 1.45     |
| 11  | cA    | 803 | CLA  | C3B-C2B | 2.39  | 1.49        | 1.41     |
| 11  | bA    | 838 | CLA  | C3D-C4D | -2.39 | 1.38        | 1.44     |
| 11  | bA    | 841 | CLA  | C4C-C3C | 2.39  | 1.49        | 1.45     |
| 11  | bB    | 805 | CLA  | C3D-C4D | -2.39 | 1.38        | 1.44     |
| 11  | cA    | 831 | CLA  | C4C-C3C | 2.39  | 1.49        | 1.45     |
| 12  | bA    | 827 | F6C  | C2B-C1B | 2.39  | 1.49        | 1.44     |
| 11  | bA    | 839 | CLA  | C4C-C3C | 2.38  | 1.49        | 1.45     |
| 11  | bB    | 836 | CLA  | C3B-C4B | 2.38  | 1.49        | 1.42     |
| 11  | aB    | 826 | CLA  | C1B-C2B | 2.38  | 1.48        | 1.43     |
| 11  | cA    | 811 | CLA  | C1B-C2B | 2.38  | 1.48        | 1.43     |
| 11  | cA    | 820 | CLA  | C4C-C3C | 2.38  | 1.49        | 1.45     |
| 11  | aA    | 803 | CLA  | C3B-C2B | 2.38  | 1.49        | 1.41     |
| 11  | cA    | 833 | CLA  | C3D-C4D | -2.38 | 1.38        | 1.44     |
| 11  | aA    | 820 | CLA  | C4C-C3C | 2.38  | 1.49        | 1.45     |
| 11  | bA    | 831 | CLA  | C4C-C3C | 2.38  | 1.49        | 1.45     |
| 11  | cA    | 837 | CLA  | C3B-C2B | 2.38  | 1.49        | 1.41     |
| 12  | bL    | 202 | F6C  | C4A-NA  | -2.38 | 1.34        | 1.37     |
| 11  | cA    | 816 | CLA  | C4C-C3C | 2.38  | 1.49        | 1.45     |
| 15  | bL    | 203 | BCR  | C33-C5  | -2.38 | 1.47        | 1.50     |
| 11  | aA    | 805 | CLA  | C1B-C2B | 2.38  | 1.48        | 1.43     |
| 11  | cB    | 809 | CLA  | C3D-C4D | -2.38 | 1.38        | 1.44     |
| 11  | bK    | 101 | CLA  | C4C-C3C | 2.38  | 1.49        | 1.45     |
| 11  | bA    | 829 | CLA  | C4C-C3C | 2.38  | 1.49        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | bA    | 843 | CLA  | C1B-C2B | 2.38  | 1.48        | 1.43     |
| 12  | cA    | 827 | F6C  | C2B-C1B | 2.38  | 1.49        | 1.44     |
| 12  | cA    | 844 | F6C  | C1A-C2A | 2.38  | 1.50        | 1.45     |
| 12  | aA    | 844 | F6C  | C1A-C2A | 2.38  | 1.50        | 1.45     |
| 11  | bB    | 838 | CLA  | C4C-C3C | 2.38  | 1.49        | 1.45     |
| 11  | cB    | 831 | CLA  | C4C-C3C | 2.38  | 1.49        | 1.45     |
| 11  | aA    | 822 | CLA  | C1B-C2B | 2.38  | 1.48        | 1.43     |
| 11  | aA    | 811 | CLA  | C1B-C2B | 2.38  | 1.48        | 1.43     |
| 11  | aB    | 807 | CLA  | C4C-C3C | 2.37  | 1.49        | 1.45     |
| 11  | cB    | 839 | CLA  | C1C-C2C | 2.37  | 1.49        | 1.44     |
| 11  | cA    | 829 | CLA  | C4C-C3C | 2.37  | 1.49        | 1.45     |
| 11  | cA    | 840 | CLA  | C1B-C2B | 2.37  | 1.48        | 1.43     |
| 11  | aA    | 816 | CLA  | C4C-C3C | 2.37  | 1.49        | 1.45     |
| 11  | aA    | 831 | CLA  | C4C-C3C | 2.37  | 1.49        | 1.45     |
| 11  | bB    | 807 | CLA  | C4C-C3C | 2.37  | 1.49        | 1.45     |
| 11  | bA    | 802 | CLA  | C1B-C2B | 2.37  | 1.48        | 1.43     |
| 11  | aB    | 805 | CLA  | C3D-C4D | -2.37 | 1.38        | 1.44     |
| 11  | aA    | 833 | CLA  | C3D-C4D | -2.37 | 1.38        | 1.44     |
| 11  | bA    | 808 | CLA  | C4C-C3C | 2.37  | 1.49        | 1.45     |
| 11  | bA    | 820 | CLA  | C4C-C3C | 2.37  | 1.49        | 1.45     |
| 11  | cA    | 811 | CLA  | C4C-C3C | 2.37  | 1.49        | 1.45     |
| 11  | cA    | 806 | CLA  | C1B-C2B | 2.37  | 1.48        | 1.43     |
| 11  | cA    | 802 | CLA  | C3D-C4D | -2.37 | 1.38        | 1.44     |
| 11  | bK    | 101 | CLA  | C3B-C4B | 2.37  | 1.49        | 1.42     |
| 11  | cA    | 817 | CLA  | C4C-C3C | 2.37  | 1.49        | 1.45     |
| 11  | cB    | 840 | CLA  | C3D-C4D | -2.37 | 1.38        | 1.44     |
| 11  | bA    | 840 | CLA  | C1B-C2B | 2.37  | 1.48        | 1.43     |
| 11  | cB    | 818 | CLA  | C3B-C4B | 2.37  | 1.49        | 1.42     |
| 11  | bA    | 829 | CLA  | C3B-C2B | 2.37  | 1.49        | 1.41     |
| 11  | cA    | 833 | CLA  | C1B-C2B | 2.37  | 1.48        | 1.43     |
| 11  | cB    | 808 | CLA  | C1B-C2B | 2.37  | 1.48        | 1.43     |
| 11  | bA    | 819 | CLA  | C1C-C2C | 2.36  | 1.49        | 1.44     |
| 11  | bB    | 826 | CLA  | C1B-C2B | 2.36  | 1.48        | 1.43     |
| 11  | cA    | 802 | CLA  | C1B-C2B | 2.36  | 1.48        | 1.43     |
| 11  | cA    | 841 | CLA  | C4C-C3C | 2.36  | 1.49        | 1.45     |
| 11  | aB    | 836 | CLA  | C3B-C4B | 2.36  | 1.49        | 1.42     |
| 11  | cB    | 826 | CLA  | C1B-C2B | 2.36  | 1.48        | 1.43     |
| 11  | cA    | 808 | CLA  | C4C-C3C | 2.36  | 1.49        | 1.45     |
| 11  | aA    | 802 | CLA  | C3D-C4D | -2.36 | 1.38        | 1.44     |
| 11  | bA    | 811 | CLA  | C1B-C2B | 2.36  | 1.48        | 1.43     |
| 11  | bA    | 822 | CLA  | C1B-C2B | 2.36  | 1.48        | 1.43     |
| 11  | cA    | 815 | CLA  | C4C-C3C | 2.36  | 1.49        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | aA    | 837 | CLA  | C3B-C2B | 2.36  | 1.49        | 1.41     |
| 11  | aA    | 841 | CLA  | C4C-C3C | 2.36  | 1.49        | 1.45     |
| 11  | cB    | 833 | CLA  | C4C-C3C | 2.36  | 1.49        | 1.45     |
| 11  | bA    | 821 | CLA  | C3B-C4B | 2.36  | 1.49        | 1.42     |
| 11  | aB    | 814 | CLA  | C3B-C4B | 2.36  | 1.49        | 1.42     |
| 11  | aA    | 818 | CLA  | C1C-C2C | 2.36  | 1.49        | 1.44     |
| 12  | bB    | 824 | F6C  | CHB-C4A | -2.36 | 1.33        | 1.38     |
| 11  | bA    | 816 | CLA  | C4C-C3C | 2.36  | 1.49        | 1.45     |
| 11  | aA    | 829 | CLA  | C3B-C2B | 2.36  | 1.49        | 1.41     |
| 11  | aA    | 815 | CLA  | C4C-C3C | 2.36  | 1.49        | 1.45     |
| 11  | cB    | 816 | CLA  | C3B-C4B | 2.35  | 1.49        | 1.42     |
| 11  | bA    | 805 | CLA  | C1B-C2B | 2.35  | 1.48        | 1.43     |
| 11  | cA    | 818 | CLA  | C1C-C2C | 2.35  | 1.49        | 1.44     |
| 11  | aB    | 839 | CLA  | C1C-C2C | 2.35  | 1.49        | 1.44     |
| 11  | bA    | 817 | CLA  | C4C-C3C | 2.35  | 1.49        | 1.45     |
| 12  | cB    | 824 | F6C  | CHB-C4A | -2.35 | 1.33        | 1.38     |
| 11  | aA    | 825 | CLA  | C4C-C3C | 2.35  | 1.49        | 1.45     |
| 11  | bA    | 810 | CLA  | C4C-C3C | 2.35  | 1.49        | 1.45     |
| 11  | cB    | 806 | CLA  | C3D-C4D | -2.35 | 1.38        | 1.44     |
| 11  | aA    | 821 | CLA  | C3B-C4B | 2.35  | 1.49        | 1.42     |
| 11  | bA    | 834 | CLA  | C3D-C4D | -2.35 | 1.38        | 1.44     |
| 11  | bB    | 806 | CLA  | C3D-C4D | -2.35 | 1.38        | 1.44     |
| 12  | bA    | 844 | F6C  | C1A-C2A | 2.35  | 1.50        | 1.45     |
| 11  | aA    | 842 | CLA  | C1B-C2B | 2.35  | 1.48        | 1.43     |
| 11  | bA    | 837 | CLA  | C3B-C2B | 2.35  | 1.49        | 1.41     |
| 11  | bB    | 833 | CLA  | C4C-C3C | 2.35  | 1.49        | 1.45     |
| 11  | bB    | 825 | CLA  | C3D-C4D | -2.35 | 1.38        | 1.44     |
| 11  | aA    | 806 | CLA  | C1B-C2B | 2.35  | 1.48        | 1.43     |
| 11  | aA    | 816 | CLA  | C1B-C2B | 2.35  | 1.48        | 1.43     |
| 11  | cA    | 829 | CLA  | C3B-C2B | 2.35  | 1.49        | 1.41     |
| 11  | bA    | 818 | CLA  | C1C-C2C | 2.35  | 1.49        | 1.44     |
| 11  | bB    | 815 | CLA  | C1C-C2C | 2.35  | 1.49        | 1.44     |
| 11  | bA    | 811 | CLA  | C4C-C3C | 2.35  | 1.49        | 1.45     |
| 11  | bB    | 816 | CLA  | C3B-C4B | 2.35  | 1.49        | 1.42     |
| 11  | cA    | 821 | CLA  | C3B-C4B | 2.35  | 1.49        | 1.42     |
| 11  | cA    | 837 | CLA  | C1C-C2C | 2.35  | 1.49        | 1.44     |
| 11  | bA    | 813 | CLA  | C4C-C3C | 2.35  | 1.49        | 1.45     |
| 11  | aA    | 810 | CLA  | C4C-C3C | 2.35  | 1.49        | 1.45     |
| 11  | bA    | 802 | CLA  | C4C-C3C | 2.35  | 1.49        | 1.45     |
| 11  | cA    | 819 | CLA  | C1C-C2C | 2.35  | 1.49        | 1.44     |
| 11  | aA    | 802 | CLA  | C1B-C2B | 2.35  | 1.48        | 1.43     |
| 11  | cB    | 836 | CLA  | C3B-C4B | 2.34  | 1.49        | 1.42     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | cB    | 819 | CLA  | C1C-C2C | 2.34  | 1.49        | 1.44     |
| 15  | aA    | 847 | BCR  | C30-C25 | -2.34 | 1.50        | 1.53     |
| 15  | cB    | 848 | BCR  | C30-C25 | -2.34 | 1.50        | 1.53     |
| 11  | cB    | 825 | CLA  | C3B-C2B | 2.34  | 1.49        | 1.41     |
| 11  | aA    | 833 | CLA  | C1B-C2B | 2.34  | 1.48        | 1.43     |
| 11  | aB    | 805 | CLA  | C4C-C3C | 2.34  | 1.49        | 1.45     |
| 11  | bB    | 802 | CLA  | C1C-C2C | 2.34  | 1.49        | 1.44     |
| 11  | aK    | 101 | CLA  | C3B-C4B | 2.34  | 1.49        | 1.42     |
| 11  | aA    | 811 | CLA  | C4C-C3C | 2.34  | 1.49        | 1.45     |
| 15  | aL    | 203 | BCR  | C33-C5  | -2.34 | 1.47        | 1.50     |
| 11  | cB    | 836 | CLA  | C1B-C2B | 2.34  | 1.48        | 1.43     |
| 11  | aA    | 840 | CLA  | C1B-C2B | 2.34  | 1.48        | 1.43     |
| 11  | cA    | 814 | CLA  | C4C-C3C | 2.34  | 1.49        | 1.45     |
| 11  | aB    | 836 | CLA  | C1B-C2B | 2.34  | 1.48        | 1.43     |
| 11  | aB    | 816 | CLA  | C4C-C3C | 2.34  | 1.49        | 1.45     |
| 11  | aA    | 825 | CLA  | C1B-C2B | 2.34  | 1.48        | 1.43     |
| 11  | cA    | 805 | CLA  | C1B-C2B | 2.34  | 1.48        | 1.43     |
| 11  | cK    | 101 | CLA  | C3B-C4B | 2.34  | 1.49        | 1.42     |
| 11  | bB    | 808 | CLA  | C1B-C2B | 2.34  | 1.48        | 1.43     |
| 11  | cA    | 839 | CLA  | C3D-C4D | -2.34 | 1.38        | 1.44     |
| 11  | bB    | 811 | CLA  | C3B-C4B | 2.34  | 1.49        | 1.42     |
| 11  | cA    | 825 | CLA  | C1B-C2B | 2.34  | 1.48        | 1.43     |
| 11  | aB    | 815 | CLA  | C1C-C2C | 2.34  | 1.49        | 1.44     |
| 12  | cA    | 844 | F6C  | CHB-C4A | -2.34 | 1.33        | 1.38     |
| 11  | cB    | 821 | CLA  | C3B-C4B | 2.34  | 1.49        | 1.42     |
| 11  | bB    | 831 | CLA  | C4C-C3C | 2.34  | 1.49        | 1.45     |
| 12  | aA    | 832 | F6C  | CHB-C4A | -2.34 | 1.33        | 1.38     |
| 11  | bB    | 802 | CLA  | C1B-C2B | 2.34  | 1.48        | 1.43     |
| 11  | aA    | 819 | CLA  | C3D-C4D | -2.34 | 1.38        | 1.44     |
| 11  | bB    | 839 | CLA  | C1C-C2C | 2.34  | 1.49        | 1.44     |
| 11  | cA    | 813 | CLA  | C4C-C3C | 2.33  | 1.49        | 1.45     |
| 11  | cA    | 825 | CLA  | C4C-C3C | 2.33  | 1.49        | 1.45     |
| 11  | aB    | 821 | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 11  | bB    | 810 | CLA  | C3D-C4D | -2.33 | 1.38        | 1.44     |
| 11  | aA    | 842 | CLA  | C1C-C2C | 2.33  | 1.49        | 1.44     |
| 11  | cA    | 822 | CLA  | C1B-C2B | 2.33  | 1.48        | 1.43     |
| 11  | aA    | 808 | CLA  | C4C-C3C | 2.33  | 1.49        | 1.45     |
| 11  | bA    | 843 | CLA  | C3D-C4D | -2.33 | 1.38        | 1.44     |
| 11  | cB    | 805 | CLA  | C3D-C4D | -2.33 | 1.38        | 1.44     |
| 11  | bA    | 814 | CLA  | C4C-C3C | 2.33  | 1.49        | 1.45     |
| 11  | bA    | 804 | CLA  | C1C-C2C | 2.33  | 1.49        | 1.44     |
| 15  | bK    | 102 | BCR  | C30-C25 | -2.33 | 1.50        | 1.53     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | aB    | 838 | CLA  | C4C-C3C | 2.33  | 1.49        | 1.45     |
| 11  | aB    | 810 | CLA  | C3D-C4D | -2.33 | 1.38        | 1.44     |
| 11  | cB    | 814 | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 11  | cA    | 816 | CLA  | C1B-C2B | 2.33  | 1.48        | 1.43     |
| 11  | cB    | 815 | CLA  | C1C-C2C | 2.33  | 1.49        | 1.44     |
| 11  | bA    | 842 | CLA  | C1B-C2B | 2.33  | 1.48        | 1.43     |
| 11  | bA    | 842 | CLA  | C1C-C2C | 2.33  | 1.49        | 1.44     |
| 11  | aB    | 818 | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 11  | bB    | 814 | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 11  | aB    | 840 | CLA  | C3D-C4D | -2.33 | 1.38        | 1.44     |
| 11  | cA    | 819 | CLA  | C3D-C4D | -2.33 | 1.38        | 1.44     |
| 11  | bB    | 818 | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 11  | cB    | 802 | CLA  | C1B-C2B | 2.33  | 1.48        | 1.43     |
| 12  | bA    | 832 | F6C  | C1C-C2C | 2.33  | 1.48        | 1.43     |
| 11  | bB    | 825 | CLA  | C3B-C2B | 2.33  | 1.49        | 1.41     |
| 11  | bA    | 843 | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 12  | aA    | 832 | F6C  | C1C-C2C | 2.33  | 1.48        | 1.43     |
| 11  | aA    | 843 | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 15  | cL    | 203 | BCR  | C33-C5  | -2.33 | 1.47        | 1.50     |
| 11  | aB    | 825 | CLA  | C3B-C2B | 2.33  | 1.49        | 1.41     |
| 12  | aA    | 830 | F6C  | CMB-C2B | 2.33  | 1.50        | 1.45     |
| 11  | bB    | 821 | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 11  | bA    | 816 | CLA  | C1B-C2B | 2.33  | 1.48        | 1.43     |
| 11  | aA    | 806 | CLA  | C4C-C3C | 2.33  | 1.49        | 1.45     |
| 11  | bA    | 825 | CLA  | C4C-C3C | 2.33  | 1.49        | 1.45     |
| 11  | bA    | 833 | CLA  | C1B-C2B | 2.33  | 1.48        | 1.43     |
| 11  | aA    | 834 | CLA  | C3D-C4D | -2.33 | 1.39        | 1.44     |
| 11  | bB    | 837 | CLA  | C3D-C4D | -2.33 | 1.39        | 1.44     |
| 11  | cA    | 843 | CLA  | C3D-C4D | -2.33 | 1.39        | 1.44     |
| 11  | bB    | 836 | CLA  | C1B-C2B | 2.33  | 1.48        | 1.43     |
| 11  | bA    | 802 | CLA  | C3D-C4D | -2.32 | 1.39        | 1.44     |
| 11  | cA    | 833 | CLA  | C3B-C2B | 2.32  | 1.49        | 1.41     |
| 11  | aB    | 802 | CLA  | C1B-C2B | 2.32  | 1.48        | 1.43     |
| 11  | bA    | 814 | CLA  | C3D-C4D | -2.32 | 1.39        | 1.44     |
| 12  | aA    | 827 | F6C  | C2B-C1B | 2.32  | 1.49        | 1.44     |
| 11  | bB    | 840 | CLA  | C3D-C4D | -2.32 | 1.39        | 1.44     |
| 11  | cA    | 814 | CLA  | C3D-C4D | -2.32 | 1.39        | 1.44     |
| 11  | cA    | 842 | CLA  | C1B-C2B | 2.32  | 1.48        | 1.43     |
| 11  | cA    | 804 | CLA  | C1C-C2C | 2.32  | 1.49        | 1.44     |
| 11  | aA    | 837 | CLA  | C1C-C2C | 2.32  | 1.49        | 1.44     |
| 11  | cA    | 810 | CLA  | C4C-C3C | 2.32  | 1.49        | 1.45     |
| 11  | bA    | 825 | CLA  | C1B-C2B | 2.32  | 1.48        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 15  | bB    | 842 | BCR  | C30-C25 | -2.32 | 1.50        | 1.53     |
| 11  | aA    | 829 | CLA  | C4C-C3C | 2.32  | 1.49        | 1.45     |
| 11  | bB    | 837 | CLA  | C1C-C2C | 2.32  | 1.49        | 1.44     |
| 12  | aB    | 824 | F6C  | CHB-C4A | -2.32 | 1.33        | 1.38     |
| 11  | aA    | 833 | CLA  | C3B-C2B | 2.32  | 1.49        | 1.41     |
| 11  | aB    | 816 | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 11  | aB    | 806 | CLA  | C3D-C4D | -2.32 | 1.39        | 1.44     |
| 11  | aA    | 814 | CLA  | C4C-C3C | 2.32  | 1.49        | 1.45     |
| 11  | cB    | 825 | CLA  | C4C-C3C | 2.32  | 1.49        | 1.45     |
| 12  | bA    | 826 | F6C  | CHB-C4A | -2.32 | 1.33        | 1.38     |
| 11  | bB    | 804 | CLA  | C3B-C2B | 2.32  | 1.49        | 1.41     |
| 11  | cA    | 828 | CLA  | C3D-C4D | -2.32 | 1.39        | 1.44     |
| 11  | bA    | 828 | CLA  | C3D-C4D | -2.32 | 1.39        | 1.44     |
| 11  | cB    | 809 | CLA  | C1B-C2B | 2.32  | 1.48        | 1.43     |
| 11  | aA    | 817 | CLA  | C4C-C3C | 2.32  | 1.49        | 1.45     |
| 12  | cL    | 202 | F6C  | C2B-C1B | 2.32  | 1.49        | 1.44     |
| 11  | cB    | 837 | CLA  | C1C-C2C | 2.32  | 1.49        | 1.44     |
| 12  | bA    | 844 | F6C  | CHB-C4A | -2.32 | 1.33        | 1.38     |
| 11  | bB    | 832 | CLA  | C3B-C4B | 2.31  | 1.49        | 1.42     |
| 11  | aA    | 813 | CLA  | C4C-C3C | 2.31  | 1.49        | 1.45     |
| 11  | bA    | 810 | CLA  | C3D-C4D | -2.31 | 1.39        | 1.44     |
| 12  | aA    | 844 | F6C  | CMB-C2B | 2.31  | 1.50        | 1.45     |
| 11  | aA    | 840 | CLA  | C3D-C4D | -2.31 | 1.39        | 1.44     |
| 12  | cA    | 844 | F6C  | CMB-C2B | 2.31  | 1.50        | 1.45     |
| 11  | aA    | 814 | CLA  | C3D-C4D | -2.31 | 1.39        | 1.44     |
| 11  | aB    | 834 | CLA  | C1B-C2B | 2.31  | 1.48        | 1.43     |
| 11  | cA    | 843 | CLA  | C3B-C4B | 2.31  | 1.49        | 1.42     |
| 11  | aA    | 839 | CLA  | C3D-C4D | -2.31 | 1.39        | 1.44     |
| 11  | bA    | 833 | CLA  | C3B-C2B | 2.31  | 1.49        | 1.41     |
| 11  | cB    | 825 | CLA  | C3D-C4D | -2.31 | 1.39        | 1.44     |
| 11  | aB    | 837 | CLA  | C1C-C2C | 2.31  | 1.49        | 1.44     |
| 11  | cA    | 834 | CLA  | C3D-C4D | -2.31 | 1.39        | 1.44     |
| 12  | cA    | 832 | F6C  | C1C-C2C | 2.31  | 1.48        | 1.43     |
| 11  | aB    | 833 | CLA  | C4C-C3C | 2.31  | 1.49        | 1.45     |
| 11  | bB    | 819 | CLA  | C1C-C2C | 2.31  | 1.49        | 1.44     |
| 11  | bA    | 815 | CLA  | C3B-C2B | 2.31  | 1.49        | 1.41     |
| 11  | bB    | 838 | CLA  | C3D-C4D | -2.31 | 1.39        | 1.44     |
| 11  | bA    | 840 | CLA  | C3D-C4D | -2.31 | 1.39        | 1.44     |
| 11  | cA    | 840 | CLA  | C3D-C4D | -2.31 | 1.39        | 1.44     |
| 11  | bB    | 825 | CLA  | C4C-C3C | 2.31  | 1.49        | 1.45     |
| 15  | cB    | 842 | BCR  | C30-C25 | -2.31 | 1.50        | 1.53     |
| 12  | aA    | 844 | F6C  | CHB-C4A | -2.31 | 1.33        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | bA    | 833 | CLA  | C3D-C4D | -2.31 | 1.39        | 1.44     |
| 11  | aA    | 804 | CLA  | C1C-C2C | 2.31  | 1.49        | 1.44     |
| 11  | aA    | 819 | CLA  | C1C-C2C | 2.31  | 1.49        | 1.44     |
| 11  | bB    | 805 | CLA  | C4C-C3C | 2.31  | 1.49        | 1.45     |
| 11  | cB    | 805 | CLA  | C4C-C3C | 2.31  | 1.49        | 1.45     |
| 11  | cB    | 832 | CLA  | C3B-C4B | 2.31  | 1.49        | 1.42     |
| 12  | bA    | 830 | F6C  | CMB-C2B | 2.31  | 1.50        | 1.45     |
| 11  | cA    | 828 | CLA  | C3B-C2B | 2.31  | 1.49        | 1.41     |
| 12  | aA    | 844 | F6C  | C4A-C3A | 2.31  | 1.49        | 1.45     |
| 11  | aB    | 812 | CLA  | C3D-C4D | -2.31 | 1.39        | 1.44     |
| 11  | bA    | 839 | CLA  | C3D-C4D | -2.31 | 1.39        | 1.44     |
| 11  | cA    | 806 | CLA  | C3D-C4D | -2.31 | 1.39        | 1.44     |
| 12  | aA    | 826 | F6C  | CHB-C4A | -2.30 | 1.33        | 1.38     |
| 11  | cB    | 816 | CLA  | C4C-C3C | 2.30  | 1.48        | 1.45     |
| 11  | cB    | 811 | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 12  | bA    | 832 | F6C  | CHB-C4A | -2.30 | 1.33        | 1.38     |
| 12  | aA    | 844 | F6C  | C4B-NB  | -2.30 | 1.34        | 1.37     |
| 11  | cA    | 802 | CLA  | C4C-C3C | 2.30  | 1.48        | 1.45     |
| 11  | cB    | 812 | CLA  | C3D-C4D | -2.30 | 1.39        | 1.44     |
| 11  | aB    | 817 | CLA  | C1B-C2B | 2.30  | 1.48        | 1.43     |
| 12  | cA    | 844 | F6C  | C4A-C3A | 2.30  | 1.49        | 1.45     |
| 11  | aB    | 825 | CLA  | C3D-C4D | -2.30 | 1.39        | 1.44     |
| 15  | aB    | 848 | BCR  | C30-C25 | -2.30 | 1.50        | 1.53     |
| 11  | aA    | 828 | CLA  | C3D-C4D | -2.30 | 1.39        | 1.44     |
| 12  | bA    | 844 | F6C  | CMB-C2B | 2.30  | 1.50        | 1.45     |
| 12  | cB    | 824 | F6C  | C4C-C3C | 2.30  | 1.49        | 1.44     |
| 11  | bB    | 812 | CLA  | C3D-C4D | -2.30 | 1.39        | 1.44     |
| 11  | aB    | 808 | CLA  | C1B-C2B | 2.30  | 1.48        | 1.43     |
| 11  | aA    | 828 | CLA  | C3B-C2B | 2.30  | 1.48        | 1.41     |
| 11  | aA    | 802 | CLA  | C4C-C3C | 2.30  | 1.48        | 1.45     |
| 11  | aB    | 819 | CLA  | C1C-C2C | 2.30  | 1.49        | 1.44     |
| 11  | cA    | 815 | CLA  | C3B-C2B | 2.30  | 1.48        | 1.41     |
| 11  | cB    | 802 | CLA  | C3B-C2B | 2.30  | 1.48        | 1.41     |
| 11  | cB    | 802 | CLA  | C1C-C2C | 2.30  | 1.49        | 1.44     |
| 11  | aB    | 832 | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 18  | bB    | 847 | LMG  | O7-C8   | -2.30 | 1.41        | 1.46     |
| 11  | cB    | 810 | CLA  | C3D-C4D | -2.29 | 1.39        | 1.44     |
| 11  | aA    | 840 | CLA  | C4C-C3C | 2.29  | 1.48        | 1.45     |
| 11  | cB    | 823 | CLA  | C1C-C2C | 2.29  | 1.49        | 1.44     |
| 11  | bB    | 839 | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 11  | cB    | 840 | CLA  | C1B-C2B | 2.29  | 1.48        | 1.43     |
| 11  | cA    | 824 | CLA  | C1B-C2B | 2.29  | 1.48        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | cA    | 835 | CLA  | C3D-C4D | -2.29 | 1.39        | 1.44     |
| 11  | cB    | 804 | CLA  | C3B-C2B | 2.29  | 1.48        | 1.41     |
| 11  | cA    | 841 | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 11  | cB    | 837 | CLA  | C3D-C4D | -2.29 | 1.39        | 1.44     |
| 12  | aA    | 844 | F6C  | C1C-NC  | -2.29 | 1.34        | 1.37     |
| 11  | aB    | 802 | CLA  | C1C-C2C | 2.29  | 1.49        | 1.44     |
| 11  | bB    | 823 | CLA  | C1C-C2C | 2.29  | 1.49        | 1.44     |
| 11  | bA    | 843 | CLA  | C4C-C3C | 2.29  | 1.48        | 1.45     |
| 11  | bB    | 810 | CLA  | C4C-C3C | 2.29  | 1.48        | 1.45     |
| 11  | bB    | 834 | CLA  | C1B-C2B | 2.29  | 1.48        | 1.43     |
| 12  | cA    | 844 | F6C  | C4B-NB  | -2.29 | 1.34        | 1.37     |
| 11  | cB    | 828 | CLA  | C3B-C2B | 2.29  | 1.48        | 1.41     |
| 11  | aL    | 206 | CLA  | C3D-C4D | -2.29 | 1.39        | 1.44     |
| 11  | aA    | 818 | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 11  | aA    | 843 | CLA  | C3D-C4D | -2.29 | 1.39        | 1.44     |
| 11  | bA    | 841 | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 11  | bB    | 828 | CLA  | C3B-C2B | 2.29  | 1.48        | 1.41     |
| 11  | aA    | 806 | CLA  | C3D-C4D | -2.29 | 1.39        | 1.44     |
| 11  | bA    | 837 | CLA  | C1C-C2C | 2.29  | 1.49        | 1.44     |
| 11  | aB    | 837 | CLA  | C3D-C4D | -2.29 | 1.39        | 1.44     |
| 11  | bL    | 206 | CLA  | C3D-C4D | -2.29 | 1.39        | 1.44     |
| 12  | cA    | 832 | F6C  | CHB-C4A | -2.29 | 1.33        | 1.38     |
| 11  | aB    | 823 | CLA  | C1C-C2C | 2.29  | 1.49        | 1.44     |
| 11  | bA    | 808 | CLA  | C1C-C2C | 2.29  | 1.49        | 1.44     |
| 11  | bB    | 802 | CLA  | C3B-C2B | 2.29  | 1.48        | 1.41     |
| 11  | cA    | 820 | CLA  | C1B-C2B | 2.29  | 1.48        | 1.43     |
| 15  | aB    | 842 | BCR  | C30-C25 | -2.29 | 1.50        | 1.53     |
| 11  | bA    | 819 | CLA  | C3D-C4D | -2.29 | 1.39        | 1.44     |
| 11  | aA    | 824 | CLA  | C1B-C2B | 2.29  | 1.48        | 1.43     |
| 11  | aA    | 815 | CLA  | C3B-C2B | 2.29  | 1.48        | 1.41     |
| 11  | aB    | 802 | CLA  | C3B-C2B | 2.29  | 1.48        | 1.41     |
| 11  | bA    | 806 | CLA  | C4C-C3C | 2.29  | 1.48        | 1.45     |
| 11  | bB    | 816 | CLA  | C4C-C3C | 2.29  | 1.48        | 1.45     |
| 11  | bB    | 805 | CLA  | C3B-C2B | 2.29  | 1.48        | 1.41     |
| 11  | bB    | 822 | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 11  | aB    | 809 | CLA  | C1B-C2B | 2.29  | 1.48        | 1.43     |
| 11  | bA    | 804 | CLA  | C4C-C3C | 2.29  | 1.48        | 1.45     |
| 11  | cB    | 817 | CLA  | C1B-C2B | 2.28  | 1.48        | 1.43     |
| 11  | bA    | 818 | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |
| 11  | cB    | 817 | CLA  | C3D-C4D | -2.28 | 1.39        | 1.44     |
| 11  | bA    | 835 | CLA  | C3D-C4D | -2.28 | 1.39        | 1.44     |
| 15  | cA    | 847 | BCR  | C30-C25 | -2.28 | 1.50        | 1.53     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | aB    | 811 | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |
| 11  | cA    | 818 | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |
| 15  | bB    | 846 | BCR  | C1-C6   | -2.28 | 1.50        | 1.53     |
| 11  | aB    | 830 | CLA  | C1B-C2B | 2.28  | 1.48        | 1.43     |
| 11  | aB    | 810 | CLA  | C4C-C3C | 2.28  | 1.48        | 1.45     |
| 12  | aB    | 824 | F6C  | C4C-C3C | 2.28  | 1.49        | 1.44     |
| 12  | aL    | 202 | F6C  | C2B-C1B | 2.28  | 1.49        | 1.44     |
| 12  | bA    | 844 | F6C  | C4A-C3A | 2.28  | 1.49        | 1.45     |
| 11  | aB    | 817 | CLA  | C3D-C4D | -2.28 | 1.39        | 1.44     |
| 11  | bA    | 820 | CLA  | C1B-C2B | 2.28  | 1.48        | 1.43     |
| 15  | aB    | 846 | BCR  | C1-C6   | -2.28 | 1.50        | 1.53     |
| 11  | cB    | 838 | CLA  | C3D-C4D | -2.28 | 1.39        | 1.44     |
| 11  | aA    | 843 | CLA  | C4C-C3C | 2.28  | 1.48        | 1.45     |
| 11  | bA    | 806 | CLA  | C3D-C4D | -2.28 | 1.39        | 1.44     |
| 11  | bA    | 824 | CLA  | C1B-C2B | 2.28  | 1.48        | 1.43     |
| 11  | cB    | 830 | CLA  | C1B-C2B | 2.28  | 1.48        | 1.43     |
| 11  | aB    | 804 | CLA  | C3B-C2B | 2.28  | 1.48        | 1.41     |
| 11  | aA    | 810 | CLA  | C1C-C2C | 2.27  | 1.49        | 1.44     |
| 11  | aB    | 828 | CLA  | C3B-C2B | 2.27  | 1.48        | 1.41     |
| 18  | cB    | 847 | LMG  | O7-C8   | -2.27 | 1.41        | 1.46     |
| 11  | cA    | 836 | CLA  | C1B-C2B | 2.27  | 1.48        | 1.43     |
| 11  | aA    | 831 | CLA  | C3B-C2B | 2.27  | 1.48        | 1.41     |
| 11  | cA    | 843 | CLA  | C4C-C3C | 2.27  | 1.48        | 1.45     |
| 11  | aA    | 841 | CLA  | C1C-C2C | 2.27  | 1.49        | 1.44     |
| 11  | bA    | 805 | CLA  | C3B-C2B | 2.27  | 1.48        | 1.41     |
| 11  | cA    | 810 | CLA  | C1C-C2C | 2.27  | 1.49        | 1.44     |
| 11  | cB    | 805 | CLA  | C3B-C2B | 2.27  | 1.48        | 1.41     |
| 11  | bA    | 840 | CLA  | C4C-C3C | 2.27  | 1.48        | 1.45     |
| 11  | bB    | 840 | CLA  | C1B-C2B | 2.27  | 1.48        | 1.43     |
| 11  | aL    | 205 | CLA  | C4C-C3C | 2.27  | 1.48        | 1.45     |
| 12  | bB    | 824 | F6C  | C4C-C3C | 2.27  | 1.49        | 1.44     |
| 11  | bB    | 809 | CLA  | C1B-C2B | 2.27  | 1.48        | 1.43     |
| 11  | bA    | 822 | CLA  | C4C-C3C | 2.27  | 1.48        | 1.45     |
| 11  | aB    | 825 | CLA  | C4C-C3C | 2.27  | 1.48        | 1.45     |
| 12  | bA    | 844 | F6C  | C4B-NB  | -2.27 | 1.34        | 1.37     |
| 11  | aB    | 838 | CLA  | C3D-C4D | -2.27 | 1.39        | 1.44     |
| 11  | cA    | 806 | CLA  | C4C-C3C | 2.27  | 1.48        | 1.45     |
| 11  | bB    | 817 | CLA  | C1B-C2B | 2.27  | 1.48        | 1.43     |
| 11  | cB    | 834 | CLA  | C1B-C2B | 2.27  | 1.48        | 1.43     |
| 11  | bB    | 831 | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |
| 11  | aB    | 830 | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |
| 11  | cB    | 839 | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | bB    | 830 | CLA  | C1B-C2B | 2.27  | 1.48        | 1.43     |
| 12  | aB    | 824 | F6C  | C1C-C2C | 2.27  | 1.48        | 1.43     |
| 15  | bB    | 848 | BCR  | C30-C25 | -2.27 | 1.50        | 1.53     |
| 12  | cA    | 826 | F6C  | CHB-C4A | -2.27 | 1.33        | 1.38     |
| 11  | cA    | 842 | CLA  | C1C-C2C | 2.27  | 1.49        | 1.44     |
| 11  | aA    | 841 | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |
| 11  | bA    | 828 | CLA  | C3B-C2B | 2.27  | 1.48        | 1.41     |
| 11  | cA    | 805 | CLA  | C3B-C2B | 2.27  | 1.48        | 1.41     |
| 11  | aA    | 808 | CLA  | C1C-C2C | 2.27  | 1.49        | 1.44     |
| 12  | cA    | 827 | F6C  | CHB-C4A | -2.27 | 1.33        | 1.38     |
| 11  | aB    | 839 | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 12  | cA    | 844 | F6C  | C1C-NC  | -2.26 | 1.34        | 1.37     |
| 12  | cA    | 830 | F6C  | CMB-C2B | 2.26  | 1.50        | 1.45     |
| 11  | cA    | 817 | CLA  | C3B-C2B | 2.26  | 1.48        | 1.41     |
| 11  | aA    | 807 | CLA  | C3D-C4D | -2.26 | 1.39        | 1.44     |
| 11  | aA    | 809 | CLA  | C3B-C2B | 2.26  | 1.48        | 1.41     |
| 11  | cL    | 206 | CLA  | C3D-C4D | -2.26 | 1.39        | 1.44     |
| 11  | aB    | 840 | CLA  | C1B-C2B | 2.26  | 1.48        | 1.43     |
| 15  | bA    | 847 | BCR  | C30-C25 | -2.26 | 1.50        | 1.53     |
| 11  | cB    | 818 | CLA  | C4C-C3C | 2.26  | 1.48        | 1.45     |
| 12  | bL    | 202 | F6C  | C4C-C3C | 2.26  | 1.49        | 1.44     |
| 18  | aB    | 847 | LMG  | O7-C8   | -2.26 | 1.41        | 1.46     |
| 11  | bB    | 830 | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 11  | aA    | 804 | CLA  | C4C-C3C | 2.26  | 1.48        | 1.45     |
| 11  | aB    | 822 | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 12  | bB    | 824 | F6C  | C1C-C2C | 2.26  | 1.48        | 1.43     |
| 12  | bL    | 202 | F6C  | C2B-C1B | 2.26  | 1.49        | 1.44     |
| 11  | aA    | 838 | CLA  | C1C-C2C | 2.26  | 1.49        | 1.44     |
| 11  | cA    | 838 | CLA  | C1C-C2C | 2.26  | 1.49        | 1.44     |
| 11  | aA    | 836 | CLA  | C1B-C2B | 2.26  | 1.48        | 1.43     |
| 11  | aA    | 804 | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 11  | aA    | 820 | CLA  | C1B-C2B | 2.26  | 1.48        | 1.43     |
| 11  | cA    | 804 | CLA  | C4C-C3C | 2.26  | 1.48        | 1.45     |
| 11  | cB    | 810 | CLA  | C4C-C3C | 2.26  | 1.48        | 1.45     |
| 11  | aA    | 812 | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 11  | cB    | 812 | CLA  | C3B-C2B | 2.26  | 1.48        | 1.41     |
| 11  | aB    | 805 | CLA  | C3B-C2B | 2.26  | 1.48        | 1.41     |
| 11  | aA    | 817 | CLA  | C1B-C2B | 2.26  | 1.48        | 1.43     |
| 11  | cA    | 807 | CLA  | C3D-C4D | -2.26 | 1.39        | 1.44     |
| 11  | bA    | 809 | CLA  | C3B-C2B | 2.26  | 1.48        | 1.41     |
| 11  | bB    | 818 | CLA  | C4C-C3C | 2.25  | 1.48        | 1.45     |
| 11  | cA    | 804 | CLA  | C3B-C4B | 2.25  | 1.49        | 1.42     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | cB    | 815 | CLA  | C3B-C4B | 2.25  | 1.49        | 1.42     |
| 11  | cL    | 205 | CLA  | C4C-C3C | 2.25  | 1.48        | 1.45     |
| 11  | cB    | 822 | CLA  | C3B-C4B | 2.25  | 1.49        | 1.42     |
| 11  | bA    | 817 | CLA  | C3B-C2B | 2.25  | 1.48        | 1.41     |
| 11  | cA    | 840 | CLA  | C4C-C3C | 2.25  | 1.48        | 1.45     |
| 11  | aB    | 831 | CLA  | C3B-C4B | 2.25  | 1.49        | 1.42     |
| 11  | aA    | 817 | CLA  | C3B-C2B | 2.25  | 1.48        | 1.41     |
| 12  | aA    | 827 | F6C  | C1C-NC  | -2.25 | 1.34        | 1.37     |
| 11  | cA    | 810 | CLA  | C3D-C4D | -2.25 | 1.39        | 1.44     |
| 11  | bA    | 838 | CLA  | C1C-C2C | 2.25  | 1.49        | 1.44     |
| 11  | aB    | 802 | CLA  | C3D-C4D | -2.25 | 1.39        | 1.44     |
| 11  | cA    | 831 | CLA  | C3B-C2B | 2.25  | 1.48        | 1.41     |
| 15  | cB    | 846 | BCR  | C1-C6   | -2.25 | 1.50        | 1.53     |
| 12  | cB    | 824 | F6C  | C4A-C3A | 2.25  | 1.49        | 1.45     |
| 11  | aL    | 205 | CLA  | C3D-C4D | -2.25 | 1.39        | 1.44     |
| 11  | bB    | 831 | CLA  | C3D-C4D | -2.25 | 1.39        | 1.44     |
| 11  | cA    | 822 | CLA  | C1C-C2C | 2.25  | 1.49        | 1.44     |
| 11  | aA    | 810 | CLA  | C3D-C4D | -2.25 | 1.39        | 1.44     |
| 11  | cA    | 809 | CLA  | C3B-C2B | 2.25  | 1.48        | 1.41     |
| 11  | bB    | 811 | CLA  | C1C-C2C | 2.25  | 1.49        | 1.44     |
| 11  | aB    | 813 | CLA  | C3B-C2B | 2.25  | 1.48        | 1.41     |
| 11  | cA    | 833 | CLA  | C4C-C3C | 2.25  | 1.48        | 1.45     |
| 15  | cL    | 208 | BCR  | C1-C6   | -2.25 | 1.50        | 1.53     |
| 11  | bB    | 813 | CLA  | C3D-C4D | -2.25 | 1.39        | 1.44     |
| 11  | bA    | 831 | CLA  | C3B-C2B | 2.25  | 1.48        | 1.41     |
| 11  | cB    | 813 | CLA  | C3D-C4D | -2.25 | 1.39        | 1.44     |
| 11  | bB    | 813 | CLA  | C3B-C2B | 2.25  | 1.48        | 1.41     |
| 11  | aA    | 809 | CLA  | C4C-C3C | 2.25  | 1.48        | 1.45     |
| 11  | bA    | 810 | CLA  | C1C-C2C | 2.25  | 1.49        | 1.44     |
| 11  | bL    | 205 | CLA  | C3D-C4D | -2.25 | 1.39        | 1.44     |
| 11  | bB    | 816 | CLA  | C1B-C2B | 2.25  | 1.48        | 1.43     |
| 11  | aB    | 837 | CLA  | C4C-C3C | 2.25  | 1.48        | 1.45     |
| 12  | bB    | 824 | F6C  | C4A-C3A | 2.25  | 1.49        | 1.45     |
| 11  | cA    | 841 | CLA  | C1C-C2C | 2.25  | 1.49        | 1.44     |
| 11  | bA    | 822 | CLA  | C1C-C2C | 2.24  | 1.49        | 1.44     |
| 11  | cA    | 808 | CLA  | C1C-C2C | 2.24  | 1.49        | 1.44     |
| 11  | bL    | 205 | CLA  | C4C-C3C | 2.24  | 1.48        | 1.45     |
| 11  | aA    | 837 | CLA  | C4C-C3C | 2.24  | 1.48        | 1.45     |
| 11  | cA    | 817 | CLA  | C1B-C2B | 2.24  | 1.48        | 1.43     |
| 11  | aB    | 815 | CLA  | C3B-C4B | 2.24  | 1.49        | 1.42     |
| 11  | cB    | 831 | CLA  | C3B-C4B | 2.24  | 1.49        | 1.42     |
| 11  | bA    | 841 | CLA  | C1C-C2C | 2.24  | 1.49        | 1.44     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | cA    | 842 | CLA  | C4C-C3C | 2.24  | 1.48        | 1.45     |
| 11  | aK    | 103 | CLA  | C3B-C4B | 2.24  | 1.49        | 1.42     |
| 11  | cB    | 833 | CLA  | C1C-C2C | 2.24  | 1.49        | 1.44     |
| 11  | aA    | 822 | CLA  | C1C-C2C | 2.24  | 1.49        | 1.44     |
| 11  | aA    | 835 | CLA  | C3D-C4D | -2.24 | 1.39        | 1.44     |
| 11  | bB    | 812 | CLA  | C3B-C2B | 2.24  | 1.48        | 1.41     |
| 11  | aA    | 828 | CLA  | C1C-NC  | -2.24 | 1.34        | 1.37     |
| 11  | bA    | 809 | CLA  | C1C-C2C | 2.24  | 1.49        | 1.44     |
| 11  | cB    | 821 | CLA  | C1C-C2C | 2.24  | 1.49        | 1.44     |
| 11  | bA    | 809 | CLA  | C4C-C3C | 2.24  | 1.48        | 1.45     |
| 11  | aB    | 812 | CLA  | C3B-C2B | 2.24  | 1.48        | 1.41     |
| 11  | aB    | 813 | CLA  | C3D-C4D | -2.24 | 1.39        | 1.44     |
| 11  | bB    | 817 | CLA  | C3D-C4D | -2.24 | 1.39        | 1.44     |
| 11  | bB    | 837 | CLA  | C4C-C3C | 2.24  | 1.48        | 1.45     |
| 11  | cB    | 819 | CLA  | C4C-C3C | 2.24  | 1.48        | 1.45     |
| 11  | bA    | 833 | CLA  | C4C-C3C | 2.23  | 1.48        | 1.45     |
| 11  | cA    | 822 | CLA  | C4C-C3C | 2.23  | 1.48        | 1.45     |
| 11  | cA    | 812 | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 11  | bA    | 836 | CLA  | C1B-C2B | 2.23  | 1.48        | 1.43     |
| 11  | aB    | 831 | CLA  | C3D-C4D | -2.23 | 1.39        | 1.44     |
| 12  | cA    | 827 | F6C  | C1C-NC  | -2.23 | 1.34        | 1.37     |
| 11  | bA    | 807 | CLA  | C3D-C4D | -2.23 | 1.39        | 1.44     |
| 12  | cB    | 824 | F6C  | C1C-C2C | 2.23  | 1.48        | 1.43     |
| 11  | bA    | 804 | CLA  | C3B-C2B | 2.23  | 1.48        | 1.41     |
| 11  | cL    | 206 | CLA  | C4C-C3C | 2.23  | 1.48        | 1.45     |
| 11  | bK    | 103 | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 11  | bA    | 804 | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 11  | cB    | 813 | CLA  | C3B-C2B | 2.23  | 1.48        | 1.41     |
| 11  | cB    | 831 | CLA  | C3D-C4D | -2.23 | 1.39        | 1.44     |
| 11  | aB    | 818 | CLA  | C4C-C3C | 2.23  | 1.48        | 1.45     |
| 11  | cA    | 837 | CLA  | C4C-C3C | 2.23  | 1.48        | 1.45     |
| 11  | aA    | 822 | CLA  | C4C-C3C | 2.23  | 1.48        | 1.45     |
| 11  | bB    | 815 | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 11  | cB    | 830 | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 11  | cA    | 828 | CLA  | C1C-NC  | -2.23 | 1.34        | 1.37     |
| 12  | aA    | 826 | F6C  | C1C-NC  | -2.23 | 1.34        | 1.37     |
| 11  | aA    | 805 | CLA  | C3B-C2B | 2.23  | 1.48        | 1.41     |
| 11  | bB    | 821 | CLA  | C3B-C2B | 2.23  | 1.48        | 1.41     |
| 11  | bA    | 823 | CLA  | C1A-CHA | 2.23  | 1.52        | 1.43     |
| 11  | cA    | 810 | CLA  | C3B-C2B | 2.23  | 1.48        | 1.41     |
| 11  | aA    | 833 | CLA  | C4C-C3C | 2.22  | 1.48        | 1.45     |
| 11  | aL    | 206 | CLA  | C4C-C3C | 2.22  | 1.48        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | bA    | 837 | CLA  | C4C-C3C | 2.22  | 1.48        | 1.45     |
| 11  | cA    | 823 | CLA  | C1A-CHA | 2.22  | 1.52        | 1.43     |
| 11  | cK    | 103 | CLA  | C3B-C4B | 2.22  | 1.49        | 1.42     |
| 11  | bA    | 817 | CLA  | C1B-C2B | 2.22  | 1.48        | 1.43     |
| 11  | bA    | 810 | CLA  | C3B-C2B | 2.22  | 1.48        | 1.41     |
| 11  | cB    | 837 | CLA  | C3B-C4B | 2.22  | 1.49        | 1.42     |
| 11  | bB    | 822 | CLA  | C3D-C4D | -2.22 | 1.39        | 1.44     |
| 11  | aB    | 821 | CLA  | C1C-C2C | 2.22  | 1.49        | 1.44     |
| 11  | cB    | 836 | CLA  | C1C-C2C | 2.22  | 1.49        | 1.44     |
| 11  | aA    | 842 | CLA  | C4C-C3C | 2.22  | 1.48        | 1.45     |
| 11  | bA    | 812 | CLA  | C3B-C4B | 2.22  | 1.49        | 1.42     |
| 11  | aB    | 827 | CLA  | C3D-C4D | -2.22 | 1.39        | 1.44     |
| 11  | cL    | 205 | CLA  | C3D-C4D | -2.22 | 1.39        | 1.44     |
| 12  | bA    | 844 | F6C  | C4C-C3C | 2.22  | 1.49        | 1.44     |
| 11  | aB    | 816 | CLA  | C1B-C2B | 2.22  | 1.48        | 1.43     |
| 11  | bB    | 821 | CLA  | C1C-C2C | 2.22  | 1.49        | 1.44     |
| 11  | bB    | 816 | CLA  | C3D-C4D | -2.22 | 1.39        | 1.44     |
| 12  | aB    | 824 | F6C  | C4A-C3A | 2.22  | 1.49        | 1.45     |
| 11  | cA    | 814 | CLA  | C3B-C4B | 2.22  | 1.49        | 1.42     |
| 11  | cB    | 802 | CLA  | C4C-C3C | 2.22  | 1.48        | 1.45     |
| 11  | bB    | 827 | CLA  | C3D-C4D | -2.22 | 1.39        | 1.44     |
| 11  | cA    | 808 | CLA  | C3B-C2B | 2.22  | 1.48        | 1.41     |
| 11  | cA    | 836 | CLA  | C4C-C3C | 2.22  | 1.48        | 1.45     |
| 11  | aA    | 809 | CLA  | C1C-C2C | 2.21  | 1.49        | 1.44     |
| 11  | cB    | 827 | CLA  | C3D-C4D | -2.21 | 1.39        | 1.44     |
| 11  | aB    | 819 | CLA  | C4C-C3C | 2.21  | 1.48        | 1.45     |
| 11  | aA    | 811 | CLA  | C1C-C2C | 2.21  | 1.49        | 1.44     |
| 11  | aB    | 823 | CLA  | C3D-C4D | -2.21 | 1.39        | 1.44     |
| 11  | cA    | 809 | CLA  | C1C-C2C | 2.21  | 1.49        | 1.44     |
| 12  | cA    | 832 | F6C  | C2B-C1B | 2.21  | 1.49        | 1.44     |
| 11  | bB    | 819 | CLA  | C4C-C3C | 2.21  | 1.48        | 1.45     |
| 11  | bA    | 813 | CLA  | C1B-C2B | 2.21  | 1.48        | 1.43     |
| 11  | cA    | 813 | CLA  | C1C-C2C | 2.21  | 1.49        | 1.44     |
| 11  | cA    | 816 | CLA  | C3D-C4D | -2.21 | 1.39        | 1.44     |
| 11  | cB    | 802 | CLA  | C3D-C4D | -2.21 | 1.39        | 1.44     |
| 12  | aA    | 832 | F6C  | C4C-C3C | 2.21  | 1.49        | 1.44     |
| 11  | aA    | 829 | CLA  | C3D-C4D | -2.21 | 1.39        | 1.44     |
| 11  | bA    | 836 | CLA  | C4C-C3C | 2.21  | 1.48        | 1.45     |
| 11  | bL    | 206 | CLA  | C4C-C3C | 2.21  | 1.48        | 1.45     |
| 12  | aA    | 844 | F6C  | C4C-C3C | 2.21  | 1.49        | 1.44     |
| 11  | aA    | 816 | CLA  | C3B-C2B | 2.21  | 1.48        | 1.41     |
| 11  | aB    | 811 | CLA  | C1C-C2C | 2.21  | 1.49        | 1.44     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | aA    | 805 | CLA  | C4C-C3C | 2.21  | 1.48        | 1.45     |
| 11  | bA    | 828 | CLA  | C1C-NC  | -2.21 | 1.34        | 1.37     |
| 11  | bA    | 805 | CLA  | C4C-C3C | 2.21  | 1.48        | 1.45     |
| 11  | aK    | 101 | CLA  | C1C-C2C | 2.21  | 1.49        | 1.44     |
| 12  | aA    | 832 | F6C  | C2B-C1B | 2.21  | 1.49        | 1.44     |
| 11  | aB    | 820 | CLA  | C3B-C2B | 2.21  | 1.48        | 1.41     |
| 11  | bA    | 808 | CLA  | C3B-C2B | 2.21  | 1.48        | 1.41     |
| 11  | cA    | 805 | CLA  | C4C-C3C | 2.21  | 1.48        | 1.45     |
| 11  | aB    | 833 | CLA  | C1C-C2C | 2.21  | 1.49        | 1.44     |
| 11  | bB    | 823 | CLA  | C3B-C2B | 2.21  | 1.48        | 1.41     |
| 12  | bA    | 832 | F6C  | C2B-C1B | 2.21  | 1.49        | 1.44     |
| 12  | bA    | 832 | F6C  | C4C-C3C | 2.21  | 1.49        | 1.44     |
| 11  | aA    | 823 | CLA  | C1A-CHA | 2.21  | 1.52        | 1.43     |
| 11  | bA    | 821 | CLA  | C1C-C2C | 2.21  | 1.49        | 1.44     |
| 11  | bB    | 820 | CLA  | C3B-C2B | 2.21  | 1.48        | 1.41     |
| 11  | cB    | 821 | CLA  | C3B-C2B | 2.21  | 1.48        | 1.41     |
| 11  | bA    | 837 | CLA  | C3D-C4D | -2.21 | 1.39        | 1.44     |
| 11  | bA    | 803 | CLA  | C3B-C4B | 2.21  | 1.49        | 1.42     |
| 12  | cA    | 844 | F6C  | C4C-C3C | 2.21  | 1.49        | 1.44     |
| 11  | cB    | 802 | CLA  | C3B-C4B | 2.21  | 1.49        | 1.42     |
| 11  | cB    | 813 | CLA  | C4C-C3C | 2.21  | 1.48        | 1.45     |
| 15  | aL    | 208 | BCR  | C1-C6   | -2.21 | 1.51        | 1.53     |
| 12  | cL    | 202 | F6C  | C4C-C3C | 2.21  | 1.49        | 1.44     |
| 12  | bB    | 824 | F6C  | C1A-C2A | 2.20  | 1.50        | 1.45     |
| 11  | aA    | 810 | CLA  | C3B-C2B | 2.20  | 1.48        | 1.41     |
| 11  | aB    | 823 | CLA  | C3B-C2B | 2.20  | 1.48        | 1.41     |
| 11  | cA    | 804 | CLA  | C3B-C2B | 2.20  | 1.48        | 1.41     |
| 11  | aA    | 814 | CLA  | C3B-C4B | 2.20  | 1.49        | 1.42     |
| 11  | bB    | 813 | CLA  | C4C-C3C | 2.20  | 1.48        | 1.45     |
| 11  | cA    | 809 | CLA  | C4C-C3C | 2.20  | 1.48        | 1.45     |
| 11  | cB    | 837 | CLA  | C4C-C3C | 2.20  | 1.48        | 1.45     |
| 11  | aB    | 821 | CLA  | C3B-C2B | 2.20  | 1.48        | 1.41     |
| 11  | cB    | 816 | CLA  | C3D-C4D | -2.20 | 1.39        | 1.44     |
| 11  | cK    | 101 | CLA  | C3B-C2B | 2.20  | 1.48        | 1.41     |
| 12  | bA    | 844 | F6C  | C1C-NC  | -2.20 | 1.35        | 1.37     |
| 11  | aA    | 803 | CLA  | C3B-C4B | 2.20  | 1.49        | 1.42     |
| 12  | bA    | 827 | F6C  | CHB-C4A | -2.20 | 1.34        | 1.38     |
| 11  | aB    | 826 | CLA  | C1C-C2C | 2.20  | 1.49        | 1.44     |
| 11  | bB    | 823 | CLA  | C3D-C4D | -2.20 | 1.39        | 1.44     |
| 11  | cA    | 837 | CLA  | C3D-C4D | -2.20 | 1.39        | 1.44     |
| 15  | bL    | 208 | BCR  | C1-C6   | -2.20 | 1.51        | 1.53     |
| 11  | cB    | 811 | CLA  | C1C-C2C | 2.20  | 1.49        | 1.44     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12  | bB    | 824 | F6C  | C1D-C2D | 2.20  | 1.49        | 1.44     |
| 11  | aA    | 819 | CLA  | C3B-C2B | 2.20  | 1.48        | 1.41     |
| 11  | aA    | 804 | CLA  | C3B-C2B | 2.20  | 1.48        | 1.41     |
| 11  | bA    | 813 | CLA  | C3B-C2B | 2.20  | 1.48        | 1.41     |
| 12  | bL    | 202 | F6C  | CHB-C4A | -2.20 | 1.34        | 1.38     |
| 11  | aA    | 813 | CLA  | C1B-C2B | 2.20  | 1.48        | 1.43     |
| 11  | bK    | 101 | CLA  | C3B-C2B | 2.20  | 1.48        | 1.41     |
| 11  | bA    | 842 | CLA  | C4C-C3C | 2.20  | 1.48        | 1.45     |
| 11  | bB    | 837 | CLA  | C3B-C4B | 2.20  | 1.49        | 1.42     |
| 11  | aA    | 808 | CLA  | C3D-C4D | -2.20 | 1.39        | 1.44     |
| 11  | aA    | 820 | CLA  | C3D-C4D | -2.20 | 1.39        | 1.44     |
| 11  | aB    | 816 | CLA  | C3D-C4D | -2.20 | 1.39        | 1.44     |
| 12  | cA    | 832 | F6C  | C4C-C3C | 2.20  | 1.49        | 1.44     |
| 11  | cB    | 827 | CLA  | C3B-C2B | 2.20  | 1.48        | 1.41     |
| 11  | cB    | 816 | CLA  | C1B-C2B | 2.20  | 1.48        | 1.43     |
| 11  | cK    | 101 | CLA  | C1C-C2C | 2.20  | 1.49        | 1.44     |
| 11  | aA    | 804 | CLA  | C3D-C4D | -2.20 | 1.39        | 1.44     |
| 11  | aB    | 837 | CLA  | C3B-C4B | 2.20  | 1.49        | 1.42     |
| 11  | aA    | 825 | CLA  | C3D-C4D | -2.19 | 1.39        | 1.44     |
| 11  | aB    | 826 | CLA  | C3D-C4D | -2.19 | 1.39        | 1.44     |
| 11  | cB    | 823 | CLA  | C4C-C3C | 2.19  | 1.48        | 1.45     |
| 11  | bA    | 825 | CLA  | C3D-C4D | -2.19 | 1.39        | 1.44     |
| 11  | aB    | 822 | CLA  | C3D-C4D | -2.19 | 1.39        | 1.44     |
| 11  | cA    | 822 | CLA  | C3D-C4D | -2.19 | 1.39        | 1.44     |
| 11  | bA    | 837 | CLA  | C3B-C4B | 2.19  | 1.49        | 1.42     |
| 11  | cB    | 823 | CLA  | C3D-C4D | -2.19 | 1.39        | 1.44     |
| 11  | bA    | 813 | CLA  | C1C-C2C | 2.19  | 1.49        | 1.44     |
| 11  | bK    | 101 | CLA  | C3D-C4D | -2.19 | 1.39        | 1.44     |
| 11  | aB    | 827 | CLA  | C3B-C2B | 2.19  | 1.48        | 1.41     |
| 11  | bB    | 826 | CLA  | C1C-C2C | 2.19  | 1.49        | 1.44     |
| 11  | bB    | 833 | CLA  | C1C-C2C | 2.19  | 1.49        | 1.44     |
| 11  | cB    | 822 | CLA  | C3D-C4D | -2.19 | 1.39        | 1.44     |
| 11  | cA    | 837 | CLA  | C3B-C4B | 2.19  | 1.49        | 1.42     |
| 11  | aA    | 836 | CLA  | C4C-C3C | 2.19  | 1.48        | 1.45     |
| 11  | bL    | 205 | CLA  | C1C-C2C | 2.19  | 1.49        | 1.44     |
| 11  | bB    | 826 | CLA  | C3B-C2B | 2.19  | 1.48        | 1.41     |
| 11  | aL    | 204 | CLA  | C4C-C3C | 2.19  | 1.48        | 1.45     |
| 12  | bA    | 827 | F6C  | C1C-NC  | -2.19 | 1.35        | 1.37     |
| 11  | cA    | 813 | CLA  | C1B-C2B | 2.19  | 1.48        | 1.43     |
| 11  | bA    | 816 | CLA  | C3D-C4D | -2.19 | 1.39        | 1.44     |
| 11  | aB    | 813 | CLA  | C4C-C3C | 2.19  | 1.48        | 1.45     |
| 11  | aA    | 807 | CLA  | C3B-C2B | 2.19  | 1.48        | 1.41     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12  | cA    | 826 | F6C  | C1C-NC  | -2.19 | 1.35        | 1.37     |
| 11  | bA    | 814 | CLA  | C3B-C4B | 2.19  | 1.49        | 1.42     |
| 11  | cL    | 204 | CLA  | C4C-C3C | 2.19  | 1.48        | 1.45     |
| 11  | aA    | 813 | CLA  | C3B-C2B | 2.19  | 1.48        | 1.41     |
| 11  | bA    | 804 | CLA  | C3D-C4D | -2.19 | 1.39        | 1.44     |
| 11  | cA    | 825 | CLA  | C3D-C4D | -2.19 | 1.39        | 1.44     |
| 11  | cA    | 813 | CLA  | C3B-C2B | 2.19  | 1.48        | 1.41     |
| 11  | cK    | 103 | CLA  | C3D-C4D | -2.19 | 1.39        | 1.44     |
| 11  | cB    | 820 | CLA  | C3B-C2B | 2.19  | 1.48        | 1.41     |
| 11  | cL    | 204 | CLA  | C3D-C4D | -2.19 | 1.39        | 1.44     |
| 11  | aA    | 817 | CLA  | C3D-C4D | -2.19 | 1.39        | 1.44     |
| 11  | bB    | 836 | CLA  | C1C-C2C | 2.19  | 1.49        | 1.44     |
| 11  | cA    | 819 | CLA  | C3B-C2B | 2.19  | 1.48        | 1.41     |
| 11  | cA    | 816 | CLA  | C3B-C2B | 2.18  | 1.48        | 1.41     |
| 11  | bL    | 204 | CLA  | C4C-C3C | 2.18  | 1.48        | 1.45     |
| 11  | bB    | 826 | CLA  | C3D-C4D | -2.18 | 1.39        | 1.44     |
| 11  | cB    | 823 | CLA  | C3B-C2B | 2.18  | 1.48        | 1.41     |
| 11  | aK    | 101 | CLA  | C3B-C2B | 2.18  | 1.48        | 1.41     |
| 11  | bA    | 807 | CLA  | C3B-C2B | 2.18  | 1.48        | 1.41     |
| 11  | bK    | 103 | CLA  | C3D-C4D | -2.18 | 1.39        | 1.44     |
| 11  | aB    | 802 | CLA  | C3B-C4B | 2.18  | 1.49        | 1.42     |
| 11  | cB    | 819 | CLA  | C3D-C4D | -2.18 | 1.39        | 1.44     |
| 11  | cA    | 820 | CLA  | C3D-C4D | -2.18 | 1.39        | 1.44     |
| 11  | bB    | 827 | CLA  | C3B-C2B | 2.18  | 1.48        | 1.41     |
| 11  | cK    | 101 | CLA  | C3D-C4D | -2.18 | 1.39        | 1.44     |
| 11  | bA    | 838 | CLA  | C4C-C3C | 2.18  | 1.48        | 1.45     |
| 11  | bA    | 814 | CLA  | C3B-C2B | 2.18  | 1.48        | 1.41     |
| 11  | bA    | 816 | CLA  | C3B-C2B | 2.18  | 1.48        | 1.41     |
| 11  | cA    | 804 | CLA  | C3D-C4D | -2.18 | 1.39        | 1.44     |
| 11  | cA    | 811 | CLA  | C1C-C2C | 2.18  | 1.48        | 1.44     |
| 11  | cB    | 831 | CLA  | C1C-C2C | 2.18  | 1.48        | 1.44     |
| 11  | cB    | 804 | CLA  | C3B-C4B | 2.18  | 1.49        | 1.42     |
| 11  | cB    | 827 | CLA  | C1C-C2C | 2.18  | 1.48        | 1.44     |
| 11  | cL    | 206 | CLA  | C1C-C2C | 2.18  | 1.48        | 1.44     |
| 12  | aA    | 827 | F6C  | CHB-C4A | -2.18 | 1.34        | 1.38     |
| 11  | aA    | 821 | CLA  | C3D-C4D | -2.18 | 1.39        | 1.44     |
| 11  | bB    | 802 | CLA  | C3D-C4D | -2.18 | 1.39        | 1.44     |
| 11  | bA    | 822 | CLA  | C3D-C4D | -2.18 | 1.39        | 1.44     |
| 11  | aA    | 837 | CLA  | C3B-C4B | 2.18  | 1.49        | 1.42     |
| 11  | cA    | 829 | CLA  | C3D-C4D | -2.18 | 1.39        | 1.44     |
| 11  | bB    | 804 | CLA  | C3B-C4B | 2.18  | 1.49        | 1.42     |
| 11  | cB    | 819 | CLA  | C3B-C2B | 2.18  | 1.48        | 1.41     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | aB    | 836 | CLA  | C1C-C2C | 2.18  | 1.48        | 1.44     |
| 11  | cB    | 815 | CLA  | C3D-C4D | -2.18 | 1.39        | 1.44     |
| 11  | cB    | 835 | CLA  | C3B-C4B | 2.18  | 1.49        | 1.42     |
| 11  | bB    | 819 | CLA  | C3B-C2B | 2.18  | 1.48        | 1.41     |
| 11  | bB    | 802 | CLA  | C3B-C4B | 2.18  | 1.49        | 1.42     |
| 11  | aA    | 808 | CLA  | C3B-C2B | 2.18  | 1.48        | 1.41     |
| 11  | cA    | 812 | CLA  | C3B-C2B | 2.18  | 1.48        | 1.41     |
| 11  | aA    | 816 | CLA  | C3D-C4D | -2.18 | 1.39        | 1.44     |
| 11  | cA    | 808 | CLA  | C3B-C4B | 2.18  | 1.49        | 1.42     |
| 11  | aA    | 821 | CLA  | C1C-C2C | 2.18  | 1.48        | 1.44     |
| 11  | cA    | 816 | CLA  | C1C-C2C | 2.18  | 1.48        | 1.44     |
| 12  | bA    | 826 | F6C  | C1C-NC  | -2.18 | 1.35        | 1.37     |
| 11  | aB    | 821 | CLA  | C3D-C4D | -2.18 | 1.39        | 1.44     |
| 11  | aB    | 819 | CLA  | C3B-C4B | 2.18  | 1.49        | 1.42     |
| 11  | aA    | 815 | CLA  | C1A-CHA | 2.18  | 1.52        | 1.43     |
| 11  | cA    | 821 | CLA  | C3D-C4D | -2.17 | 1.39        | 1.44     |
| 11  | aB    | 819 | CLA  | C3B-C2B | 2.17  | 1.48        | 1.41     |
| 11  | cA    | 839 | CLA  | C3B-C4B | 2.17  | 1.49        | 1.42     |
| 11  | bA    | 821 | CLA  | C3D-C4D | -2.17 | 1.39        | 1.44     |
| 11  | aA    | 813 | CLA  | C1C-C2C | 2.17  | 1.48        | 1.44     |
| 12  | bA    | 830 | F6C  | CHB-C4A | -2.17 | 1.34        | 1.38     |
| 11  | cB    | 819 | CLA  | C3B-C4B | 2.17  | 1.49        | 1.42     |
| 11  | aB    | 826 | CLA  | C4C-C3C | 2.17  | 1.48        | 1.45     |
| 11  | cA    | 807 | CLA  | C3B-C2B | 2.17  | 1.48        | 1.41     |
| 11  | aB    | 804 | CLA  | C3B-C4B | 2.17  | 1.49        | 1.42     |
| 11  | bB    | 815 | CLA  | C3D-C4D | -2.17 | 1.39        | 1.44     |
| 11  | cB    | 833 | CLA  | C3D-C4D | -2.17 | 1.39        | 1.44     |
| 11  | cB    | 826 | CLA  | C1C-C2C | 2.17  | 1.48        | 1.44     |
| 11  | cB    | 806 | CLA  | C1C-C2C | 2.17  | 1.48        | 1.44     |
| 11  | bA    | 823 | CLA  | C3B-C2B | 2.17  | 1.48        | 1.41     |
| 12  | aL    | 202 | F6C  | C4C-C3C | 2.17  | 1.48        | 1.44     |
| 11  | cB    | 838 | CLA  | C1C-C2C | 2.17  | 1.48        | 1.44     |
| 11  | aB    | 838 | CLA  | C3B-C2B | 2.17  | 1.48        | 1.41     |
| 11  | cB    | 833 | CLA  | C3B-C2B | 2.17  | 1.48        | 1.41     |
| 11  | aA    | 809 | CLA  | C3D-C4D | -2.17 | 1.39        | 1.44     |
| 11  | cA    | 843 | CLA  | C3B-C2B | 2.17  | 1.48        | 1.41     |
| 11  | cB    | 834 | CLA  | C1A-CHA | 2.17  | 1.52        | 1.43     |
| 11  | bB    | 835 | CLA  | C3B-C4B | 2.17  | 1.49        | 1.42     |
| 11  | aA    | 821 | CLA  | C3B-C2B | 2.17  | 1.48        | 1.41     |
| 11  | aA    | 814 | CLA  | C3B-C2B | 2.17  | 1.48        | 1.41     |
| 11  | cB    | 826 | CLA  | C3B-C2B | 2.17  | 1.48        | 1.41     |
| 11  | cB    | 838 | CLA  | C3B-C2B | 2.17  | 1.48        | 1.41     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12  | cB    | 824 | F6C  | C1A-C2A | 2.17  | 1.50        | 1.45     |
| 11  | aB    | 839 | CLA  | C3B-C2B | 2.17  | 1.48        | 1.41     |
| 11  | cA    | 808 | CLA  | C3D-C4D | -2.17 | 1.39        | 1.44     |
| 11  | bB    | 822 | CLA  | C3B-C2B | 2.17  | 1.48        | 1.41     |
| 11  | aB    | 822 | CLA  | C3B-C2B | 2.17  | 1.48        | 1.41     |
| 11  | cB    | 826 | CLA  | C3D-C4D | -2.17 | 1.39        | 1.44     |
| 12  | aB    | 824 | F6C  | C1D-C2D | 2.17  | 1.48        | 1.44     |
| 11  | aB    | 819 | CLA  | C1A-CHA | 2.17  | 1.52        | 1.43     |
| 11  | aB    | 826 | CLA  | C3B-C2B | 2.17  | 1.48        | 1.41     |
| 11  | cA    | 803 | CLA  | C3B-C4B | 2.17  | 1.49        | 1.42     |
| 11  | bA    | 819 | CLA  | C3B-C2B | 2.16  | 1.48        | 1.41     |
| 11  | cA    | 815 | CLA  | C1A-CHA | 2.16  | 1.52        | 1.43     |
| 11  | aB    | 827 | CLA  | C1C-C2C | 2.16  | 1.48        | 1.44     |
| 11  | bB    | 821 | CLA  | C3D-C4D | -2.16 | 1.39        | 1.44     |
| 11  | aB    | 825 | CLA  | C3B-C4B | 2.16  | 1.49        | 1.42     |
| 11  | bB    | 833 | CLA  | C3D-C4D | -2.16 | 1.39        | 1.44     |
| 11  | bA    | 821 | CLA  | C3B-C2B | 2.16  | 1.48        | 1.41     |
| 11  | bB    | 811 | CLA  | C3B-C2B | 2.16  | 1.48        | 1.41     |
| 11  | aA    | 823 | CLA  | C3B-C2B | 2.16  | 1.48        | 1.41     |
| 11  | bB    | 838 | CLA  | C3B-C2B | 2.16  | 1.48        | 1.41     |
| 11  | bA    | 829 | CLA  | C3D-C4D | -2.16 | 1.39        | 1.44     |
| 11  | cA    | 821 | CLA  | C1C-C2C | 2.16  | 1.48        | 1.44     |
| 11  | aK    | 103 | CLA  | C3D-C4D | -2.16 | 1.39        | 1.44     |
| 11  | bB    | 827 | CLA  | C1C-C2C | 2.16  | 1.48        | 1.44     |
| 12  | cB    | 824 | F6C  | C2B-C1B | 2.16  | 1.49        | 1.44     |
| 11  | aA    | 839 | CLA  | C3B-C4B | 2.16  | 1.49        | 1.42     |
| 11  | bB    | 818 | CLA  | C3D-C4D | -2.16 | 1.39        | 1.44     |
| 11  | aB    | 823 | CLA  | C4C-C3C | 2.16  | 1.48        | 1.45     |
| 11  | aA    | 837 | CLA  | C3D-C4D | -2.16 | 1.39        | 1.44     |
| 11  | bB    | 817 | CLA  | C3B-C2B | 2.16  | 1.48        | 1.41     |
| 11  | cB    | 822 | CLA  | C3B-C2B | 2.16  | 1.48        | 1.41     |
| 11  | aL    | 205 | CLA  | C3B-C4B | 2.16  | 1.49        | 1.42     |
| 11  | aB    | 806 | CLA  | C3B-C2B | 2.16  | 1.48        | 1.41     |
| 11  | aA    | 822 | CLA  | C3D-C4D | -2.16 | 1.39        | 1.44     |
| 11  | aB    | 808 | CLA  | C3D-C4D | -2.16 | 1.39        | 1.44     |
| 11  | aB    | 815 | CLA  | C3D-C4D | -2.16 | 1.39        | 1.44     |
| 11  | bA    | 812 | CLA  | C3B-C2B | 2.16  | 1.48        | 1.41     |
| 11  | cA    | 825 | CLA  | C3B-C4B | 2.16  | 1.49        | 1.42     |
| 11  | cB    | 821 | CLA  | C3D-C4D | -2.16 | 1.39        | 1.44     |
| 12  | cL    | 202 | F6C  | CHB-C4A | -2.16 | 1.34        | 1.38     |
| 11  | bA    | 841 | CLA  | C3B-C2B | 2.16  | 1.48        | 1.41     |
| 11  | aB    | 818 | CLA  | C3D-C4D | -2.16 | 1.39        | 1.44     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | cL    | 205 | CLA  | C1C-C2C | 2.16  | 1.48        | 1.44     |
| 11  | bB    | 815 | CLA  | C3B-C2B | 2.16  | 1.48        | 1.41     |
| 11  | cB    | 815 | CLA  | C3B-C2B | 2.16  | 1.48        | 1.41     |
| 11  | aB    | 835 | CLA  | C3B-C4B | 2.16  | 1.49        | 1.42     |
| 11  | cA    | 814 | CLA  | C3B-C2B | 2.16  | 1.48        | 1.41     |
| 11  | cB    | 806 | CLA  | C3B-C2B | 2.16  | 1.48        | 1.41     |
| 11  | aB    | 819 | CLA  | C3D-C4D | -2.16 | 1.39        | 1.44     |
| 11  | cB    | 818 | CLA  | C3D-C4D | -2.16 | 1.39        | 1.44     |
| 11  | cA    | 817 | CLA  | C3D-C4D | -2.16 | 1.39        | 1.44     |
| 11  | cB    | 839 | CLA  | C3B-C2B | 2.15  | 1.48        | 1.41     |
| 11  | bB    | 819 | CLA  | C3B-C4B | 2.15  | 1.49        | 1.42     |
| 11  | cA    | 841 | CLA  | C3B-C2B | 2.15  | 1.48        | 1.41     |
| 11  | cB    | 811 | CLA  | C3B-C2B | 2.15  | 1.48        | 1.41     |
| 11  | cB    | 809 | CLA  | C4C-C3C | 2.15  | 1.48        | 1.45     |
| 11  | aA    | 813 | CLA  | C3D-C4D | -2.15 | 1.39        | 1.44     |
| 12  | bB    | 824 | F6C  | C2B-C1B | 2.15  | 1.49        | 1.44     |
| 11  | bB    | 826 | CLA  | C4C-C3C | 2.15  | 1.48        | 1.45     |
| 11  | aA    | 843 | CLA  | C3B-C2B | 2.15  | 1.48        | 1.41     |
| 11  | bB    | 806 | CLA  | C1C-C2C | 2.15  | 1.48        | 1.44     |
| 11  | bK    | 101 | CLA  | C1C-C2C | 2.15  | 1.48        | 1.44     |
| 11  | cB    | 816 | CLA  | C1C-C2C | 2.15  | 1.48        | 1.44     |
| 11  | cB    | 825 | CLA  | C3B-C4B | 2.15  | 1.49        | 1.42     |
| 11  | aB    | 811 | CLA  | C3B-C2B | 2.15  | 1.48        | 1.41     |
| 12  | cA    | 830 | F6C  | CHB-C4A | -2.15 | 1.34        | 1.38     |
| 11  | bA    | 811 | CLA  | C3B-C4B | 2.15  | 1.49        | 1.42     |
| 11  | cB    | 839 | CLA  | C1B-C2B | 2.15  | 1.48        | 1.43     |
| 11  | aK    | 101 | CLA  | C3D-C4D | -2.15 | 1.39        | 1.44     |
| 11  | bA    | 808 | CLA  | C3D-C4D | -2.15 | 1.39        | 1.44     |
| 11  | bK    | 103 | CLA  | C3B-C2B | 2.15  | 1.48        | 1.41     |
| 11  | aA    | 808 | CLA  | C3B-C4B | 2.15  | 1.49        | 1.42     |
| 11  | aB    | 827 | CLA  | C4C-C3C | 2.15  | 1.48        | 1.45     |
| 11  | bB    | 820 | CLA  | C1C-C2C | 2.15  | 1.48        | 1.44     |
| 11  | aB    | 802 | CLA  | C4C-C3C | 2.15  | 1.48        | 1.45     |
| 11  | bA    | 811 | CLA  | C1C-C2C | 2.15  | 1.48        | 1.44     |
| 11  | cA    | 823 | CLA  | C3B-C2B | 2.15  | 1.48        | 1.41     |
| 11  | aB    | 833 | CLA  | C3B-C2B | 2.15  | 1.48        | 1.41     |
| 11  | aB    | 834 | CLA  | C3B-C4B | 2.15  | 1.49        | 1.42     |
| 11  | bA    | 808 | CLA  | C3B-C4B | 2.15  | 1.49        | 1.42     |
| 11  | bL    | 204 | CLA  | C3D-C4D | -2.15 | 1.39        | 1.44     |
| 11  | cA    | 809 | CLA  | C3D-C4D | -2.15 | 1.39        | 1.44     |
| 11  | aA    | 816 | CLA  | C1C-C2C | 2.15  | 1.48        | 1.44     |
| 11  | cA    | 840 | CLA  | C1C-C2C | 2.15  | 1.48        | 1.44     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | bA    | 835 | CLA  | C4C-C3C | 2.15  | 1.48        | 1.45     |
| 11  | aB    | 839 | CLA  | C1B-C2B | 2.15  | 1.48        | 1.43     |
| 11  | cA    | 824 | CLA  | C3B-C4B | 2.15  | 1.49        | 1.42     |
| 11  | bA    | 820 | CLA  | C3D-C4D | -2.15 | 1.39        | 1.44     |
| 11  | cB    | 814 | CLA  | C3B-C2B | 2.15  | 1.48        | 1.41     |
| 11  | cA    | 834 | CLA  | C4C-C3C | 2.15  | 1.48        | 1.45     |
| 11  | bA    | 817 | CLA  | C3D-C4D | -2.15 | 1.39        | 1.44     |
| 11  | bA    | 825 | CLA  | C3B-C4B | 2.15  | 1.49        | 1.42     |
| 11  | aB    | 815 | CLA  | C3B-C2B | 2.15  | 1.48        | 1.41     |
| 11  | bB    | 806 | CLA  | C3B-C2B | 2.15  | 1.48        | 1.41     |
| 12  | aB    | 824 | F6C  | C1A-C2A | 2.15  | 1.50        | 1.45     |
| 11  | bB    | 819 | CLA  | C1A-CHA | 2.15  | 1.51        | 1.43     |
| 11  | aB    | 825 | CLA  | C1C-C2C | 2.15  | 1.48        | 1.44     |
| 11  | bA    | 816 | CLA  | C1C-C2C | 2.15  | 1.48        | 1.44     |
| 11  | aA    | 824 | CLA  | C3B-C4B | 2.15  | 1.49        | 1.42     |
| 11  | bA    | 839 | CLA  | C3B-C4B | 2.15  | 1.49        | 1.42     |
| 12  | aL    | 202 | F6C  | CHB-C4A | -2.15 | 1.34        | 1.38     |
| 11  | bB    | 801 | CLA  | C3D-C4D | -2.15 | 1.39        | 1.44     |
| 11  | bB    | 833 | CLA  | C3B-C2B | 2.15  | 1.48        | 1.41     |
| 11  | cA    | 835 | CLA  | C4C-C3C | 2.15  | 1.48        | 1.45     |
| 16  | bA    | 852 | LHG  | P-O6    | 2.15  | 1.67        | 1.59     |
| 11  | bB    | 823 | CLA  | C4C-C3C | 2.15  | 1.48        | 1.45     |
| 16  | aA    | 852 | LHG  | P-O6    | 2.15  | 1.67        | 1.59     |
| 11  | aB    | 833 | CLA  | C3D-C4D | -2.15 | 1.39        | 1.44     |
| 11  | aA    | 838 | CLA  | C4C-C3C | 2.15  | 1.48        | 1.45     |
| 11  | bB    | 838 | CLA  | C1C-C2C | 2.14  | 1.48        | 1.44     |
| 11  | aB    | 830 | CLA  | C3B-C2B | 2.14  | 1.48        | 1.41     |
| 11  | cA    | 838 | CLA  | C4C-C3C | 2.14  | 1.48        | 1.45     |
| 11  | bA    | 815 | CLA  | C1A-CHA | 2.14  | 1.51        | 1.43     |
| 11  | bA    | 813 | CLA  | C3D-C4D | -2.14 | 1.39        | 1.44     |
| 11  | bB    | 819 | CLA  | C3D-C4D | -2.14 | 1.39        | 1.44     |
| 11  | bB    | 832 | CLA  | C1C-C2C | 2.14  | 1.48        | 1.44     |
| 11  | cB    | 820 | CLA  | C1C-C2C | 2.14  | 1.48        | 1.44     |
| 11  | aB    | 834 | CLA  | C1A-CHA | 2.14  | 1.51        | 1.43     |
| 11  | aA    | 829 | CLA  | C1C-C2C | 2.14  | 1.48        | 1.44     |
| 11  | aL    | 204 | CLA  | C1C-C2C | 2.14  | 1.48        | 1.44     |
| 12  | cB    | 824 | F6C  | C1D-C2D | 2.14  | 1.48        | 1.44     |
| 11  | bA    | 834 | CLA  | C4C-C3C | 2.14  | 1.48        | 1.45     |
| 11  | aB    | 816 | CLA  | C1C-C2C | 2.14  | 1.48        | 1.44     |
| 11  | aA    | 825 | CLA  | C3B-C4B | 2.14  | 1.49        | 1.42     |
| 11  | bB    | 834 | CLA  | C1A-CHA | 2.14  | 1.51        | 1.43     |
| 11  | cB    | 819 | CLA  | C1A-CHA | 2.14  | 1.51        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | aA    | 811 | CLA  | C3B-C4B | 2.14  | 1.49        | 1.42     |
| 11  | cB    | 826 | CLA  | C4C-C3C | 2.14  | 1.48        | 1.45     |
| 12  | aB    | 824 | F6C  | C2B-C1B | 2.14  | 1.49        | 1.44     |
| 11  | bA    | 824 | CLA  | C3B-C4B | 2.14  | 1.49        | 1.42     |
| 11  | cA    | 829 | CLA  | C1C-C2C | 2.14  | 1.48        | 1.44     |
| 11  | cK    | 103 | CLA  | C3B-C2B | 2.14  | 1.48        | 1.41     |
| 11  | cB    | 808 | CLA  | C3D-C4D | -2.14 | 1.39        | 1.44     |
| 11  | bA    | 828 | CLA  | C3B-C4B | 2.14  | 1.49        | 1.42     |
| 11  | aA    | 818 | CLA  | C1A-CHA | 2.14  | 1.51        | 1.43     |
| 11  | aA    | 812 | CLA  | C3B-C2B | 2.14  | 1.48        | 1.41     |
| 11  | bB    | 839 | CLA  | C3B-C2B | 2.14  | 1.48        | 1.41     |
| 11  | aA    | 843 | CLA  | C1C-C2C | 2.14  | 1.48        | 1.44     |
| 11  | aB    | 806 | CLA  | C1C-C2C | 2.14  | 1.48        | 1.44     |
| 11  | cB    | 801 | CLA  | C3D-C4D | -2.14 | 1.39        | 1.44     |
| 11  | bB    | 802 | CLA  | C4C-C3C | 2.14  | 1.48        | 1.45     |
| 11  | bL    | 205 | CLA  | C3B-C4B | 2.14  | 1.49        | 1.42     |
| 11  | bA    | 843 | CLA  | C3B-C2B | 2.14  | 1.48        | 1.41     |
| 11  | cB    | 803 | CLA  | C3B-C2B | 2.14  | 1.48        | 1.41     |
| 11  | cB    | 827 | CLA  | C4C-C3C | 2.14  | 1.48        | 1.45     |
| 11  | aB    | 823 | CLA  | C3B-C4B | 2.14  | 1.49        | 1.42     |
| 12  | aA    | 830 | F6C  | CHB-C4A | -2.14 | 1.34        | 1.38     |
| 11  | bB    | 808 | CLA  | C3D-C4D | -2.14 | 1.39        | 1.44     |
| 11  | bA    | 818 | CLA  | C3D-C4D | -2.14 | 1.39        | 1.44     |
| 11  | cB    | 830 | CLA  | C1C-C2C | 2.14  | 1.48        | 1.44     |
| 11  | cL    | 204 | CLA  | C1C-C2C | 2.14  | 1.48        | 1.44     |
| 11  | bB    | 803 | CLA  | C3B-C2B | 2.14  | 1.48        | 1.41     |
| 11  | bB    | 814 | CLA  | C3B-C2B | 2.14  | 1.48        | 1.41     |
| 11  | aL    | 205 | CLA  | C1C-C2C | 2.14  | 1.48        | 1.44     |
| 11  | cB    | 832 | CLA  | C1C-C2C | 2.14  | 1.48        | 1.44     |
| 12  | aB    | 824 | F6C  | C1C-NC  | -2.14 | 1.35        | 1.37     |
| 11  | aB    | 803 | CLA  | C3B-C2B | 2.14  | 1.48        | 1.41     |
| 11  | bB    | 825 | CLA  | C3B-C4B | 2.13  | 1.49        | 1.42     |
| 11  | cB    | 835 | CLA  | C1C-C2C | 2.13  | 1.48        | 1.44     |
| 11  | cB    | 830 | CLA  | C3B-C2B | 2.13  | 1.48        | 1.41     |
| 11  | bB    | 820 | CLA  | C3B-C4B | 2.13  | 1.49        | 1.42     |
| 11  | bA    | 819 | CLA  | C1B-C2B | 2.13  | 1.48        | 1.43     |
| 11  | bB    | 811 | CLA  | C3D-C4D | -2.13 | 1.39        | 1.44     |
| 11  | cA    | 813 | CLA  | C3D-C4D | -2.13 | 1.39        | 1.44     |
| 11  | aA    | 824 | CLA  | C4C-C3C | 2.13  | 1.48        | 1.45     |
| 16  | cA    | 852 | LHG  | P-O6    | 2.13  | 1.67        | 1.59     |
| 11  | aL    | 204 | CLA  | C3D-C4D | -2.13 | 1.39        | 1.44     |
| 11  | aB    | 829 | CLA  | C1A-CHA | 2.13  | 1.51        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | aB    | 817 | CLA  | C3B-C2B | 2.13  | 1.48        | 1.41     |
| 11  | aB    | 814 | CLA  | C3B-C2B | 2.13  | 1.48        | 1.41     |
| 11  | cB    | 837 | CLA  | C3B-C2B | 2.13  | 1.48        | 1.41     |
| 11  | aA    | 811 | CLA  | C3D-C4D | -2.13 | 1.39        | 1.44     |
| 11  | cA    | 811 | CLA  | C3B-C4B | 2.13  | 1.49        | 1.42     |
| 11  | bB    | 835 | CLA  | C1C-C2C | 2.13  | 1.48        | 1.44     |
| 12  | bA    | 844 | F6C  | C1D-C2D | 2.13  | 1.48        | 1.44     |
| 11  | cA    | 821 | CLA  | C3B-C2B | 2.13  | 1.48        | 1.41     |
| 12  | bB    | 824 | F6C  | C1C-NC  | -2.13 | 1.35        | 1.37     |
| 11  | aA    | 841 | CLA  | C3B-C2B | 2.13  | 1.48        | 1.41     |
| 11  | aA    | 840 | CLA  | C1C-C2C | 2.13  | 1.48        | 1.44     |
| 11  | aB    | 820 | CLA  | C3B-C4B | 2.13  | 1.48        | 1.42     |
| 12  | cA    | 832 | F6C  | C1C-NC  | -2.13 | 1.35        | 1.37     |
| 11  | aA    | 834 | CLA  | C4C-C3C | 2.13  | 1.48        | 1.45     |
| 11  | cL    | 205 | CLA  | C3B-C4B | 2.13  | 1.48        | 1.42     |
| 11  | bA    | 809 | CLA  | C3D-C4D | -2.13 | 1.39        | 1.44     |
| 11  | aB    | 838 | CLA  | C1C-C2C | 2.13  | 1.48        | 1.44     |
| 11  | bB    | 816 | CLA  | C1C-C2C | 2.13  | 1.48        | 1.44     |
| 15  | aM    | 101 | BCR  | C30-C25 | -2.13 | 1.51        | 1.53     |
| 11  | bA    | 840 | CLA  | C1C-C2C | 2.13  | 1.48        | 1.44     |
| 11  | cA    | 811 | CLA  | C3D-C4D | -2.13 | 1.39        | 1.44     |
| 11  | aK    | 103 | CLA  | C3B-C2B | 2.13  | 1.48        | 1.41     |
| 11  | cA    | 828 | CLA  | C3B-C4B | 2.13  | 1.48        | 1.42     |
| 11  | bA    | 823 | CLA  | C1C-C2C | 2.13  | 1.48        | 1.44     |
| 11  | bL    | 204 | CLA  | C1C-C2C | 2.13  | 1.48        | 1.44     |
| 12  | aA    | 827 | F6C  | C4C-C3C | 2.12  | 1.48        | 1.44     |
| 11  | cB    | 817 | CLA  | C3B-C2B | 2.12  | 1.48        | 1.41     |
| 11  | aA    | 828 | CLA  | C3B-C4B | 2.12  | 1.48        | 1.42     |
| 11  | aA    | 842 | CLA  | C3B-C2B | 2.12  | 1.48        | 1.41     |
| 11  | aA    | 836 | CLA  | C1C-C2C | 2.12  | 1.48        | 1.44     |
| 11  | bB    | 808 | CLA  | C3B-C2B | 2.12  | 1.48        | 1.41     |
| 11  | aB    | 832 | CLA  | C3B-C2B | 2.12  | 1.48        | 1.41     |
| 11  | bB    | 839 | CLA  | C1B-C2B | 2.12  | 1.48        | 1.43     |
| 11  | bB    | 827 | CLA  | C4C-C3C | 2.12  | 1.48        | 1.45     |
| 11  | bB    | 831 | CLA  | C1C-C2C | 2.12  | 1.48        | 1.44     |
| 11  | cB    | 829 | CLA  | C1A-CHA | 2.12  | 1.51        | 1.43     |
| 11  | bB    | 829 | CLA  | C1A-CHA | 2.12  | 1.51        | 1.43     |
| 11  | aL    | 206 | CLA  | C1C-C2C | 2.12  | 1.48        | 1.44     |
| 11  | bB    | 834 | CLA  | C3D-C4D | -2.12 | 1.39        | 1.44     |
| 11  | cB    | 834 | CLA  | C3B-C4B | 2.12  | 1.48        | 1.42     |
| 11  | cA    | 818 | CLA  | C1A-CHA | 2.12  | 1.51        | 1.43     |
| 11  | cB    | 820 | CLA  | C1A-CHA | 2.12  | 1.51        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | bB    | 823 | CLA  | C3B-C4B | 2.12  | 1.48        | 1.42     |
| 11  | aA    | 835 | CLA  | C4C-C3C | 2.12  | 1.48        | 1.45     |
| 11  | aB    | 820 | CLA  | C3D-C4D | -2.12 | 1.39        | 1.44     |
| 11  | bA    | 843 | CLA  | C1C-C2C | 2.12  | 1.48        | 1.44     |
| 11  | aB    | 832 | CLA  | C1C-C2C | 2.12  | 1.48        | 1.44     |
| 11  | cB    | 820 | CLA  | C3B-C4B | 2.12  | 1.48        | 1.42     |
| 11  | bB    | 830 | CLA  | C1C-C2C | 2.11  | 1.48        | 1.44     |
| 11  | cB    | 804 | CLA  | C4C-C3C | 2.11  | 1.48        | 1.45     |
| 11  | bA    | 833 | CLA  | C1C-C2C | 2.11  | 1.48        | 1.44     |
| 11  | bB    | 830 | CLA  | C3B-C2B | 2.11  | 1.48        | 1.41     |
| 12  | cL    | 202 | F6C  | C3B-C4B | 2.11  | 1.49        | 1.44     |
| 11  | aB    | 808 | CLA  | C3B-C2B | 2.11  | 1.48        | 1.41     |
| 12  | aA    | 844 | F6C  | C1D-C2D | 2.11  | 1.48        | 1.44     |
| 11  | bA    | 836 | CLA  | C3D-C4D | -2.11 | 1.39        | 1.44     |
| 11  | cA    | 821 | CLA  | C1A-CHA | 2.11  | 1.51        | 1.43     |
| 11  | aB    | 801 | CLA  | C3D-C4D | -2.11 | 1.39        | 1.44     |
| 11  | aB    | 811 | CLA  | C3D-C4D | -2.11 | 1.39        | 1.44     |
| 11  | aA    | 809 | CLA  | C1A-CHA | 2.11  | 1.51        | 1.43     |
| 11  | cA    | 819 | CLA  | C1B-C2B | 2.11  | 1.48        | 1.43     |
| 11  | cA    | 807 | CLA  | C1C-C2C | 2.11  | 1.48        | 1.44     |
| 12  | bL    | 202 | F6C  | C3B-C4B | 2.11  | 1.49        | 1.44     |
| 11  | bB    | 804 | CLA  | C4C-C3C | 2.11  | 1.48        | 1.45     |
| 11  | aA    | 819 | CLA  | C1B-C2B | 2.11  | 1.48        | 1.43     |
| 11  | bL    | 206 | CLA  | C1C-C2C | 2.11  | 1.48        | 1.44     |
| 11  | bA    | 811 | CLA  | C3D-C4D | -2.11 | 1.39        | 1.44     |
| 11  | cA    | 818 | CLA  | C3D-C4D | -2.11 | 1.39        | 1.44     |
| 11  | bA    | 829 | CLA  | C1C-C2C | 2.11  | 1.48        | 1.44     |
| 11  | cB    | 831 | CLA  | C3B-C2B | 2.11  | 1.48        | 1.41     |
| 12  | aA    | 832 | F6C  | C3D-C4D | -2.11 | 1.38        | 1.44     |
| 11  | bB    | 820 | CLA  | C1A-CHA | 2.11  | 1.51        | 1.43     |
| 11  | cB    | 818 | CLA  | C1B-C2B | 2.11  | 1.48        | 1.43     |
| 11  | bB    | 835 | CLA  | C3D-C4D | -2.11 | 1.39        | 1.44     |
| 11  | bA    | 818 | CLA  | C1A-CHA | 2.11  | 1.51        | 1.43     |
| 11  | bA    | 836 | CLA  | C1C-C2C | 2.11  | 1.48        | 1.44     |
| 11  | bA    | 835 | CLA  | C1C-C2C | 2.11  | 1.48        | 1.44     |
| 12  | bA    | 832 | F6C  | C3D-C4D | -2.11 | 1.38        | 1.44     |
| 11  | bB    | 809 | CLA  | C4C-C3C | 2.11  | 1.48        | 1.45     |
| 11  | cA    | 835 | CLA  | C1C-C2C | 2.11  | 1.48        | 1.44     |
| 11  | bA    | 815 | CLA  | C3D-C4D | -2.11 | 1.39        | 1.44     |
| 11  | aB    | 831 | CLA  | C1C-C2C | 2.11  | 1.48        | 1.44     |
| 11  | bB    | 806 | CLA  | C3B-C4B | 2.11  | 1.48        | 1.42     |
| 11  | aB    | 820 | CLA  | C1A-CHA | 2.11  | 1.51        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | aB    | 835 | CLA  | C1C-C2C | 2.11  | 1.48        | 1.44     |
| 11  | cA    | 807 | CLA  | C3B-C4B | 2.11  | 1.48        | 1.42     |
| 11  | bA    | 842 | CLA  | C3B-C2B | 2.11  | 1.48        | 1.41     |
| 11  | bA    | 803 | CLA  | C1B-C2B | 2.11  | 1.48        | 1.43     |
| 11  | bB    | 834 | CLA  | C3B-C4B | 2.11  | 1.48        | 1.42     |
| 11  | aB    | 832 | CLA  | C3D-C4D | -2.11 | 1.39        | 1.44     |
| 11  | bA    | 824 | CLA  | C4C-C3C | 2.11  | 1.48        | 1.45     |
| 11  | aB    | 806 | CLA  | C3B-C4B | 2.11  | 1.48        | 1.42     |
| 11  | aA    | 818 | CLA  | C3D-C4D | -2.11 | 1.39        | 1.44     |
| 11  | cB    | 832 | CLA  | C3B-C2B | 2.11  | 1.48        | 1.41     |
| 11  | bA    | 811 | CLA  | C3B-C2B | 2.10  | 1.48        | 1.41     |
| 11  | cA    | 842 | CLA  | C3B-C2B | 2.10  | 1.48        | 1.41     |
| 11  | aB    | 820 | CLA  | C1C-C2C | 2.10  | 1.48        | 1.44     |
| 11  | aB    | 835 | CLA  | C3D-C4D | -2.10 | 1.39        | 1.44     |
| 11  | bB    | 832 | CLA  | C3D-C4D | -2.10 | 1.39        | 1.44     |
| 11  | aB    | 809 | CLA  | C4C-C3C | 2.10  | 1.48        | 1.45     |
| 11  | aB    | 837 | CLA  | C3B-C2B | 2.10  | 1.48        | 1.41     |
| 11  | aB    | 830 | CLA  | C1C-C2C | 2.10  | 1.48        | 1.44     |
| 11  | aA    | 814 | CLA  | C1C-C2C | 2.10  | 1.48        | 1.44     |
| 11  | aA    | 834 | CLA  | C1C-C2C | 2.10  | 1.48        | 1.44     |
| 12  | aA    | 830 | F6C  | C1C-NC  | -2.10 | 1.35        | 1.37     |
| 11  | cA    | 834 | CLA  | C1C-C2C | 2.10  | 1.48        | 1.44     |
| 12  | aL    | 202 | F6C  | C3B-C4B | 2.10  | 1.49        | 1.44     |
| 11  | aA    | 841 | CLA  | C1A-CHA | 2.10  | 1.51        | 1.43     |
| 11  | bA    | 820 | CLA  | C1A-CHA | 2.10  | 1.51        | 1.43     |
| 12  | bA    | 832 | F6C  | C1C-NC  | -2.10 | 1.35        | 1.37     |
| 11  | aB    | 831 | CLA  | C3B-C2B | 2.10  | 1.48        | 1.41     |
| 11  | bB    | 832 | CLA  | C3B-C2B | 2.10  | 1.48        | 1.41     |
| 11  | bB    | 829 | CLA  | C3D-C4D | -2.10 | 1.39        | 1.44     |
| 11  | cB    | 804 | CLA  | C1A-CHA | 2.10  | 1.51        | 1.43     |
| 11  | cA    | 803 | CLA  | C1B-C2B | 2.10  | 1.48        | 1.43     |
| 11  | cA    | 812 | CLA  | C3D-C4D | -2.10 | 1.39        | 1.44     |
| 11  | bA    | 834 | CLA  | C1C-C2C | 2.10  | 1.48        | 1.44     |
| 15  | bM    | 101 | BCR  | C30-C25 | -2.10 | 1.51        | 1.53     |
| 11  | aB    | 803 | CLA  | C1A-CHA | 2.10  | 1.51        | 1.43     |
| 11  | bA    | 807 | CLA  | C1C-C2C | 2.10  | 1.48        | 1.44     |
| 11  | cA    | 843 | CLA  | C1C-C2C | 2.10  | 1.48        | 1.44     |
| 11  | cB    | 830 | CLA  | C3D-C4D | -2.10 | 1.39        | 1.44     |
| 11  | bB    | 825 | CLA  | C1C-C2C | 2.10  | 1.48        | 1.44     |
| 11  | bA    | 807 | CLA  | C3B-C4B | 2.10  | 1.48        | 1.42     |
| 11  | aB    | 830 | CLA  | C3D-C4D | -2.10 | 1.39        | 1.44     |
| 11  | aB    | 807 | CLA  | C1C-C2C | 2.10  | 1.48        | 1.44     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | cB    | 823 | CLA  | C1A-CHA | 2.10  | 1.51        | 1.43     |
| 11  | cB    | 830 | CLA  | C1A-CHA | 2.10  | 1.51        | 1.43     |
| 11  | cA    | 824 | CLA  | C4C-C3C | 2.10  | 1.48        | 1.45     |
| 12  | cA    | 827 | F6C  | C4C-C3C | 2.10  | 1.48        | 1.44     |
| 11  | aA    | 823 | CLA  | C3B-C4B | 2.10  | 1.48        | 1.42     |
| 11  | aA    | 821 | CLA  | C1A-CHA | 2.10  | 1.51        | 1.43     |
| 11  | aA    | 835 | CLA  | C1C-C2C | 2.10  | 1.48        | 1.44     |
| 11  | aB    | 834 | CLA  | C1C-C2C | 2.10  | 1.48        | 1.44     |
| 11  | aB    | 823 | CLA  | C1A-CHA | 2.10  | 1.51        | 1.43     |
| 11  | cA    | 824 | CLA  | C3B-C2B | 2.10  | 1.48        | 1.41     |
| 12  | bA    | 827 | F6C  | C4C-C3C | 2.10  | 1.48        | 1.44     |
| 11  | bB    | 809 | CLA  | C1C-NC  | -2.10 | 1.34        | 1.37     |
| 11  | cB    | 825 | CLA  | C1C-C2C | 2.10  | 1.48        | 1.44     |
| 11  | bB    | 837 | CLA  | C3B-C2B | 2.10  | 1.48        | 1.41     |
| 11  | cA    | 836 | CLA  | C3D-C4D | -2.10 | 1.39        | 1.44     |
| 11  | aA    | 803 | CLA  | C1B-C2B | 2.10  | 1.48        | 1.43     |
| 11  | cA    | 829 | CLA  | C1A-CHA | 2.10  | 1.51        | 1.43     |
| 12  | cA    | 844 | F6C  | C1D-C2D | 2.10  | 1.48        | 1.44     |
| 11  | bA    | 833 | CLA  | C3B-C4B | 2.10  | 1.48        | 1.42     |
| 11  | bB    | 804 | CLA  | C1A-CHA | 2.10  | 1.51        | 1.43     |
| 11  | aA    | 807 | CLA  | C1C-C2C | 2.10  | 1.48        | 1.44     |
| 11  | cB    | 816 | CLA  | C3B-C2B | 2.10  | 1.48        | 1.41     |
| 11  | aB    | 804 | CLA  | C3D-C4D | -2.10 | 1.39        | 1.44     |
| 11  | cA    | 839 | CLA  | CBD-CAD | -2.10 | 1.47        | 1.56     |
| 11  | cA    | 823 | CLA  | C3B-C4B | 2.10  | 1.48        | 1.42     |
| 11  | bA    | 823 | CLA  | C3B-C4B | 2.09  | 1.48        | 1.42     |
| 11  | cA    | 811 | CLA  | C3B-C2B | 2.09  | 1.48        | 1.41     |
| 11  | bB    | 830 | CLA  | C1A-CHA | 2.09  | 1.51        | 1.43     |
| 11  | cA    | 815 | CLA  | C3D-C4D | -2.09 | 1.39        | 1.44     |
| 11  | cB    | 835 | CLA  | C3D-C4D | -2.09 | 1.39        | 1.44     |
| 11  | bA    | 839 | CLA  | CBD-CAD | -2.09 | 1.47        | 1.56     |
| 11  | aA    | 839 | CLA  | CBD-CAD | -2.09 | 1.47        | 1.56     |
| 11  | cA    | 823 | CLA  | C1C-C2C | 2.09  | 1.48        | 1.44     |
| 11  | bA    | 805 | CLA  | C1A-CHA | 2.09  | 1.51        | 1.43     |
| 11  | bB    | 816 | CLA  | C3B-C2B | 2.09  | 1.48        | 1.41     |
| 11  | cB    | 808 | CLA  | C1A-CHA | 2.09  | 1.51        | 1.43     |
| 11  | aA    | 833 | CLA  | C1C-C2C | 2.09  | 1.48        | 1.44     |
| 11  | bB    | 817 | CLA  | C4C-C3C | 2.09  | 1.48        | 1.45     |
| 11  | aA    | 811 | CLA  | C3B-C2B | 2.09  | 1.48        | 1.41     |
| 11  | bB    | 818 | CLA  | C1B-C2B | 2.09  | 1.48        | 1.43     |
| 11  | bA    | 821 | CLA  | C1A-CHA | 2.09  | 1.51        | 1.43     |
| 11  | aA    | 823 | CLA  | C1C-C2C | 2.09  | 1.48        | 1.44     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | cA    | 841 | CLA  | C1A-CHA | 2.09  | 1.51        | 1.43     |
| 11  | aB    | 816 | CLA  | C3B-C2B | 2.09  | 1.48        | 1.41     |
| 11  | aA    | 815 | CLA  | C3D-C4D | -2.09 | 1.39        | 1.44     |
| 11  | cB    | 829 | CLA  | C3D-C4D | -2.09 | 1.39        | 1.44     |
| 11  | cA    | 833 | CLA  | C1C-C2C | 2.09  | 1.48        | 1.44     |
| 11  | cA    | 820 | CLA  | C1A-CHA | 2.09  | 1.51        | 1.43     |
| 11  | aB    | 830 | CLA  | C1A-CHA | 2.09  | 1.51        | 1.43     |
| 12  | cA    | 832 | F6C  | C3D-C4D | -2.09 | 1.38        | 1.44     |
| 11  | cB    | 823 | CLA  | C3B-C4B | 2.09  | 1.48        | 1.42     |
| 11  | aB    | 813 | CLA  | C1C-C2C | 2.09  | 1.48        | 1.44     |
| 11  | cA    | 836 | CLA  | C1C-C2C | 2.09  | 1.48        | 1.44     |
| 11  | bB    | 831 | CLA  | C3B-C2B | 2.09  | 1.48        | 1.41     |
| 11  | bA    | 829 | CLA  | C1A-CHA | 2.09  | 1.51        | 1.43     |
| 11  | bB    | 834 | CLA  | C1C-C2C | 2.09  | 1.48        | 1.44     |
| 11  | cB    | 812 | CLA  | C1C-C2C | 2.09  | 1.48        | 1.44     |
| 11  | cA    | 809 | CLA  | C1A-CHA | 2.09  | 1.51        | 1.43     |
| 11  | bA    | 824 | CLA  | C3B-C2B | 2.09  | 1.48        | 1.41     |
| 11  | bB    | 821 | CLA  | C1A-CHA | 2.09  | 1.51        | 1.43     |
| 11  | cB    | 804 | CLA  | C3D-C4D | -2.09 | 1.39        | 1.44     |
| 11  | cB    | 806 | CLA  | C3B-C4B | 2.09  | 1.48        | 1.42     |
| 11  | aA    | 820 | CLA  | C1A-CHA | 2.09  | 1.51        | 1.43     |
| 11  | aB    | 810 | CLA  | C1C-C2C | 2.09  | 1.48        | 1.44     |
| 11  | bA    | 814 | CLA  | C1C-C2C | 2.09  | 1.48        | 1.44     |
| 11  | aB    | 804 | CLA  | C1A-CHA | 2.09  | 1.51        | 1.43     |
| 11  | cB    | 803 | CLA  | C1A-CHA | 2.09  | 1.51        | 1.43     |
| 11  | aA    | 829 | CLA  | C1A-CHA | 2.09  | 1.51        | 1.43     |
| 11  | cB    | 817 | CLA  | C4C-C3C | 2.09  | 1.48        | 1.45     |
| 11  | cB    | 809 | CLA  | C1C-NC  | -2.08 | 1.34        | 1.37     |
| 11  | aB    | 829 | CLA  | C3D-C4D | -2.08 | 1.39        | 1.44     |
| 12  | cA    | 832 | F6C  | C1D-C2D | 2.08  | 1.48        | 1.44     |
| 11  | aA    | 831 | CLA  | C3D-C4D | -2.08 | 1.39        | 1.44     |
| 11  | bL    | 205 | CLA  | C3B-C2B | 2.08  | 1.48        | 1.41     |
| 11  | bB    | 807 | CLA  | C1C-C2C | 2.08  | 1.48        | 1.44     |
| 11  | aA    | 833 | CLA  | C3B-C4B | 2.08  | 1.48        | 1.42     |
| 11  | cB    | 808 | CLA  | C3B-C2B | 2.08  | 1.48        | 1.41     |
| 11  | bA    | 841 | CLA  | C1A-CHA | 2.08  | 1.51        | 1.43     |
| 11  | bA    | 809 | CLA  | C1A-CHA | 2.08  | 1.51        | 1.43     |
| 11  | cA    | 834 | CLA  | C3B-C4B | 2.08  | 1.48        | 1.42     |
| 11  | aL    | 205 | CLA  | C3B-C2B | 2.08  | 1.48        | 1.41     |
| 11  | cB    | 834 | CLA  | C3D-C4D | -2.08 | 1.39        | 1.44     |
| 11  | cB    | 815 | CLA  | C4C-C3C | 2.08  | 1.48        | 1.45     |
| 11  | aA    | 807 | CLA  | C3B-C4B | 2.08  | 1.48        | 1.42     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | aA    | 817 | CLA  | C1A-CHA | 2.08  | 1.51        | 1.43     |
| 11  | aB    | 826 | CLA  | C3B-C4B | 2.08  | 1.48        | 1.42     |
| 12  | bA    | 832 | F6C  | C1D-C2D | 2.08  | 1.48        | 1.44     |
| 12  | cA    | 830 | F6C  | C4C-C3C | 2.08  | 1.48        | 1.44     |
| 11  | aB    | 808 | CLA  | C1A-CHA | 2.08  | 1.51        | 1.43     |
| 11  | bA    | 817 | CLA  | C1A-CHA | 2.08  | 1.51        | 1.43     |
| 11  | bB    | 823 | CLA  | C1A-CHA | 2.08  | 1.51        | 1.43     |
| 11  | cB    | 821 | CLA  | C1A-CHA | 2.08  | 1.51        | 1.43     |
| 11  | aB    | 807 | CLA  | C3B-C2B | 2.08  | 1.48        | 1.41     |
| 11  | bL    | 204 | CLA  | C1A-CHA | 2.08  | 1.51        | 1.43     |
| 11  | cB    | 832 | CLA  | C3D-C4D | -2.08 | 1.39        | 1.44     |
| 11  | aB    | 809 | CLA  | C1C-NC  | -2.08 | 1.34        | 1.37     |
| 11  | aA    | 805 | CLA  | C1A-CHA | 2.08  | 1.51        | 1.43     |
| 11  | cA    | 805 | CLA  | C1A-CHA | 2.08  | 1.51        | 1.43     |
| 11  | aB    | 805 | CLA  | C3B-C4B | 2.08  | 1.48        | 1.42     |
| 11  | bB    | 803 | CLA  | C1A-CHA | 2.08  | 1.51        | 1.43     |
| 12  | bA    | 830 | F6C  | C1C-NC  | -2.08 | 1.35        | 1.37     |
| 11  | bB    | 830 | CLA  | C3D-C4D | -2.08 | 1.39        | 1.44     |
| 11  | aA    | 837 | CLA  | C1A-CHA | 2.08  | 1.51        | 1.43     |
| 12  | bA    | 832 | F6C  | CMB-C2B | 2.08  | 1.50        | 1.45     |
| 11  | bB    | 805 | CLA  | C3B-C4B | 2.08  | 1.48        | 1.42     |
| 11  | aA    | 812 | CLA  | C3D-C4D | -2.08 | 1.39        | 1.44     |
| 11  | cA    | 802 | CLA  | C3B-C2B | 2.07  | 1.48        | 1.41     |
| 11  | aB    | 817 | CLA  | C4C-C3C | 2.07  | 1.48        | 1.45     |
| 11  | cB    | 815 | CLA  | C1A-CHA | 2.07  | 1.51        | 1.43     |
| 11  | aA    | 824 | CLA  | C3B-C2B | 2.07  | 1.48        | 1.41     |
| 11  | bB    | 815 | CLA  | C1A-CHA | 2.07  | 1.51        | 1.43     |
| 11  | cB    | 826 | CLA  | C1A-CHA | 2.07  | 1.51        | 1.43     |
| 11  | bA    | 812 | CLA  | C3D-C4D | -2.07 | 1.39        | 1.44     |
| 12  | aA    | 832 | F6C  | C1C-NC  | -2.07 | 1.35        | 1.37     |
| 11  | cA    | 817 | CLA  | C1C-C2C | 2.07  | 1.48        | 1.44     |
| 11  | aA    | 805 | CLA  | C3D-C4D | -2.07 | 1.39        | 1.44     |
| 11  | bB    | 807 | CLA  | C3B-C2B | 2.07  | 1.48        | 1.41     |
| 11  | cL    | 205 | CLA  | C3B-C2B | 2.07  | 1.48        | 1.41     |
| 11  | cB    | 811 | CLA  | C3D-C4D | -2.07 | 1.39        | 1.44     |
| 11  | cA    | 806 | CLA  | C3B-C2B | 2.07  | 1.48        | 1.41     |
| 11  | cK    | 103 | CLA  | C1C-C2C | 2.07  | 1.48        | 1.44     |
| 11  | bA    | 802 | CLA  | CBD-CAD | -2.07 | 1.47        | 1.56     |
| 11  | cB    | 835 | CLA  | C1A-CHA | 2.07  | 1.51        | 1.43     |
| 11  | aA    | 806 | CLA  | C3B-C2B | 2.07  | 1.48        | 1.41     |
| 12  | cA    | 832 | F6C  | CMB-C2B | 2.07  | 1.50        | 1.45     |
| 11  | bB    | 835 | CLA  | C3B-C2B | 2.07  | 1.48        | 1.41     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | bA    | 823 | CLA  | C3D-C4D | -2.07 | 1.39        | 1.44     |
| 11  | aB    | 821 | CLA  | C1A-CHA | 2.07  | 1.51        | 1.43     |
| 11  | bB    | 808 | CLA  | C1A-CHA | 2.07  | 1.51        | 1.43     |
| 11  | bB    | 826 | CLA  | C3B-C4B | 2.07  | 1.48        | 1.42     |
| 11  | aB    | 804 | CLA  | C4C-C3C | 2.07  | 1.48        | 1.45     |
| 12  | aA    | 832 | F6C  | CMB-C2B | 2.07  | 1.50        | 1.45     |
| 11  | cB    | 810 | CLA  | C3B-C2B | 2.07  | 1.48        | 1.41     |
| 11  | bB    | 818 | CLA  | C1C-C2C | 2.07  | 1.48        | 1.44     |
| 11  | bA    | 842 | CLA  | C3D-C4D | -2.07 | 1.39        | 1.44     |
| 11  | aA    | 802 | CLA  | CBD-CAD | -2.07 | 1.47        | 1.56     |
| 11  | cA    | 842 | CLA  | C3D-C4D | -2.07 | 1.39        | 1.44     |
| 11  | bB    | 835 | CLA  | C1A-CHA | 2.07  | 1.51        | 1.43     |
| 11  | aB    | 810 | CLA  | C3B-C2B | 2.06  | 1.48        | 1.41     |
| 11  | aB    | 835 | CLA  | C1A-CHA | 2.06  | 1.51        | 1.43     |
| 11  | cB    | 805 | CLA  | C3B-C4B | 2.06  | 1.48        | 1.42     |
| 11  | aA    | 839 | CLA  | C1C-C2C | 2.06  | 1.48        | 1.44     |
| 12  | bA    | 827 | F6C  | C1D-C2D | 2.06  | 1.48        | 1.44     |
| 15  | cM    | 101 | BCR  | C30-C25 | -2.06 | 1.51        | 1.53     |
| 11  | aB    | 834 | CLA  | C3D-C4D | -2.06 | 1.39        | 1.44     |
| 11  | cB    | 820 | CLA  | C3D-C4D | -2.06 | 1.39        | 1.44     |
| 12  | cA    | 827 | F6C  | C1D-C2D | 2.06  | 1.48        | 1.44     |
| 11  | cB    | 826 | CLA  | C3B-C4B | 2.06  | 1.48        | 1.42     |
| 11  | bA    | 805 | CLA  | C3D-C4D | -2.06 | 1.39        | 1.44     |
| 11  | aA    | 817 | CLA  | C1C-C2C | 2.06  | 1.48        | 1.44     |
| 11  | bK    | 103 | CLA  | C1C-C2C | 2.06  | 1.48        | 1.44     |
| 11  | cA    | 833 | CLA  | C3B-C4B | 2.06  | 1.48        | 1.42     |
| 12  | cA    | 830 | F6C  | C1C-NC  | -2.06 | 1.35        | 1.37     |
| 11  | aB    | 818 | CLA  | C1C-C2C | 2.06  | 1.48        | 1.44     |
| 11  | aB    | 832 | CLA  | C1A-CHA | 2.06  | 1.51        | 1.43     |
| 11  | cA    | 802 | CLA  | CBD-CAD | -2.06 | 1.47        | 1.56     |
| 11  | bA    | 825 | CLA  | C3B-C2B | 2.06  | 1.48        | 1.41     |
| 11  | bB    | 810 | CLA  | C3B-C2B | 2.06  | 1.48        | 1.41     |
| 11  | cB    | 840 | CLA  | C3B-C2B | 2.06  | 1.48        | 1.41     |
| 11  | aB    | 815 | CLA  | C1A-CHA | 2.06  | 1.51        | 1.43     |
| 11  | bA    | 837 | CLA  | C1A-CHA | 2.06  | 1.51        | 1.43     |
| 11  | aA    | 836 | CLA  | C3D-C4D | -2.06 | 1.39        | 1.44     |
| 11  | cB    | 807 | CLA  | C1C-C2C | 2.06  | 1.48        | 1.44     |
| 11  | bB    | 826 | CLA  | C1A-CHA | 2.06  | 1.51        | 1.43     |
| 11  | bA    | 822 | CLA  | C3B-C4B | 2.06  | 1.48        | 1.42     |
| 11  | bB    | 814 | CLA  | C3D-C4D | -2.06 | 1.39        | 1.44     |
| 11  | cL    | 204 | CLA  | C1A-CHA | 2.06  | 1.51        | 1.43     |
| 11  | bB    | 804 | CLA  | C3D-C4D | -2.06 | 1.39        | 1.44     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | aL    | 204 | CLA  | C1A-CHA | 2.06  | 1.51        | 1.43     |
| 11  | cA    | 817 | CLA  | C1A-CHA | 2.06  | 1.51        | 1.43     |
| 12  | aA    | 832 | F6C  | C1D-C2D | 2.06  | 1.48        | 1.44     |
| 11  | aB    | 818 | CLA  | C1B-C2B | 2.06  | 1.48        | 1.43     |
| 11  | bA    | 806 | CLA  | C3B-C2B | 2.06  | 1.48        | 1.41     |
| 11  | bB    | 813 | CLA  | C1C-C2C | 2.06  | 1.48        | 1.44     |
| 11  | cA    | 835 | CLA  | C3B-C4B | 2.06  | 1.48        | 1.42     |
| 11  | aB    | 826 | CLA  | C1A-CHA | 2.06  | 1.51        | 1.43     |
| 11  | cB    | 834 | CLA  | C1C-C2C | 2.06  | 1.48        | 1.44     |
| 11  | aB    | 835 | CLA  | C3B-C2B | 2.06  | 1.48        | 1.41     |
| 11  | bB    | 820 | CLA  | C3D-C4D | -2.06 | 1.39        | 1.44     |
| 11  | bB    | 810 | CLA  | C1C-C2C | 2.06  | 1.48        | 1.44     |
| 11  | aA    | 835 | CLA  | C3B-C4B | 2.06  | 1.48        | 1.42     |
| 11  | aB    | 812 | CLA  | C1C-C2C | 2.05  | 1.48        | 1.44     |
| 11  | cB    | 807 | CLA  | C3B-C2B | 2.05  | 1.48        | 1.41     |
| 11  | cB    | 810 | CLA  | C1C-C2C | 2.05  | 1.48        | 1.44     |
| 11  | aA    | 822 | CLA  | C3B-C4B | 2.05  | 1.48        | 1.42     |
| 11  | bA    | 834 | CLA  | C3B-C4B | 2.05  | 1.48        | 1.42     |
| 11  | cA    | 810 | CLA  | C3B-C4B | 2.05  | 1.48        | 1.42     |
| 11  | aA    | 825 | CLA  | C3B-C2B | 2.05  | 1.48        | 1.41     |
| 11  | bL    | 206 | CLA  | C3B-C2B | 2.05  | 1.48        | 1.41     |
| 11  | bA    | 839 | CLA  | C1C-C2C | 2.05  | 1.48        | 1.44     |
| 11  | cB    | 813 | CLA  | C1C-C2C | 2.05  | 1.48        | 1.44     |
| 15  | cI    | 103 | BCR  | C33-C5  | -2.05 | 1.47        | 1.50     |
| 11  | bB    | 815 | CLA  | C4C-C3C | 2.05  | 1.48        | 1.45     |
| 11  | bA    | 841 | CLA  | C3D-C4D | -2.05 | 1.39        | 1.44     |
| 11  | aA    | 842 | CLA  | C1A-CHA | 2.05  | 1.51        | 1.43     |
| 11  | aB    | 801 | CLA  | C1C-C2C | 2.05  | 1.48        | 1.44     |
| 11  | bA    | 810 | CLA  | C3B-C4B | 2.05  | 1.48        | 1.42     |
| 11  | cB    | 832 | CLA  | C1A-CHA | 2.05  | 1.51        | 1.43     |
| 11  | bA    | 831 | CLA  | C1C-NC  | -2.05 | 1.34        | 1.37     |
| 15  | bI    | 101 | BCR  | C33-C5  | -2.05 | 1.47        | 1.50     |
| 12  | bA    | 830 | F6C  | C4C-C3C | 2.05  | 1.48        | 1.44     |
| 11  | aA    | 834 | CLA  | C3B-C4B | 2.05  | 1.48        | 1.42     |
| 11  | bA    | 831 | CLA  | C3D-C4D | -2.05 | 1.39        | 1.44     |
| 11  | bA    | 842 | CLA  | C1A-CHA | 2.05  | 1.51        | 1.43     |
| 11  | cA    | 808 | CLA  | C1A-CHA | 2.05  | 1.51        | 1.43     |
| 11  | bB    | 840 | CLA  | C3B-C2B | 2.05  | 1.48        | 1.41     |
| 12  | aA    | 830 | F6C  | C4C-C3C | 2.05  | 1.48        | 1.44     |
| 11  | bK    | 103 | CLA  | C1A-CHA | 2.05  | 1.51        | 1.43     |
| 11  | aA    | 842 | CLA  | C3D-C4D | -2.05 | 1.39        | 1.44     |
| 11  | aB    | 814 | CLA  | C3D-C4D | -2.05 | 1.39        | 1.44     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | cA    | 823 | CLA  | C3D-C4D | -2.04 | 1.39        | 1.44     |
| 11  | aK    | 103 | CLA  | C1C-C2C | 2.04  | 1.48        | 1.44     |
| 11  | cA    | 805 | CLA  | C3D-C4D | -2.04 | 1.39        | 1.44     |
| 11  | bA    | 835 | CLA  | C3B-C4B | 2.04  | 1.48        | 1.42     |
| 12  | cL    | 202 | F6C  | C4D-CHA | 2.04  | 1.47        | 1.42     |
| 11  | cB    | 835 | CLA  | C3B-C2B | 2.04  | 1.48        | 1.41     |
| 16  | aA    | 852 | LHG  | O7-C5   | -2.04 | 1.41        | 1.46     |
| 11  | cA    | 822 | CLA  | C3B-C4B | 2.04  | 1.48        | 1.42     |
| 11  | bB    | 801 | CLA  | C3B-C2B | 2.04  | 1.48        | 1.41     |
| 11  | cB    | 818 | CLA  | C1C-C2C | 2.04  | 1.48        | 1.44     |
| 11  | aL    | 206 | CLA  | C3B-C2B | 2.04  | 1.48        | 1.41     |
| 11  | cB    | 814 | CLA  | C3D-C4D | -2.04 | 1.39        | 1.44     |
| 11  | cA    | 842 | CLA  | C1A-CHA | 2.04  | 1.51        | 1.43     |
| 11  | aA    | 802 | CLA  | C3B-C2B | 2.04  | 1.48        | 1.41     |
| 11  | cA    | 839 | CLA  | C1C-C2C | 2.04  | 1.48        | 1.44     |
| 15  | cK    | 102 | BCR  | C33-C5  | -2.04 | 1.47        | 1.50     |
| 11  | aA    | 823 | CLA  | C3D-C4D | -2.04 | 1.39        | 1.44     |
| 11  | aA    | 840 | CLA  | C3B-C2B | 2.04  | 1.48        | 1.41     |
| 11  | aL    | 206 | CLA  | C3B-C4B | 2.04  | 1.48        | 1.42     |
| 11  | bB    | 832 | CLA  | C1A-CHA | 2.04  | 1.51        | 1.43     |
| 11  | cA    | 809 | CLA  | C3B-C4B | 2.04  | 1.48        | 1.42     |
| 11  | bA    | 840 | CLA  | C3B-C2B | 2.04  | 1.48        | 1.41     |
| 11  | cA    | 837 | CLA  | C1A-CHA | 2.04  | 1.51        | 1.43     |
| 11  | cA    | 825 | CLA  | C1A-CHA | 2.04  | 1.51        | 1.43     |
| 11  | aB    | 840 | CLA  | C3B-C2B | 2.04  | 1.48        | 1.41     |
| 11  | bA    | 808 | CLA  | C1A-CHA | 2.04  | 1.51        | 1.43     |
| 11  | cA    | 807 | CLA  | C1A-CHA | 2.04  | 1.51        | 1.43     |
| 12  | aA    | 827 | F6C  | C1D-C2D | 2.04  | 1.48        | 1.44     |
| 11  | cA    | 834 | CLA  | C3B-C2B | 2.04  | 1.48        | 1.41     |
| 11  | aB    | 815 | CLA  | C4C-C3C | 2.04  | 1.48        | 1.45     |
| 11  | bA    | 825 | CLA  | C1A-CHA | 2.04  | 1.51        | 1.43     |
| 11  | aA    | 810 | CLA  | C3B-C4B | 2.04  | 1.48        | 1.42     |
| 11  | aB    | 801 | CLA  | C3B-C2B | 2.04  | 1.48        | 1.41     |
| 12  | bL    | 202 | F6C  | C4D-CHA | 2.04  | 1.47        | 1.42     |
| 11  | aB    | 814 | CLA  | C1A-CHA | 2.04  | 1.51        | 1.43     |
| 11  | bB    | 812 | CLA  | C1C-C2C | 2.03  | 1.48        | 1.44     |
| 11  | aA    | 810 | CLA  | C1A-CHA | 2.03  | 1.51        | 1.43     |
| 11  | aA    | 816 | CLA  | C1A-CHA | 2.03  | 1.51        | 1.43     |
| 12  | cB    | 824 | F6C  | C1C-NC  | -2.03 | 1.35        | 1.37     |
| 11  | bB    | 840 | CLA  | C1C-C2C | 2.03  | 1.48        | 1.44     |
| 11  | bB    | 813 | CLA  | C3B-C4B | 2.03  | 1.48        | 1.42     |
| 11  | cL    | 206 | CLA  | C3B-C2B | 2.03  | 1.48        | 1.41     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 16  | cA    | 852 | LHG  | O7-C5   | -2.03 | 1.41        | 1.46     |
| 11  | aB    | 828 | CLA  | C1B-C2B | 2.03  | 1.47        | 1.43     |
| 11  | cA    | 803 | CLA  | C1A-CHA | 2.03  | 1.51        | 1.43     |
| 11  | bA    | 802 | CLA  | C3B-C2B | 2.03  | 1.48        | 1.41     |
| 11  | aA    | 825 | CLA  | C1A-CHA | 2.03  | 1.51        | 1.43     |
| 11  | aB    | 813 | CLA  | C1A-CHA | 2.03  | 1.51        | 1.43     |
| 11  | bA    | 810 | CLA  | C1A-CHA | 2.03  | 1.51        | 1.43     |
| 11  | cB    | 836 | CLA  | C3B-C2B | 2.03  | 1.48        | 1.41     |
| 11  | bB    | 801 | CLA  | C1C-C2C | 2.03  | 1.48        | 1.44     |
| 11  | bA    | 812 | CLA  | C1A-CHA | 2.03  | 1.51        | 1.43     |
| 11  | cA    | 820 | CLA  | C3B-C4B | 2.03  | 1.48        | 1.42     |
| 11  | aB    | 818 | CLA  | C3B-C2B | 2.03  | 1.48        | 1.41     |
| 11  | bB    | 809 | CLA  | C3B-C2B | 2.03  | 1.48        | 1.41     |
| 11  | cB    | 801 | CLA  | C3B-C2B | 2.03  | 1.48        | 1.41     |
| 12  | aL    | 202 | F6C  | C4D-CHA | 2.03  | 1.47        | 1.42     |
| 11  | aB    | 811 | CLA  | C1A-CHA | 2.03  | 1.51        | 1.43     |
| 11  | bB    | 813 | CLA  | C1A-CHA | 2.03  | 1.51        | 1.43     |
| 11  | cB    | 809 | CLA  | C3B-C2B | 2.03  | 1.48        | 1.41     |
| 11  | aA    | 809 | CLA  | C3B-C4B | 2.03  | 1.48        | 1.42     |
| 11  | bB    | 808 | CLA  | C3B-C4B | 2.03  | 1.48        | 1.42     |
| 11  | bA    | 820 | CLA  | C3B-C4B | 2.03  | 1.48        | 1.42     |
| 11  | bA    | 817 | CLA  | C1C-C2C | 2.03  | 1.48        | 1.44     |
| 11  | aB    | 808 | CLA  | C3B-C4B | 2.02  | 1.48        | 1.42     |
| 11  | cA    | 812 | CLA  | C1A-CHA | 2.02  | 1.51        | 1.43     |
| 11  | cA    | 814 | CLA  | C1C-C2C | 2.02  | 1.48        | 1.44     |
| 11  | bB    | 805 | CLA  | CBD-CAD | -2.02 | 1.47        | 1.56     |
| 11  | aA    | 841 | CLA  | C3D-C4D | -2.02 | 1.39        | 1.44     |
| 11  | aA    | 812 | CLA  | C1A-CHA | 2.02  | 1.51        | 1.43     |
| 11  | aA    | 819 | CLA  | C1A-CHA | 2.02  | 1.51        | 1.43     |
| 11  | aA    | 808 | CLA  | C1A-CHA | 2.02  | 1.51        | 1.43     |
| 11  | aA    | 815 | CLA  | C3B-C4B | 2.02  | 1.48        | 1.42     |
| 11  | bB    | 828 | CLA  | C1B-C2B | 2.02  | 1.47        | 1.43     |
| 11  | aA    | 807 | CLA  | C1A-CHA | 2.02  | 1.51        | 1.43     |
| 11  | aB    | 805 | CLA  | CBD-CAD | -2.02 | 1.47        | 1.56     |
| 15  | bK    | 102 | BCR  | C33-C5  | -2.02 | 1.47        | 1.50     |
| 11  | bL    | 206 | CLA  | C3B-C4B | 2.02  | 1.48        | 1.42     |
| 11  | bB    | 814 | CLA  | C1A-CHA | 2.02  | 1.51        | 1.43     |
| 11  | aB    | 840 | CLA  | C1C-C2C | 2.02  | 1.48        | 1.44     |
| 11  | cB    | 813 | CLA  | C1A-CHA | 2.02  | 1.51        | 1.43     |
| 11  | bB    | 805 | CLA  | C1C-C2C | 2.02  | 1.48        | 1.44     |
| 11  | bA    | 809 | CLA  | C3B-C4B | 2.02  | 1.48        | 1.42     |
| 11  | cA    | 816 | CLA  | C1A-CHA | 2.02  | 1.51        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | cA    | 840 | CLA  | C3B-C2B | 2.02  | 1.48        | 1.41     |
| 11  | bA    | 834 | CLA  | C3B-C2B | 2.02  | 1.48        | 1.41     |
| 11  | bA    | 807 | CLA  | C1A-CHA | 2.02  | 1.51        | 1.43     |
| 15  | aI    | 101 | BCR  | C33-C5  | -2.02 | 1.47        | 1.50     |
| 11  | cB    | 840 | CLA  | C1C-C2C | 2.02  | 1.48        | 1.44     |
| 11  | aK    | 103 | CLA  | C1A-CHA | 2.02  | 1.51        | 1.43     |
| 11  | cA    | 819 | CLA  | C1A-CHA | 2.02  | 1.51        | 1.43     |
| 11  | cK    | 103 | CLA  | C1A-CHA | 2.02  | 1.51        | 1.43     |
| 11  | cL    | 204 | CLA  | C3B-C4B | 2.02  | 1.48        | 1.42     |
| 11  | aL    | 205 | CLA  | C1A-CHA | 2.02  | 1.51        | 1.43     |
| 11  | cB    | 808 | CLA  | C3B-C4B | 2.02  | 1.48        | 1.42     |
| 11  | aA    | 834 | CLA  | C3B-C2B | 2.02  | 1.48        | 1.41     |
| 11  | bL    | 204 | CLA  | C3B-C4B | 2.02  | 1.48        | 1.42     |
| 11  | cB    | 805 | CLA  | CBD-CAD | -2.02 | 1.47        | 1.56     |
| 11  | aB    | 839 | CLA  | C4C-C3C | 2.02  | 1.48        | 1.45     |
| 11  | aB    | 817 | CLA  | C1A-CHA | 2.02  | 1.51        | 1.43     |
| 11  | cA    | 841 | CLA  | C3D-C4D | -2.02 | 1.39        | 1.44     |
| 11  | cA    | 825 | CLA  | C3B-C2B | 2.01  | 1.48        | 1.41     |
| 11  | bB    | 836 | CLA  | C3B-C2B | 2.01  | 1.48        | 1.41     |
| 11  | aA    | 803 | CLA  | C1A-CHA | 2.01  | 1.51        | 1.43     |
| 11  | cB    | 801 | CLA  | C1C-C2C | 2.01  | 1.48        | 1.44     |
| 11  | cL    | 206 | CLA  | C3B-C4B | 2.01  | 1.48        | 1.42     |
| 11  | cA    | 810 | CLA  | C1A-CHA | 2.01  | 1.51        | 1.43     |
| 11  | bB    | 839 | CLA  | C4C-C3C | 2.01  | 1.48        | 1.45     |
| 12  | cA    | 844 | F6C  | C3D-C4D | -2.01 | 1.38        | 1.44     |
| 11  | cB    | 817 | CLA  | C1A-CHA | 2.01  | 1.51        | 1.43     |
| 11  | cA    | 831 | CLA  | C1B-C2B | 2.01  | 1.47        | 1.43     |
| 11  | bB    | 811 | CLA  | C1A-CHA | 2.01  | 1.51        | 1.43     |
| 12  | aA    | 827 | F6C  | C3D-C4D | -2.01 | 1.38        | 1.44     |
| 12  | cL    | 202 | F6C  | C3D-C4D | -2.01 | 1.38        | 1.44     |
| 11  | cB    | 813 | CLA  | C3B-C4B | 2.01  | 1.48        | 1.42     |
| 11  | aB    | 805 | CLA  | C1C-C2C | 2.01  | 1.48        | 1.44     |
| 11  | aL    | 204 | CLA  | C3B-C4B | 2.01  | 1.48        | 1.42     |
| 11  | cA    | 828 | CLA  | C1A-CHA | 2.01  | 1.51        | 1.43     |
| 11  | bA    | 806 | CLA  | C1A-CHA | 2.01  | 1.51        | 1.43     |
| 11  | cB    | 814 | CLA  | C1A-CHA | 2.01  | 1.51        | 1.43     |
| 11  | cA    | 806 | CLA  | C1A-CHA | 2.01  | 1.51        | 1.43     |
| 11  | cB    | 818 | CLA  | C1A-CHA | 2.01  | 1.51        | 1.43     |
| 11  | bA    | 829 | CLA  | C3B-C4B | 2.01  | 1.48        | 1.42     |
| 11  | bA    | 816 | CLA  | C1A-CHA | 2.01  | 1.51        | 1.43     |
| 11  | cA    | 831 | CLA  | C3D-C4D | -2.01 | 1.39        | 1.44     |
| 12  | aL    | 202 | F6C  | C3D-C4D | -2.01 | 1.38        | 1.44     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | cB    | 828 | CLA  | C1B-C2B | 2.01  | 1.47        | 1.43     |
| 11  | cB    | 808 | CLA  | C4C-C3C | 2.01  | 1.48        | 1.45     |
| 11  | cB    | 839 | CLA  | C4C-C3C | 2.01  | 1.48        | 1.45     |
| 11  | aA    | 820 | CLA  | C3B-C4B | 2.01  | 1.48        | 1.42     |
| 11  | bA    | 831 | CLA  | C1B-C2B | 2.01  | 1.47        | 1.43     |
| 11  | cB    | 811 | CLA  | C1A-CHA | 2.01  | 1.51        | 1.43     |
| 11  | bA    | 831 | CLA  | C1A-CHA | 2.01  | 1.51        | 1.43     |
| 11  | bB    | 822 | CLA  | C1A-CHA | 2.01  | 1.51        | 1.43     |
| 11  | cB    | 816 | CLA  | C1A-CHA | 2.01  | 1.51        | 1.43     |
| 11  | aB    | 836 | CLA  | C3B-C2B | 2.01  | 1.47        | 1.41     |
| 11  | bB    | 817 | CLA  | C1A-CHA | 2.01  | 1.51        | 1.43     |
| 11  | aB    | 809 | CLA  | C3B-C2B | 2.00  | 1.47        | 1.41     |
| 11  | bB    | 831 | CLA  | C1A-CHA | 2.00  | 1.51        | 1.43     |
| 11  | aB    | 818 | CLA  | C1A-CHA | 2.00  | 1.51        | 1.43     |
| 11  | aA    | 831 | CLA  | C1B-C2B | 2.00  | 1.47        | 1.43     |
| 11  | aA    | 829 | CLA  | C3B-C4B | 2.00  | 1.48        | 1.42     |
| 11  | bA    | 803 | CLA  | C1A-CHA | 2.00  | 1.51        | 1.43     |
| 11  | bB    | 816 | CLA  | C1A-CHA | 2.00  | 1.51        | 1.43     |
| 11  | cB    | 831 | CLA  | C1A-CHA | 2.00  | 1.51        | 1.43     |
| 11  | cA    | 831 | CLA  | C1A-CHA | 2.00  | 1.51        | 1.43     |
| 11  | bB    | 840 | CLA  | C3B-C4B | 2.00  | 1.48        | 1.42     |
| 11  | bB    | 801 | CLA  | CBD-CAD | -2.00 | 1.47        | 1.56     |
| 11  | bB    | 814 | CLA  | C1C-NC  | -2.00 | 1.34        | 1.37     |
| 11  | bA    | 819 | CLA  | C1A-CHA | 2.00  | 1.51        | 1.43     |
| 12  | bL    | 202 | F6C  | C3D-C4D | -2.00 | 1.38        | 1.44     |

All (8351) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 11  | aA    | 829 | CLA  | C4-C3-C5   | -21.23 | 78.37       | 115.23   |
| 11  | cA    | 829 | CLA  | C4-C3-C5   | -21.23 | 78.38       | 115.23   |
| 11  | bA    | 829 | CLA  | C4-C3-C5   | -21.21 | 78.42       | 115.23   |
| 11  | bA    | 829 | CLA  | C5-C3-C2   | 17.13  | 159.62      | 121.17   |
| 11  | aA    | 829 | CLA  | C5-C3-C2   | 17.11  | 159.57      | 121.17   |
| 11  | cA    | 829 | CLA  | C5-C3-C2   | 17.11  | 159.57      | 121.17   |
| 11  | cA    | 829 | CLA  | C4-C3-C2   | -16.47 | 81.32       | 123.63   |
| 11  | bA    | 829 | CLA  | C4-C3-C2   | -16.47 | 81.34       | 123.63   |
| 11  | aA    | 829 | CLA  | C4-C3-C2   | -16.47 | 81.34       | 123.63   |
| 12  | aA    | 827 | F6C  | C1D-ND-C4D | -14.94 | 99.86       | 106.68   |
| 12  | bA    | 827 | F6C  | C1D-ND-C4D | -14.88 | 99.89       | 106.68   |
| 12  | cA    | 844 | F6C  | C1D-ND-C4D | -14.88 | 99.89       | 106.68   |
| 12  | cA    | 827 | F6C  | C1D-ND-C4D | -14.82 | 99.92       | 106.68   |

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| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 12  | bA    | 844 | F6C  | C1D-ND-C4D  | -14.80 | 99.93       | 106.68   |
| 12  | aA    | 844 | F6C  | C1D-ND-C4D  | -14.71 | 99.97       | 106.68   |
| 12  | aA    | 832 | F6C  | C1D-ND-C4D  | -14.35 | 100.13      | 106.68   |
| 12  | bA    | 826 | F6C  | C1D-ND-C4D  | -14.32 | 100.15      | 106.68   |
| 12  | aA    | 826 | F6C  | C1D-ND-C4D  | -14.31 | 100.15      | 106.68   |
| 12  | bA    | 832 | F6C  | C1D-ND-C4D  | -14.29 | 100.16      | 106.68   |
| 12  | cA    | 826 | F6C  | C1D-ND-C4D  | -14.25 | 100.18      | 106.68   |
| 12  | aA    | 830 | F6C  | C1D-ND-C4D  | -14.21 | 100.19      | 106.68   |
| 12  | cA    | 832 | F6C  | C1D-ND-C4D  | -14.17 | 100.22      | 106.68   |
| 12  | cA    | 830 | F6C  | C1D-ND-C4D  | -14.14 | 100.23      | 106.68   |
| 12  | bA    | 830 | F6C  | C1D-ND-C4D  | -14.11 | 100.24      | 106.68   |
| 12  | cL    | 202 | F6C  | C1D-ND-C4D  | -14.04 | 100.28      | 106.68   |
| 12  | aL    | 202 | F6C  | C1D-ND-C4D  | -14.03 | 100.28      | 106.68   |
| 12  | bL    | 202 | F6C  | C1D-ND-C4D  | -13.96 | 100.31      | 106.68   |
| 12  | cB    | 824 | F6C  | C1D-ND-C4D  | -13.85 | 100.36      | 106.68   |
| 12  | aB    | 824 | F6C  | C1D-ND-C4D  | -13.78 | 100.39      | 106.68   |
| 12  | bB    | 824 | F6C  | C1D-ND-C4D  | -13.71 | 100.42      | 106.68   |
| 12  | aB    | 824 | F6C  | CAA-C2A-C3A | -12.72 | 104.04      | 127.87   |
| 12  | cB    | 824 | F6C  | CAA-C2A-C3A | -12.72 | 104.05      | 127.87   |
| 12  | bB    | 824 | F6C  | CAA-C2A-C3A | -12.70 | 104.09      | 127.87   |
| 12  | cA    | 827 | F6C  | CAA-C2A-C3A | -12.12 | 105.17      | 127.87   |
| 12  | bA    | 827 | F6C  | CAA-C2A-C3A | -12.10 | 105.20      | 127.87   |
| 12  | aA    | 827 | F6C  | CAA-C2A-C3A | -12.10 | 105.20      | 127.87   |
| 12  | cA    | 832 | F6C  | CAA-C2A-C3A | -10.69 | 107.85      | 127.87   |
| 12  | bA    | 832 | F6C  | CAA-C2A-C3A | -10.69 | 107.85      | 127.87   |
| 12  | aA    | 832 | F6C  | CAA-C2A-C3A | -10.66 | 107.90      | 127.87   |
| 12  | aA    | 830 | F6C  | CAA-C2A-C3A | -10.23 | 108.71      | 127.87   |
| 12  | bA    | 830 | F6C  | CAA-C2A-C3A | -10.19 | 108.78      | 127.87   |
| 12  | cA    | 830 | F6C  | CAA-C2A-C3A | -10.18 | 108.81      | 127.87   |
| 12  | cA    | 844 | F6C  | CAA-C2A-C3A | -10.12 | 108.92      | 127.87   |
| 12  | bA    | 844 | F6C  | CAA-C2A-C3A | -10.11 | 108.94      | 127.87   |
| 12  | aA    | 844 | F6C  | CAA-C2A-C3A | -10.10 | 108.96      | 127.87   |
| 12  | aA    | 844 | F6C  | CMA-C3A-C4A | -10.06 | 107.02      | 124.73   |
| 12  | cA    | 844 | F6C  | CMA-C3A-C4A | -10.05 | 107.03      | 124.73   |
| 12  | bA    | 844 | F6C  | CMA-C3A-C4A | -10.03 | 107.06      | 124.73   |
| 12  | bA    | 826 | F6C  | C3B-C2B-C1B | -9.78  | 101.42      | 106.46   |
| 11  | bB    | 822 | CLA  | C1D-ND-C4D  | -9.73  | 99.48       | 106.31   |
| 12  | aA    | 826 | F6C  | C3B-C2B-C1B | -9.70  | 101.45      | 106.46   |
| 11  | aB    | 822 | CLA  | C1D-ND-C4D  | -9.68  | 99.52       | 106.31   |
| 12  | cA    | 826 | F6C  | C3B-C2B-C1B | -9.67  | 101.47      | 106.46   |
| 11  | cA    | 818 | CLA  | C1D-ND-C4D  | -9.67  | 99.52       | 106.31   |
| 11  | cB    | 822 | CLA  | C1D-ND-C4D  | -9.64  | 99.55       | 106.31   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12  | cA    | 832 | F6C  | CMA-C3A-C4A | -9.62 | 107.79      | 124.73   |
| 11  | bA    | 818 | CLA  | C1D-ND-C4D  | -9.61 | 99.57       | 106.31   |
| 11  | aA    | 818 | CLA  | C1D-ND-C4D  | -9.59 | 99.58       | 106.31   |
| 12  | aA    | 832 | F6C  | CMA-C3A-C4A | -9.59 | 107.84      | 124.73   |
| 12  | bB    | 824 | F6C  | CMA-C3A-C4A | -9.59 | 107.84      | 124.73   |
| 12  | bA    | 832 | F6C  | CMA-C3A-C4A | -9.57 | 107.87      | 124.73   |
| 12  | aB    | 824 | F6C  | CMA-C3A-C4A | -9.57 | 107.88      | 124.73   |
| 12  | cB    | 824 | F6C  | CMA-C3A-C4A | -9.57 | 107.88      | 124.73   |
| 11  | aB    | 820 | CLA  | C1D-ND-C4D  | -9.53 | 99.62       | 106.31   |
| 12  | cA    | 827 | F6C  | C3B-C2B-C1B | -9.49 | 101.56      | 106.46   |
| 11  | cB    | 820 | CLA  | C1D-ND-C4D  | -9.47 | 99.67       | 106.31   |
| 12  | bA    | 827 | F6C  | C3B-C2B-C1B | -9.47 | 101.58      | 106.46   |
| 12  | cL    | 202 | F6C  | C3B-C2B-C1B | -9.43 | 101.59      | 106.46   |
| 11  | cA    | 808 | CLA  | C1D-ND-C4D  | -9.43 | 99.70       | 106.31   |
| 11  | aA    | 808 | CLA  | C1D-ND-C4D  | -9.43 | 99.70       | 106.31   |
| 11  | bB    | 820 | CLA  | C1D-ND-C4D  | -9.42 | 99.70       | 106.31   |
| 11  | aA    | 803 | CLA  | C1D-ND-C4D  | -9.41 | 99.71       | 106.31   |
| 12  | aL    | 202 | F6C  | C3B-C2B-C1B | -9.39 | 101.61      | 106.46   |
| 11  | cA    | 803 | CLA  | C1D-ND-C4D  | -9.39 | 99.72       | 106.31   |
| 11  | bA    | 808 | CLA  | C1D-ND-C4D  | -9.39 | 99.72       | 106.31   |
| 11  | bA    | 803 | CLA  | C1D-ND-C4D  | -9.37 | 99.74       | 106.31   |
| 12  | bL    | 202 | F6C  | C3B-C2B-C1B | -9.36 | 101.63      | 106.46   |
| 11  | bA    | 828 | CLA  | C1D-ND-C4D  | -9.36 | 99.75       | 106.31   |
| 11  | aA    | 828 | CLA  | C1D-ND-C4D  | -9.35 | 99.75       | 106.31   |
| 11  | cA    | 823 | CLA  | C1D-ND-C4D  | -9.35 | 99.75       | 106.31   |
| 11  | bB    | 838 | CLA  | C1D-ND-C4D  | -9.34 | 99.76       | 106.31   |
| 11  | cB    | 838 | CLA  | C1D-ND-C4D  | -9.34 | 99.76       | 106.31   |
| 11  | aA    | 840 | CLA  | C1D-ND-C4D  | -9.34 | 99.76       | 106.31   |
| 11  | cL    | 206 | CLA  | C1D-ND-C4D  | -9.34 | 99.76       | 106.31   |
| 11  | bL    | 206 | CLA  | C1D-ND-C4D  | -9.33 | 99.76       | 106.31   |
| 12  | aA    | 827 | F6C  | C3B-C2B-C1B | -9.32 | 101.65      | 106.46   |
| 11  | cA    | 828 | CLA  | C1D-ND-C4D  | -9.32 | 99.78       | 106.31   |
| 11  | bA    | 823 | CLA  | C1D-ND-C4D  | -9.31 | 99.78       | 106.31   |
| 11  | aL    | 206 | CLA  | C1D-ND-C4D  | -9.31 | 99.78       | 106.31   |
| 11  | bA    | 840 | CLA  | C1D-ND-C4D  | -9.31 | 99.78       | 106.31   |
| 11  | bA    | 841 | CLA  | C1D-ND-C4D  | -9.31 | 99.78       | 106.31   |
| 11  | cA    | 840 | CLA  | C1D-ND-C4D  | -9.31 | 99.78       | 106.31   |
| 11  | aA    | 841 | CLA  | C1D-ND-C4D  | -9.30 | 99.78       | 106.31   |
| 11  | aB    | 838 | CLA  | C1D-ND-C4D  | -9.30 | 99.79       | 106.31   |
| 11  | aB    | 804 | CLA  | C1D-ND-C4D  | -9.29 | 99.79       | 106.31   |
| 11  | cB    | 818 | CLA  | C1D-ND-C4D  | -9.29 | 99.79       | 106.31   |
| 11  | aB    | 818 | CLA  | C1D-ND-C4D  | -9.28 | 99.80       | 106.31   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aA    | 823 | CLA  | C1D-ND-C4D  | -9.28 | 99.80       | 106.31   |
| 11  | bB    | 801 | CLA  | C1D-ND-C4D  | -9.28 | 99.80       | 106.31   |
| 11  | bB    | 818 | CLA  | C1D-ND-C4D  | -9.26 | 99.82       | 106.31   |
| 11  | cA    | 841 | CLA  | C1D-ND-C4D  | -9.25 | 99.82       | 106.31   |
| 11  | aB    | 801 | CLA  | C1D-ND-C4D  | -9.24 | 99.83       | 106.31   |
| 11  | cK    | 103 | CLA  | C1D-ND-C4D  | -9.21 | 99.85       | 106.31   |
| 11  | cB    | 801 | CLA  | C1D-ND-C4D  | -9.20 | 99.85       | 106.31   |
| 11  | cB    | 804 | CLA  | C1D-ND-C4D  | -9.20 | 99.86       | 106.31   |
| 11  | bK    | 103 | CLA  | C1D-ND-C4D  | -9.19 | 99.86       | 106.31   |
| 11  | bB    | 804 | CLA  | C1D-ND-C4D  | -9.18 | 99.87       | 106.31   |
| 11  | aA    | 837 | CLA  | C1D-ND-C4D  | -9.18 | 99.87       | 106.31   |
| 11  | cA    | 837 | CLA  | C1D-ND-C4D  | -9.17 | 99.88       | 106.31   |
| 11  | aA    | 806 | CLA  | C1D-ND-C4D  | -9.16 | 99.89       | 106.31   |
| 11  | aB    | 833 | CLA  | C1D-ND-C4D  | -9.16 | 99.89       | 106.31   |
| 11  | bB    | 833 | CLA  | C1D-ND-C4D  | -9.15 | 99.89       | 106.31   |
| 11  | aL    | 205 | CLA  | C1D-ND-C4D  | -9.15 | 99.89       | 106.31   |
| 11  | cB    | 833 | CLA  | C1D-ND-C4D  | -9.15 | 99.89       | 106.31   |
| 11  | cA    | 806 | CLA  | C1D-ND-C4D  | -9.14 | 99.90       | 106.31   |
| 11  | aK    | 103 | CLA  | C1D-ND-C4D  | -9.13 | 99.91       | 106.31   |
| 11  | bA    | 806 | CLA  | C1D-ND-C4D  | -9.13 | 99.91       | 106.31   |
| 11  | cL    | 205 | CLA  | C1D-ND-C4D  | -9.13 | 99.91       | 106.31   |
| 11  | bL    | 205 | CLA  | C1D-ND-C4D  | -9.12 | 99.91       | 106.31   |
| 11  | cB    | 825 | CLA  | C1D-ND-C4D  | -9.12 | 99.91       | 106.31   |
| 11  | bA    | 837 | CLA  | C1D-ND-C4D  | -9.11 | 99.92       | 106.31   |
| 12  | cA    | 830 | F6C  | C3B-C2B-C1B | -9.11 | 101.76      | 106.46   |
| 12  | bA    | 830 | F6C  | C3B-C2B-C1B | -9.10 | 101.77      | 106.46   |
| 12  | bA    | 830 | F6C  | CMA-C3A-C4A | -9.08 | 108.74      | 124.73   |
| 11  | bB    | 825 | CLA  | C1D-ND-C4D  | -9.07 | 99.95       | 106.31   |
| 12  | aA    | 830 | F6C  | CMA-C3A-C4A | -9.06 | 108.78      | 124.73   |
| 11  | cA    | 842 | CLA  | C1D-ND-C4D  | -9.06 | 99.96       | 106.31   |
| 11  | aB    | 825 | CLA  | C1D-ND-C4D  | -9.05 | 99.96       | 106.31   |
| 12  | cA    | 830 | F6C  | CMA-C3A-C4A | -9.05 | 108.80      | 124.73   |
| 11  | bA    | 807 | CLA  | C1D-ND-C4D  | -9.04 | 99.97       | 106.31   |
| 11  | cA    | 807 | CLA  | C1D-ND-C4D  | -9.04 | 99.97       | 106.31   |
| 11  | cA    | 819 | CLA  | C1D-ND-C4D  | -9.04 | 99.97       | 106.31   |
| 11  | cA    | 813 | CLA  | C1D-ND-C4D  | -9.02 | 99.98       | 106.31   |
| 12  | aA    | 830 | F6C  | C3B-C2B-C1B | -9.02 | 101.81      | 106.46   |
| 10  | aA    | 801 | CL0  | C1B-CHB-C4A | 9.02  | 127.12      | 121.32   |
| 11  | bA    | 842 | CLA  | C1D-ND-C4D  | -9.01 | 99.99       | 106.31   |
| 11  | aA    | 842 | CLA  | C1D-ND-C4D  | -9.01 | 99.99       | 106.31   |
| 11  | bL    | 204 | CLA  | C1D-ND-C4D  | -9.01 | 99.99       | 106.31   |
| 11  | aA    | 814 | CLA  | C1D-ND-C4D  | -9.00 | 99.99       | 106.31   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bA    | 816 | CLA  | C1D-ND-C4D  | -8.99 | 100.00      | 106.31   |
| 11  | cL    | 204 | CLA  | C1D-ND-C4D  | -8.99 | 100.00      | 106.31   |
| 11  | bA    | 819 | CLA  | C1D-ND-C4D  | -8.99 | 100.00      | 106.31   |
| 11  | aA    | 807 | CLA  | C1D-ND-C4D  | -8.99 | 100.01      | 106.31   |
| 11  | bB    | 817 | CLA  | C1D-ND-C4D  | -8.99 | 100.01      | 106.31   |
| 10  | bA    | 801 | CL0  | C1B-CHB-C4A | 8.99  | 127.10      | 121.32   |
| 11  | aA    | 819 | CLA  | C1D-ND-C4D  | -8.98 | 100.01      | 106.31   |
| 11  | bB    | 826 | CLA  | C1D-ND-C4D  | -8.98 | 100.01      | 106.31   |
| 11  | cB    | 826 | CLA  | C1D-ND-C4D  | -8.98 | 100.01      | 106.31   |
| 11  | cA    | 816 | CLA  | C1D-ND-C4D  | -8.97 | 100.02      | 106.31   |
| 10  | cA    | 801 | CL0  | C1B-CHB-C4A | 8.97  | 127.09      | 121.32   |
| 11  | aA    | 816 | CLA  | C1D-ND-C4D  | -8.97 | 100.02      | 106.31   |
| 11  | cB    | 817 | CLA  | C1D-ND-C4D  | -8.96 | 100.02      | 106.31   |
| 11  | aA    | 813 | CLA  | C1D-ND-C4D  | -8.96 | 100.03      | 106.31   |
| 11  | bA    | 813 | CLA  | C1D-ND-C4D  | -8.96 | 100.03      | 106.31   |
| 11  | aB    | 807 | CLA  | C1D-ND-C4D  | -8.96 | 100.03      | 106.31   |
| 11  | cA    | 814 | CLA  | C1D-ND-C4D  | -8.95 | 100.03      | 106.31   |
| 11  | aB    | 817 | CLA  | C1D-ND-C4D  | -8.95 | 100.03      | 106.31   |
| 11  | bB    | 807 | CLA  | C1D-ND-C4D  | -8.94 | 100.04      | 106.31   |
| 11  | aB    | 826 | CLA  | C1D-ND-C4D  | -8.93 | 100.05      | 106.31   |
| 11  | bA    | 804 | CLA  | C1D-ND-C4D  | -8.93 | 100.05      | 106.31   |
| 11  | bA    | 835 | CLA  | C1D-ND-C4D  | -8.93 | 100.05      | 106.31   |
| 11  | bB    | 803 | CLA  | C1D-ND-C4D  | -8.93 | 100.05      | 106.31   |
| 11  | bA    | 814 | CLA  | C1D-ND-C4D  | -8.93 | 100.05      | 106.31   |
| 11  | aB    | 803 | CLA  | C1D-ND-C4D  | -8.92 | 100.05      | 106.31   |
| 11  | bB    | 832 | CLA  | C1D-ND-C4D  | -8.92 | 100.05      | 106.31   |
| 11  | cK    | 101 | CLA  | C1D-ND-C4D  | -8.92 | 100.05      | 106.31   |
| 11  | bA    | 839 | CLA  | C1D-ND-C4D  | -8.92 | 100.06      | 106.31   |
| 11  | aA    | 839 | CLA  | C1D-ND-C4D  | -8.91 | 100.06      | 106.31   |
| 11  | aL    | 204 | CLA  | C1D-ND-C4D  | -8.91 | 100.06      | 106.31   |
| 11  | cB    | 807 | CLA  | C1D-ND-C4D  | -8.91 | 100.06      | 106.31   |
| 11  | cA    | 839 | CLA  | C1D-ND-C4D  | -8.91 | 100.06      | 106.31   |
| 11  | bB    | 837 | CLA  | C1D-ND-C4D  | -8.91 | 100.06      | 106.31   |
| 11  | aB    | 832 | CLA  | C1D-ND-C4D  | -8.90 | 100.07      | 106.31   |
| 11  | aB    | 816 | CLA  | C1D-ND-C4D  | -8.90 | 100.07      | 106.31   |
| 11  | aA    | 810 | CLA  | C1D-ND-C4D  | -8.90 | 100.07      | 106.31   |
| 11  | cB    | 803 | CLA  | C1D-ND-C4D  | -8.90 | 100.07      | 106.31   |
| 11  | bK    | 101 | CLA  | C1D-ND-C4D  | -8.89 | 100.07      | 106.31   |
| 11  | bA    | 810 | CLA  | C1D-ND-C4D  | -8.89 | 100.07      | 106.31   |
| 11  | aK    | 101 | CLA  | C1D-ND-C4D  | -8.89 | 100.08      | 106.31   |
| 11  | bB    | 806 | CLA  | C1D-ND-C4D  | -8.89 | 100.08      | 106.31   |
| 11  | cB    | 832 | CLA  | C1D-ND-C4D  | -8.89 | 100.08      | 106.31   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 11  | cA    | 835 | CLA  | C1D-ND-C4D | -8.88 | 100.08      | 106.31   |
| 11  | aA    | 804 | CLA  | C1D-ND-C4D | -8.88 | 100.08      | 106.31   |
| 11  | aB    | 806 | CLA  | C1D-ND-C4D | -8.88 | 100.08      | 106.31   |
| 11  | aB    | 836 | CLA  | C1D-ND-C4D | -8.87 | 100.09      | 106.31   |
| 11  | bB    | 809 | CLA  | C1D-ND-C4D | -8.87 | 100.09      | 106.31   |
| 11  | aB    | 815 | CLA  | C1D-ND-C4D | -8.87 | 100.09      | 106.31   |
| 11  | aA    | 835 | CLA  | C1D-ND-C4D | -8.86 | 100.09      | 106.31   |
| 11  | aB    | 821 | CLA  | C1D-ND-C4D | -8.86 | 100.09      | 106.31   |
| 11  | cB    | 816 | CLA  | C1D-ND-C4D | -8.86 | 100.10      | 106.31   |
| 11  | cA    | 804 | CLA  | C1D-ND-C4D | -8.85 | 100.10      | 106.31   |
| 11  | cB    | 806 | CLA  | C1D-ND-C4D | -8.85 | 100.11      | 106.31   |
| 11  | cB    | 815 | CLA  | C1D-ND-C4D | -8.85 | 100.11      | 106.31   |
| 11  | bB    | 815 | CLA  | C1D-ND-C4D | -8.84 | 100.11      | 106.31   |
| 11  | cA    | 810 | CLA  | C1D-ND-C4D | -8.84 | 100.11      | 106.31   |
| 11  | aB    | 809 | CLA  | C1D-ND-C4D | -8.83 | 100.12      | 106.31   |
| 11  | cB    | 809 | CLA  | C1D-ND-C4D | -8.82 | 100.12      | 106.31   |
| 11  | aB    | 837 | CLA  | C1D-ND-C4D | -8.82 | 100.12      | 106.31   |
| 11  | cB    | 835 | CLA  | C1D-ND-C4D | -8.82 | 100.13      | 106.31   |
| 11  | cA    | 811 | CLA  | C1D-ND-C4D | -8.82 | 100.13      | 106.31   |
| 11  | cA    | 833 | CLA  | C1D-ND-C4D | -8.82 | 100.13      | 106.31   |
| 11  | aA    | 824 | CLA  | C1D-ND-C4D | -8.81 | 100.13      | 106.31   |
| 11  | aA    | 811 | CLA  | C1D-ND-C4D | -8.81 | 100.13      | 106.31   |
| 11  | bA    | 811 | CLA  | C1D-ND-C4D | -8.80 | 100.14      | 106.31   |
| 11  | bB    | 836 | CLA  | C1D-ND-C4D | -8.80 | 100.14      | 106.31   |
| 11  | aB    | 805 | CLA  | C1D-ND-C4D | -8.80 | 100.14      | 106.31   |
| 11  | aA    | 833 | CLA  | C1D-ND-C4D | -8.80 | 100.14      | 106.31   |
| 11  | bA    | 833 | CLA  | C1D-ND-C4D | -8.80 | 100.14      | 106.31   |
| 11  | bB    | 816 | CLA  | C1D-ND-C4D | -8.80 | 100.14      | 106.31   |
| 11  | cB    | 837 | CLA  | C1D-ND-C4D | -8.79 | 100.14      | 106.31   |
| 11  | cB    | 821 | CLA  | C1D-ND-C4D | -8.78 | 100.15      | 106.31   |
| 11  | bA    | 834 | CLA  | C1D-ND-C4D | -8.77 | 100.16      | 106.31   |
| 11  | cA    | 834 | CLA  | C1D-ND-C4D | -8.77 | 100.16      | 106.31   |
| 11  | aA    | 809 | CLA  | C1D-ND-C4D | -8.77 | 100.16      | 106.31   |
| 11  | bB    | 805 | CLA  | C1D-ND-C4D | -8.77 | 100.16      | 106.31   |
| 11  | bA    | 805 | CLA  | C1D-ND-C4D | -8.77 | 100.16      | 106.31   |
| 11  | aA    | 834 | CLA  | C1D-ND-C4D | -8.76 | 100.16      | 106.31   |
| 11  | aB    | 835 | CLA  | C1D-ND-C4D | -8.76 | 100.17      | 106.31   |
| 11  | bB    | 835 | CLA  | C1D-ND-C4D | -8.76 | 100.17      | 106.31   |
| 11  | cB    | 836 | CLA  | C1D-ND-C4D | -8.76 | 100.17      | 106.31   |
| 11  | cA    | 805 | CLA  | C1D-ND-C4D | -8.76 | 100.17      | 106.31   |
| 11  | cB    | 840 | CLA  | C1D-ND-C4D | -8.76 | 100.17      | 106.31   |
| 11  | bA    | 824 | CLA  | C1D-ND-C4D | -8.75 | 100.17      | 106.31   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 11  | aB    | 814 | CLA  | C1D-ND-C4D | -8.75 | 100.17      | 106.31   |
| 11  | cA    | 824 | CLA  | C1D-ND-C4D | -8.75 | 100.17      | 106.31   |
| 11  | bA    | 821 | CLA  | C1D-ND-C4D | -8.75 | 100.18      | 106.31   |
| 11  | bB    | 821 | CLA  | C1D-ND-C4D | -8.75 | 100.18      | 106.31   |
| 11  | aA    | 805 | CLA  | C1D-ND-C4D | -8.74 | 100.18      | 106.31   |
| 11  | bB    | 811 | CLA  | C1D-ND-C4D | -8.74 | 100.18      | 106.31   |
| 11  | cA    | 821 | CLA  | C1D-ND-C4D | -8.74 | 100.18      | 106.31   |
| 11  | cA    | 809 | CLA  | C1D-ND-C4D | -8.73 | 100.18      | 106.31   |
| 11  | cB    | 805 | CLA  | C1D-ND-C4D | -8.73 | 100.19      | 106.31   |
| 11  | bB    | 839 | CLA  | C1D-ND-C4D | -8.73 | 100.19      | 106.31   |
| 11  | aA    | 836 | CLA  | C1D-ND-C4D | -8.72 | 100.19      | 106.31   |
| 11  | bB    | 810 | CLA  | C1D-ND-C4D | -8.72 | 100.19      | 106.31   |
| 11  | aA    | 821 | CLA  | C1D-ND-C4D | -8.72 | 100.19      | 106.31   |
| 11  | bB    | 840 | CLA  | C1D-ND-C4D | -8.72 | 100.19      | 106.31   |
| 11  | cB    | 811 | CLA  | C1D-ND-C4D | -8.72 | 100.20      | 106.31   |
| 11  | cB    | 839 | CLA  | C1D-ND-C4D | -8.72 | 100.20      | 106.31   |
| 11  | cA    | 829 | CLA  | C1D-ND-C4D | -8.71 | 100.20      | 106.31   |
| 11  | bA    | 829 | CLA  | C1D-ND-C4D | -8.71 | 100.20      | 106.31   |
| 11  | bA    | 809 | CLA  | C1D-ND-C4D | -8.71 | 100.20      | 106.31   |
| 11  | aB    | 839 | CLA  | C1D-ND-C4D | -8.70 | 100.20      | 106.31   |
| 11  | aB    | 811 | CLA  | C1D-ND-C4D | -8.70 | 100.21      | 106.31   |
| 11  | cB    | 814 | CLA  | C1D-ND-C4D | -8.70 | 100.21      | 106.31   |
| 11  | bB    | 814 | CLA  | C1D-ND-C4D | -8.69 | 100.21      | 106.31   |
| 11  | aA    | 822 | CLA  | C1D-ND-C4D | -8.68 | 100.22      | 106.31   |
| 11  | aB    | 840 | CLA  | C1D-ND-C4D | -8.68 | 100.22      | 106.31   |
| 11  | aB    | 810 | CLA  | C1D-ND-C4D | -8.68 | 100.22      | 106.31   |
| 11  | cA    | 836 | CLA  | C1D-ND-C4D | -8.67 | 100.23      | 106.31   |
| 11  | aA    | 829 | CLA  | C1D-ND-C4D | -8.66 | 100.23      | 106.31   |
| 11  | bA    | 836 | CLA  | C1D-ND-C4D | -8.66 | 100.24      | 106.31   |
| 11  | aB    | 813 | CLA  | C1D-ND-C4D | -8.65 | 100.24      | 106.31   |
| 11  | bB    | 813 | CLA  | C1D-ND-C4D | -8.65 | 100.24      | 106.31   |
| 11  | cA    | 822 | CLA  | C1D-ND-C4D | -8.65 | 100.24      | 106.31   |
| 11  | cB    | 810 | CLA  | C1D-ND-C4D | -8.65 | 100.25      | 106.31   |
| 11  | bA    | 822 | CLA  | C1D-ND-C4D | -8.65 | 100.25      | 106.31   |
| 11  | cB    | 813 | CLA  | C1D-ND-C4D | -8.64 | 100.25      | 106.31   |
| 11  | cB    | 819 | CLA  | C1D-ND-C4D | -8.63 | 100.25      | 106.31   |
| 11  | bA    | 812 | CLA  | C1D-ND-C4D | -8.63 | 100.26      | 106.31   |
| 11  | bA    | 838 | CLA  | C1D-ND-C4D | -8.61 | 100.27      | 106.31   |
| 11  | aA    | 838 | CLA  | C1D-ND-C4D | -8.60 | 100.28      | 106.31   |
| 11  | bB    | 819 | CLA  | C1D-ND-C4D | -8.60 | 100.28      | 106.31   |
| 11  | aB    | 819 | CLA  | C1D-ND-C4D | -8.59 | 100.28      | 106.31   |
| 11  | cB    | 831 | CLA  | C1D-ND-C4D | -8.59 | 100.28      | 106.31   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aA    | 812 | CLA  | C1D-ND-C4D  | -8.58 | 100.29      | 106.31   |
| 11  | cA    | 838 | CLA  | C1D-ND-C4D  | -8.58 | 100.29      | 106.31   |
| 11  | cA    | 843 | CLA  | C1D-ND-C4D  | -8.58 | 100.29      | 106.31   |
| 11  | aA    | 843 | CLA  | C1D-ND-C4D  | -8.56 | 100.30      | 106.31   |
| 11  | bB    | 831 | CLA  | C1D-ND-C4D  | -8.56 | 100.30      | 106.31   |
| 12  | cA    | 827 | F6C  | CAA-C2A-C1A | -8.56 | 104.11      | 128.01   |
| 12  | bA    | 832 | F6C  | C3B-C2B-C1B | -8.55 | 102.05      | 106.46   |
| 12  | bA    | 827 | F6C  | CAA-C2A-C1A | -8.55 | 104.14      | 128.01   |
| 12  | aA    | 827 | F6C  | CAA-C2A-C1A | -8.54 | 104.14      | 128.01   |
| 11  | bA    | 843 | CLA  | C1D-ND-C4D  | -8.54 | 100.32      | 106.31   |
| 11  | aB    | 831 | CLA  | C1D-ND-C4D  | -8.53 | 100.33      | 106.31   |
| 11  | cA    | 812 | CLA  | C1D-ND-C4D  | -8.52 | 100.33      | 106.31   |
| 12  | aA    | 832 | F6C  | C3B-C2B-C1B | -8.51 | 102.07      | 106.46   |
| 12  | cA    | 832 | F6C  | C3B-C2B-C1B | -8.51 | 102.07      | 106.46   |
| 11  | aB    | 808 | CLA  | C1D-ND-C4D  | -8.50 | 100.35      | 106.31   |
| 11  | cB    | 808 | CLA  | C1D-ND-C4D  | -8.49 | 100.35      | 106.31   |
| 11  | aB    | 802 | CLA  | C1D-ND-C4D  | -8.47 | 100.37      | 106.31   |
| 11  | bA    | 831 | CLA  | C1D-ND-C4D  | -8.47 | 100.37      | 106.31   |
| 12  | bA    | 844 | F6C  | C3B-C2B-C1B | -8.46 | 102.09      | 106.46   |
| 11  | bB    | 808 | CLA  | C1D-ND-C4D  | -8.45 | 100.38      | 106.31   |
| 11  | aB    | 830 | CLA  | C1D-ND-C4D  | -8.44 | 100.39      | 106.31   |
| 12  | cA    | 844 | F6C  | C3B-C2B-C1B | -8.44 | 102.11      | 106.46   |
| 11  | cB    | 802 | CLA  | C1D-ND-C4D  | -8.42 | 100.41      | 106.31   |
| 11  | bB    | 823 | CLA  | C1D-ND-C4D  | -8.41 | 100.41      | 106.31   |
| 11  | bB    | 830 | CLA  | C1D-ND-C4D  | -8.40 | 100.42      | 106.31   |
| 12  | aA    | 844 | F6C  | C3B-C2B-C1B | -8.40 | 102.13      | 106.46   |
| 11  | cB    | 830 | CLA  | C1D-ND-C4D  | -8.39 | 100.42      | 106.31   |
| 11  | aA    | 831 | CLA  | C1D-ND-C4D  | -8.38 | 100.43      | 106.31   |
| 11  | aB    | 823 | CLA  | C1D-ND-C4D  | -8.37 | 100.44      | 106.31   |
| 11  | bB    | 802 | CLA  | C1D-ND-C4D  | -8.36 | 100.44      | 106.31   |
| 11  | bB    | 834 | CLA  | C1D-ND-C4D  | -8.34 | 100.46      | 106.31   |
| 11  | cA    | 831 | CLA  | C1D-ND-C4D  | -8.33 | 100.46      | 106.31   |
| 11  | cB    | 823 | CLA  | C1D-ND-C4D  | -8.33 | 100.46      | 106.31   |
| 11  | bA    | 825 | CLA  | C1D-ND-C4D  | -8.31 | 100.48      | 106.31   |
| 11  | aB    | 834 | CLA  | C1D-ND-C4D  | -8.31 | 100.48      | 106.31   |
| 11  | aA    | 825 | CLA  | C1D-ND-C4D  | -8.31 | 100.48      | 106.31   |
| 11  | cA    | 825 | CLA  | C1D-ND-C4D  | -8.30 | 100.49      | 106.31   |
| 11  | bB    | 827 | CLA  | C1D-ND-C4D  | -8.30 | 100.49      | 106.31   |
| 11  | bA    | 820 | CLA  | C1D-ND-C4D  | -8.30 | 100.49      | 106.31   |
| 11  | cB    | 834 | CLA  | C1D-ND-C4D  | -8.29 | 100.50      | 106.31   |
| 11  | bA    | 817 | CLA  | C1D-ND-C4D  | -8.27 | 100.51      | 106.31   |
| 11  | aA    | 817 | CLA  | C1D-ND-C4D  | -8.27 | 100.51      | 106.31   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cB    | 827 | CLA  | C1D-ND-C4D  | -8.26 | 100.52      | 106.31   |
| 11  | aA    | 820 | CLA  | C1D-ND-C4D  | -8.24 | 100.53      | 106.31   |
| 11  | aA    | 802 | CLA  | C1D-ND-C4D  | -8.23 | 100.53      | 106.31   |
| 11  | aB    | 827 | CLA  | C1D-ND-C4D  | -8.23 | 100.53      | 106.31   |
| 11  | cA    | 820 | CLA  | C1D-ND-C4D  | -8.23 | 100.54      | 106.31   |
| 11  | cA    | 802 | CLA  | C1D-ND-C4D  | -8.22 | 100.55      | 106.31   |
| 11  | cA    | 817 | CLA  | C1D-ND-C4D  | -8.18 | 100.57      | 106.31   |
| 11  | bA    | 802 | CLA  | C1D-ND-C4D  | -8.16 | 100.59      | 106.31   |
| 11  | bA    | 815 | CLA  | C1D-ND-C4D  | -8.14 | 100.60      | 106.31   |
| 11  | aA    | 815 | CLA  | C1D-ND-C4D  | -8.12 | 100.62      | 106.31   |
| 11  | cA    | 815 | CLA  | C1D-ND-C4D  | -8.11 | 100.62      | 106.31   |
| 12  | aA    | 827 | F6C  | CMA-C3A-C4A | -8.06 | 110.53      | 124.73   |
| 12  | bA    | 827 | F6C  | CMA-C3A-C4A | -8.06 | 110.54      | 124.73   |
| 12  | cA    | 827 | F6C  | CMA-C3A-C4A | -8.05 | 110.55      | 124.73   |
| 11  | aB    | 812 | CLA  | C1D-ND-C4D  | -8.04 | 100.67      | 106.31   |
| 11  | bB    | 829 | CLA  | C1D-ND-C4D  | -7.99 | 100.71      | 106.31   |
| 11  | cB    | 829 | CLA  | C1D-ND-C4D  | -7.98 | 100.71      | 106.31   |
| 11  | bB    | 812 | CLA  | C1D-ND-C4D  | -7.96 | 100.72      | 106.31   |
| 12  | aB    | 824 | F6C  | C3B-C2B-C1B | -7.95 | 102.36      | 106.46   |
| 11  | cB    | 812 | CLA  | C1D-ND-C4D  | -7.92 | 100.76      | 106.31   |
| 11  | aB    | 829 | CLA  | C1D-ND-C4D  | -7.91 | 100.77      | 106.31   |
| 12  | cB    | 824 | F6C  | C3B-C2B-C1B | -7.87 | 102.40      | 106.46   |
| 12  | bB    | 824 | F6C  | C3B-C2B-C1B | -7.85 | 102.41      | 106.46   |
| 12  | bL    | 202 | F6C  | CMA-C3A-C4A | -7.82 | 110.96      | 124.73   |
| 12  | aL    | 202 | F6C  | CMA-C3A-C4A | -7.82 | 110.96      | 124.73   |
| 12  | cL    | 202 | F6C  | CMA-C3A-C4A | -7.80 | 110.99      | 124.73   |
| 11  | bB    | 828 | CLA  | C1D-ND-C4D  | -7.71 | 100.91      | 106.31   |
| 12  | aA    | 826 | F6C  | CAA-C2A-C3A | -7.70 | 113.45      | 127.87   |
| 12  | cA    | 826 | F6C  | CAA-C2A-C3A | -7.69 | 113.47      | 127.87   |
| 11  | cB    | 828 | CLA  | C1D-ND-C4D  | -7.69 | 100.92      | 106.31   |
| 11  | aB    | 828 | CLA  | C1D-ND-C4D  | -7.68 | 100.92      | 106.31   |
| 12  | bA    | 826 | F6C  | CAA-C2A-C3A | -7.68 | 113.48      | 127.87   |
| 12  | cB    | 824 | F6C  | CAA-C2A-C1A | -7.67 | 106.60      | 128.01   |
| 12  | aB    | 824 | F6C  | CAA-C2A-C1A | -7.66 | 106.61      | 128.01   |
| 12  | bB    | 824 | F6C  | CAA-C2A-C1A | -7.66 | 106.62      | 128.01   |
| 11  | cB    | 831 | CLA  | CAA-C2A-C3A | -7.61 | 92.42       | 113.00   |
| 11  | bB    | 831 | CLA  | CAA-C2A-C3A | -7.61 | 92.43       | 113.00   |
| 11  | aB    | 831 | CLA  | CAA-C2A-C3A | -7.58 | 92.51       | 113.00   |
| 12  | cL    | 202 | F6C  | C3A-C4A-NA  | 7.54  | 117.59      | 110.13   |
| 12  | bL    | 202 | F6C  | C3A-C4A-NA  | 7.51  | 117.55      | 110.13   |
| 12  | aL    | 202 | F6C  | C3A-C4A-NA  | 7.50  | 117.55      | 110.13   |
| 12  | cA    | 844 | F6C  | CMA-C3A-C2A | -7.38 | 106.18      | 126.15   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12  | bA    | 844 | F6C  | CMA-C3A-C2A | -7.38 | 106.19      | 126.15   |
| 12  | aA    | 844 | F6C  | CMA-C3A-C2A | -7.38 | 106.20      | 126.15   |
| 11  | bA    | 840 | CLA  | CAA-C2A-C3A | -7.32 | 93.22       | 113.00   |
| 11  | cA    | 840 | CLA  | CAA-C2A-C3A | -7.31 | 93.26       | 113.00   |
| 11  | aA    | 840 | CLA  | CAA-C2A-C3A | -7.30 | 93.28       | 113.00   |
| 10  | cA    | 801 | CL0  | CMA-C3A-C4A | -7.27 | 98.94       | 114.61   |
| 10  | aA    | 801 | CL0  | CMA-C3A-C4A | -7.26 | 98.96       | 114.61   |
| 10  | bA    | 801 | CL0  | CMA-C3A-C4A | -7.25 | 98.98       | 114.61   |
| 12  | aA    | 830 | F6C  | CMA-C3A-C2A | -7.16 | 106.79      | 126.15   |
| 12  | cA    | 830 | F6C  | CMA-C3A-C2A | -7.15 | 106.81      | 126.15   |
| 12  | bA    | 830 | F6C  | CMA-C3A-C2A | -7.15 | 106.82      | 126.15   |
| 11  | aA    | 803 | CLA  | C2D-C1D-ND  | 7.13  | 117.19      | 110.13   |
| 11  | bA    | 803 | CLA  | C2D-C1D-ND  | 7.13  | 117.18      | 110.13   |
| 11  | cA    | 803 | CLA  | C2D-C1D-ND  | 7.10  | 117.15      | 110.13   |
| 11  | cA    | 823 | CLA  | C2D-C1D-ND  | 7.03  | 117.08      | 110.13   |
| 11  | aA    | 823 | CLA  | C2D-C1D-ND  | 7.00  | 117.05      | 110.13   |
| 11  | bA    | 823 | CLA  | C2D-C1D-ND  | 7.00  | 117.05      | 110.13   |
| 12  | cB    | 824 | F6C  | CMA-C3A-C2A | -6.98 | 107.28      | 126.15   |
| 12  | cA    | 832 | F6C  | CMD-C2D-C1D | 6.97  | 135.92      | 125.03   |
| 12  | bA    | 832 | F6C  | CMD-C2D-C1D | 6.97  | 135.92      | 125.03   |
| 12  | aB    | 824 | F6C  | CMA-C3A-C2A | -6.96 | 107.31      | 126.15   |
| 12  | cL    | 202 | F6C  | CMD-C2D-C1D | 6.96  | 135.91      | 125.03   |
| 12  | bB    | 824 | F6C  | CMA-C3A-C2A | -6.96 | 107.33      | 126.15   |
| 12  | aA    | 832 | F6C  | CMD-C2D-C1D | 6.95  | 135.89      | 125.03   |
| 12  | aL    | 202 | F6C  | CMD-C2D-C1D | 6.95  | 135.89      | 125.03   |
| 12  | bL    | 202 | F6C  | CMD-C2D-C1D | 6.94  | 135.88      | 125.03   |
| 11  | aB    | 828 | CLA  | CMD-C2D-C1D | 6.92  | 136.91      | 124.73   |
| 11  | cB    | 828 | CLA  | CMD-C2D-C1D | 6.91  | 136.89      | 124.73   |
| 11  | bB    | 828 | CLA  | CMD-C2D-C1D | 6.89  | 136.87      | 124.73   |
| 10  | cA    | 801 | CL0  | C4D-ND-C1D  | -6.89 | 99.99       | 105.22   |
| 12  | aB    | 824 | F6C  | C3A-C4A-NA  | 6.87  | 116.93      | 110.13   |
| 12  | cB    | 824 | F6C  | C3A-C4A-NA  | 6.83  | 116.88      | 110.13   |
| 10  | aA    | 801 | CL0  | C4D-ND-C1D  | -6.83 | 100.04      | 105.22   |
| 10  | bA    | 801 | CL0  | C4D-ND-C1D  | -6.82 | 100.04      | 105.22   |
| 11  | cA    | 818 | CLA  | C2D-C1D-ND  | 6.82  | 116.88      | 110.13   |
| 12  | bA    | 844 | F6C  | C3A-C4A-NA  | 6.82  | 116.88      | 110.13   |
| 12  | cA    | 844 | F6C  | CMD-C2D-C1D | 6.82  | 135.69      | 125.03   |
| 12  | aA    | 830 | F6C  | C3A-C4A-NA  | 6.81  | 116.87      | 110.13   |
| 12  | cA    | 826 | F6C  | C3A-C4A-NA  | 6.81  | 116.86      | 110.13   |
| 12  | bB    | 824 | F6C  | C3A-C4A-NA  | 6.80  | 116.86      | 110.13   |
| 12  | aA    | 844 | F6C  | C3A-C4A-NA  | 6.80  | 116.86      | 110.13   |
| 12  | cA    | 844 | F6C  | C3A-C4A-NA  | 6.80  | 116.86      | 110.13   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12  | aA    | 844 | F6C  | CMD-C2D-C1D | 6.80  | 135.66      | 125.03   |
| 11  | aA    | 818 | CLA  | C2D-C1D-ND  | 6.79  | 116.85      | 110.13   |
| 12  | bA    | 844 | F6C  | CMD-C2D-C1D | 6.78  | 135.63      | 125.03   |
| 11  | bA    | 818 | CLA  | C2D-C1D-ND  | 6.78  | 116.83      | 110.13   |
| 12  | bA    | 826 | F6C  | C3A-C4A-NA  | 6.77  | 116.83      | 110.13   |
| 12  | cA    | 830 | F6C  | C3A-C4A-NA  | 6.77  | 116.83      | 110.13   |
| 12  | aA    | 826 | F6C  | C3A-C4A-NA  | 6.76  | 116.82      | 110.13   |
| 11  | aB    | 833 | CLA  | CMD-C2D-C1D | 6.75  | 136.61      | 124.73   |
| 11  | cB    | 833 | CLA  | CMD-C2D-C1D | 6.74  | 136.59      | 124.73   |
| 12  | bA    | 830 | F6C  | C3A-C4A-NA  | 6.73  | 116.79      | 110.13   |
| 11  | bB    | 833 | CLA  | CMD-C2D-C1D | 6.73  | 136.57      | 124.73   |
| 11  | bB    | 831 | CLA  | CMD-C2D-C1D | 6.72  | 136.56      | 124.73   |
| 11  | aB    | 803 | CLA  | C2D-C1D-ND  | 6.72  | 116.77      | 110.13   |
| 11  | aB    | 831 | CLA  | CMD-C2D-C1D | 6.71  | 136.54      | 124.73   |
| 11  | cB    | 831 | CLA  | CMD-C2D-C1D | 6.70  | 136.52      | 124.73   |
| 12  | aA    | 827 | F6C  | C3A-C4A-NA  | 6.69  | 116.75      | 110.13   |
| 12  | bA    | 827 | F6C  | C3A-C4A-NA  | 6.68  | 116.74      | 110.13   |
| 12  | cA    | 832 | F6C  | CMA-C3A-C2A | -6.68 | 108.09      | 126.15   |
| 11  | aA    | 828 | CLA  | CHD-C4C-C3C | -6.67 | 115.04      | 124.77   |
| 11  | cA    | 818 | CLA  | O2D-CGD-CBD | 6.67  | 122.89      | 111.23   |
| 11  | cA    | 828 | CLA  | CHD-C4C-C3C | -6.67 | 115.05      | 124.77   |
| 12  | aA    | 832 | F6C  | CMA-C3A-C2A | -6.66 | 108.12      | 126.15   |
| 11  | bA    | 818 | CLA  | O2D-CGD-CBD | 6.66  | 122.88      | 111.23   |
| 11  | bB    | 803 | CLA  | C2D-C1D-ND  | 6.66  | 116.72      | 110.13   |
| 11  | cB    | 803 | CLA  | C2D-C1D-ND  | 6.66  | 116.72      | 110.13   |
| 12  | bA    | 832 | F6C  | CMA-C3A-C2A | -6.66 | 108.15      | 126.15   |
| 11  | bA    | 828 | CLA  | CHD-C4C-C3C | -6.65 | 115.08      | 124.77   |
| 11  | aA    | 818 | CLA  | O2D-CGD-CBD | 6.64  | 122.84      | 111.23   |
| 12  | aB    | 824 | F6C  | CMD-C2D-C1D | 6.64  | 135.41      | 125.03   |
| 12  | bB    | 824 | F6C  | CMD-C2D-C1D | 6.64  | 135.41      | 125.03   |
| 12  | cB    | 824 | F6C  | CMD-C2D-C1D | 6.64  | 135.41      | 125.03   |
| 11  | aA    | 824 | CLA  | CMD-C2D-C1D | 6.62  | 136.39      | 124.73   |
| 12  | cA    | 832 | F6C  | C3A-C4A-NA  | 6.62  | 116.68      | 110.13   |
| 11  | bB    | 806 | CLA  | CMD-C2D-C1D | 6.62  | 136.38      | 124.73   |
| 11  | bA    | 828 | CLA  | C2D-C1D-ND  | 6.62  | 116.68      | 110.13   |
| 11  | cA    | 824 | CLA  | CMD-C2D-C1D | 6.61  | 136.38      | 124.73   |
| 12  | bB    | 824 | F6C  | C2B-C3B-C4B | -6.61 | 103.05      | 106.46   |
| 12  | aA    | 832 | F6C  | C3A-C4A-NA  | 6.61  | 116.67      | 110.13   |
| 12  | cB    | 824 | F6C  | C2B-C3B-C4B | -6.61 | 103.05      | 106.46   |
| 12  | aA    | 827 | F6C  | CMD-C2D-C1D | 6.60  | 135.35      | 125.03   |
| 12  | bA    | 832 | F6C  | C3A-C4A-NA  | 6.60  | 116.66      | 110.13   |
| 11  | bA    | 824 | CLA  | CMD-C2D-C1D | 6.60  | 136.35      | 124.73   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cA    | 807 | CLA  | CMD-C2D-C1D | 6.60  | 136.35      | 124.73   |
| 12  | bA    | 826 | F6C  | CMD-C2D-C1D | 6.60  | 135.34      | 125.03   |
| 12  | bA    | 827 | F6C  | CMD-C2D-C1D | 6.60  | 135.34      | 125.03   |
| 12  | cA    | 827 | F6C  | C3A-C4A-NA  | 6.59  | 116.65      | 110.13   |
| 12  | aA    | 826 | F6C  | CMD-C2D-C1D | 6.59  | 135.34      | 125.03   |
| 12  | cA    | 826 | F6C  | CMD-C2D-C1D | 6.59  | 135.34      | 125.03   |
| 11  | aB    | 806 | CLA  | CMD-C2D-C1D | 6.59  | 136.33      | 124.73   |
| 12  | cA    | 827 | F6C  | CMD-C2D-C1D | 6.59  | 135.33      | 125.03   |
| 11  | cB    | 806 | CLA  | CMD-C2D-C1D | 6.59  | 136.33      | 124.73   |
| 11  | cA    | 828 | CLA  | C2D-C1D-ND  | 6.59  | 116.64      | 110.13   |
| 11  | bA    | 807 | CLA  | CMD-C2D-C1D | 6.58  | 136.32      | 124.73   |
| 11  | aA    | 807 | CLA  | CMD-C2D-C1D | 6.56  | 136.28      | 124.73   |
| 11  | aA    | 838 | CLA  | CMD-C2D-C1D | 6.56  | 136.28      | 124.73   |
| 12  | aB    | 824 | F6C  | C2B-C3B-C4B | -6.56 | 103.08      | 106.46   |
| 11  | aB    | 822 | CLA  | C2D-C1D-ND  | 6.56  | 116.61      | 110.13   |
| 11  | cA    | 838 | CLA  | CMD-C2D-C1D | 6.55  | 136.27      | 124.73   |
| 11  | cB    | 822 | CLA  | CMD-C2D-C1D | 6.55  | 136.27      | 124.73   |
| 11  | aB    | 822 | CLA  | CMD-C2D-C1D | 6.55  | 136.26      | 124.73   |
| 11  | bA    | 838 | CLA  | CMD-C2D-C1D | 6.55  | 136.26      | 124.73   |
| 11  | bB    | 822 | CLA  | C2D-C1D-ND  | 6.55  | 116.61      | 110.13   |
| 11  | aA    | 828 | CLA  | C2D-C1D-ND  | 6.54  | 116.60      | 110.13   |
| 11  | bB    | 822 | CLA  | CMD-C2D-C1D | 6.53  | 136.23      | 124.73   |
| 11  | cB    | 822 | CLA  | C2D-C1D-ND  | 6.52  | 116.58      | 110.13   |
| 11  | bA    | 828 | CLA  | CMD-C2D-C1D | 6.52  | 136.22      | 124.73   |
| 11  | aA    | 818 | CLA  | CHD-C4C-C3C | -6.50 | 115.30      | 124.77   |
| 11  | cA    | 828 | CLA  | CMD-C2D-C1D | 6.49  | 136.16      | 124.73   |
| 11  | bB    | 822 | CLA  | CHD-C4C-C3C | -6.49 | 115.31      | 124.77   |
| 11  | aB    | 834 | CLA  | CMD-C2D-C1D | 6.48  | 136.14      | 124.73   |
| 11  | cB    | 810 | CLA  | CMD-C2D-C1D | 6.48  | 136.14      | 124.73   |
| 10  | aA    | 801 | CL0  | O2D-CGD-CBD | 6.48  | 118.07      | 110.95   |
| 11  | aB    | 822 | CLA  | CHD-C4C-C3C | -6.48 | 115.33      | 124.77   |
| 11  | bA    | 808 | CLA  | CMD-C2D-C1D | 6.47  | 136.13      | 124.73   |
| 11  | bA    | 814 | CLA  | CMD-C2D-C1D | 6.47  | 136.13      | 124.73   |
| 11  | cB    | 825 | CLA  | CMD-C2D-C1D | 6.47  | 136.13      | 124.73   |
| 11  | cB    | 834 | CLA  | CMD-C2D-C1D | 6.47  | 136.13      | 124.73   |
| 10  | bA    | 801 | CL0  | O2D-CGD-CBD | 6.47  | 118.06      | 110.95   |
| 11  | cB    | 822 | CLA  | CHD-C4C-C3C | -6.47 | 115.34      | 124.77   |
| 11  | bA    | 818 | CLA  | CHD-C4C-C3C | -6.47 | 115.34      | 124.77   |
| 11  | aA    | 808 | CLA  | CMD-C2D-C1D | 6.47  | 136.12      | 124.73   |
| 11  | bB    | 810 | CLA  | CMD-C2D-C1D | 6.47  | 136.12      | 124.73   |
| 11  | bB    | 834 | CLA  | CMD-C2D-C1D | 6.47  | 136.12      | 124.73   |
| 11  | aA    | 814 | CLA  | CMD-C2D-C1D | 6.46  | 136.11      | 124.73   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bB    | 826 | CLA  | C2D-C1D-ND  | 6.46  | 116.52      | 110.13   |
| 11  | aA    | 828 | CLA  | CMD-C2D-C1D | 6.46  | 136.10      | 124.73   |
| 11  | aB    | 825 | CLA  | CMD-C2D-C1D | 6.46  | 136.10      | 124.73   |
| 11  | cB    | 826 | CLA  | C2D-C1D-ND  | 6.46  | 116.52      | 110.13   |
| 11  | bB    | 825 | CLA  | CMD-C2D-C1D | 6.45  | 136.09      | 124.73   |
| 10  | cA    | 801 | CL0  | O2D-CGD-CBD | 6.45  | 118.04      | 110.95   |
| 11  | aB    | 817 | CLA  | CMD-C2D-C1D | 6.45  | 136.09      | 124.73   |
| 11  | cA    | 814 | CLA  | CMD-C2D-C1D | 6.45  | 136.09      | 124.73   |
| 11  | aB    | 810 | CLA  | CMD-C2D-C1D | 6.45  | 136.09      | 124.73   |
| 11  | cA    | 808 | CLA  | CMD-C2D-C1D | 6.45  | 136.09      | 124.73   |
| 11  | aB    | 801 | CLA  | CHD-C4C-C3C | -6.44 | 115.38      | 124.77   |
| 11  | bA    | 841 | CLA  | C2D-C1D-ND  | 6.44  | 116.50      | 110.13   |
| 11  | aA    | 809 | CLA  | CMD-C2D-C1D | 6.44  | 136.07      | 124.73   |
| 11  | bA    | 829 | CLA  | CMD-C2D-C1D | 6.44  | 136.07      | 124.73   |
| 11  | cA    | 804 | CLA  | CMD-C2D-C1D | 6.44  | 136.07      | 124.73   |
| 11  | cB    | 801 | CLA  | CHD-C4C-C3C | -6.44 | 115.39      | 124.77   |
| 11  | aA    | 819 | CLA  | CMD-C2D-C1D | 6.44  | 136.06      | 124.73   |
| 11  | bA    | 804 | CLA  | CMD-C2D-C1D | 6.44  | 136.06      | 124.73   |
| 11  | cA    | 829 | CLA  | CMD-C2D-C1D | 6.44  | 136.06      | 124.73   |
| 11  | aA    | 829 | CLA  | CMD-C2D-C1D | 6.44  | 136.06      | 124.73   |
| 11  | bA    | 819 | CLA  | CMD-C2D-C1D | 6.44  | 136.06      | 124.73   |
| 11  | cA    | 818 | CLA  | CHD-C4C-C3C | -6.43 | 115.39      | 124.77   |
| 11  | aB    | 816 | CLA  | CMD-C2D-C1D | 6.43  | 136.05      | 124.73   |
| 11  | aA    | 841 | CLA  | C2D-C1D-ND  | 6.43  | 116.49      | 110.13   |
| 11  | cB    | 817 | CLA  | CMD-C2D-C1D | 6.43  | 136.05      | 124.73   |
| 11  | cB    | 816 | CLA  | CMD-C2D-C1D | 6.43  | 136.05      | 124.73   |
| 11  | bB    | 801 | CLA  | CHD-C4C-C3C | -6.43 | 115.40      | 124.77   |
| 11  | cA    | 809 | CLA  | CMD-C2D-C1D | 6.43  | 136.04      | 124.73   |
| 11  | bB    | 816 | CLA  | CMD-C2D-C1D | 6.42  | 136.04      | 124.73   |
| 11  | aB    | 820 | CLA  | C2D-C1D-ND  | 6.42  | 116.48      | 110.13   |
| 11  | aB    | 835 | CLA  | CMD-C2D-C1D | 6.42  | 136.03      | 124.73   |
| 11  | bB    | 832 | CLA  | CMD-C2D-C1D | 6.42  | 136.03      | 124.73   |
| 11  | cB    | 835 | CLA  | CMD-C2D-C1D | 6.42  | 136.03      | 124.73   |
| 11  | bA    | 809 | CLA  | CMD-C2D-C1D | 6.42  | 136.03      | 124.73   |
| 11  | bB    | 835 | CLA  | CMD-C2D-C1D | 6.42  | 136.03      | 124.73   |
| 11  | cB    | 829 | CLA  | CMD-C2D-C1D | 6.42  | 136.03      | 124.73   |
| 11  | bB    | 817 | CLA  | CMD-C2D-C1D | 6.41  | 136.03      | 124.73   |
| 11  | cA    | 819 | CLA  | CMD-C2D-C1D | 6.41  | 136.03      | 124.73   |
| 11  | bB    | 829 | CLA  | CMD-C2D-C1D | 6.41  | 136.02      | 124.73   |
| 11  | aA    | 804 | CLA  | CMD-C2D-C1D | 6.41  | 136.02      | 124.73   |
| 11  | bB    | 815 | CLA  | CMD-C2D-C1D | 6.41  | 136.02      | 124.73   |
| 11  | bA    | 819 | CLA  | CHD-C4C-C3C | -6.41 | 115.43      | 124.77   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cA    | 819 | CLA  | CHD-C4C-C3C | -6.41 | 115.43      | 124.77   |
| 11  | cA    | 841 | CLA  | C2D-C1D-ND  | 6.41  | 116.47      | 110.13   |
| 11  | aB    | 826 | CLA  | C2D-C1D-ND  | 6.41  | 116.47      | 110.13   |
| 11  | bA    | 820 | CLA  | CMD-C2D-C1D | 6.41  | 136.01      | 124.73   |
| 11  | bK    | 103 | CLA  | CMD-C2D-C1D | 6.41  | 136.01      | 124.73   |
| 11  | bB    | 840 | CLA  | CMD-C2D-C1D | 6.40  | 136.00      | 124.73   |
| 11  | cB    | 840 | CLA  | CMD-C2D-C1D | 6.40  | 136.00      | 124.73   |
| 11  | aB    | 829 | CLA  | CMD-C2D-C1D | 6.40  | 136.00      | 124.73   |
| 11  | cA    | 837 | CLA  | CMD-C2D-C1D | 6.40  | 135.99      | 124.73   |
| 11  | aA    | 834 | CLA  | CMD-C2D-C1D | 6.40  | 135.99      | 124.73   |
| 11  | aB    | 840 | CLA  | CMD-C2D-C1D | 6.40  | 135.99      | 124.73   |
| 11  | cA    | 812 | CLA  | CMD-C2D-C1D | 6.40  | 135.99      | 124.73   |
| 11  | cB    | 832 | CLA  | CMD-C2D-C1D | 6.39  | 135.99      | 124.73   |
| 11  | aK    | 103 | CLA  | CMD-C2D-C1D | 6.39  | 135.99      | 124.73   |
| 11  | bA    | 812 | CLA  | CMD-C2D-C1D | 6.39  | 135.99      | 124.73   |
| 11  | aB    | 832 | CLA  | CMD-C2D-C1D | 6.39  | 135.98      | 124.73   |
| 11  | bA    | 834 | CLA  | CMD-C2D-C1D | 6.39  | 135.98      | 124.73   |
| 11  | cA    | 811 | CLA  | CMD-C2D-C1D | 6.39  | 135.98      | 124.73   |
| 11  | bA    | 837 | CLA  | CMD-C2D-C1D | 6.39  | 135.98      | 124.73   |
| 11  | bA    | 811 | CLA  | CMD-C2D-C1D | 6.39  | 135.98      | 124.73   |
| 11  | aA    | 820 | CLA  | CMD-C2D-C1D | 6.39  | 135.98      | 124.73   |
| 11  | cK    | 103 | CLA  | CMD-C2D-C1D | 6.39  | 135.97      | 124.73   |
| 11  | cA    | 820 | CLA  | CMD-C2D-C1D | 6.39  | 135.97      | 124.73   |
| 11  | aA    | 819 | CLA  | CHD-C4C-C3C | -6.39 | 115.46      | 124.77   |
| 11  | aB    | 815 | CLA  | CMD-C2D-C1D | 6.38  | 135.97      | 124.73   |
| 11  | cB    | 820 | CLA  | C2D-C1D-ND  | 6.38  | 116.44      | 110.13   |
| 11  | aA    | 842 | CLA  | CMD-C2D-C1D | 6.38  | 135.96      | 124.73   |
| 11  | bB    | 820 | CLA  | C2D-C1D-ND  | 6.38  | 116.44      | 110.13   |
| 11  | aB    | 812 | CLA  | CMD-C2D-C1D | 6.38  | 135.96      | 124.73   |
| 11  | cB    | 839 | CLA  | CMD-C2D-C1D | 6.38  | 135.96      | 124.73   |
| 11  | cB    | 815 | CLA  | CMD-C2D-C1D | 6.38  | 135.96      | 124.73   |
| 11  | bB    | 839 | CLA  | CMD-C2D-C1D | 6.37  | 135.95      | 124.73   |
| 11  | aB    | 804 | CLA  | CMD-C2D-C1D | 6.37  | 135.95      | 124.73   |
| 11  | cK    | 101 | CLA  | CMD-C2D-C1D | 6.37  | 135.95      | 124.73   |
| 11  | aA    | 812 | CLA  | CMD-C2D-C1D | 6.37  | 135.95      | 124.73   |
| 11  | aB    | 839 | CLA  | CMD-C2D-C1D | 6.37  | 135.94      | 124.73   |
| 11  | cA    | 834 | CLA  | CMD-C2D-C1D | 6.37  | 135.94      | 124.73   |
| 11  | bB    | 804 | CLA  | CMD-C2D-C1D | 6.37  | 135.94      | 124.73   |
| 11  | cB    | 825 | CLA  | C2D-C1D-ND  | 6.37  | 116.43      | 110.13   |
| 11  | aK    | 101 | CLA  | CMD-C2D-C1D | 6.36  | 135.93      | 124.73   |
| 11  | cA    | 840 | CLA  | CMD-C2D-C1D | 6.36  | 135.93      | 124.73   |
| 11  | aA    | 811 | CLA  | CMD-C2D-C1D | 6.36  | 135.92      | 124.73   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bA    | 806 | CLA  | CMD-C2D-C1D | 6.35  | 135.92      | 124.73   |
| 11  | cA    | 842 | CLA  | CMD-C2D-C1D | 6.35  | 135.92      | 124.73   |
| 11  | cB    | 804 | CLA  | CMD-C2D-C1D | 6.35  | 135.91      | 124.73   |
| 11  | aA    | 837 | CLA  | CMD-C2D-C1D | 6.35  | 135.91      | 124.73   |
| 11  | bA    | 842 | CLA  | CMD-C2D-C1D | 6.35  | 135.91      | 124.73   |
| 11  | cB    | 804 | CLA  | CHD-C4C-C3C | -6.35 | 115.51      | 124.77   |
| 11  | bK    | 101 | CLA  | CMD-C2D-C1D | 6.35  | 135.91      | 124.73   |
| 11  | cB    | 802 | CLA  | O2D-CGD-CBD | 6.35  | 122.33      | 111.23   |
| 11  | aA    | 840 | CLA  | CMD-C2D-C1D | 6.34  | 135.89      | 124.73   |
| 11  | cB    | 812 | CLA  | CMD-C2D-C1D | 6.34  | 135.89      | 124.73   |
| 11  | bB    | 804 | CLA  | CHD-C4C-C3C | -6.33 | 115.54      | 124.77   |
| 11  | aB    | 820 | CLA  | CMD-C2D-C1D | 6.33  | 135.88      | 124.73   |
| 11  | aA    | 806 | CLA  | CMD-C2D-C1D | 6.33  | 135.88      | 124.73   |
| 11  | bA    | 840 | CLA  | CMD-C2D-C1D | 6.33  | 135.88      | 124.73   |
| 11  | cA    | 806 | CLA  | CMD-C2D-C1D | 6.33  | 135.87      | 124.73   |
| 11  | bB    | 820 | CLA  | CMD-C2D-C1D | 6.33  | 135.87      | 124.73   |
| 11  | aB    | 802 | CLA  | O2D-CGD-CBD | 6.33  | 122.29      | 111.23   |
| 11  | bB    | 802 | CLA  | O2D-CGD-CBD | 6.33  | 122.29      | 111.23   |
| 11  | cB    | 820 | CLA  | CMD-C2D-C1D | 6.33  | 135.87      | 124.73   |
| 11  | aB    | 804 | CLA  | CHD-C4C-C3C | -6.32 | 115.56      | 124.77   |
| 11  | bB    | 812 | CLA  | CMD-C2D-C1D | 6.32  | 135.85      | 124.73   |
| 11  | bB    | 825 | CLA  | C2D-C1D-ND  | 6.31  | 116.37      | 110.13   |
| 11  | bB    | 839 | CLA  | CHD-C4C-C3C | -6.31 | 115.57      | 124.77   |
| 11  | aB    | 825 | CLA  | C2D-C1D-ND  | 6.31  | 116.37      | 110.13   |
| 12  | cA    | 844 | F6C  | C2B-C3B-C4B | -6.31 | 103.20      | 106.46   |
| 11  | aA    | 833 | CLA  | CMD-C2D-C1D | 6.30  | 135.81      | 124.73   |
| 11  | cA    | 833 | CLA  | CMD-C2D-C1D | 6.29  | 135.81      | 124.73   |
| 11  | aB    | 839 | CLA  | CHD-C4C-C3C | -6.29 | 115.61      | 124.77   |
| 11  | bA    | 833 | CLA  | CMD-C2D-C1D | 6.29  | 135.80      | 124.73   |
| 11  | aB    | 830 | CLA  | CMD-C2D-C1D | 6.28  | 135.80      | 124.73   |
| 11  | cA    | 823 | CLA  | CHD-C4C-C3C | -6.28 | 115.62      | 124.77   |
| 11  | bB    | 830 | CLA  | CMD-C2D-C1D | 6.28  | 135.79      | 124.73   |
| 11  | cB    | 815 | CLA  | CHD-C4C-C3C | -6.28 | 115.62      | 124.77   |
| 12  | bA    | 844 | F6C  | C2B-C3B-C4B | -6.28 | 103.22      | 106.46   |
| 11  | cB    | 839 | CLA  | CHD-C4C-C3C | -6.28 | 115.62      | 124.77   |
| 11  | bB    | 815 | CLA  | CHD-C4C-C3C | -6.28 | 115.62      | 124.77   |
| 12  | aA    | 844 | F6C  | C2B-C3B-C4B | -6.27 | 103.22      | 106.46   |
| 11  | aA    | 823 | CLA  | CHD-C4C-C3C | -6.27 | 115.63      | 124.77   |
| 11  | bA    | 823 | CLA  | CHD-C4C-C3C | -6.27 | 115.64      | 124.77   |
| 11  | aB    | 815 | CLA  | CHD-C4C-C3C | -6.26 | 115.64      | 124.77   |
| 12  | cA    | 826 | F6C  | O2D-CGD-CBD | 6.26  | 122.18      | 111.23   |
| 11  | aA    | 817 | CLA  | CMD-C2D-C1D | 6.26  | 135.75      | 124.73   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12  | bA    | 826 | F6C  | O2D-CGD-CBD | 6.26  | 122.17      | 111.23   |
| 11  | bB    | 821 | CLA  | CMD-C2D-C1D | 6.26  | 135.75      | 124.73   |
| 11  | cB    | 830 | CLA  | CMD-C2D-C1D | 6.26  | 135.75      | 124.73   |
| 12  | aA    | 826 | F6C  | O2D-CGD-CBD | 6.25  | 122.16      | 111.23   |
| 11  | bA    | 825 | CLA  | CMD-C2D-C1D | 6.25  | 135.74      | 124.73   |
| 11  | cA    | 817 | CLA  | CMD-C2D-C1D | 6.25  | 135.74      | 124.73   |
| 11  | bA    | 817 | CLA  | CMD-C2D-C1D | 6.25  | 135.73      | 124.73   |
| 11  | cB    | 837 | CLA  | CMD-C2D-C1D | 6.25  | 135.73      | 124.73   |
| 11  | aB    | 821 | CLA  | CMD-C2D-C1D | 6.23  | 135.70      | 124.73   |
| 11  | aA    | 825 | CLA  | CMD-C2D-C1D | 6.23  | 135.70      | 124.73   |
| 11  | cA    | 825 | CLA  | CMD-C2D-C1D | 6.23  | 135.69      | 124.73   |
| 11  | bB    | 837 | CLA  | CMD-C2D-C1D | 6.23  | 135.69      | 124.73   |
| 11  | aA    | 839 | CLA  | CMD-C2D-C1D | 6.22  | 135.68      | 124.73   |
| 11  | bB    | 826 | CLA  | CHD-C4C-C3C | -6.22 | 115.71      | 124.77   |
| 11  | bA    | 839 | CLA  | CMD-C2D-C1D | 6.22  | 135.67      | 124.73   |
| 11  | bB    | 806 | CLA  | CHD-C4C-C3C | -6.21 | 115.71      | 124.77   |
| 11  | bL    | 204 | CLA  | C2D-C1D-ND  | 6.21  | 116.28      | 110.13   |
| 11  | aB    | 837 | CLA  | CMD-C2D-C1D | 6.21  | 135.67      | 124.73   |
| 11  | aB    | 804 | CLA  | C2D-C1D-ND  | 6.21  | 116.27      | 110.13   |
| 12  | bA    | 827 | F6C  | CMA-C3A-C2A | -6.21 | 109.35      | 126.15   |
| 11  | cK    | 103 | CLA  | C2D-C1D-ND  | 6.21  | 116.27      | 110.13   |
| 11  | cA    | 839 | CLA  | CMD-C2D-C1D | 6.21  | 135.66      | 124.73   |
| 12  | aA    | 827 | F6C  | CMA-C3A-C2A | -6.20 | 109.37      | 126.15   |
| 12  | cA    | 827 | F6C  | CMA-C3A-C2A | -6.20 | 109.38      | 126.15   |
| 11  | cB    | 821 | CLA  | CMD-C2D-C1D | 6.20  | 135.65      | 124.73   |
| 11  | cB    | 806 | CLA  | CHD-C4C-C3C | -6.20 | 115.73      | 124.77   |
| 11  | cB    | 838 | CLA  | C2D-C1D-ND  | 6.19  | 116.26      | 110.13   |
| 11  | cB    | 826 | CLA  | CHD-C4C-C3C | -6.19 | 115.74      | 124.77   |
| 11  | aB    | 806 | CLA  | CHD-C4C-C3C | -6.19 | 115.75      | 124.77   |
| 11  | aB    | 826 | CLA  | CHD-C4C-C3C | -6.19 | 115.75      | 124.77   |
| 12  | cA    | 832 | F6C  | CAA-C2A-C1A | -6.19 | 110.72      | 128.01   |
| 11  | bK    | 103 | CLA  | C2D-C1D-ND  | 6.19  | 116.25      | 110.13   |
| 11  | aB    | 838 | CLA  | C2D-C1D-ND  | 6.18  | 116.24      | 110.13   |
| 11  | bA    | 815 | CLA  | CMD-C2D-C1D | 6.18  | 135.61      | 124.73   |
| 11  | bA    | 808 | CLA  | C2D-C1D-ND  | 6.18  | 116.24      | 110.13   |
| 11  | bB    | 838 | CLA  | C2D-C1D-ND  | 6.18  | 116.24      | 110.13   |
| 12  | aA    | 832 | F6C  | CAA-C2A-C1A | -6.17 | 110.76      | 128.01   |
| 11  | cB    | 818 | CLA  | C2D-C1D-ND  | 6.17  | 116.24      | 110.13   |
| 11  | aB    | 818 | CLA  | C2D-C1D-ND  | 6.17  | 116.23      | 110.13   |
| 11  | cL    | 204 | CLA  | C2D-C1D-ND  | 6.17  | 116.23      | 110.13   |
| 11  | bB    | 801 | CLA  | C2D-C1D-ND  | 6.17  | 116.23      | 110.13   |
| 11  | aA    | 835 | CLA  | CMD-C2D-C1D | 6.17  | 135.59      | 124.73   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12  | bA    | 832 | F6C  | CAA-C2A-C1A | -6.17 | 110.78      | 128.01   |
| 11  | cA    | 815 | CLA  | CMD-C2D-C1D | 6.17  | 135.59      | 124.73   |
| 11  | bA    | 819 | CLA  | C2D-C1D-ND  | 6.17  | 116.23      | 110.13   |
| 11  | cB    | 801 | CLA  | C2D-C1D-ND  | 6.17  | 116.23      | 110.13   |
| 11  | bB    | 818 | CLA  | C2D-C1D-ND  | 6.16  | 116.23      | 110.13   |
| 11  | aA    | 815 | CLA  | CMD-C2D-C1D | 6.16  | 135.58      | 124.73   |
| 11  | aA    | 808 | CLA  | C2D-C1D-ND  | 6.16  | 116.23      | 110.13   |
| 11  | aA    | 819 | CLA  | C2D-C1D-ND  | 6.16  | 116.22      | 110.13   |
| 11  | cA    | 823 | CLA  | O2D-CGD-CBD | 6.16  | 121.99      | 111.23   |
| 11  | aB    | 801 | CLA  | C2D-C1D-ND  | 6.15  | 116.22      | 110.13   |
| 11  | cA    | 808 | CLA  | C2D-C1D-ND  | 6.15  | 116.21      | 110.13   |
| 11  | cA    | 835 | CLA  | CMD-C2D-C1D | 6.15  | 135.56      | 124.73   |
| 11  | cL    | 205 | CLA  | C2D-C1D-ND  | 6.15  | 116.21      | 110.13   |
| 11  | bB    | 804 | CLA  | C2D-C1D-ND  | 6.15  | 116.21      | 110.13   |
| 11  | cA    | 819 | CLA  | C2D-C1D-ND  | 6.15  | 116.21      | 110.13   |
| 11  | aL    | 204 | CLA  | C2D-C1D-ND  | 6.14  | 116.21      | 110.13   |
| 11  | cB    | 805 | CLA  | CMD-C2D-C1D | 6.14  | 135.54      | 124.73   |
| 11  | bB    | 805 | CLA  | CMD-C2D-C1D | 6.14  | 135.54      | 124.73   |
| 11  | bA    | 835 | CLA  | CMD-C2D-C1D | 6.14  | 135.54      | 124.73   |
| 11  | bA    | 823 | CLA  | O2D-CGD-CBD | 6.14  | 121.96      | 111.23   |
| 11  | bL    | 205 | CLA  | C2D-C1D-ND  | 6.14  | 116.20      | 110.13   |
| 11  | aK    | 103 | CLA  | C2D-C1D-ND  | 6.13  | 116.20      | 110.13   |
| 11  | aA    | 842 | CLA  | C2D-C1D-ND  | 6.13  | 116.20      | 110.13   |
| 11  | cA    | 805 | CLA  | CMD-C2D-C1D | 6.13  | 135.52      | 124.73   |
| 11  | cL    | 206 | CLA  | C2D-C1D-ND  | 6.13  | 116.19      | 110.13   |
| 11  | cB    | 838 | CLA  | CMD-C2D-C1D | 6.13  | 135.52      | 124.73   |
| 11  | aB    | 829 | CLA  | C2C-C1C-NC  | 6.12  | 116.41      | 109.98   |
| 11  | aB    | 805 | CLA  | CMD-C2D-C1D | 6.12  | 135.51      | 124.73   |
| 11  | aA    | 823 | CLA  | O2D-CGD-CBD | 6.12  | 121.93      | 111.23   |
| 11  | cB    | 804 | CLA  | C2D-C1D-ND  | 6.12  | 116.19      | 110.13   |
| 11  | aA    | 805 | CLA  | CMD-C2D-C1D | 6.12  | 135.51      | 124.73   |
| 11  | bB    | 815 | CLA  | C2D-C1D-ND  | 6.12  | 116.18      | 110.13   |
| 11  | bB    | 838 | CLA  | CMD-C2D-C1D | 6.12  | 135.50      | 124.73   |
| 11  | bA    | 842 | CLA  | C2D-C1D-ND  | 6.12  | 116.18      | 110.13   |
| 11  | cA    | 842 | CLA  | C2D-C1D-ND  | 6.12  | 116.18      | 110.13   |
| 11  | cA    | 840 | CLA  | C2D-C1D-ND  | 6.12  | 116.18      | 110.13   |
| 11  | bA    | 805 | CLA  | CMD-C2D-C1D | 6.12  | 135.50      | 124.73   |
| 11  | cB    | 811 | CLA  | CMD-C2D-C1D | 6.12  | 135.50      | 124.73   |
| 11  | aB    | 838 | CLA  | CMD-C2D-C1D | 6.12  | 135.50      | 124.73   |
| 11  | bB    | 811 | CLA  | CMD-C2D-C1D | 6.12  | 135.50      | 124.73   |
| 11  | cB    | 829 | CLA  | C2C-C1C-NC  | 6.11  | 116.40      | 109.98   |
| 11  | bB    | 823 | CLA  | CHD-C4C-C3C | -6.11 | 115.86      | 124.77   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aL    | 205 | CLA  | C2D-C1D-ND  | 6.11  | 116.18      | 110.13   |
| 11  | aB    | 806 | CLA  | C2D-C1D-ND  | 6.11  | 116.17      | 110.13   |
| 11  | cB    | 823 | CLA  | CHD-C4C-C3C | -6.11 | 115.87      | 124.77   |
| 11  | aB    | 823 | CLA  | CHD-C4C-C3C | -6.10 | 115.88      | 124.77   |
| 11  | cA    | 816 | CLA  | CMD-C2D-C1D | 6.10  | 135.47      | 124.73   |
| 11  | aB    | 815 | CLA  | C2D-C1D-ND  | 6.10  | 116.16      | 110.13   |
| 11  | cB    | 815 | CLA  | C2D-C1D-ND  | 6.10  | 116.16      | 110.13   |
| 11  | cB    | 836 | CLA  | CMD-C2D-C1D | 6.10  | 135.46      | 124.73   |
| 11  | aA    | 813 | CLA  | CMD-C2D-C1D | 6.10  | 135.46      | 124.73   |
| 11  | aL    | 206 | CLA  | C2D-C1D-ND  | 6.09  | 116.16      | 110.13   |
| 11  | cA    | 843 | CLA  | CMD-C2D-C1D | 6.09  | 135.46      | 124.73   |
| 11  | bL    | 206 | CLA  | C2D-C1D-ND  | 6.09  | 116.16      | 110.13   |
| 11  | aB    | 836 | CLA  | CMD-C2D-C1D | 6.09  | 135.45      | 124.73   |
| 11  | aA    | 816 | CLA  | CMD-C2D-C1D | 6.09  | 135.45      | 124.73   |
| 11  | bA    | 813 | CLA  | CMD-C2D-C1D | 6.09  | 135.45      | 124.73   |
| 11  | bB    | 806 | CLA  | C2D-C1D-ND  | 6.08  | 116.15      | 110.13   |
| 11  | bA    | 837 | CLA  | CHD-C4C-C3C | -6.08 | 115.90      | 124.77   |
| 11  | cA    | 813 | CLA  | CMD-C2D-C1D | 6.08  | 135.44      | 124.73   |
| 11  | bA    | 840 | CLA  | C2D-C1D-ND  | 6.08  | 116.15      | 110.13   |
| 11  | cB    | 813 | CLA  | CMD-C2D-C1D | 6.08  | 135.44      | 124.73   |
| 11  | cB    | 801 | CLA  | CMD-C2D-C1D | 6.08  | 135.44      | 124.73   |
| 11  | aB    | 811 | CLA  | CMD-C2D-C1D | 6.08  | 135.43      | 124.73   |
| 11  | cA    | 837 | CLA  | CHD-C4C-C3C | -6.08 | 115.91      | 124.77   |
| 11  | aA    | 843 | CLA  | CMD-C2D-C1D | 6.08  | 135.43      | 124.73   |
| 11  | bA    | 816 | CLA  | CMD-C2D-C1D | 6.08  | 135.43      | 124.73   |
| 11  | aA    | 840 | CLA  | C2D-C1D-ND  | 6.08  | 116.14      | 110.13   |
| 11  | aB    | 808 | CLA  | CHD-C4C-C3C | -6.08 | 115.91      | 124.77   |
| 11  | bB    | 808 | CLA  | CHD-C4C-C3C | -6.07 | 115.92      | 124.77   |
| 11  | bA    | 807 | CLA  | C2D-C1D-ND  | 6.07  | 116.14      | 110.13   |
| 11  | cB    | 808 | CLA  | CHD-C4C-C3C | -6.07 | 115.92      | 124.77   |
| 11  | bB    | 829 | CLA  | C2C-C1C-NC  | 6.07  | 116.36      | 109.98   |
| 11  | bB    | 801 | CLA  | CMD-C2D-C1D | 6.07  | 135.41      | 124.73   |
| 11  | aL    | 204 | CLA  | O2D-CGD-CBD | 6.07  | 121.84      | 111.23   |
| 11  | aA    | 836 | CLA  | C2D-C1D-ND  | 6.06  | 116.13      | 110.13   |
| 11  | aB    | 807 | CLA  | C2D-C1D-ND  | 6.06  | 116.12      | 110.13   |
| 11  | bB    | 836 | CLA  | CMD-C2D-C1D | 6.06  | 135.40      | 124.73   |
| 11  | aB    | 801 | CLA  | CMD-C2D-C1D | 6.05  | 135.39      | 124.73   |
| 11  | cA    | 807 | CLA  | C2D-C1D-ND  | 6.05  | 116.12      | 110.13   |
| 11  | bA    | 843 | CLA  | CMD-C2D-C1D | 6.05  | 135.38      | 124.73   |
| 11  | aB    | 836 | CLA  | C2D-C1D-ND  | 6.05  | 116.11      | 110.13   |
| 11  | bL    | 204 | CLA  | O2D-CGD-CBD | 6.05  | 121.80      | 111.23   |
| 11  | aB    | 813 | CLA  | CMD-C2D-C1D | 6.04  | 135.37      | 124.73   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bB    | 814 | CLA  | CMD-C2D-C1D | 6.04  | 135.36      | 124.73   |
| 11  | cL    | 204 | CLA  | O2D-CGD-CBD | 6.04  | 121.79      | 111.23   |
| 11  | bA    | 831 | CLA  | C2D-C1D-ND  | 6.04  | 116.10      | 110.13   |
| 11  | bB    | 807 | CLA  | C2D-C1D-ND  | 6.04  | 116.10      | 110.13   |
| 11  | cB    | 806 | CLA  | C2D-C1D-ND  | 6.04  | 116.10      | 110.13   |
| 11  | cA    | 836 | CLA  | C2D-C1D-ND  | 6.03  | 116.10      | 110.13   |
| 11  | cA    | 836 | CLA  | CHD-C4C-C3C | -6.03 | 115.98      | 124.77   |
| 12  | bL    | 202 | F6C  | O2D-CGD-CBD | 6.03  | 121.77      | 111.23   |
| 11  | aB    | 814 | CLA  | CMD-C2D-C1D | 6.03  | 135.35      | 124.73   |
| 11  | aA    | 837 | CLA  | CHD-C4C-C3C | -6.03 | 115.98      | 124.77   |
| 11  | bB    | 813 | CLA  | CMD-C2D-C1D | 6.03  | 135.34      | 124.73   |
| 11  | aA    | 807 | CLA  | C2D-C1D-ND  | 6.03  | 116.09      | 110.13   |
| 12  | aL    | 202 | F6C  | O2D-CGD-CBD | 6.02  | 121.76      | 111.23   |
| 11  | bA    | 836 | CLA  | CHD-C4C-C3C | -6.02 | 115.99      | 124.77   |
| 11  | aA    | 805 | CLA  | CHD-C4C-C3C | -6.02 | 116.00      | 124.77   |
| 11  | cB    | 814 | CLA  | CMD-C2D-C1D | 6.01  | 135.32      | 124.73   |
| 11  | cB    | 836 | CLA  | C2D-C1D-ND  | 6.01  | 116.08      | 110.13   |
| 11  | aA    | 835 | CLA  | C2D-C1D-ND  | 6.01  | 116.08      | 110.13   |
| 11  | cA    | 813 | CLA  | C2D-C1D-ND  | 6.01  | 116.08      | 110.13   |
| 12  | cL    | 202 | F6C  | O2D-CGD-CBD | 6.01  | 121.73      | 111.23   |
| 11  | cA    | 837 | CLA  | C2D-C1D-ND  | 6.01  | 116.07      | 110.13   |
| 11  | cB    | 807 | CLA  | C2D-C1D-ND  | 6.00  | 116.07      | 110.13   |
| 12  | cA    | 844 | F6C  | CAA-C2A-C1A | -6.00 | 111.24      | 128.01   |
| 11  | aA    | 831 | CLA  | C2D-C1D-ND  | 6.00  | 116.07      | 110.13   |
| 11  | bA    | 836 | CLA  | C2D-C1D-ND  | 6.00  | 116.06      | 110.13   |
| 11  | aA    | 836 | CLA  | CHD-C4C-C3C | -6.00 | 116.02      | 124.77   |
| 11  | cB    | 802 | CLA  | CHD-C4C-C3C | -6.00 | 116.03      | 124.77   |
| 11  | bA    | 831 | CLA  | O2D-CGD-CBD | 5.99  | 121.71      | 111.23   |
| 11  | aA    | 805 | CLA  | C2D-C1D-ND  | 5.99  | 116.06      | 110.13   |
| 11  | cA    | 805 | CLA  | C2D-C1D-ND  | 5.99  | 116.06      | 110.13   |
| 11  | bA    | 835 | CLA  | C2D-C1D-ND  | 5.99  | 116.05      | 110.13   |
| 11  | cA    | 831 | CLA  | C2D-C1D-ND  | 5.99  | 116.05      | 110.13   |
| 11  | bA    | 805 | CLA  | CHD-C4C-C3C | -5.99 | 116.05      | 124.77   |
| 11  | aA    | 813 | CLA  | C2D-C1D-ND  | 5.98  | 116.05      | 110.13   |
| 11  | aB    | 817 | CLA  | C2D-C1D-ND  | 5.98  | 116.05      | 110.13   |
| 11  | cB    | 817 | CLA  | C2D-C1D-ND  | 5.98  | 116.05      | 110.13   |
| 11  | bA    | 813 | CLA  | C2D-C1D-ND  | 5.98  | 116.05      | 110.13   |
| 11  | cA    | 805 | CLA  | CHD-C4C-C3C | -5.98 | 116.05      | 124.77   |
| 12  | bA    | 844 | F6C  | CAA-C2A-C1A | -5.98 | 111.30      | 128.01   |
| 11  | bB    | 802 | CLA  | CHD-C4C-C3C | -5.98 | 116.05      | 124.77   |
| 11  | cA    | 807 | CLA  | CHD-C4C-C3C | -5.98 | 116.05      | 124.77   |
| 11  | bA    | 805 | CLA  | C2D-C1D-ND  | 5.98  | 116.04      | 110.13   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aA    | 837 | CLA  | C2D-C1D-ND  | 5.98  | 116.04      | 110.13   |
| 11  | bB    | 836 | CLA  | C2D-C1D-ND  | 5.98  | 116.04      | 110.13   |
| 11  | bB    | 817 | CLA  | C2D-C1D-ND  | 5.98  | 116.04      | 110.13   |
| 12  | aA    | 844 | F6C  | CAA-C2A-C1A | -5.97 | 111.32      | 128.01   |
| 11  | bB    | 825 | CLA  | CHD-C4C-C3C | -5.97 | 116.06      | 124.77   |
| 11  | cB    | 840 | CLA  | CHD-C4C-C3C | -5.97 | 116.06      | 124.77   |
| 11  | cA    | 831 | CLA  | O2D-CGD-CBD | 5.97  | 121.67      | 111.23   |
| 11  | cA    | 835 | CLA  | C2D-C1D-ND  | 5.97  | 116.03      | 110.13   |
| 11  | bB    | 840 | CLA  | CHD-C4C-C3C | -5.97 | 116.07      | 124.77   |
| 11  | aA    | 831 | CLA  | O2D-CGD-CBD | 5.97  | 121.66      | 111.23   |
| 11  | bA    | 837 | CLA  | C2D-C1D-ND  | 5.97  | 116.03      | 110.13   |
| 11  | aB    | 802 | CLA  | CHD-C4C-C3C | -5.96 | 116.08      | 124.77   |
| 11  | aB    | 840 | CLA  | CHD-C4C-C3C | -5.96 | 116.08      | 124.77   |
| 11  | aB    | 825 | CLA  | CHD-C4C-C3C | -5.96 | 116.08      | 124.77   |
| 11  | bA    | 822 | CLA  | CHD-C4C-C3C | -5.96 | 116.08      | 124.77   |
| 11  | cB    | 825 | CLA  | CHD-C4C-C3C | -5.96 | 116.08      | 124.77   |
| 11  | aA    | 822 | CLA  | CHD-C4C-C3C | -5.96 | 116.09      | 124.77   |
| 11  | bA    | 807 | CLA  | CHD-C4C-C3C | -5.94 | 116.11      | 124.77   |
| 11  | aA    | 835 | CLA  | CHD-C4C-C3C | -5.94 | 116.11      | 124.77   |
| 11  | bB    | 823 | CLA  | O2D-CGD-CBD | 5.94  | 121.62      | 111.23   |
| 11  | bA    | 835 | CLA  | CHD-C4C-C3C | -5.94 | 116.11      | 124.77   |
| 11  | cA    | 835 | CLA  | CHD-C4C-C3C | -5.94 | 116.11      | 124.77   |
| 11  | aA    | 807 | CLA  | CHD-C4C-C3C | -5.93 | 116.12      | 124.77   |
| 11  | cB    | 823 | CLA  | O2D-CGD-CBD | 5.93  | 121.60      | 111.23   |
| 11  | cA    | 822 | CLA  | CHD-C4C-C3C | -5.93 | 116.13      | 124.77   |
| 11  | aA    | 809 | CLA  | C2D-C1D-ND  | 5.93  | 115.99      | 110.13   |
| 11  | aB    | 833 | CLA  | C2D-C1D-ND  | 5.93  | 115.99      | 110.13   |
| 11  | aB    | 823 | CLA  | O2D-CGD-CBD | 5.92  | 121.59      | 111.23   |
| 11  | cB    | 818 | CLA  | CHD-C4C-C3C | -5.92 | 116.14      | 124.77   |
| 11  | bA    | 822 | CLA  | CMD-C2D-C1D | 5.92  | 135.15      | 124.73   |
| 11  | aB    | 818 | CLA  | CHD-C4C-C3C | -5.91 | 116.15      | 124.77   |
| 11  | bB    | 818 | CLA  | CHD-C4C-C3C | -5.91 | 116.15      | 124.77   |
| 11  | bB    | 809 | CLA  | C2D-C1D-ND  | 5.91  | 115.98      | 110.13   |
| 12  | cA    | 830 | F6C  | CAA-C2A-C1A | -5.91 | 111.50      | 128.01   |
| 11  | cB    | 827 | CLA  | CHD-C4C-C3C | -5.91 | 116.16      | 124.77   |
| 11  | bB    | 819 | CLA  | CHD-C4C-C3C | -5.91 | 116.16      | 124.77   |
| 11  | cB    | 809 | CLA  | C2D-C1D-ND  | 5.90  | 115.97      | 110.13   |
| 11  | cB    | 837 | CLA  | CHD-C4C-C3C | -5.90 | 116.17      | 124.77   |
| 11  | cA    | 809 | CLA  | C2D-C1D-ND  | 5.90  | 115.97      | 110.13   |
| 11  | cA    | 822 | CLA  | CMD-C2D-C1D | 5.90  | 135.12      | 124.73   |
| 11  | cB    | 833 | CLA  | C2D-C1D-ND  | 5.90  | 115.97      | 110.13   |
| 12  | aA    | 830 | F6C  | CAA-C2A-C1A | -5.90 | 111.53      | 128.01   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aL    | 206 | CLA  | CHD-C4C-C3C | -5.90 | 116.17      | 124.77   |
| 11  | aB    | 807 | CLA  | CMD-C2D-C1D | 5.90  | 135.11      | 124.73   |
| 11  | aB    | 809 | CLA  | C2D-C1D-ND  | 5.90  | 115.96      | 110.13   |
| 11  | cL    | 206 | CLA  | CHD-C4C-C3C | -5.90 | 116.18      | 124.77   |
| 11  | aA    | 822 | CLA  | CMD-C2D-C1D | 5.89  | 135.11      | 124.73   |
| 11  | cL    | 204 | CLA  | CMD-C2D-C1D | 5.89  | 135.11      | 124.73   |
| 11  | bB    | 833 | CLA  | C2D-C1D-ND  | 5.89  | 115.96      | 110.13   |
| 12  | bA    | 830 | F6C  | CAA-C2A-C1A | -5.89 | 111.55      | 128.01   |
| 11  | cB    | 819 | CLA  | CHD-C4C-C3C | -5.89 | 116.19      | 124.77   |
| 11  | bA    | 810 | CLA  | CHD-C4C-C3C | -5.89 | 116.19      | 124.77   |
| 12  | cL    | 202 | F6C  | C4A-C3A-C2A | -5.89 | 98.23       | 106.97   |
| 11  | bB    | 827 | CLA  | CHD-C4C-C3C | -5.89 | 116.19      | 124.77   |
| 11  | bB    | 807 | CLA  | CMD-C2D-C1D | 5.89  | 135.09      | 124.73   |
| 12  | aL    | 202 | F6C  | C4A-C3A-C2A | -5.88 | 98.24       | 106.97   |
| 11  | aL    | 204 | CLA  | CMD-C2D-C1D | 5.88  | 135.09      | 124.73   |
| 11  | bA    | 834 | CLA  | CHD-C4C-C3C | -5.88 | 116.20      | 124.77   |
| 11  | cA    | 804 | CLA  | CHD-C4C-C3C | -5.88 | 116.20      | 124.77   |
| 11  | bL    | 204 | CLA  | CMD-C2D-C1D | 5.88  | 135.08      | 124.73   |
| 11  | aA    | 810 | CLA  | CHD-C4C-C3C | -5.88 | 116.20      | 124.77   |
| 11  | cB    | 807 | CLA  | CMD-C2D-C1D | 5.88  | 135.08      | 124.73   |
| 11  | bA    | 809 | CLA  | C2D-C1D-ND  | 5.88  | 115.94      | 110.13   |
| 11  | cA    | 810 | CLA  | CHD-C4C-C3C | -5.87 | 116.21      | 124.77   |
| 11  | aA    | 838 | CLA  | CHD-C4C-C3C | -5.87 | 116.21      | 124.77   |
| 11  | bB    | 837 | CLA  | CHD-C4C-C3C | -5.87 | 116.21      | 124.77   |
| 11  | bL    | 206 | CLA  | CHD-C4C-C3C | -5.87 | 116.21      | 124.77   |
| 11  | cA    | 816 | CLA  | C2D-C1D-ND  | 5.87  | 115.94      | 110.13   |
| 11  | aA    | 834 | CLA  | CHD-C4C-C3C | -5.87 | 116.21      | 124.77   |
| 11  | aB    | 837 | CLA  | CHD-C4C-C3C | -5.87 | 116.22      | 124.77   |
| 11  | bA    | 821 | CLA  | C2D-C1D-ND  | 5.87  | 115.94      | 110.13   |
| 11  | aB    | 814 | CLA  | C2D-C1D-ND  | 5.87  | 115.93      | 110.13   |
| 11  | bA    | 838 | CLA  | CHD-C4C-C3C | -5.87 | 116.22      | 124.77   |
| 11  | aB    | 827 | CLA  | CHD-C4C-C3C | -5.87 | 116.22      | 124.77   |
| 11  | bA    | 804 | CLA  | CHD-C4C-C3C | -5.86 | 116.22      | 124.77   |
| 11  | cA    | 834 | CLA  | CHD-C4C-C3C | -5.86 | 116.22      | 124.77   |
| 11  | cA    | 838 | CLA  | CHD-C4C-C3C | -5.86 | 116.23      | 124.77   |
| 11  | aA    | 839 | CLA  | C2D-C1D-ND  | 5.86  | 115.92      | 110.13   |
| 11  | bA    | 839 | CLA  | C2D-C1D-ND  | 5.85  | 115.92      | 110.13   |
| 11  | aB    | 813 | CLA  | CHD-C4C-C3C | -5.85 | 116.24      | 124.77   |
| 11  | aB    | 819 | CLA  | CHD-C4C-C3C | -5.85 | 116.24      | 124.77   |
| 11  | cA    | 842 | CLA  | CHD-C4C-C3C | -5.85 | 116.24      | 124.77   |
| 11  | cA    | 821 | CLA  | C2D-C1D-ND  | 5.85  | 115.92      | 110.13   |
| 12  | bL    | 202 | F6C  | C4A-C3A-C2A | -5.85 | 98.29       | 106.97   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bB    | 821 | CLA  | C2D-C1D-ND  | 5.85  | 115.92      | 110.13   |
| 11  | cB    | 820 | CLA  | CHD-C4C-C3C | -5.85 | 116.25      | 124.77   |
| 11  | aA    | 821 | CLA  | C2D-C1D-ND  | 5.85  | 115.91      | 110.13   |
| 11  | aB    | 816 | CLA  | C2D-C1D-ND  | 5.85  | 115.91      | 110.13   |
| 11  | cA    | 843 | CLA  | CHD-C4C-C3C | -5.85 | 116.25      | 124.77   |
| 11  | cA    | 810 | CLA  | CMD-C2D-C1D | 5.84  | 135.02      | 124.73   |
| 11  | bA    | 810 | CLA  | CMD-C2D-C1D | 5.84  | 135.02      | 124.73   |
| 11  | aA    | 816 | CLA  | C2D-C1D-ND  | 5.84  | 115.91      | 110.13   |
| 11  | cB    | 813 | CLA  | CHD-C4C-C3C | -5.84 | 116.26      | 124.77   |
| 11  | bA    | 816 | CLA  | C2D-C1D-ND  | 5.84  | 115.91      | 110.13   |
| 11  | aA    | 804 | CLA  | CHD-C4C-C3C | -5.84 | 116.26      | 124.77   |
| 11  | aA    | 810 | CLA  | CMD-C2D-C1D | 5.84  | 135.00      | 124.73   |
| 11  | aA    | 842 | CLA  | CHD-C4C-C3C | -5.83 | 116.27      | 124.77   |
| 11  | aB    | 821 | CLA  | C2D-C1D-ND  | 5.83  | 115.90      | 110.13   |
| 11  | bB    | 814 | CLA  | C2D-C1D-ND  | 5.83  | 115.90      | 110.13   |
| 11  | bB    | 816 | CLA  | C2D-C1D-ND  | 5.82  | 115.89      | 110.13   |
| 11  | aB    | 820 | CLA  | CHD-C4C-C3C | -5.82 | 116.29      | 124.77   |
| 11  | cB    | 816 | CLA  | C2D-C1D-ND  | 5.82  | 115.88      | 110.13   |
| 11  | cB    | 814 | CLA  | C2D-C1D-ND  | 5.82  | 115.88      | 110.13   |
| 11  | bA    | 843 | CLA  | CHD-C4C-C3C | -5.82 | 116.29      | 124.77   |
| 11  | bB    | 820 | CLA  | CHD-C4C-C3C | -5.81 | 116.30      | 124.77   |
| 11  | bL    | 204 | CLA  | CHD-C4C-C3C | -5.81 | 116.30      | 124.77   |
| 11  | cA    | 839 | CLA  | C2D-C1D-ND  | 5.81  | 115.88      | 110.13   |
| 11  | aA    | 806 | CLA  | C2B-C1B-NB  | 5.81  | 116.35      | 110.33   |
| 11  | aA    | 843 | CLA  | CHD-C4C-C3C | -5.81 | 116.30      | 124.77   |
| 11  | bA    | 842 | CLA  | CHD-C4C-C3C | -5.81 | 116.30      | 124.77   |
| 11  | bA    | 806 | CLA  | C2D-C1D-ND  | 5.81  | 115.87      | 110.13   |
| 11  | bB    | 832 | CLA  | C2D-C1D-ND  | 5.81  | 115.87      | 110.13   |
| 11  | cL    | 204 | CLA  | CHD-C4C-C3C | -5.81 | 116.31      | 124.77   |
| 11  | bA    | 833 | CLA  | C2D-C1D-ND  | 5.80  | 115.87      | 110.13   |
| 11  | cA    | 829 | CLA  | C2D-C1D-ND  | 5.80  | 115.87      | 110.13   |
| 11  | cB    | 821 | CLA  | C2D-C1D-ND  | 5.80  | 115.86      | 110.13   |
| 11  | bB    | 837 | CLA  | C2D-C1D-ND  | 5.80  | 115.86      | 110.13   |
| 11  | aL    | 204 | CLA  | CHD-C4C-C3C | -5.80 | 116.32      | 124.77   |
| 11  | bB    | 813 | CLA  | CHD-C4C-C3C | -5.80 | 116.32      | 124.77   |
| 11  | aA    | 806 | CLA  | C2D-C1D-ND  | 5.79  | 115.86      | 110.13   |
| 11  | cA    | 833 | CLA  | C2D-C1D-ND  | 5.79  | 115.86      | 110.13   |
| 11  | cB    | 840 | CLA  | C2D-C1D-ND  | 5.79  | 115.86      | 110.13   |
| 11  | bA    | 804 | CLA  | C2D-C1D-ND  | 5.79  | 115.86      | 110.13   |
| 11  | cA    | 806 | CLA  | C2B-C1B-NB  | 5.79  | 116.33      | 110.33   |
| 11  | bA    | 806 | CLA  | C2B-C1B-NB  | 5.78  | 116.33      | 110.33   |
| 11  | aA    | 833 | CLA  | C2D-C1D-ND  | 5.78  | 115.85      | 110.13   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cB    | 837 | CLA  | C2D-C1D-ND  | 5.78  | 115.85      | 110.13   |
| 11  | bA    | 803 | CLA  | CHD-C4C-C3C | -5.78 | 116.34      | 124.77   |
| 11  | aA    | 802 | CLA  | CMD-C2D-C1D | 5.78  | 134.91      | 124.73   |
| 11  | bB    | 802 | CLA  | C2B-C1B-NB  | 5.78  | 116.32      | 110.33   |
| 11  | bA    | 829 | CLA  | C2D-C1D-ND  | 5.77  | 115.84      | 110.13   |
| 11  | bB    | 840 | CLA  | C2D-C1D-ND  | 5.77  | 115.84      | 110.13   |
| 11  | aB    | 802 | CLA  | C2D-C1D-ND  | 5.77  | 115.84      | 110.13   |
| 11  | aB    | 832 | CLA  | C2D-C1D-ND  | 5.77  | 115.84      | 110.13   |
| 11  | cA    | 802 | CLA  | CMD-C2D-C1D | 5.77  | 134.89      | 124.73   |
| 11  | aB    | 805 | CLA  | C2D-C1D-ND  | 5.77  | 115.83      | 110.13   |
| 11  | cB    | 811 | CLA  | C2D-C1D-ND  | 5.77  | 115.83      | 110.13   |
| 11  | cA    | 843 | CLA  | C2D-C1D-ND  | 5.76  | 115.83      | 110.13   |
| 11  | cK    | 101 | CLA  | C2D-C1D-ND  | 5.76  | 115.83      | 110.13   |
| 11  | aA    | 813 | CLA  | CHD-C4C-C3C | -5.76 | 116.37      | 124.77   |
| 11  | aB    | 830 | CLA  | C2D-C1D-ND  | 5.76  | 115.83      | 110.13   |
| 11  | bA    | 802 | CLA  | CMD-C2D-C1D | 5.76  | 134.87      | 124.73   |
| 11  | cB    | 802 | CLA  | C2B-C1B-NB  | 5.75  | 116.29      | 110.33   |
| 11  | bB    | 811 | CLA  | C2D-C1D-ND  | 5.75  | 115.82      | 110.13   |
| 11  | bB    | 830 | CLA  | C2D-C1D-ND  | 5.75  | 115.82      | 110.13   |
| 11  | cA    | 804 | CLA  | C2D-C1D-ND  | 5.75  | 115.82      | 110.13   |
| 11  | cA    | 803 | CLA  | CHD-C4C-C3C | -5.75 | 116.38      | 124.77   |
| 11  | aA    | 810 | CLA  | C2D-C1D-ND  | 5.75  | 115.82      | 110.13   |
| 11  | cB    | 832 | CLA  | C2D-C1D-ND  | 5.75  | 115.82      | 110.13   |
| 11  | bB    | 805 | CLA  | C2D-C1D-ND  | 5.75  | 115.82      | 110.13   |
| 11  | bA    | 813 | CLA  | CHD-C4C-C3C | -5.75 | 116.39      | 124.77   |
| 11  | aB    | 840 | CLA  | C2D-C1D-ND  | 5.75  | 115.82      | 110.13   |
| 11  | cB    | 802 | CLA  | C2D-C1D-ND  | 5.75  | 115.81      | 110.13   |
| 11  | cB    | 826 | CLA  | CMD-C2D-C1D | 5.75  | 134.85      | 124.73   |
| 11  | aK    | 101 | CLA  | C2D-C1D-ND  | 5.75  | 115.81      | 110.13   |
| 11  | cB    | 805 | CLA  | C2D-C1D-ND  | 5.75  | 115.81      | 110.13   |
| 11  | aA    | 843 | CLA  | C2D-C1D-ND  | 5.75  | 115.81      | 110.13   |
| 11  | bA    | 810 | CLA  | C2D-C1D-ND  | 5.75  | 115.81      | 110.13   |
| 11  | bB    | 811 | CLA  | CHD-C4C-C3C | -5.74 | 116.40      | 124.77   |
| 11  | bK    | 101 | CLA  | C2D-C1D-ND  | 5.74  | 115.81      | 110.13   |
| 11  | cA    | 811 | CLA  | C2D-C1D-ND  | 5.74  | 115.81      | 110.13   |
| 11  | aB    | 819 | CLA  | C2D-C1D-ND  | 5.74  | 115.81      | 110.13   |
| 11  | aA    | 803 | CLA  | CHD-C4C-C3C | -5.74 | 116.40      | 124.77   |
| 11  | cB    | 819 | CLA  | C2D-C1D-ND  | 5.74  | 115.81      | 110.13   |
| 11  | cA    | 816 | CLA  | CHD-C4C-C3C | -5.74 | 116.41      | 124.77   |
| 11  | cB    | 821 | CLA  | CHD-C4C-C3C | -5.74 | 116.41      | 124.77   |
| 11  | cA    | 806 | CLA  | C2D-C1D-ND  | 5.74  | 115.80      | 110.13   |
| 11  | bB    | 836 | CLA  | CHD-C4C-C3C | -5.74 | 116.41      | 124.77   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bB    | 826 | CLA  | CMD-C2D-C1D | 5.73  | 134.82      | 124.73   |
| 11  | cA    | 828 | CLA  | O2D-CGD-CBD | 5.73  | 121.25      | 111.23   |
| 11  | aA    | 829 | CLA  | C2D-C1D-ND  | 5.73  | 115.80      | 110.13   |
| 11  | aA    | 840 | CLA  | CHD-C4C-C3C | -5.73 | 116.42      | 124.77   |
| 11  | bA    | 828 | CLA  | O2D-CGD-CBD | 5.73  | 121.25      | 111.23   |
| 12  | bB    | 824 | F6C  | O2D-CGD-CBD | 5.73  | 121.25      | 111.23   |
| 11  | cL    | 205 | CLA  | CHD-C4C-C3C | -5.73 | 116.42      | 124.77   |
| 11  | bB    | 821 | CLA  | CHD-C4C-C3C | -5.73 | 116.42      | 124.77   |
| 11  | aA    | 822 | CLA  | C2D-C1D-ND  | 5.73  | 115.79      | 110.13   |
| 11  | bA    | 843 | CLA  | C2D-C1D-ND  | 5.73  | 115.79      | 110.13   |
| 11  | aB    | 811 | CLA  | CHD-C4C-C3C | -5.73 | 116.42      | 124.77   |
| 11  | cA    | 840 | CLA  | CHD-C4C-C3C | -5.73 | 116.42      | 124.77   |
| 11  | aB    | 837 | CLA  | C2D-C1D-ND  | 5.73  | 115.79      | 110.13   |
| 12  | cB    | 824 | F6C  | O2D-CGD-CBD | 5.73  | 121.24      | 111.23   |
| 11  | aA    | 804 | CLA  | C2D-C1D-ND  | 5.72  | 115.79      | 110.13   |
| 11  | aA    | 816 | CLA  | CHD-C4C-C3C | -5.72 | 116.43      | 124.77   |
| 11  | cA    | 813 | CLA  | CHD-C4C-C3C | -5.72 | 116.43      | 124.77   |
| 11  | bA    | 811 | CLA  | C2D-C1D-ND  | 5.72  | 115.79      | 110.13   |
| 11  | aB    | 821 | CLA  | CHD-C4C-C3C | -5.72 | 116.43      | 124.77   |
| 11  | bB    | 831 | CLA  | CHD-C4C-C3C | -5.72 | 116.43      | 124.77   |
| 11  | bB    | 817 | CLA  | CHD-C4C-C3C | -5.72 | 116.44      | 124.77   |
| 11  | cA    | 817 | CLA  | CHD-C4C-C3C | -5.72 | 116.44      | 124.77   |
| 12  | cL    | 202 | F6C  | C2D-C1D-ND  | 5.72  | 115.98      | 109.98   |
| 12  | aB    | 824 | F6C  | O2D-CGD-CBD | 5.72  | 121.22      | 111.23   |
| 11  | bB    | 819 | CLA  | C2D-C1D-ND  | 5.71  | 115.78      | 110.13   |
| 11  | cA    | 810 | CLA  | C2D-C1D-ND  | 5.71  | 115.78      | 110.13   |
| 11  | cB    | 835 | CLA  | CHD-C4C-C3C | -5.71 | 116.44      | 124.77   |
| 11  | aA    | 828 | CLA  | O2D-CGD-CBD | 5.71  | 121.22      | 111.23   |
| 11  | bA    | 816 | CLA  | CHD-C4C-C3C | -5.71 | 116.44      | 124.77   |
| 11  | aA    | 811 | CLA  | C2D-C1D-ND  | 5.71  | 115.78      | 110.13   |
| 11  | aB    | 817 | CLA  | CHD-C4C-C3C | -5.71 | 116.44      | 124.77   |
| 11  | bA    | 840 | CLA  | CHD-C4C-C3C | -5.71 | 116.45      | 124.77   |
| 11  | bB    | 835 | CLA  | CHD-C4C-C3C | -5.71 | 116.45      | 124.77   |
| 11  | aB    | 811 | CLA  | C2D-C1D-ND  | 5.71  | 115.78      | 110.13   |
| 11  | cA    | 822 | CLA  | C2D-C1D-ND  | 5.71  | 115.78      | 110.13   |
| 11  | bB    | 802 | CLA  | C2D-C1D-ND  | 5.71  | 115.77      | 110.13   |
| 11  | cB    | 830 | CLA  | C2D-C1D-ND  | 5.71  | 115.77      | 110.13   |
| 11  | aB    | 835 | CLA  | CHD-C4C-C3C | -5.71 | 116.45      | 124.77   |
| 11  | bA    | 822 | CLA  | C2D-C1D-ND  | 5.70  | 115.77      | 110.13   |
| 11  | aB    | 802 | CLA  | C2B-C1B-NB  | 5.70  | 116.24      | 110.33   |
| 11  | aB    | 826 | CLA  | CMD-C2D-C1D | 5.70  | 134.77      | 124.73   |
| 11  | bA    | 817 | CLA  | CHD-C4C-C3C | -5.70 | 116.46      | 124.77   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cB    | 818 | CLA  | CMD-C2D-C1D | 5.70  | 134.76      | 124.73   |
| 11  | cB    | 831 | CLA  | CHD-C4C-C3C | -5.70 | 116.47      | 124.77   |
| 11  | cB    | 835 | CLA  | C2D-C1D-ND  | 5.70  | 115.76      | 110.13   |
| 11  | aB    | 831 | CLA  | CHD-C4C-C3C | -5.70 | 116.47      | 124.77   |
| 11  | aA    | 808 | CLA  | CHD-C4C-C3C | -5.70 | 116.47      | 124.77   |
| 11  | aB    | 810 | CLA  | CHD-C4C-C3C | -5.69 | 116.47      | 124.77   |
| 11  | aL    | 205 | CLA  | CHD-C4C-C3C | -5.69 | 116.47      | 124.77   |
| 11  | cB    | 811 | CLA  | CHD-C4C-C3C | -5.69 | 116.47      | 124.77   |
| 11  | aA    | 817 | CLA  | CHD-C4C-C3C | -5.69 | 116.47      | 124.77   |
| 11  | cB    | 838 | CLA  | CHD-C4C-C3C | -5.69 | 116.47      | 124.77   |
| 11  | bA    | 838 | CLA  | C2D-C1D-ND  | 5.69  | 115.76      | 110.13   |
| 11  | cB    | 817 | CLA  | CHD-C4C-C3C | -5.69 | 116.47      | 124.77   |
| 11  | cB    | 810 | CLA  | CHD-C4C-C3C | -5.69 | 116.47      | 124.77   |
| 11  | bB    | 810 | CLA  | CHD-C4C-C3C | -5.69 | 116.47      | 124.77   |
| 12  | bL    | 202 | F6C  | C2D-C1D-ND  | 5.69  | 115.96      | 109.98   |
| 12  | aL    | 202 | F6C  | C2D-C1D-ND  | 5.69  | 115.95      | 109.98   |
| 11  | aB    | 836 | CLA  | CHD-C4C-C3C | -5.69 | 116.48      | 124.77   |
| 11  | cB    | 836 | CLA  | CHD-C4C-C3C | -5.68 | 116.49      | 124.77   |
| 11  | aB    | 835 | CLA  | C2D-C1D-ND  | 5.68  | 115.75      | 110.13   |
| 11  | bB    | 835 | CLA  | C2D-C1D-ND  | 5.68  | 115.75      | 110.13   |
| 11  | aB    | 814 | CLA  | O2D-CGD-CBD | 5.68  | 121.17      | 111.23   |
| 11  | bL    | 205 | CLA  | CHD-C4C-C3C | -5.68 | 116.49      | 124.77   |
| 11  | aA    | 811 | CLA  | CHD-C4C-C3C | -5.68 | 116.49      | 124.77   |
| 11  | bB    | 818 | CLA  | CMD-C2D-C1D | 5.68  | 134.73      | 124.73   |
| 11  | aB    | 838 | CLA  | CHD-C4C-C3C | -5.68 | 116.49      | 124.77   |
| 11  | cA    | 811 | CLA  | CHD-C4C-C3C | -5.67 | 116.50      | 124.77   |
| 11  | aB    | 818 | CLA  | CMD-C2D-C1D | 5.67  | 134.72      | 124.73   |
| 11  | bA    | 808 | CLA  | CHD-C4C-C3C | -5.67 | 116.50      | 124.77   |
| 12  | bA    | 826 | F6C  | C2D-C1D-ND  | 5.67  | 115.94      | 109.98   |
| 11  | bA    | 824 | CLA  | CHD-C4C-C3C | -5.67 | 116.51      | 124.77   |
| 11  | bK    | 103 | CLA  | CHD-C4C-C3C | -5.67 | 116.51      | 124.77   |
| 11  | cA    | 838 | CLA  | C2D-C1D-ND  | 5.66  | 115.73      | 110.13   |
| 11  | cA    | 809 | CLA  | CHD-C4C-C3C | -5.66 | 116.52      | 124.77   |
| 11  | aK    | 103 | CLA  | CHD-C4C-C3C | -5.66 | 116.52      | 124.77   |
| 11  | cB    | 808 | CLA  | C2D-C1D-ND  | 5.66  | 115.73      | 110.13   |
| 11  | cA    | 808 | CLA  | CHD-C4C-C3C | -5.66 | 116.52      | 124.77   |
| 11  | bB    | 830 | CLA  | CHD-C4C-C3C | -5.66 | 116.53      | 124.77   |
| 11  | aA    | 838 | CLA  | C2D-C1D-ND  | 5.65  | 115.72      | 110.13   |
| 11  | aB    | 808 | CLA  | C2D-C1D-ND  | 5.65  | 115.72      | 110.13   |
| 12  | cA    | 826 | F6C  | C2D-C1D-ND  | 5.65  | 115.91      | 109.98   |
| 11  | bB    | 838 | CLA  | CHD-C4C-C3C | -5.65 | 116.54      | 124.77   |
| 11  | aB    | 802 | CLA  | CMD-C2D-C1D | 5.65  | 134.67      | 124.73   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aA    | 824 | CLA  | CHD-C4C-C3C | -5.64 | 116.55      | 124.77   |
| 11  | bA    | 811 | CLA  | CHD-C4C-C3C | -5.64 | 116.55      | 124.77   |
| 12  | bA    | 832 | F6C  | C1A-C2A-C3A | -5.64 | 101.03      | 106.97   |
| 11  | bA    | 809 | CLA  | CHD-C4C-C3C | -5.64 | 116.55      | 124.77   |
| 11  | aA    | 829 | CLA  | CHD-C4C-C3C | -5.64 | 116.55      | 124.77   |
| 11  | cK    | 103 | CLA  | CHD-C4C-C3C | -5.64 | 116.55      | 124.77   |
| 11  | aA    | 833 | CLA  | CHD-C4C-C3C | -5.64 | 116.55      | 124.77   |
| 11  | bB    | 810 | CLA  | C2D-C1D-ND  | 5.64  | 115.71      | 110.13   |
| 11  | bA    | 841 | CLA  | CHD-C4C-C3C | -5.64 | 116.55      | 124.77   |
| 11  | cA    | 824 | CLA  | CHD-C4C-C3C | -5.64 | 116.55      | 124.77   |
| 11  | bB    | 828 | CLA  | C2C-C1C-NC  | 5.64  | 115.90      | 109.98   |
| 12  | aA    | 826 | F6C  | C2D-C1D-ND  | 5.64  | 115.90      | 109.98   |
| 11  | bA    | 829 | CLA  | CHD-C4C-C3C | -5.63 | 116.56      | 124.77   |
| 11  | cA    | 829 | CLA  | CHD-C4C-C3C | -5.63 | 116.56      | 124.77   |
| 11  | cA    | 833 | CLA  | CHD-C4C-C3C | -5.63 | 116.56      | 124.77   |
| 11  | bA    | 833 | CLA  | CHD-C4C-C3C | -5.63 | 116.56      | 124.77   |
| 11  | aA    | 809 | CLA  | CHD-C4C-C3C | -5.63 | 116.56      | 124.77   |
| 11  | cB    | 802 | CLA  | CMD-C2D-C1D | 5.63  | 134.65      | 124.73   |
| 11  | aA    | 814 | CLA  | O2D-CGD-CBD | 5.63  | 121.08      | 111.23   |
| 11  | aK    | 101 | CLA  | CHD-C4C-C3C | -5.63 | 116.56      | 124.77   |
| 11  | bB    | 814 | CLA  | O2D-CGD-CBD | 5.63  | 121.07      | 111.23   |
| 11  | cA    | 821 | CLA  | CHD-C4C-C3C | -5.63 | 116.56      | 124.77   |
| 11  | cK    | 101 | CLA  | CHD-C4C-C3C | -5.63 | 116.56      | 124.77   |
| 11  | bB    | 802 | CLA  | CMD-C2D-C1D | 5.63  | 134.64      | 124.73   |
| 11  | aB    | 830 | CLA  | CHD-C4C-C3C | -5.63 | 116.56      | 124.77   |
| 11  | cB    | 814 | CLA  | O2D-CGD-CBD | 5.63  | 121.07      | 111.23   |
| 11  | cA    | 802 | CLA  | C2C-C1C-NC  | 5.63  | 115.89      | 109.98   |
| 11  | bA    | 814 | CLA  | O2D-CGD-CBD | 5.63  | 121.06      | 111.23   |
| 11  | cB    | 830 | CLA  | CHD-C4C-C3C | -5.62 | 116.57      | 124.77   |
| 12  | aA    | 832 | F6C  | C1A-C2A-C3A | -5.62 | 101.05      | 106.97   |
| 11  | aB    | 823 | CLA  | C2D-C1D-ND  | 5.62  | 115.69      | 110.13   |
| 11  | bA    | 821 | CLA  | O2D-CGD-CBD | 5.62  | 121.06      | 111.23   |
| 11  | bB    | 823 | CLA  | C2D-C1D-ND  | 5.62  | 115.69      | 110.13   |
| 11  | aA    | 841 | CLA  | CHD-C4C-C3C | -5.62 | 116.58      | 124.77   |
| 11  | aA    | 834 | CLA  | C2D-C1D-ND  | 5.61  | 115.68      | 110.13   |
| 11  | bA    | 834 | CLA  | C2D-C1D-ND  | 5.61  | 115.68      | 110.13   |
| 12  | cA    | 832 | F6C  | C1A-C2A-C3A | -5.61 | 101.06      | 106.97   |
| 11  | aA    | 821 | CLA  | CHD-C4C-C3C | -5.61 | 116.60      | 124.77   |
| 11  | bK    | 101 | CLA  | CHD-C4C-C3C | -5.61 | 116.60      | 124.77   |
| 11  | cA    | 841 | CLA  | CHD-C4C-C3C | -5.61 | 116.60      | 124.77   |
| 11  | bB    | 808 | CLA  | C2D-C1D-ND  | 5.60  | 115.67      | 110.13   |
| 11  | cB    | 810 | CLA  | C2D-C1D-ND  | 5.60  | 115.67      | 110.13   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cA    | 834 | CLA  | C2D-C1D-ND  | 5.60  | 115.67      | 110.13   |
| 11  | cB    | 828 | CLA  | C2C-C1C-NC  | 5.60  | 115.87      | 109.98   |
| 12  | aA    | 826 | F6C  | CMA-C3A-C4A | -5.60 | 114.86      | 124.73   |
| 11  | bA    | 821 | CLA  | CHD-C4C-C3C | -5.60 | 116.61      | 124.77   |
| 11  | cB    | 809 | CLA  | CHD-C4C-C3C | -5.60 | 116.61      | 124.77   |
| 11  | cA    | 814 | CLA  | O2D-CGD-CBD | 5.60  | 121.02      | 111.23   |
| 11  | cA    | 821 | CLA  | O2D-CGD-CBD | 5.60  | 121.02      | 111.23   |
| 11  | bA    | 812 | CLA  | C2D-C1D-ND  | 5.60  | 115.67      | 110.13   |
| 11  | bB    | 827 | CLA  | C2D-C1D-ND  | 5.60  | 115.67      | 110.13   |
| 11  | bB    | 831 | CLA  | C2D-C1D-ND  | 5.60  | 115.66      | 110.13   |
| 11  | bB    | 809 | CLA  | CHD-C4C-C3C | -5.60 | 116.61      | 124.77   |
| 12  | bA    | 827 | F6C  | C2D-C1D-ND  | 5.59  | 115.86      | 109.98   |
| 12  | aA    | 827 | F6C  | C2D-C1D-ND  | 5.59  | 115.86      | 109.98   |
| 11  | aB    | 831 | CLA  | C2D-C1D-ND  | 5.59  | 115.66      | 110.13   |
| 11  | cA    | 821 | CLA  | CMD-C2D-C1D | 5.59  | 134.58      | 124.73   |
| 12  | cA    | 827 | F6C  | C2D-C1D-ND  | 5.59  | 115.86      | 109.98   |
| 11  | aA    | 821 | CLA  | CMD-C2D-C1D | 5.59  | 134.57      | 124.73   |
| 12  | cA    | 826 | F6C  | CMA-C3A-C4A | -5.59 | 114.88      | 124.73   |
| 12  | bA    | 826 | F6C  | CMA-C3A-C4A | -5.59 | 114.89      | 124.73   |
| 11  | aA    | 802 | CLA  | C2C-C1C-NC  | 5.59  | 115.85      | 109.98   |
| 11  | bA    | 821 | CLA  | CMD-C2D-C1D | 5.58  | 134.56      | 124.73   |
| 11  | aA    | 821 | CLA  | O2D-CGD-CBD | 5.58  | 120.99      | 111.23   |
| 11  | cB    | 831 | CLA  | C2D-C1D-ND  | 5.58  | 115.65      | 110.13   |
| 11  | aB    | 810 | CLA  | C2D-C1D-ND  | 5.58  | 115.65      | 110.13   |
| 11  | aB    | 807 | CLA  | O2D-CGD-CBD | 5.58  | 120.98      | 111.23   |
| 11  | cB    | 807 | CLA  | O2D-CGD-CBD | 5.57  | 120.97      | 111.23   |
| 11  | aB    | 813 | CLA  | C2D-C1D-ND  | 5.57  | 115.64      | 110.13   |
| 11  | bB    | 807 | CLA  | O2D-CGD-CBD | 5.57  | 120.96      | 111.23   |
| 11  | aB    | 809 | CLA  | CHD-C4C-C3C | -5.56 | 116.66      | 124.77   |
| 11  | cB    | 833 | CLA  | CHD-C4C-C3C | -5.56 | 116.66      | 124.77   |
| 11  | cB    | 827 | CLA  | C2D-C1D-ND  | 5.56  | 115.63      | 110.13   |
| 11  | aA    | 812 | CLA  | C2D-C1D-ND  | 5.56  | 115.63      | 110.13   |
| 11  | cB    | 813 | CLA  | C2D-C1D-ND  | 5.56  | 115.63      | 110.13   |
| 11  | aB    | 828 | CLA  | C2C-C1C-NC  | 5.56  | 115.82      | 109.98   |
| 11  | cA    | 812 | CLA  | C2D-C1D-ND  | 5.56  | 115.62      | 110.13   |
| 11  | cB    | 823 | CLA  | C2D-C1D-ND  | 5.55  | 115.62      | 110.13   |
| 11  | bA    | 817 | CLA  | C2D-C1D-ND  | 5.55  | 115.62      | 110.13   |
| 11  | aB    | 833 | CLA  | CHD-C4C-C3C | -5.55 | 116.69      | 124.77   |
| 11  | bA    | 820 | CLA  | C2D-C1D-ND  | 5.55  | 115.61      | 110.13   |
| 11  | bB    | 813 | CLA  | C2D-C1D-ND  | 5.54  | 115.61      | 110.13   |
| 11  | aA    | 815 | CLA  | C2D-C1D-ND  | 5.53  | 115.60      | 110.13   |
| 11  | aA    | 817 | CLA  | C2D-C1D-ND  | 5.53  | 115.60      | 110.13   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aA    | 839 | CLA  | CHD-C4C-C3C | -5.53 | 116.71      | 124.77   |
| 11  | cA    | 815 | CLA  | C2D-C1D-ND  | 5.53  | 115.60      | 110.13   |
| 11  | bB    | 833 | CLA  | CHD-C4C-C3C | -5.53 | 116.72      | 124.77   |
| 11  | aA    | 820 | CLA  | C2D-C1D-ND  | 5.53  | 115.59      | 110.13   |
| 11  | bA    | 815 | CLA  | C2D-C1D-ND  | 5.52  | 115.59      | 110.13   |
| 11  | aB    | 827 | CLA  | C2D-C1D-ND  | 5.52  | 115.59      | 110.13   |
| 12  | aA    | 832 | F6C  | C2B-C3B-C4B | -5.52 | 103.61      | 106.46   |
| 11  | bA    | 802 | CLA  | C2C-C1C-NC  | 5.52  | 115.78      | 109.98   |
| 11  | bB    | 834 | CLA  | C2D-C1D-ND  | 5.52  | 115.59      | 110.13   |
| 11  | bA    | 814 | CLA  | CHD-C4C-C3C | -5.52 | 116.73      | 124.77   |
| 12  | bA    | 832 | F6C  | C2B-C3B-C4B | -5.51 | 103.62      | 106.46   |
| 11  | cA    | 817 | CLA  | C2D-C1D-ND  | 5.51  | 115.58      | 110.13   |
| 11  | cA    | 820 | CLA  | C2D-C1D-ND  | 5.51  | 115.58      | 110.13   |
| 11  | bB    | 805 | CLA  | CHD-C4C-C3C | -5.51 | 116.75      | 124.77   |
| 11  | bB    | 807 | CLA  | C2C-C1C-NC  | 5.50  | 115.76      | 109.98   |
| 11  | bA    | 839 | CLA  | CHD-C4C-C3C | -5.50 | 116.75      | 124.77   |
| 11  | cB    | 805 | CLA  | CHD-C4C-C3C | -5.50 | 116.75      | 124.77   |
| 11  | aB    | 816 | CLA  | CHD-C4C-C3C | -5.50 | 116.76      | 124.77   |
| 11  | cA    | 839 | CLA  | CHD-C4C-C3C | -5.50 | 116.76      | 124.77   |
| 11  | cB    | 807 | CLA  | C2C-C1C-NC  | 5.50  | 115.75      | 109.98   |
| 11  | aA    | 814 | CLA  | C2D-C1D-ND  | 5.49  | 115.56      | 110.13   |
| 11  | aA    | 824 | CLA  | C2D-C1D-ND  | 5.49  | 115.56      | 110.13   |
| 11  | cA    | 824 | CLA  | C2D-C1D-ND  | 5.49  | 115.56      | 110.13   |
| 11  | aA    | 803 | CLA  | C2B-C1B-NB  | 5.49  | 116.02      | 110.33   |
| 12  | cA    | 832 | F6C  | C2B-C3B-C4B | -5.49 | 103.63      | 106.46   |
| 11  | aB    | 807 | CLA  | C2C-C1C-NC  | 5.49  | 115.75      | 109.98   |
| 11  | bA    | 802 | CLA  | O2D-CGD-CBD | 5.49  | 120.83      | 111.23   |
| 11  | bA    | 814 | CLA  | C2D-C1D-ND  | 5.49  | 115.56      | 110.13   |
| 10  | aA    | 801 | CL0  | CHA-C1A-C2A | -5.49 | 120.42      | 133.31   |
| 11  | aA    | 802 | CLA  | O2D-CGD-CBD | 5.49  | 120.82      | 111.23   |
| 11  | aB    | 823 | CLA  | CMD-C2D-C1D | 5.49  | 134.39      | 124.73   |
| 11  | cA    | 802 | CLA  | CHD-C4C-C3C | -5.49 | 116.77      | 124.77   |
| 11  | cA    | 814 | CLA  | CHD-C4C-C3C | -5.49 | 116.77      | 124.77   |
| 11  | cA    | 802 | CLA  | C2D-C1D-ND  | 5.49  | 115.56      | 110.13   |
| 11  | cB    | 834 | CLA  | C2D-C1D-ND  | 5.49  | 115.56      | 110.13   |
| 11  | cA    | 803 | CLA  | C2B-C1B-NB  | 5.48  | 116.01      | 110.33   |
| 11  | aB    | 834 | CLA  | C2D-C1D-ND  | 5.48  | 115.55      | 110.13   |
| 10  | bA    | 801 | CL0  | CHA-C1A-C2A | -5.48 | 120.43      | 133.31   |
| 11  | aB    | 805 | CLA  | CHD-C4C-C3C | -5.48 | 116.78      | 124.77   |
| 11  | bB    | 816 | CLA  | CHD-C4C-C3C | -5.48 | 116.78      | 124.77   |
| 10  | cA    | 801 | CL0  | CHA-C1A-C2A | -5.48 | 120.44      | 133.31   |
| 11  | bB    | 808 | CLA  | O2D-CGD-CBD | 5.48  | 120.81      | 111.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cA    | 802 | CLA  | O2D-CGD-CBD | 5.48  | 120.81      | 111.23   |
| 11  | aB    | 807 | CLA  | CHD-C4C-C3C | -5.48 | 116.79      | 124.77   |
| 11  | cB    | 816 | CLA  | CHD-C4C-C3C | -5.47 | 116.79      | 124.77   |
| 11  | aA    | 802 | CLA  | CHD-C4C-C3C | -5.47 | 116.80      | 124.77   |
| 11  | cL    | 206 | CLA  | CMD-C2D-C1D | 5.47  | 134.36      | 124.73   |
| 11  | bA    | 802 | CLA  | CHD-C4C-C3C | -5.47 | 116.80      | 124.77   |
| 11  | bB    | 823 | CLA  | CMD-C2D-C1D | 5.47  | 134.36      | 124.73   |
| 11  | aA    | 802 | CLA  | C2D-C1D-ND  | 5.47  | 115.54      | 110.13   |
| 11  | bA    | 803 | CLA  | C2B-C1B-NB  | 5.47  | 115.99      | 110.33   |
| 11  | bB    | 834 | CLA  | C2C-C1C-NC  | 5.46  | 115.72      | 109.98   |
| 11  | aA    | 814 | CLA  | CHD-C4C-C3C | -5.46 | 116.81      | 124.77   |
| 11  | bB    | 807 | CLA  | CHD-C4C-C3C | -5.46 | 116.81      | 124.77   |
| 11  | bA    | 815 | CLA  | CHD-C4C-C3C | -5.46 | 116.81      | 124.77   |
| 11  | cA    | 814 | CLA  | C2D-C1D-ND  | 5.46  | 115.53      | 110.13   |
| 11  | bL    | 206 | CLA  | CMD-C2D-C1D | 5.46  | 134.34      | 124.73   |
| 11  | aA    | 841 | CLA  | CMD-C2D-C1D | 5.45  | 134.33      | 124.73   |
| 11  | cB    | 808 | CLA  | O2D-CGD-CBD | 5.45  | 120.76      | 111.23   |
| 11  | cB    | 807 | CLA  | CHD-C4C-C3C | -5.45 | 116.83      | 124.77   |
| 11  | bA    | 825 | CLA  | C2D-C1D-ND  | 5.45  | 115.52      | 110.13   |
| 11  | aL    | 206 | CLA  | CMD-C2D-C1D | 5.45  | 134.32      | 124.73   |
| 11  | aB    | 808 | CLA  | O2D-CGD-CBD | 5.45  | 120.75      | 111.23   |
| 11  | bA    | 841 | CLA  | CMD-C2D-C1D | 5.45  | 134.32      | 124.73   |
| 11  | cA    | 841 | CLA  | CMD-C2D-C1D | 5.45  | 134.32      | 124.73   |
| 11  | cB    | 823 | CLA  | CMD-C2D-C1D | 5.45  | 134.32      | 124.73   |
| 11  | cB    | 834 | CLA  | C2C-C1C-NC  | 5.45  | 115.70      | 109.98   |
| 11  | aB    | 819 | CLA  | CMD-C2D-C1D | 5.44  | 134.32      | 124.73   |
| 11  | bA    | 824 | CLA  | C2D-C1D-ND  | 5.44  | 115.51      | 110.13   |
| 11  | aA    | 840 | CLA  | O2D-CGD-CBD | 5.44  | 120.75      | 111.23   |
| 11  | aA    | 815 | CLA  | CHD-C4C-C3C | -5.44 | 116.84      | 124.77   |
| 11  | cA    | 809 | CLA  | O2D-CGD-CBD | 5.44  | 120.74      | 111.23   |
| 11  | bA    | 840 | CLA  | O2D-CGD-CBD | 5.44  | 120.74      | 111.23   |
| 11  | bA    | 802 | CLA  | C2D-C1D-ND  | 5.44  | 115.51      | 110.13   |
| 11  | aB    | 834 | CLA  | C2C-C1C-NC  | 5.44  | 115.69      | 109.98   |
| 11  | aA    | 809 | CLA  | O2D-CGD-CBD | 5.43  | 120.73      | 111.23   |
| 12  | cA    | 844 | F6C  | C2D-C1D-ND  | 5.43  | 115.69      | 109.98   |
| 11  | bA    | 809 | CLA  | O2D-CGD-CBD | 5.43  | 120.72      | 111.23   |
| 11  | bA    | 805 | CLA  | O2D-CGD-CBD | 5.43  | 120.72      | 111.23   |
| 12  | aA    | 830 | F6C  | C2B-C3B-C4B | -5.43 | 103.66      | 106.46   |
| 11  | bA    | 831 | CLA  | C2C-C1C-NC  | 5.42  | 115.68      | 109.98   |
| 11  | cA    | 840 | CLA  | O2D-CGD-CBD | 5.42  | 120.71      | 111.23   |
| 11  | cB    | 819 | CLA  | CMD-C2D-C1D | 5.42  | 134.26      | 124.73   |
| 12  | cA    | 830 | F6C  | C2B-C3B-C4B | -5.41 | 103.67      | 106.46   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cA    | 815 | CLA  | CHD-C4C-C3C | -5.41 | 116.88      | 124.77   |
| 11  | cA    | 805 | CLA  | O2D-CGD-CBD | 5.41  | 120.69      | 111.23   |
| 11  | bB    | 840 | CLA  | C2C-C1C-NC  | 5.41  | 115.66      | 109.98   |
| 11  | aA    | 825 | CLA  | C2D-C1D-ND  | 5.41  | 115.48      | 110.13   |
| 11  | aA    | 836 | CLA  | C2C-C1C-NC  | 5.41  | 115.66      | 109.98   |
| 11  | aA    | 831 | CLA  | C2C-C1C-NC  | 5.40  | 115.66      | 109.98   |
| 11  | cA    | 831 | CLA  | C2C-C1C-NC  | 5.40  | 115.66      | 109.98   |
| 11  | aA    | 805 | CLA  | O2D-CGD-CBD | 5.40  | 120.67      | 111.23   |
| 11  | bB    | 819 | CLA  | CMD-C2D-C1D | 5.40  | 134.24      | 124.73   |
| 12  | aA    | 844 | F6C  | C2D-C1D-ND  | 5.39  | 115.65      | 109.98   |
| 11  | bB    | 812 | CLA  | O2D-CGD-CBD | 5.39  | 120.66      | 111.23   |
| 11  | cA    | 825 | CLA  | C2D-C1D-ND  | 5.39  | 115.46      | 110.13   |
| 11  | cB    | 834 | CLA  | CHD-C4C-C3C | -5.39 | 116.92      | 124.77   |
| 12  | bA    | 830 | F6C  | C2B-C3B-C4B | -5.39 | 103.68      | 106.46   |
| 11  | bB    | 834 | CLA  | CHD-C4C-C3C | -5.39 | 116.92      | 124.77   |
| 11  | aB    | 834 | CLA  | CHD-C4C-C3C | -5.38 | 116.92      | 124.77   |
| 12  | aA    | 830 | F6C  | C2D-C1D-ND  | 5.38  | 115.64      | 109.98   |
| 11  | aB    | 840 | CLA  | C2C-C1C-NC  | 5.38  | 115.63      | 109.98   |
| 12  | bA    | 844 | F6C  | C2D-C1D-ND  | 5.38  | 115.63      | 109.98   |
| 11  | cA    | 836 | CLA  | C2C-C1C-NC  | 5.38  | 115.63      | 109.98   |
| 12  | cA    | 826 | F6C  | C2B-C3B-C4B | -5.37 | 103.69      | 106.46   |
| 11  | bA    | 836 | CLA  | C2C-C1C-NC  | 5.37  | 115.62      | 109.98   |
| 11  | cB    | 804 | CLA  | O2D-CGD-CBD | 5.37  | 120.62      | 111.23   |
| 12  | cA    | 844 | F6C  | C1A-C2A-C3A | -5.37 | 101.32      | 106.97   |
| 11  | aB    | 812 | CLA  | O2D-CGD-CBD | 5.36  | 120.61      | 111.23   |
| 12  | cA    | 830 | F6C  | C2D-C1D-ND  | 5.36  | 115.61      | 109.98   |
| 11  | bA    | 817 | CLA  | C2C-C1C-NC  | 5.36  | 115.61      | 109.98   |
| 11  | cB    | 840 | CLA  | C2C-C1C-NC  | 5.36  | 115.61      | 109.98   |
| 11  | aB    | 804 | CLA  | O2D-CGD-CBD | 5.36  | 120.59      | 111.23   |
| 11  | cA    | 805 | CLA  | C2B-C1B-NB  | 5.35  | 115.88      | 110.33   |
| 12  | cA    | 826 | F6C  | C1A-C2A-C3A | -5.35 | 101.33      | 106.97   |
| 12  | aA    | 826 | F6C  | C2B-C3B-C4B | -5.35 | 103.70      | 106.46   |
| 11  | cB    | 812 | CLA  | O2D-CGD-CBD | 5.35  | 120.58      | 111.23   |
| 12  | aA    | 844 | F6C  | C1A-C2A-C3A | -5.35 | 101.34      | 106.97   |
| 12  | bA    | 830 | F6C  | C2D-C1D-ND  | 5.35  | 115.60      | 109.98   |
| 11  | bB    | 802 | CLA  | C3B-C2B-C1B | -5.35 | 100.87      | 107.17   |
| 11  | bA    | 805 | CLA  | C2B-C1B-NB  | 5.35  | 115.87      | 110.33   |
| 11  | cA    | 825 | CLA  | CHD-C4C-C3C | -5.34 | 116.98      | 124.77   |
| 11  | bL    | 205 | CLA  | CMD-C2D-C1D | 5.34  | 134.14      | 124.73   |
| 12  | bA    | 832 | F6C  | O2D-CGD-CBD | 5.34  | 120.57      | 111.23   |
| 12  | bL    | 202 | F6C  | C2B-C3B-C4B | -5.34 | 103.71      | 106.46   |
| 11  | bB    | 832 | CLA  | CHD-C4C-C3C | -5.34 | 116.99      | 124.77   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aB    | 832 | CLA  | CHD-C4C-C3C | -5.34 | 116.99      | 124.77   |
| 11  | bA    | 825 | CLA  | CHD-C4C-C3C | -5.34 | 116.99      | 124.77   |
| 11  | bB    | 804 | CLA  | O2D-CGD-CBD | 5.33  | 120.56      | 111.23   |
| 11  | aA    | 812 | CLA  | CHD-C4C-C3C | -5.33 | 117.00      | 124.77   |
| 12  | cA    | 830 | F6C  | C1A-C2A-C3A | -5.33 | 101.36      | 106.97   |
| 12  | aA    | 832 | F6C  | O2D-CGD-CBD | 5.33  | 120.55      | 111.23   |
| 12  | aA    | 830 | F6C  | C1A-C2A-C3A | -5.33 | 101.36      | 106.97   |
| 11  | cB    | 832 | CLA  | CHD-C4C-C3C | -5.33 | 117.01      | 124.77   |
| 11  | aA    | 817 | CLA  | C2C-C1C-NC  | 5.33  | 115.58      | 109.98   |
| 11  | bB    | 832 | CLA  | C2B-C1B-NB  | 5.32  | 115.85      | 110.33   |
| 12  | bA    | 830 | F6C  | C1A-C2A-C3A | -5.32 | 101.36      | 106.97   |
| 11  | aA    | 825 | CLA  | CHD-C4C-C3C | -5.32 | 117.01      | 124.77   |
| 12  | cA    | 832 | F6C  | O2D-CGD-CBD | 5.32  | 120.53      | 111.23   |
| 11  | cA    | 817 | CLA  | C2C-C1C-NC  | 5.32  | 115.57      | 109.98   |
| 12  | aA    | 826 | F6C  | C1A-C2A-C3A | -5.32 | 101.37      | 106.97   |
| 11  | bA    | 812 | CLA  | CHD-C4C-C3C | -5.32 | 117.02      | 124.77   |
| 12  | bA    | 844 | F6C  | C1A-C2A-C3A | -5.31 | 101.38      | 106.97   |
| 11  | cB    | 802 | CLA  | C3B-C2B-C1B | -5.31 | 100.91      | 107.17   |
| 11  | bA    | 802 | CLA  | CAA-C2A-C3A | -5.31 | 98.65       | 113.00   |
| 11  | aA    | 802 | CLA  | CAA-C2A-C3A | -5.31 | 98.65       | 113.00   |
| 11  | aL    | 205 | CLA  | CMD-C2D-C1D | 5.31  | 134.08      | 124.73   |
| 11  | aB    | 814 | CLA  | CHD-C4C-C3C | -5.31 | 117.03      | 124.77   |
| 11  | cA    | 812 | CLA  | CHD-C4C-C3C | -5.31 | 117.04      | 124.77   |
| 11  | cL    | 205 | CLA  | CMD-C2D-C1D | 5.31  | 134.07      | 124.73   |
| 11  | bB    | 809 | CLA  | CMD-C2D-C1D | 5.30  | 134.07      | 124.73   |
| 11  | cA    | 802 | CLA  | CAA-C2A-C3A | -5.30 | 98.67       | 113.00   |
| 11  | cA    | 807 | CLA  | O2D-CGD-CBD | 5.30  | 120.50      | 111.23   |
| 11  | bB    | 814 | CLA  | CHD-C4C-C3C | -5.30 | 117.04      | 124.77   |
| 11  | aA    | 820 | CLA  | C2C-C1C-NC  | 5.30  | 115.55      | 109.98   |
| 11  | aB    | 809 | CLA  | CMD-C2D-C1D | 5.30  | 134.06      | 124.73   |
| 11  | aB    | 825 | CLA  | O2D-CGD-CBD | 5.30  | 120.49      | 111.23   |
| 11  | cA    | 838 | CLA  | O2D-CGD-CBD | 5.30  | 120.49      | 111.23   |
| 11  | cB    | 814 | CLA  | CHD-C4C-C3C | -5.30 | 117.05      | 124.77   |
| 11  | aB    | 802 | CLA  | C3B-C2B-C1B | -5.30 | 100.93      | 107.17   |
| 12  | bA    | 826 | F6C  | C1A-C2A-C3A | -5.29 | 101.39      | 106.97   |
| 11  | cB    | 809 | CLA  | CMD-C2D-C1D | 5.29  | 134.05      | 124.73   |
| 11  | aA    | 805 | CLA  | C2B-C1B-NB  | 5.29  | 115.81      | 110.33   |
| 12  | bA    | 832 | F6C  | C2D-C1D-ND  | 5.28  | 115.53      | 109.98   |
| 11  | bA    | 838 | CLA  | O2D-CGD-CBD | 5.28  | 120.47      | 111.23   |
| 11  | bB    | 825 | CLA  | O2D-CGD-CBD | 5.28  | 120.47      | 111.23   |
| 12  | aA    | 832 | F6C  | C2D-C1D-ND  | 5.28  | 115.53      | 109.98   |
| 11  | cB    | 829 | CLA  | C2D-C1D-ND  | 5.28  | 115.35      | 110.13   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bA    | 807 | CLA  | O2D-CGD-CBD | 5.28  | 120.46      | 111.23   |
| 11  | aA    | 838 | CLA  | O2D-CGD-CBD | 5.28  | 120.46      | 111.23   |
| 11  | bA    | 809 | CLA  | C3B-C2B-C1B | -5.28 | 100.95      | 107.17   |
| 11  | cB    | 825 | CLA  | O2D-CGD-CBD | 5.28  | 120.45      | 111.23   |
| 11  | cB    | 832 | CLA  | C2B-C1B-NB  | 5.27  | 115.80      | 110.33   |
| 11  | bA    | 820 | CLA  | C2C-C1C-NC  | 5.27  | 115.52      | 109.98   |
| 11  | cA    | 820 | CLA  | C2C-C1C-NC  | 5.27  | 115.52      | 109.98   |
| 11  | bB    | 829 | CLA  | C2D-C1D-ND  | 5.27  | 115.34      | 110.13   |
| 12  | bA    | 826 | F6C  | C3C-C4C-NC  | 5.27  | 116.09      | 110.32   |
| 11  | aA    | 835 | CLA  | O2D-CGD-CBD | 5.27  | 120.44      | 111.23   |
| 11  | cA    | 835 | CLA  | O2D-CGD-CBD | 5.26  | 120.43      | 111.23   |
| 11  | bA    | 835 | CLA  | O2D-CGD-CBD | 5.26  | 120.43      | 111.23   |
| 11  | aB    | 832 | CLA  | C2B-C1B-NB  | 5.26  | 115.78      | 110.33   |
| 11  | cA    | 828 | CLA  | C3D-C2D-C1D | -5.26 | 98.65       | 105.83   |
| 11  | aA    | 807 | CLA  | O2D-CGD-CBD | 5.26  | 120.42      | 111.23   |
| 12  | bA    | 826 | F6C  | C2B-C3B-C4B | -5.25 | 103.75      | 106.46   |
| 11  | bA    | 828 | CLA  | C3D-C2D-C1D | -5.25 | 98.67       | 105.83   |
| 12  | aA    | 826 | F6C  | C3C-C4C-NC  | 5.25  | 116.07      | 110.32   |
| 11  | cA    | 809 | CLA  | C3B-C2B-C1B | -5.25 | 100.98      | 107.17   |
| 11  | cA    | 821 | CLA  | C2C-C1C-NC  | 5.24  | 115.49      | 109.98   |
| 11  | aA    | 820 | CLA  | CHD-C4C-C3C | -5.24 | 117.13      | 124.77   |
| 11  | cA    | 831 | CLA  | CHD-C4C-C3C | -5.24 | 117.13      | 124.77   |
| 11  | aA    | 809 | CLA  | C3B-C2B-C1B | -5.24 | 100.99      | 107.17   |
| 12  | cA    | 832 | F6C  | C2D-C1D-ND  | 5.24  | 115.48      | 109.98   |
| 11  | cA    | 820 | CLA  | CHD-C4C-C3C | -5.24 | 117.14      | 124.77   |
| 11  | bB    | 821 | CLA  | C2C-C1C-NC  | 5.24  | 115.48      | 109.98   |
| 11  | bA    | 821 | CLA  | C2C-C1C-NC  | 5.23  | 115.48      | 109.98   |
| 12  | aL    | 202 | F6C  | C2B-C3B-C4B | -5.23 | 103.76      | 106.46   |
| 11  | cA    | 815 | CLA  | C2C-C1C-NC  | 5.23  | 115.48      | 109.98   |
| 11  | aA    | 831 | CLA  | CHD-C4C-C3C | -5.23 | 117.15      | 124.77   |
| 11  | aL    | 205 | CLA  | O2D-CGD-CBD | 5.23  | 120.37      | 111.23   |
| 11  | aA    | 821 | CLA  | C2C-C1C-NC  | 5.23  | 115.47      | 109.98   |
| 11  | bL    | 205 | CLA  | O2D-CGD-CBD | 5.23  | 120.37      | 111.23   |
| 12  | cA    | 826 | F6C  | C3C-C4C-NC  | 5.23  | 116.05      | 110.32   |
| 11  | bA    | 831 | CLA  | CHD-C4C-C3C | -5.23 | 117.15      | 124.77   |
| 11  | bB    | 812 | CLA  | CHD-C4C-C3C | -5.22 | 117.16      | 124.77   |
| 11  | bA    | 820 | CLA  | CHD-C4C-C3C | -5.22 | 117.16      | 124.77   |
| 11  | aB    | 821 | CLA  | C2C-C1C-NC  | 5.22  | 115.47      | 109.98   |
| 11  | cB    | 829 | CLA  | O2D-CGD-CBD | 5.22  | 120.36      | 111.23   |
| 11  | aA    | 815 | CLA  | C2C-C1C-NC  | 5.22  | 115.47      | 109.98   |
| 11  | aB    | 829 | CLA  | C2D-C1D-ND  | 5.22  | 115.29      | 110.13   |
| 11  | aB    | 802 | CLA  | C4A-NA-C1A  | -5.22 | 104.30      | 106.68   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cL    | 205 | CLA  | O2D-CGD-CBD | 5.22  | 120.35      | 111.23   |
| 11  | aB    | 805 | CLA  | C2B-C1B-NB  | 5.21  | 115.73      | 110.33   |
| 11  | aB    | 829 | CLA  | O2D-CGD-CBD | 5.21  | 120.34      | 111.23   |
| 11  | bB    | 835 | CLA  | C2C-C1C-NC  | 5.21  | 115.45      | 109.98   |
| 11  | aA    | 828 | CLA  | C3D-C2D-C1D | -5.20 | 98.73       | 105.83   |
| 11  | bB    | 823 | CLA  | C2B-C1B-NB  | 5.20  | 115.72      | 110.33   |
| 11  | bB    | 829 | CLA  | O2D-CGD-CBD | 5.20  | 120.32      | 111.23   |
| 11  | aA    | 829 | CLA  | C2B-C1B-NB  | 5.20  | 115.72      | 110.33   |
| 12  | aA    | 827 | F6C  | C4A-C3A-C2A | -5.20 | 99.26       | 106.97   |
| 11  | bA    | 815 | CLA  | O2D-CGD-CBD | 5.20  | 120.32      | 111.23   |
| 11  | aB    | 812 | CLA  | CHD-C4C-C3C | -5.20 | 117.20      | 124.77   |
| 11  | cB    | 821 | CLA  | C2C-C1C-NC  | 5.20  | 115.44      | 109.98   |
| 12  | cL    | 202 | F6C  | C2B-C3B-C4B | -5.20 | 103.78      | 106.46   |
| 11  | bB    | 802 | CLA  | C4A-NA-C1A  | -5.19 | 104.31      | 106.68   |
| 11  | aA    | 829 | CLA  | C3B-C2B-C1B | -5.19 | 101.05      | 107.17   |
| 11  | cB    | 835 | CLA  | C2C-C1C-NC  | 5.19  | 115.44      | 109.98   |
| 11  | bA    | 815 | CLA  | C2C-C1C-NC  | 5.19  | 115.44      | 109.98   |
| 11  | cB    | 823 | CLA  | C2C-C1C-NC  | 5.19  | 115.43      | 109.98   |
| 12  | bA    | 827 | F6C  | C4A-C3A-C2A | -5.19 | 99.27       | 106.97   |
| 11  | aB    | 835 | CLA  | C2C-C1C-NC  | 5.19  | 115.43      | 109.98   |
| 11  | bB    | 805 | CLA  | C2B-C1B-NB  | 5.19  | 115.71      | 110.33   |
| 11  | cA    | 815 | CLA  | O2D-CGD-CBD | 5.19  | 120.30      | 111.23   |
| 11  | aB    | 816 | CLA  | C2B-C1B-NB  | 5.19  | 115.70      | 110.33   |
| 11  | cB    | 816 | CLA  | C2B-C1B-NB  | 5.19  | 115.70      | 110.33   |
| 11  | aA    | 815 | CLA  | O2D-CGD-CBD | 5.18  | 120.28      | 111.23   |
| 11  | bA    | 823 | CLA  | C3D-C2D-C1D | -5.18 | 98.76       | 105.83   |
| 11  | aB    | 812 | CLA  | C2D-C1D-ND  | 5.18  | 115.25      | 110.13   |
| 11  | cB    | 823 | CLA  | C2B-C1B-NB  | 5.17  | 115.69      | 110.33   |
| 11  | bB    | 839 | CLA  | C2D-C1D-ND  | 5.17  | 115.25      | 110.13   |
| 11  | cA    | 829 | CLA  | C3B-C2B-C1B | -5.17 | 101.07      | 107.17   |
| 11  | cB    | 812 | CLA  | CHD-C4C-C3C | -5.17 | 117.24      | 124.77   |
| 11  | cB    | 805 | CLA  | C2B-C1B-NB  | 5.17  | 115.69      | 110.33   |
| 11  | bA    | 825 | CLA  | O2D-CGD-CBD | 5.17  | 120.26      | 111.23   |
| 11  | aA    | 810 | CLA  | C2C-C1C-NC  | 5.17  | 115.41      | 109.98   |
| 11  | bA    | 829 | CLA  | C3B-C2B-C1B | -5.16 | 101.08      | 107.17   |
| 11  | cA    | 829 | CLA  | C2B-C1B-NB  | 5.16  | 115.68      | 110.33   |
| 11  | cB    | 839 | CLA  | C2D-C1D-ND  | 5.16  | 115.23      | 110.13   |
| 11  | aA    | 823 | CLA  | C3D-C2D-C1D | -5.16 | 98.79       | 105.83   |
| 11  | aA    | 825 | CLA  | O2D-CGD-CBD | 5.16  | 120.25      | 111.23   |
| 11  | cA    | 823 | CLA  | C3D-C2D-C1D | -5.16 | 98.80       | 105.83   |
| 11  | cA    | 825 | CLA  | O2D-CGD-CBD | 5.16  | 120.24      | 111.23   |
| 11  | cB    | 822 | CLA  | O2D-CGD-CBD | 5.16  | 120.24      | 111.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cA    | 812 | CLA  | C2B-C1B-NB  | 5.15  | 115.67      | 110.33   |
| 11  | aB    | 822 | CLA  | O2D-CGD-CBD | 5.15  | 120.24      | 111.23   |
| 12  | cA    | 827 | F6C  | C4A-C3A-C2A | -5.15 | 99.33       | 106.97   |
| 11  | aB    | 839 | CLA  | C2D-C1D-ND  | 5.15  | 115.22      | 110.13   |
| 11  | bA    | 829 | CLA  | C2B-C1B-NB  | 5.14  | 115.66      | 110.33   |
| 11  | bA    | 812 | CLA  | C2B-C1B-NB  | 5.14  | 115.66      | 110.33   |
| 11  | cA    | 810 | CLA  | C2C-C1C-NC  | 5.14  | 115.38      | 109.98   |
| 11  | aA    | 818 | CLA  | CMD-C2D-C1D | 5.14  | 133.78      | 124.73   |
| 12  | bB    | 824 | F6C  | C1A-C2A-C3A | -5.14 | 101.56      | 106.97   |
| 11  | bB    | 822 | CLA  | O2D-CGD-CBD | 5.14  | 120.21      | 111.23   |
| 11  | aB    | 823 | CLA  | C2B-C1B-NB  | 5.14  | 115.65      | 110.33   |
| 12  | bL    | 202 | F6C  | C2C-C1C-NC  | 5.14  | 115.65      | 110.33   |
| 11  | aB    | 823 | CLA  | C2C-C1C-NC  | 5.14  | 115.38      | 109.98   |
| 11  | bB    | 803 | CLA  | C3B-C2B-C1B | -5.14 | 101.11      | 107.17   |
| 11  | bA    | 818 | CLA  | CMD-C2D-C1D | 5.13  | 133.77      | 124.73   |
| 11  | cA    | 818 | CLA  | CMD-C2D-C1D | 5.13  | 133.77      | 124.73   |
| 11  | bB    | 823 | CLA  | C2C-C1C-NC  | 5.13  | 115.37      | 109.98   |
| 12  | cL    | 202 | F6C  | C2C-C1C-NC  | 5.13  | 115.65      | 110.33   |
| 12  | aA    | 827 | F6C  | O2D-CGD-CBD | 5.13  | 120.19      | 111.23   |
| 11  | cB    | 803 | CLA  | C3B-C2B-C1B | -5.13 | 101.12      | 107.17   |
| 11  | bA    | 802 | CLA  | C4A-NA-C1A  | -5.13 | 104.34      | 106.68   |
| 12  | cB    | 824 | F6C  | C1A-C2A-C3A | -5.12 | 101.57      | 106.97   |
| 11  | aB    | 804 | CLA  | C3B-C2B-C1B | -5.12 | 101.13      | 107.17   |
| 12  | aL    | 202 | F6C  | CAA-C2A-C3A | -5.12 | 118.27      | 127.87   |
| 11  | cB    | 804 | CLA  | C3B-C2B-C1B | -5.12 | 101.13      | 107.17   |
| 11  | cB    | 823 | CLA  | C3B-C2B-C1B | -5.12 | 101.13      | 107.17   |
| 11  | bB    | 804 | CLA  | C3B-C2B-C1B | -5.12 | 101.14      | 107.17   |
| 12  | bA    | 827 | F6C  | O2D-CGD-CBD | 5.12  | 120.18      | 111.23   |
| 12  | bL    | 202 | F6C  | CAA-C2A-C3A | -5.12 | 118.28      | 127.87   |
| 11  | bA    | 810 | CLA  | C2C-C1C-NC  | 5.11  | 115.35      | 109.98   |
| 11  | bB    | 823 | CLA  | C3B-C2B-C1B | -5.11 | 101.14      | 107.17   |
| 11  | bB    | 816 | CLA  | C2B-C1B-NB  | 5.11  | 115.63      | 110.33   |
| 11  | aA    | 812 | CLA  | C2B-C1B-NB  | 5.11  | 115.62      | 110.33   |
| 12  | aB    | 824 | F6C  | C2D-C1D-ND  | 5.11  | 115.35      | 109.98   |
| 11  | aB    | 838 | CLA  | O2D-CGD-CBD | 5.11  | 120.16      | 111.23   |
| 12  | cL    | 202 | F6C  | CAA-C2A-C3A | -5.11 | 118.30      | 127.87   |
| 12  | cB    | 824 | F6C  | C2D-C1D-ND  | 5.11  | 115.35      | 109.98   |
| 11  | bA    | 805 | CLA  | C3B-C2B-C1B | -5.11 | 101.15      | 107.17   |
| 11  | bA    | 806 | CLA  | C3B-C2B-C1B | -5.10 | 101.15      | 107.17   |
| 11  | cA    | 806 | CLA  | C3B-C2B-C1B | -5.10 | 101.15      | 107.17   |
| 12  | aB    | 824 | F6C  | C1A-C2A-C3A | -5.10 | 101.60      | 106.97   |
| 11  | cA    | 805 | CLA  | C3B-C2B-C1B | -5.10 | 101.16      | 107.17   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aA    | 806 | CLA  | C3B-C2B-C1B | -5.10 | 101.16      | 107.17   |
| 11  | cB    | 817 | CLA  | C2C-C1C-NC  | 5.10  | 115.34      | 109.98   |
| 11  | cB    | 805 | CLA  | O2D-CGD-CBD | 5.09  | 120.14      | 111.23   |
| 11  | aB    | 803 | CLA  | C3B-C2B-C1B | -5.09 | 101.17      | 107.17   |
| 11  | cB    | 838 | CLA  | O2D-CGD-CBD | 5.09  | 120.13      | 111.23   |
| 12  | aL    | 202 | F6C  | C2C-C1C-NC  | 5.09  | 115.60      | 110.33   |
| 11  | aB    | 805 | CLA  | O2D-CGD-CBD | 5.09  | 120.12      | 111.23   |
| 12  | cA    | 827 | F6C  | O2D-CGD-CBD | 5.09  | 120.12      | 111.23   |
| 11  | aB    | 817 | CLA  | C2C-C1C-NC  | 5.08  | 115.32      | 109.98   |
| 11  | cB    | 812 | CLA  | C2D-C1D-ND  | 5.08  | 115.16      | 110.13   |
| 11  | bB    | 805 | CLA  | O2D-CGD-CBD | 5.08  | 120.11      | 111.23   |
| 11  | bB    | 838 | CLA  | O2D-CGD-CBD | 5.08  | 120.11      | 111.23   |
| 11  | aA    | 805 | CLA  | C3B-C2B-C1B | -5.08 | 101.18      | 107.17   |
| 11  | bB    | 812 | CLA  | C2D-C1D-ND  | 5.08  | 115.15      | 110.13   |
| 11  | cB    | 817 | CLA  | O2D-CGD-CBD | 5.07  | 120.10      | 111.23   |
| 12  | bB    | 824 | F6C  | C2D-C1D-ND  | 5.07  | 115.31      | 109.98   |
| 11  | bB    | 817 | CLA  | O2D-CGD-CBD | 5.07  | 120.09      | 111.23   |
| 11  | aL    | 204 | CLA  | C2C-C1C-NC  | 5.07  | 115.31      | 109.98   |
| 11  | bB    | 817 | CLA  | C2C-C1C-NC  | 5.07  | 115.31      | 109.98   |
| 11  | aB    | 817 | CLA  | O2D-CGD-CBD | 5.07  | 120.09      | 111.23   |
| 11  | cB    | 825 | CLA  | C3D-C2D-C1D | -5.07 | 98.91       | 105.83   |
| 11  | cA    | 839 | CLA  | O2D-CGD-CBD | 5.07  | 120.09      | 111.23   |
| 11  | cB    | 802 | CLA  | C4A-NA-C1A  | -5.07 | 104.37      | 106.68   |
| 11  | aA    | 823 | CLA  | CMD-C2D-C1D | 5.07  | 133.65      | 124.73   |
| 11  | bA    | 839 | CLA  | C2C-C1C-NC  | 5.07  | 115.30      | 109.98   |
| 11  | bB    | 814 | CLA  | C2C-C1C-NC  | 5.07  | 115.30      | 109.98   |
| 11  | aB    | 823 | CLA  | C3B-C2B-C1B | -5.07 | 101.20      | 107.17   |
| 11  | cA    | 823 | CLA  | CMD-C2D-C1D | 5.07  | 133.65      | 124.73   |
| 11  | bL    | 204 | CLA  | C2C-C1C-NC  | 5.07  | 115.30      | 109.98   |
| 11  | aB    | 832 | CLA  | C3B-C2B-C1B | -5.06 | 101.20      | 107.17   |
| 11  | aB    | 810 | CLA  | C2C-C1C-NC  | 5.06  | 115.30      | 109.98   |
| 11  | bB    | 832 | CLA  | C3B-C2B-C1B | -5.06 | 101.21      | 107.17   |
| 11  | cB    | 832 | CLA  | C3B-C2B-C1B | -5.06 | 101.21      | 107.17   |
| 11  | cB    | 826 | CLA  | O2D-CGD-CBD | 5.06  | 120.07      | 111.23   |
| 11  | bB    | 825 | CLA  | C3D-C2D-C1D | -5.06 | 98.93       | 105.83   |
| 11  | bA    | 823 | CLA  | CMD-C2D-C1D | 5.05  | 133.63      | 124.73   |
| 11  | aA    | 839 | CLA  | O2D-CGD-CBD | 5.05  | 120.06      | 111.23   |
| 11  | aB    | 838 | CLA  | C2C-C1C-NC  | 5.05  | 115.29      | 109.98   |
| 11  | aB    | 814 | CLA  | C2C-C1C-NC  | 5.05  | 115.28      | 109.98   |
| 11  | bB    | 838 | CLA  | C2C-C1C-NC  | 5.05  | 115.28      | 109.98   |
| 11  | bB    | 826 | CLA  | O2D-CGD-CBD | 5.05  | 120.05      | 111.23   |
| 11  | bA    | 812 | CLA  | C3B-C2B-C1B | -5.05 | 101.22      | 107.17   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bA    | 839 | CLA  | O2D-CGD-CBD | 5.05  | 120.05      | 111.23   |
| 11  | aA    | 803 | CLA  | C3B-C2B-C1B | -5.05 | 101.22      | 107.17   |
| 11  | aB    | 814 | CLA  | C2B-C1B-NB  | 5.05  | 115.56      | 110.33   |
| 11  | cL    | 204 | CLA  | C2C-C1C-NC  | 5.04  | 115.28      | 109.98   |
| 12  | bA    | 826 | F6C  | C4A-C3A-C2A | -5.04 | 99.49       | 106.97   |
| 11  | aA    | 839 | CLA  | C2C-C1C-NC  | 5.04  | 115.28      | 109.98   |
| 11  | cB    | 838 | CLA  | C2C-C1C-NC  | 5.04  | 115.28      | 109.98   |
| 11  | cA    | 803 | CLA  | C3B-C2B-C1B | -5.04 | 101.23      | 107.17   |
| 11  | aB    | 827 | CLA  | C2C-C1C-NC  | 5.04  | 115.28      | 109.98   |
| 11  | cB    | 810 | CLA  | C2C-C1C-NC  | 5.04  | 115.28      | 109.98   |
| 11  | cB    | 814 | CLA  | C2B-C1B-NB  | 5.04  | 115.55      | 110.33   |
| 12  | aA    | 826 | F6C  | C4A-C3A-C2A | -5.04 | 99.49       | 106.97   |
| 11  | aB    | 825 | CLA  | C3D-C2D-C1D | -5.04 | 98.96       | 105.83   |
| 11  | bA    | 829 | CLA  | C2C-C1C-NC  | 5.04  | 115.27      | 109.98   |
| 11  | cB    | 822 | CLA  | C3D-C2D-C1D | -5.03 | 98.96       | 105.83   |
| 11  | bB    | 827 | CLA  | C2C-C1C-NC  | 5.03  | 115.27      | 109.98   |
| 11  | cB    | 802 | CLA  | CAA-C2A-C3A | -5.03 | 99.41       | 113.00   |
| 11  | aA    | 819 | CLA  | C2B-C1B-NB  | 5.03  | 115.54      | 110.33   |
| 11  | cB    | 814 | CLA  | C2C-C1C-NC  | 5.03  | 115.26      | 109.98   |
| 11  | cA    | 812 | CLA  | C3B-C2B-C1B | -5.03 | 101.24      | 107.17   |
| 11  | cB    | 830 | CLA  | O2D-CGD-CBD | 5.03  | 120.02      | 111.23   |
| 12  | cA    | 826 | F6C  | C4A-C3A-C2A | -5.02 | 99.52       | 106.97   |
| 11  | bB    | 830 | CLA  | O2D-CGD-CBD | 5.02  | 120.01      | 111.23   |
| 11  | cB    | 813 | CLA  | C2C-C1C-NC  | 5.02  | 115.26      | 109.98   |
| 11  | bB    | 822 | CLA  | C3D-C2D-C1D | -5.02 | 98.98       | 105.83   |
| 11  | bB    | 814 | CLA  | C2B-C1B-NB  | 5.02  | 115.53      | 110.33   |
| 11  | cB    | 827 | CLA  | C2C-C1C-NC  | 5.02  | 115.25      | 109.98   |
| 11  | aB    | 802 | CLA  | CAA-C2A-C3A | -5.02 | 99.43       | 113.00   |
| 11  | aB    | 826 | CLA  | O2D-CGD-CBD | 5.02  | 120.00      | 111.23   |
| 11  | bB    | 802 | CLA  | CAA-C2A-C3A | -5.02 | 99.44       | 113.00   |
| 11  | aB    | 830 | CLA  | O2D-CGD-CBD | 5.01  | 120.00      | 111.23   |
| 11  | aA    | 834 | CLA  | C2C-C1C-NC  | 5.01  | 115.25      | 109.98   |
| 11  | cA    | 839 | CLA  | C2C-C1C-NC  | 5.01  | 115.25      | 109.98   |
| 11  | bA    | 834 | CLA  | C2C-C1C-NC  | 5.01  | 115.25      | 109.98   |
| 11  | bA    | 809 | CLA  | C2B-C1B-NB  | 5.01  | 115.52      | 110.33   |
| 11  | aB    | 822 | CLA  | C3D-C2D-C1D | -5.01 | 99.00       | 105.83   |
| 11  | bA    | 803 | CLA  | C3B-C2B-C1B | -5.01 | 101.27      | 107.17   |
| 11  | cB    | 812 | CLA  | C3B-C2B-C1B | -5.00 | 101.27      | 107.17   |
| 11  | aA    | 840 | CLA  | C2B-C1B-NB  | 5.00  | 115.51      | 110.33   |
| 11  | aB    | 812 | CLA  | C3B-C2B-C1B | -5.00 | 101.27      | 107.17   |
| 11  | aA    | 835 | CLA  | C3B-C2B-C1B | -5.00 | 101.28      | 107.17   |
| 12  | bA    | 826 | F6C  | C2C-C1C-NC  | 5.00  | 115.51      | 110.33   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cA    | 837 | CLA  | C3B-C2B-C1B | -5.00 | 101.28      | 107.17   |
| 11  | cA    | 829 | CLA  | C2C-C1C-NC  | 5.00  | 115.23      | 109.98   |
| 11  | bA    | 819 | CLA  | C2B-C1B-NB  | 4.99  | 115.50      | 110.33   |
| 11  | aA    | 812 | CLA  | C3B-C2B-C1B | -4.99 | 101.28      | 107.17   |
| 11  | cB    | 833 | CLA  | C2B-C1B-NB  | 4.99  | 115.50      | 110.33   |
| 11  | cB    | 822 | CLA  | C3B-C2B-C1B | -4.99 | 101.29      | 107.17   |
| 11  | cA    | 834 | CLA  | C2C-C1C-NC  | 4.99  | 115.22      | 109.98   |
| 11  | bB    | 810 | CLA  | C2C-C1C-NC  | 4.99  | 115.22      | 109.98   |
| 12  | aA    | 826 | F6C  | C2C-C1C-NC  | 4.99  | 115.50      | 110.33   |
| 11  | cB    | 805 | CLA  | C3B-C2B-C1B | -4.99 | 101.29      | 107.17   |
| 11  | cA    | 802 | CLA  | C4A-NA-C1A  | -4.98 | 104.41      | 106.68   |
| 11  | bB    | 831 | CLA  | C2C-C1C-NC  | 4.98  | 115.22      | 109.98   |
| 11  | cA    | 816 | CLA  | C2B-C1B-NB  | 4.98  | 115.49      | 110.33   |
| 11  | cA    | 840 | CLA  | C2C-C1C-NC  | 4.98  | 115.21      | 109.98   |
| 11  | aB    | 822 | CLA  | C3B-C2B-C1B | -4.98 | 101.30      | 107.17   |
| 11  | bA    | 840 | CLA  | C2C-C1C-NC  | 4.98  | 115.21      | 109.98   |
| 11  | cA    | 819 | CLA  | C2B-C1B-NB  | 4.98  | 115.49      | 110.33   |
| 11  | cA    | 825 | CLA  | C2C-C1C-NC  | 4.98  | 115.21      | 109.98   |
| 11  | cA    | 835 | CLA  | C3B-C2B-C1B | -4.97 | 101.31      | 107.17   |
| 11  | aA    | 816 | CLA  | C2B-C1B-NB  | 4.97  | 115.48      | 110.33   |
| 11  | aB    | 829 | CLA  | C1C-C2C-C3C | -4.97 | 101.75      | 106.98   |
| 11  | bB    | 833 | CLA  | C2B-C1B-NB  | 4.97  | 115.48      | 110.33   |
| 11  | cB    | 831 | CLA  | C2C-C1C-NC  | 4.97  | 115.20      | 109.98   |
| 11  | aB    | 831 | CLA  | C2C-C1C-NC  | 4.97  | 115.20      | 109.98   |
| 11  | aB    | 833 | CLA  | C2B-C1B-NB  | 4.97  | 115.48      | 110.33   |
| 11  | bA    | 825 | CLA  | C2C-C1C-NC  | 4.97  | 115.20      | 109.98   |
| 11  | cB    | 829 | CLA  | C1C-C2C-C3C | -4.97 | 101.75      | 106.98   |
| 11  | aA    | 808 | CLA  | C3B-C2B-C1B | -4.97 | 101.31      | 107.17   |
| 11  | cA    | 840 | CLA  | C2B-C1B-NB  | 4.97  | 115.48      | 110.33   |
| 11  | aA    | 809 | CLA  | C2B-C1B-NB  | 4.97  | 115.47      | 110.33   |
| 11  | bA    | 840 | CLA  | C2B-C1B-NB  | 4.97  | 115.47      | 110.33   |
| 11  | bB    | 829 | CLA  | C1C-C2C-C3C | -4.96 | 101.76      | 106.98   |
| 11  | cA    | 828 | CLA  | C3B-C2B-C1B | -4.96 | 101.32      | 107.17   |
| 11  | aB    | 813 | CLA  | C2C-C1C-NC  | 4.96  | 115.19      | 109.98   |
| 11  | cA    | 808 | CLA  | C3B-C2B-C1B | -4.96 | 101.32      | 107.17   |
| 11  | cA    | 809 | CLA  | C2B-C1B-NB  | 4.96  | 115.47      | 110.33   |
| 11  | bB    | 813 | CLA  | C2C-C1C-NC  | 4.96  | 115.19      | 109.98   |
| 11  | bB    | 822 | CLA  | C3B-C2B-C1B | -4.96 | 101.32      | 107.17   |
| 10  | cA    | 801 | CL0  | CAA-C2A-C3A | -4.96 | 99.60       | 113.00   |
| 11  | bB    | 812 | CLA  | C2C-C1C-NC  | 4.96  | 115.19      | 109.98   |
| 11  | cA    | 818 | CLA  | C2B-C1B-NB  | 4.96  | 115.47      | 110.33   |
| 11  | aA    | 825 | CLA  | C2C-C1C-NC  | 4.96  | 115.19      | 109.98   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bA    | 835 | CLA  | C3B-C2B-C1B | -4.96 | 101.33      | 107.17   |
| 11  | aA    | 838 | CLA  | C2C-C1C-NC  | 4.96  | 115.19      | 109.98   |
| 11  | bA    | 828 | CLA  | C3B-C2B-C1B | -4.96 | 101.33      | 107.17   |
| 11  | bB    | 812 | CLA  | C3B-C2B-C1B | -4.96 | 101.33      | 107.17   |
| 11  | cB    | 820 | CLA  | C2C-C1C-NC  | 4.95  | 115.19      | 109.98   |
| 10  | aA    | 801 | CL0  | CAA-C2A-C3A | -4.95 | 99.61       | 113.00   |
| 11  | aB    | 805 | CLA  | C3B-C2B-C1B | -4.95 | 101.33      | 107.17   |
| 11  | bB    | 806 | CLA  | C3D-C2D-C1D | -4.95 | 99.07       | 105.83   |
| 11  | aA    | 829 | CLA  | C2C-C1C-NC  | 4.95  | 115.18      | 109.98   |
| 11  | aA    | 837 | CLA  | C3B-C2B-C1B | -4.95 | 101.33      | 107.17   |
| 11  | aB    | 812 | CLA  | C2C-C1C-NC  | 4.95  | 115.18      | 109.98   |
| 11  | bB    | 830 | CLA  | C2C-C1C-NC  | 4.95  | 115.18      | 109.98   |
| 11  | aA    | 828 | CLA  | C3B-C2B-C1B | -4.95 | 101.33      | 107.17   |
| 11  | bA    | 837 | CLA  | C3B-C2B-C1B | -4.95 | 101.33      | 107.17   |
| 11  | bA    | 808 | CLA  | C3B-C2B-C1B | -4.95 | 101.34      | 107.17   |
| 11  | cA    | 842 | CLA  | C2B-C1B-NB  | 4.95  | 115.46      | 110.33   |
| 11  | aB    | 806 | CLA  | C3D-C2D-C1D | -4.95 | 99.08       | 105.83   |
| 11  | cB    | 806 | CLA  | C3D-C2D-C1D | -4.94 | 99.08       | 105.83   |
| 10  | bA    | 801 | CL0  | CAA-C2A-C3A | -4.94 | 99.64       | 113.00   |
| 11  | bB    | 805 | CLA  | C3B-C2B-C1B | -4.94 | 101.34      | 107.17   |
| 11  | bB    | 815 | CLA  | C3B-C2B-C1B | -4.94 | 101.34      | 107.17   |
| 11  | aB    | 831 | CLA  | C2B-C1B-NB  | 4.94  | 115.45      | 110.33   |
| 11  | aB    | 825 | CLA  | C3B-C2B-C1B | -4.94 | 101.34      | 107.17   |
| 11  | aB    | 830 | CLA  | C2C-C1C-NC  | 4.94  | 115.17      | 109.98   |
| 11  | aB    | 816 | CLA  | C3B-C2B-C1B | -4.94 | 101.35      | 107.17   |
| 11  | bA    | 816 | CLA  | C2B-C1B-NB  | 4.94  | 115.45      | 110.33   |
| 12  | cA    | 826 | F6C  | C2C-C1C-NC  | 4.94  | 115.45      | 110.33   |
| 11  | bA    | 816 | CLA  | O2D-CGD-CBD | 4.94  | 119.86      | 111.23   |
| 11  | aB    | 827 | CLA  | C3B-C2B-C1B | -4.93 | 101.36      | 107.17   |
| 11  | bA    | 842 | CLA  | C2B-C1B-NB  | 4.93  | 115.44      | 110.33   |
| 11  | cB    | 812 | CLA  | C2C-C1C-NC  | 4.93  | 115.16      | 109.98   |
| 11  | aA    | 842 | CLA  | C2B-C1B-NB  | 4.93  | 115.44      | 110.33   |
| 11  | aA    | 816 | CLA  | O2D-CGD-CBD | 4.93  | 119.85      | 111.23   |
| 11  | bB    | 822 | CLA  | C2B-C1B-NB  | 4.93  | 115.44      | 110.33   |
| 11  | cK    | 103 | CLA  | C2C-C1C-NC  | 4.93  | 115.16      | 109.98   |
| 11  | bB    | 819 | CLA  | O2D-CGD-CBD | 4.93  | 119.84      | 111.23   |
| 11  | aB    | 822 | CLA  | C2B-C1B-NB  | 4.93  | 115.44      | 110.33   |
| 11  | cB    | 819 | CLA  | O2D-CGD-CBD | 4.93  | 119.84      | 111.23   |
| 11  | aA    | 840 | CLA  | C2C-C1C-NC  | 4.93  | 115.16      | 109.98   |
| 11  | aA    | 807 | CLA  | C2C-C1C-NC  | 4.93  | 115.16      | 109.98   |
| 11  | aB    | 819 | CLA  | C3B-C2B-C1B | -4.92 | 101.36      | 107.17   |
| 11  | cB    | 825 | CLA  | C3B-C2B-C1B | -4.92 | 101.36      | 107.17   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cA    | 838 | CLA  | C2C-C1C-NC  | 4.92  | 115.15      | 109.98   |
| 11  | bB    | 827 | CLA  | C3B-C2B-C1B | -4.92 | 101.37      | 107.17   |
| 11  | cB    | 815 | CLA  | C3B-C2B-C1B | -4.92 | 101.37      | 107.17   |
| 11  | aB    | 819 | CLA  | O2D-CGD-CBD | 4.92  | 119.83      | 111.23   |
| 11  | aA    | 818 | CLA  | C2B-C1B-NB  | 4.92  | 115.43      | 110.33   |
| 11  | cB    | 804 | CLA  | C2B-C1B-NB  | 4.92  | 115.43      | 110.33   |
| 11  | cB    | 831 | CLA  | C2B-C1B-NB  | 4.92  | 115.43      | 110.33   |
| 11  | cA    | 816 | CLA  | O2D-CGD-CBD | 4.92  | 119.83      | 111.23   |
| 11  | cB    | 827 | CLA  | C3B-C2B-C1B | -4.92 | 101.37      | 107.17   |
| 11  | cA    | 837 | CLA  | C2B-C1B-NB  | 4.91  | 115.42      | 110.33   |
| 11  | bB    | 825 | CLA  | C3B-C2B-C1B | -4.91 | 101.38      | 107.17   |
| 11  | bA    | 838 | CLA  | C2C-C1C-NC  | 4.91  | 115.14      | 109.98   |
| 11  | aB    | 815 | CLA  | C3B-C2B-C1B | -4.91 | 101.38      | 107.17   |
| 11  | cB    | 822 | CLA  | C2B-C1B-NB  | 4.91  | 115.42      | 110.33   |
| 11  | bA    | 838 | CLA  | C3B-C2B-C1B | -4.91 | 101.38      | 107.17   |
| 11  | bA    | 804 | CLA  | C3B-C2B-C1B | -4.91 | 101.38      | 107.17   |
| 11  | bB    | 819 | CLA  | C3B-C2B-C1B | -4.91 | 101.38      | 107.17   |
| 11  | aA    | 831 | CLA  | CMD-C2D-C1D | 4.91  | 133.38      | 124.73   |
| 11  | aK    | 103 | CLA  | C2C-C1C-NC  | 4.91  | 115.14      | 109.98   |
| 12  | aB    | 824 | F6C  | C4A-C3A-C2A | -4.91 | 99.69       | 106.97   |
| 11  | bA    | 818 | CLA  | C2B-C1B-NB  | 4.91  | 115.42      | 110.33   |
| 11  | bA    | 819 | CLA  | C3D-C2D-C1D | -4.91 | 99.13       | 105.83   |
| 11  | cA    | 841 | CLA  | C3B-C2B-C1B | -4.91 | 101.39      | 107.17   |
| 11  | cB    | 811 | CLA  | C2C-C1C-NC  | 4.91  | 115.14      | 109.98   |
| 11  | aB    | 801 | CLA  | C3B-C2B-C1B | -4.91 | 101.39      | 107.17   |
| 11  | aA    | 802 | CLA  | C4A-NA-C1A  | -4.91 | 104.44      | 106.68   |
| 11  | aA    | 819 | CLA  | C3D-C2D-C1D | -4.90 | 99.14       | 105.83   |
| 11  | bB    | 801 | CLA  | C3B-C2B-C1B | -4.90 | 101.39      | 107.17   |
| 11  | aB    | 811 | CLA  | C2C-C1C-NC  | 4.90  | 115.13      | 109.98   |
| 11  | cB    | 830 | CLA  | C2C-C1C-NC  | 4.90  | 115.13      | 109.98   |
| 11  | cA    | 807 | CLA  | C2C-C1C-NC  | 4.90  | 115.13      | 109.98   |
| 11  | bK    | 103 | CLA  | C2C-C1C-NC  | 4.90  | 115.13      | 109.98   |
| 11  | cB    | 831 | CLA  | C3B-C2B-C1B | -4.90 | 101.39      | 107.17   |
| 11  | bA    | 807 | CLA  | C2C-C1C-NC  | 4.90  | 115.13      | 109.98   |
| 11  | cA    | 831 | CLA  | CMD-C2D-C1D | 4.90  | 133.36      | 124.73   |
| 11  | cB    | 831 | CLA  | O2D-CGD-CBD | 4.90  | 119.79      | 111.23   |
| 11  | cA    | 838 | CLA  | C3B-C2B-C1B | -4.90 | 101.39      | 107.17   |
| 12  | bB    | 824 | F6C  | C2C-C1C-NC  | 4.90  | 115.41      | 110.33   |
| 11  | aB    | 831 | CLA  | C3B-C2B-C1B | -4.90 | 101.40      | 107.17   |
| 11  | cB    | 816 | CLA  | C3B-C2B-C1B | -4.90 | 101.40      | 107.17   |
| 11  | bA    | 831 | CLA  | CMD-C2D-C1D | 4.89  | 133.35      | 124.73   |
| 11  | bB    | 820 | CLA  | C2C-C1C-NC  | 4.89  | 115.12      | 109.98   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bB    | 831 | CLA  | C2B-C1B-NB  | 4.89  | 115.40      | 110.33   |
| 12  | bA    | 830 | F6C  | C2C-C1C-NC  | 4.89  | 115.40      | 110.33   |
| 11  | cA    | 819 | CLA  | C3D-C2D-C1D | -4.89 | 99.16       | 105.83   |
| 11  | cA    | 822 | CLA  | C2C-C1C-NC  | 4.89  | 115.12      | 109.98   |
| 11  | cB    | 801 | CLA  | C3B-C2B-C1B | -4.89 | 101.41      | 107.17   |
| 12  | cB    | 824 | F6C  | C4A-C3A-C2A | -4.89 | 99.72       | 106.97   |
| 11  | aA    | 813 | CLA  | C2C-C1C-NC  | 4.89  | 115.12      | 109.98   |
| 11  | aB    | 820 | CLA  | C2C-C1C-NC  | 4.89  | 115.11      | 109.98   |
| 11  | bB    | 816 | CLA  | C3B-C2B-C1B | -4.89 | 101.41      | 107.17   |
| 11  | aA    | 822 | CLA  | C2C-C1C-NC  | 4.89  | 115.11      | 109.98   |
| 11  | aK    | 101 | CLA  | C2B-C1B-NB  | 4.88  | 115.39      | 110.33   |
| 11  | cA    | 808 | CLA  | O2D-CGD-CBD | 4.88  | 119.76      | 111.23   |
| 11  | bA    | 822 | CLA  | C2C-C1C-NC  | 4.88  | 115.11      | 109.98   |
| 11  | aA    | 838 | CLA  | C3B-C2B-C1B | -4.88 | 101.42      | 107.17   |
| 11  | bA    | 808 | CLA  | O2D-CGD-CBD | 4.88  | 119.76      | 111.23   |
| 11  | aA    | 808 | CLA  | O2D-CGD-CBD | 4.88  | 119.75      | 111.23   |
| 11  | cA    | 808 | CLA  | C2B-C1B-NB  | 4.88  | 115.38      | 110.33   |
| 11  | cB    | 830 | CLA  | C2B-C1B-NB  | 4.88  | 115.38      | 110.33   |
| 11  | bB    | 831 | CLA  | O2D-CGD-CBD | 4.88  | 119.75      | 111.23   |
| 11  | bA    | 808 | CLA  | C2B-C1B-NB  | 4.88  | 115.38      | 110.33   |
| 11  | bB    | 804 | CLA  | C2B-C1B-NB  | 4.88  | 115.38      | 110.33   |
| 12  | cB    | 824 | F6C  | C2C-C1C-NC  | 4.88  | 115.38      | 110.33   |
| 11  | aB    | 831 | CLA  | O2D-CGD-CBD | 4.87  | 119.75      | 111.23   |
| 11  | bK    | 101 | CLA  | C2B-C1B-NB  | 4.87  | 115.38      | 110.33   |
| 12  | aB    | 824 | F6C  | C2C-C1C-NC  | 4.87  | 115.38      | 110.33   |
| 11  | aA    | 823 | CLA  | C2C-C1C-NC  | 4.87  | 115.10      | 109.98   |
| 11  | aA    | 833 | CLA  | C2B-C1B-NB  | 4.87  | 115.38      | 110.33   |
| 12  | cA    | 830 | F6C  | C2C-C1C-NC  | 4.87  | 115.38      | 110.33   |
| 11  | aA    | 841 | CLA  | C3B-C2B-C1B | -4.87 | 101.42      | 107.17   |
| 11  | cB    | 806 | CLA  | C3B-C2B-C1B | -4.87 | 101.42      | 107.17   |
| 11  | cA    | 818 | CLA  | C3B-C2B-C1B | -4.87 | 101.43      | 107.17   |
| 11  | aB    | 806 | CLA  | C3B-C2B-C1B | -4.87 | 101.43      | 107.17   |
| 11  | bA    | 813 | CLA  | C2C-C1C-NC  | 4.87  | 115.10      | 109.98   |
| 11  | cA    | 802 | CLA  | C2B-C1B-NB  | 4.87  | 115.38      | 110.33   |
| 11  | aA    | 818 | CLA  | C3B-C2B-C1B | -4.87 | 101.43      | 107.17   |
| 11  | aA    | 823 | CLA  | C3B-C2B-C1B | -4.87 | 101.43      | 107.17   |
| 11  | bA    | 814 | CLA  | C3B-C2B-C1B | -4.87 | 101.43      | 107.17   |
| 11  | cA    | 804 | CLA  | C3B-C2B-C1B | -4.87 | 101.43      | 107.17   |
| 11  | bB    | 837 | CLA  | C3B-C2B-C1B | -4.87 | 101.43      | 107.17   |
| 11  | cB    | 819 | CLA  | C3B-C2B-C1B | -4.87 | 101.43      | 107.17   |
| 11  | cB    | 836 | CLA  | C3B-C2B-C1B | -4.87 | 101.43      | 107.17   |
| 12  | bB    | 824 | F6C  | C4A-C3A-C2A | -4.87 | 99.75       | 106.97   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bA    | 823 | CLA  | C2C-C1C-NC  | 4.87  | 115.09      | 109.98   |
| 11  | bB    | 836 | CLA  | C4A-NA-C1A  | -4.87 | 104.46      | 106.68   |
| 11  | bB    | 815 | CLA  | C2B-C1B-NB  | 4.87  | 115.37      | 110.33   |
| 11  | aK    | 101 | CLA  | C3B-C2B-C1B | -4.87 | 101.43      | 107.17   |
| 11  | bB    | 819 | CLA  | C2C-C1C-NC  | 4.87  | 115.09      | 109.98   |
| 11  | cB    | 809 | CLA  | C2C-C1C-NC  | 4.87  | 115.09      | 109.98   |
| 11  | aB    | 804 | CLA  | C2B-C1B-NB  | 4.86  | 115.37      | 110.33   |
| 11  | bK    | 103 | CLA  | C3B-C2B-C1B | -4.86 | 101.44      | 107.17   |
| 11  | aB    | 819 | CLA  | C2C-C1C-NC  | 4.86  | 115.09      | 109.98   |
| 11  | aA    | 804 | CLA  | C3B-C2B-C1B | -4.86 | 101.44      | 107.17   |
| 11  | cA    | 833 | CLA  | C3B-C2B-C1B | -4.86 | 101.44      | 107.17   |
| 11  | aA    | 808 | CLA  | C2B-C1B-NB  | 4.86  | 115.36      | 110.33   |
| 11  | aA    | 837 | CLA  | C2B-C1B-NB  | 4.86  | 115.36      | 110.33   |
| 11  | bA    | 837 | CLA  | C2B-C1B-NB  | 4.86  | 115.36      | 110.33   |
| 10  | aA    | 801 | CL0  | CMA-C3A-C2A | -4.86 | 95.37       | 114.13   |
| 11  | bA    | 841 | CLA  | C3B-C2B-C1B | -4.86 | 101.44      | 107.17   |
| 11  | cA    | 814 | CLA  | C2B-C1B-NB  | 4.86  | 115.36      | 110.33   |
| 11  | cB    | 815 | CLA  | C2B-C1B-NB  | 4.86  | 115.36      | 110.33   |
| 12  | aA    | 830 | F6C  | C2C-C1C-NC  | 4.86  | 115.36      | 110.33   |
| 11  | aB    | 820 | CLA  | C3B-C2B-C1B | -4.86 | 101.45      | 107.17   |
| 11  | cA    | 813 | CLA  | C2C-C1C-NC  | 4.85  | 115.08      | 109.98   |
| 11  | aB    | 825 | CLA  | C2C-C1C-NC  | 4.85  | 115.08      | 109.98   |
| 11  | bB    | 820 | CLA  | C3B-C2B-C1B | -4.85 | 101.45      | 107.17   |
| 11  | cK    | 101 | CLA  | C2B-C1B-NB  | 4.85  | 115.36      | 110.33   |
| 11  | cA    | 811 | CLA  | C2C-C1C-NC  | 4.85  | 115.08      | 109.98   |
| 11  | aA    | 824 | CLA  | C2C-C1C-NC  | 4.85  | 115.07      | 109.98   |
| 11  | bB    | 811 | CLA  | C2C-C1C-NC  | 4.85  | 115.07      | 109.98   |
| 11  | bB    | 825 | CLA  | C2C-C1C-NC  | 4.85  | 115.07      | 109.98   |
| 11  | cB    | 837 | CLA  | C3B-C2B-C1B | -4.85 | 101.46      | 107.17   |
| 11  | cB    | 820 | CLA  | C3B-C2B-C1B | -4.85 | 101.46      | 107.17   |
| 11  | cK    | 103 | CLA  | C3B-C2B-C1B | -4.85 | 101.46      | 107.17   |
| 11  | aB    | 830 | CLA  | C2B-C1B-NB  | 4.85  | 115.35      | 110.33   |
| 10  | cA    | 801 | CL0  | CMA-C3A-C2A | -4.84 | 95.42       | 114.13   |
| 11  | bA    | 818 | CLA  | C3B-C2B-C1B | -4.84 | 101.46      | 107.17   |
| 11  | aB    | 837 | CLA  | C3B-C2B-C1B | -4.84 | 101.46      | 107.17   |
| 11  | aK    | 103 | CLA  | C3B-C2B-C1B | -4.84 | 101.46      | 107.17   |
| 11  | cA    | 814 | CLA  | C3B-C2B-C1B | -4.84 | 101.46      | 107.17   |
| 11  | bA    | 819 | CLA  | C3B-C2B-C1B | -4.84 | 101.46      | 107.17   |
| 11  | bK    | 101 | CLA  | C3B-C2B-C1B | -4.84 | 101.46      | 107.17   |
| 11  | cK    | 101 | CLA  | C3B-C2B-C1B | -4.84 | 101.46      | 107.17   |
| 10  | bA    | 801 | CL0  | CMA-C3A-C2A | -4.84 | 95.43       | 114.13   |
| 11  | aA    | 833 | CLA  | C3B-C2B-C1B | -4.84 | 101.46      | 107.17   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cB    | 805 | CLA  | C2C-C1C-NC  | 4.84  | 115.06      | 109.98   |
| 11  | cB    | 833 | CLA  | C3B-C2B-C1B | -4.84 | 101.47      | 107.17   |
| 11  | bK    | 103 | CLA  | C3D-C2D-C1D | -4.84 | 99.23       | 105.83   |
| 11  | bB    | 830 | CLA  | C2B-C1B-NB  | 4.84  | 115.34      | 110.33   |
| 11  | bB    | 805 | CLA  | C2C-C1C-NC  | 4.84  | 115.06      | 109.98   |
| 11  | cK    | 103 | CLA  | C3D-C2D-C1D | -4.84 | 99.23       | 105.83   |
| 11  | bA    | 802 | CLA  | C2B-C1B-NB  | 4.84  | 115.34      | 110.33   |
| 11  | bB    | 838 | CLA  | C2B-C1B-NB  | 4.84  | 115.34      | 110.33   |
| 11  | aA    | 814 | CLA  | C3B-C2B-C1B | -4.84 | 101.47      | 107.17   |
| 11  | bB    | 831 | CLA  | C3B-C2B-C1B | -4.84 | 101.47      | 107.17   |
| 11  | aB    | 813 | CLA  | O2D-CGD-CBD | 4.84  | 119.68      | 111.23   |
| 11  | bB    | 813 | CLA  | O2D-CGD-CBD | 4.84  | 119.68      | 111.23   |
| 11  | cB    | 811 | CLA  | C3B-C2B-C1B | -4.84 | 101.47      | 107.17   |
| 11  | aB    | 836 | CLA  | C4A-NA-C1A  | -4.84 | 104.47      | 106.68   |
| 11  | cB    | 836 | CLA  | C3D-C2D-C1D | -4.84 | 99.23       | 105.83   |
| 11  | bB    | 811 | CLA  | C3B-C2B-C1B | -4.83 | 101.47      | 107.17   |
| 11  | bA    | 833 | CLA  | C2B-C1B-NB  | 4.83  | 115.34      | 110.33   |
| 11  | cA    | 841 | CLA  | C2B-C1B-NB  | 4.83  | 115.34      | 110.33   |
| 11  | aB    | 803 | CLA  | CMD-C2D-C1D | 4.83  | 133.24      | 124.73   |
| 11  | bB    | 836 | CLA  | C3B-C2B-C1B | -4.83 | 101.47      | 107.17   |
| 11  | aA    | 819 | CLA  | C3B-C2B-C1B | -4.83 | 101.47      | 107.17   |
| 11  | bA    | 823 | CLA  | C3B-C2B-C1B | -4.83 | 101.48      | 107.17   |
| 11  | cA    | 823 | CLA  | C3B-C2B-C1B | -4.83 | 101.48      | 107.17   |
| 11  | bB    | 836 | CLA  | C3D-C2D-C1D | -4.83 | 99.24       | 105.83   |
| 11  | cB    | 803 | CLA  | CMD-C2D-C1D | 4.83  | 133.23      | 124.73   |
| 11  | aA    | 802 | CLA  | C2B-C1B-NB  | 4.83  | 115.33      | 110.33   |
| 12  | bA    | 832 | F6C  | C2C-C1C-NC  | 4.83  | 115.33      | 110.33   |
| 11  | aB    | 833 | CLA  | C3B-C2B-C1B | -4.83 | 101.48      | 107.17   |
| 11  | aB    | 836 | CLA  | C3D-C2D-C1D | -4.83 | 99.24       | 105.83   |
| 11  | cB    | 813 | CLA  | O2D-CGD-CBD | 4.83  | 119.67      | 111.23   |
| 11  | bB    | 815 | CLA  | C3D-C2D-C1D | -4.83 | 99.25       | 105.83   |
| 11  | cA    | 823 | CLA  | C2C-C1C-NC  | 4.83  | 115.05      | 109.98   |
| 11  | bB    | 828 | CLA  | CHD-C4C-C3C | -4.83 | 117.74      | 124.77   |
| 11  | aB    | 805 | CLA  | C2C-C1C-NC  | 4.82  | 115.05      | 109.98   |
| 11  | bB    | 803 | CLA  | CMD-C2D-C1D | 4.82  | 133.22      | 124.73   |
| 11  | bA    | 833 | CLA  | C2C-C1C-NC  | 4.82  | 115.05      | 109.98   |
| 11  | aB    | 811 | CLA  | C3B-C2B-C1B | -4.82 | 101.48      | 107.17   |
| 11  | cB    | 838 | CLA  | C2B-C1B-NB  | 4.82  | 115.33      | 110.33   |
| 11  | bB    | 809 | CLA  | C2C-C1C-NC  | 4.82  | 115.05      | 109.98   |
| 11  | aB    | 820 | CLA  | C3D-C2D-C1D | -4.82 | 99.25       | 105.83   |
| 11  | bB    | 806 | CLA  | C3B-C2B-C1B | -4.82 | 101.48      | 107.17   |
| 11  | cA    | 833 | CLA  | C2B-C1B-NB  | 4.82  | 115.33      | 110.33   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aB    | 836 | CLA  | C3B-C2B-C1B | -4.82 | 101.49      | 107.17   |
| 11  | bB    | 833 | CLA  | C3B-C2B-C1B | -4.82 | 101.49      | 107.17   |
| 11  | bA    | 814 | CLA  | C2B-C1B-NB  | 4.82  | 115.33      | 110.33   |
| 12  | cA    | 832 | F6C  | C2C-C1C-NC  | 4.82  | 115.32      | 110.33   |
| 11  | aA    | 806 | CLA  | CHD-C4C-C3C | -4.82 | 117.75      | 124.77   |
| 11  | bA    | 809 | CLA  | C2C-C1C-NC  | 4.82  | 115.04      | 109.98   |
| 11  | cB    | 825 | CLA  | C2C-C1C-NC  | 4.82  | 115.04      | 109.98   |
| 11  | bA    | 841 | CLA  | C2B-C1B-NB  | 4.81  | 115.32      | 110.33   |
| 11  | cA    | 836 | CLA  | CMD-C2D-C1D | 4.81  | 133.21      | 124.73   |
| 11  | cB    | 828 | CLA  | CHD-C4C-C3C | -4.81 | 117.75      | 124.77   |
| 11  | bA    | 811 | CLA  | C2C-C1C-NC  | 4.81  | 115.04      | 109.98   |
| 11  | cB    | 815 | CLA  | C3D-C2D-C1D | -4.81 | 99.26       | 105.83   |
| 11  | aA    | 809 | CLA  | C2C-C1C-NC  | 4.81  | 115.04      | 109.98   |
| 11  | cB    | 819 | CLA  | C2C-C1C-NC  | 4.81  | 115.04      | 109.98   |
| 11  | cA    | 815 | CLA  | C2B-C1B-NB  | 4.81  | 115.32      | 110.33   |
| 11  | bB    | 820 | CLA  | C3D-C2D-C1D | -4.81 | 99.27       | 105.83   |
| 11  | aA    | 833 | CLA  | C2C-C1C-NC  | 4.81  | 115.03      | 109.98   |
| 11  | bA    | 815 | CLA  | C2B-C1B-NB  | 4.81  | 115.31      | 110.33   |
| 11  | bA    | 806 | CLA  | CHD-C4C-C3C | -4.81 | 117.76      | 124.77   |
| 11  | bA    | 824 | CLA  | C2C-C1C-NC  | 4.81  | 115.03      | 109.98   |
| 11  | cB    | 808 | CLA  | CMD-C2D-C1D | 4.81  | 133.19      | 124.73   |
| 11  | aB    | 808 | CLA  | CMD-C2D-C1D | 4.81  | 133.19      | 124.73   |
| 11  | aB    | 815 | CLA  | C2B-C1B-NB  | 4.81  | 115.31      | 110.33   |
| 11  | aA    | 836 | CLA  | CMD-C2D-C1D | 4.81  | 133.19      | 124.73   |
| 11  | cA    | 819 | CLA  | C3B-C2B-C1B | -4.81 | 101.50      | 107.17   |
| 11  | aA    | 814 | CLA  | C2B-C1B-NB  | 4.81  | 115.31      | 110.33   |
| 11  | bB    | 811 | CLA  | C2B-C1B-NB  | 4.81  | 115.31      | 110.33   |
| 11  | cA    | 806 | CLA  | CHD-C4C-C3C | -4.81 | 117.77      | 124.77   |
| 11  | aK    | 103 | CLA  | C3D-C2D-C1D | -4.81 | 99.27       | 105.83   |
| 11  | bA    | 833 | CLA  | C3B-C2B-C1B | -4.81 | 101.50      | 107.17   |
| 11  | cA    | 841 | CLA  | C2C-C1C-NC  | 4.80  | 115.03      | 109.98   |
| 11  | aB    | 828 | CLA  | CHD-C4C-C3C | -4.80 | 117.77      | 124.77   |
| 11  | bA    | 836 | CLA  | CMD-C2D-C1D | 4.80  | 133.19      | 124.73   |
| 11  | aB    | 809 | CLA  | C2C-C1C-NC  | 4.80  | 115.03      | 109.98   |
| 11  | bK    | 101 | CLA  | C2C-C1C-NC  | 4.80  | 115.03      | 109.98   |
| 11  | cA    | 808 | CLA  | C2C-C1C-NC  | 4.80  | 115.03      | 109.98   |
| 11  | cA    | 824 | CLA  | C2C-C1C-NC  | 4.80  | 115.03      | 109.98   |
| 11  | cB    | 820 | CLA  | C3D-C2D-C1D | -4.80 | 99.28       | 105.83   |
| 11  | aB    | 808 | CLA  | C2C-C1C-NC  | 4.80  | 115.02      | 109.98   |
| 11  | bK    | 103 | CLA  | C2B-C1B-NB  | 4.80  | 115.30      | 110.33   |
| 11  | bA    | 812 | CLA  | C2C-C1C-NC  | 4.80  | 115.02      | 109.98   |
| 11  | bA    | 843 | CLA  | C2C-C1C-NC  | 4.80  | 115.02      | 109.98   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aA    | 815 | CLA  | C2B-C1B-NB  | 4.80  | 115.30      | 110.33   |
| 11  | aK    | 101 | CLA  | C2C-C1C-NC  | 4.79  | 115.02      | 109.98   |
| 12  | aA    | 830 | F6C  | C4A-C3A-C2A | -4.79 | 99.86       | 106.97   |
| 11  | bA    | 841 | CLA  | C2C-C1C-NC  | 4.79  | 115.02      | 109.98   |
| 11  | cA    | 840 | CLA  | C3D-C2D-C1D | -4.79 | 99.29       | 105.83   |
| 11  | aB    | 815 | CLA  | C3D-C2D-C1D | -4.79 | 99.29       | 105.83   |
| 11  | aA    | 808 | CLA  | C2C-C1C-NC  | 4.79  | 115.02      | 109.98   |
| 11  | aA    | 843 | CLA  | C2C-C1C-NC  | 4.79  | 115.02      | 109.98   |
| 11  | cA    | 843 | CLA  | O2D-CGD-CBD | 4.79  | 119.61      | 111.23   |
| 11  | cB    | 836 | CLA  | C4A-NA-C1A  | -4.79 | 104.49      | 106.68   |
| 11  | cB    | 811 | CLA  | C2B-C1B-NB  | 4.79  | 115.29      | 110.33   |
| 11  | aA    | 811 | CLA  | C2C-C1C-NC  | 4.79  | 115.01      | 109.98   |
| 11  | cA    | 809 | CLA  | C2C-C1C-NC  | 4.79  | 115.01      | 109.98   |
| 11  | aB    | 809 | CLA  | CAA-C2A-C3A | -4.78 | 100.07      | 113.00   |
| 11  | bB    | 808 | CLA  | CMD-C2D-C1D | 4.78  | 133.15      | 124.73   |
| 12  | cA    | 830 | F6C  | C4A-C3A-C2A | -4.78 | 99.88       | 106.97   |
| 11  | bA    | 807 | CLA  | C3B-C2B-C1B | -4.78 | 101.53      | 107.17   |
| 11  | bB    | 809 | CLA  | CAA-C2A-C3A | -4.78 | 100.08      | 113.00   |
| 11  | bB    | 832 | CLA  | O2D-CGD-CBD | 4.78  | 119.58      | 111.23   |
| 11  | aA    | 807 | CLA  | C3B-C2B-C1B | -4.78 | 101.54      | 107.17   |
| 11  | bA    | 807 | CLA  | C3D-C2D-C1D | -4.78 | 99.31       | 105.83   |
| 11  | cB    | 814 | CLA  | C3B-C2B-C1B | -4.78 | 101.54      | 107.17   |
| 11  | cK    | 103 | CLA  | C2B-C1B-NB  | 4.78  | 115.28      | 110.33   |
| 12  | bA    | 844 | F6C  | C4A-C3A-C2A | -4.78 | 99.88       | 106.97   |
| 11  | cA    | 833 | CLA  | C2C-C1C-NC  | 4.78  | 115.00      | 109.98   |
| 12  | cA    | 826 | F6C  | CAA-C2A-C1A | -4.78 | 114.66      | 128.01   |
| 11  | aA    | 807 | CLA  | C3D-C2D-C1D | -4.78 | 99.31       | 105.83   |
| 11  | aL    | 206 | CLA  | C2C-C1C-NC  | 4.78  | 115.00      | 109.98   |
| 11  | cA    | 843 | CLA  | C2C-C1C-NC  | 4.78  | 115.00      | 109.98   |
| 11  | bB    | 803 | CLA  | C2B-C1B-NB  | 4.78  | 115.28      | 110.33   |
| 11  | bB    | 826 | CLA  | C3D-C2D-C1D | -4.78 | 99.31       | 105.83   |
| 12  | cA    | 844 | F6C  | C4A-C3A-C2A | -4.77 | 99.89       | 106.97   |
| 12  | aA    | 826 | F6C  | CAA-C2A-C1A | -4.77 | 114.67      | 128.01   |
| 11  | aA    | 837 | CLA  | C2C-C1C-NC  | 4.77  | 115.00      | 109.98   |
| 11  | cK    | 101 | CLA  | C2C-C1C-NC  | 4.77  | 115.00      | 109.98   |
| 11  | cA    | 807 | CLA  | C3D-C2D-C1D | -4.77 | 99.32       | 105.83   |
| 11  | cB    | 831 | CLA  | C4A-NA-C1A  | -4.77 | 104.50      | 106.68   |
| 11  | aA    | 841 | CLA  | C2B-C1B-NB  | 4.77  | 115.27      | 110.33   |
| 11  | aB    | 832 | CLA  | O2D-CGD-CBD | 4.77  | 119.57      | 111.23   |
| 12  | aA    | 844 | F6C  | C4A-C3A-C2A | -4.77 | 99.89       | 106.97   |
| 11  | bA    | 837 | CLA  | C2C-C1C-NC  | 4.77  | 114.99      | 109.98   |
| 11  | bA    | 840 | CLA  | C4A-NA-C1A  | -4.77 | 104.50      | 106.68   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aB    | 826 | CLA  | C3D-C2D-C1D | -4.77 | 99.32       | 105.83   |
| 12  | bA    | 826 | F6C  | CAA-C2A-C1A | -4.77 | 114.69      | 128.01   |
| 11  | aB    | 811 | CLA  | C2B-C1B-NB  | 4.77  | 115.27      | 110.33   |
| 11  | aB    | 838 | CLA  | C2B-C1B-NB  | 4.77  | 115.27      | 110.33   |
| 12  | bA    | 830 | F6C  | C4A-C3A-C2A | -4.77 | 99.90       | 106.97   |
| 11  | cB    | 809 | CLA  | CAA-C2A-C3A | -4.77 | 100.12      | 113.00   |
| 11  | aA    | 828 | CLA  | C2B-C1B-NB  | 4.77  | 115.27      | 110.33   |
| 11  | cA    | 828 | CLA  | C2B-C1B-NB  | 4.77  | 115.27      | 110.33   |
| 11  | cB    | 826 | CLA  | C3D-C2D-C1D | -4.77 | 99.33       | 105.83   |
| 11  | bA    | 808 | CLA  | C2C-C1C-NC  | 4.76  | 114.99      | 109.98   |
| 11  | bA    | 840 | CLA  | C3D-C2D-C1D | -4.76 | 99.33       | 105.83   |
| 11  | bB    | 814 | CLA  | C3B-C2B-C1B | -4.76 | 101.56      | 107.17   |
| 11  | aA    | 840 | CLA  | C3D-C2D-C1D | -4.76 | 99.33       | 105.83   |
| 12  | aL    | 202 | F6C  | CHB-C4A-C3A | -4.76 | 115.58      | 125.49   |
| 11  | bA    | 843 | CLA  | O2D-CGD-CBD | 4.76  | 119.55      | 111.23   |
| 11  | cB    | 832 | CLA  | O2D-CGD-CBD | 4.76  | 119.55      | 111.23   |
| 11  | aA    | 843 | CLA  | O2D-CGD-CBD | 4.76  | 119.55      | 111.23   |
| 11  | cL    | 204 | CLA  | C3B-C2B-C1B | -4.76 | 101.56      | 107.17   |
| 11  | bA    | 828 | CLA  | C2B-C1B-NB  | 4.76  | 115.26      | 110.33   |
| 11  | cA    | 842 | CLA  | C3B-C2B-C1B | -4.76 | 101.56      | 107.17   |
| 11  | aB    | 808 | CLA  | C2B-C1B-NB  | 4.76  | 115.26      | 110.33   |
| 11  | bB    | 826 | CLA  | C2C-C1C-NC  | 4.76  | 114.98      | 109.98   |
| 11  | bL    | 206 | CLA  | C2C-C1C-NC  | 4.76  | 114.98      | 109.98   |
| 12  | aA    | 832 | F6C  | C2C-C1C-NC  | 4.75  | 115.26      | 110.33   |
| 11  | cA    | 812 | CLA  | C2C-C1C-NC  | 4.75  | 114.98      | 109.98   |
| 11  | aB    | 826 | CLA  | C2C-C1C-NC  | 4.75  | 114.97      | 109.98   |
| 12  | bA    | 827 | F6C  | C1A-C2A-C3A | -4.75 | 101.96      | 106.97   |
| 11  | cA    | 831 | CLA  | C3B-C4B-NB  | 4.75  | 114.77      | 110.53   |
| 11  | aB    | 814 | CLA  | C3B-C2B-C1B | -4.75 | 101.57      | 107.17   |
| 11  | aA    | 842 | CLA  | C3B-C2B-C1B | -4.75 | 101.57      | 107.17   |
| 11  | aA    | 818 | CLA  | C3D-C2D-C1D | -4.75 | 99.35       | 105.83   |
| 11  | aA    | 831 | CLA  | C3B-C4B-NB  | 4.75  | 114.77      | 110.53   |
| 11  | cA    | 807 | CLA  | C3B-C2B-C1B | -4.75 | 101.57      | 107.17   |
| 11  | cA    | 835 | CLA  | C3D-C2D-C1D | -4.75 | 99.35       | 105.83   |
| 12  | cL    | 202 | F6C  | CHB-C4A-C3A | -4.75 | 115.61      | 125.49   |
| 11  | bL    | 205 | CLA  | C2C-C1C-NC  | 4.75  | 114.97      | 109.98   |
| 11  | cA    | 834 | CLA  | C3B-C2B-C1B | -4.74 | 101.58      | 107.17   |
| 11  | bA    | 818 | CLA  | C3D-C2D-C1D | -4.74 | 99.36       | 105.83   |
| 11  | bA    | 842 | CLA  | C3B-C2B-C1B | -4.74 | 101.58      | 107.17   |
| 11  | cB    | 803 | CLA  | C2B-C1B-NB  | 4.74  | 115.24      | 110.33   |
| 11  | bB    | 808 | CLA  | C2C-C1C-NC  | 4.74  | 114.96      | 109.98   |
| 11  | cB    | 808 | CLA  | C2C-C1C-NC  | 4.74  | 114.96      | 109.98   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bL    | 204 | CLA  | C3B-C2B-C1B | -4.74 | 101.58      | 107.17   |
| 11  | cB    | 817 | CLA  | C3D-C2D-C1D | -4.74 | 99.36       | 105.83   |
| 11  | bB    | 838 | CLA  | C3D-C2D-C1D | -4.74 | 99.36       | 105.83   |
| 11  | bB    | 820 | CLA  | O2D-CGD-CBD | 4.74  | 119.52      | 111.23   |
| 11  | aA    | 835 | CLA  | C3D-C2D-C1D | -4.74 | 99.37       | 105.83   |
| 11  | aA    | 812 | CLA  | C2C-C1C-NC  | 4.74  | 114.96      | 109.98   |
| 11  | cA    | 837 | CLA  | C2C-C1C-NC  | 4.74  | 114.96      | 109.98   |
| 12  | aA    | 827 | F6C  | C1A-C2A-C3A | -4.74 | 101.98      | 106.97   |
| 12  | cA    | 827 | F6C  | C1A-C2A-C3A | -4.74 | 101.98      | 106.97   |
| 11  | bA    | 804 | CLA  | C2B-C1B-NB  | 4.74  | 115.24      | 110.33   |
| 11  | aB    | 838 | CLA  | C3D-C2D-C1D | -4.73 | 99.37       | 105.83   |
| 11  | cL    | 205 | CLA  | C3B-C2B-C1B | -4.73 | 101.59      | 107.17   |
| 11  | aB    | 817 | CLA  | C3D-C2D-C1D | -4.73 | 99.38       | 105.83   |
| 11  | bA    | 835 | CLA  | C2C-C1C-NC  | 4.73  | 114.95      | 109.98   |
| 11  | aB    | 803 | CLA  | C2B-C1B-NB  | 4.73  | 115.23      | 110.33   |
| 11  | aK    | 103 | CLA  | C2B-C1B-NB  | 4.73  | 115.23      | 110.33   |
| 11  | bL    | 205 | CLA  | C3B-C2B-C1B | -4.73 | 101.60      | 107.17   |
| 11  | cB    | 838 | CLA  | C3D-C2D-C1D | -4.73 | 99.38       | 105.83   |
| 11  | aL    | 205 | CLA  | C2C-C1C-NC  | 4.73  | 114.95      | 109.98   |
| 11  | cL    | 205 | CLA  | C2C-C1C-NC  | 4.73  | 114.95      | 109.98   |
| 11  | cB    | 836 | CLA  | O2D-CGD-CBD | 4.72  | 119.49      | 111.23   |
| 11  | cA    | 818 | CLA  | C3D-C2D-C1D | -4.72 | 99.38       | 105.83   |
| 11  | bB    | 813 | CLA  | C3B-C2B-C1B | -4.72 | 101.60      | 107.17   |
| 11  | aA    | 840 | CLA  | C4A-NA-C1A  | -4.72 | 104.52      | 106.68   |
| 11  | bB    | 831 | CLA  | C4A-NA-C1A  | -4.72 | 104.52      | 106.68   |
| 11  | aA    | 806 | CLA  | O2D-CGD-CBD | 4.72  | 119.49      | 111.23   |
| 11  | cB    | 813 | CLA  | C3B-C2B-C1B | -4.72 | 101.60      | 107.17   |
| 11  | cB    | 821 | CLA  | O2D-CGD-CBD | 4.72  | 119.48      | 111.23   |
| 11  | cB    | 826 | CLA  | C2C-C1C-NC  | 4.72  | 114.94      | 109.98   |
| 11  | aA    | 804 | CLA  | C2B-C1B-NB  | 4.72  | 115.22      | 110.33   |
| 11  | aA    | 835 | CLA  | C2B-C1B-NB  | 4.72  | 115.22      | 110.33   |
| 12  | aA    | 827 | F6C  | C2B-C3B-C4B | -4.72 | 104.03      | 106.46   |
| 11  | aL    | 204 | CLA  | C3B-C2B-C1B | -4.72 | 101.61      | 107.17   |
| 11  | aB    | 820 | CLA  | O2D-CGD-CBD | 4.72  | 119.48      | 111.23   |
| 11  | bA    | 842 | CLA  | C3D-C2D-C1D | -4.72 | 99.40       | 105.83   |
| 11  | bA    | 835 | CLA  | C3D-C2D-C1D | -4.71 | 99.40       | 105.83   |
| 11  | cL    | 206 | CLA  | C2C-C1C-NC  | 4.71  | 114.93      | 109.98   |
| 11  | bA    | 824 | CLA  | C2B-C1B-NB  | 4.71  | 115.22      | 110.33   |
| 12  | bL    | 202 | F6C  | CHB-C4A-C3A | -4.71 | 115.68      | 125.49   |
| 11  | aK    | 103 | CLA  | O2D-CGD-CBD | 4.71  | 119.47      | 111.23   |
| 11  | cA    | 835 | CLA  | C2B-C1B-NB  | 4.71  | 115.21      | 110.33   |
| 11  | bA    | 808 | CLA  | C3D-C2D-C1D | -4.71 | 99.40       | 105.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bB    | 821 | CLA  | O2D-CGD-CBD | 4.71  | 119.46      | 111.23   |
| 11  | aA    | 834 | CLA  | C3B-C2B-C1B | -4.71 | 101.62      | 107.17   |
| 11  | aA    | 842 | CLA  | C3D-C2D-C1D | -4.71 | 99.40       | 105.83   |
| 11  | cA    | 835 | CLA  | C2C-C1C-NC  | 4.71  | 114.93      | 109.98   |
| 11  | bA    | 841 | CLA  | C3D-C2D-C1D | -4.71 | 99.40       | 105.83   |
| 11  | cA    | 808 | CLA  | C3D-C2D-C1D | -4.71 | 99.41       | 105.83   |
| 11  | aA    | 841 | CLA  | C2C-C1C-NC  | 4.71  | 114.93      | 109.98   |
| 11  | bB    | 836 | CLA  | O2D-CGD-CBD | 4.71  | 119.46      | 111.23   |
| 11  | bA    | 831 | CLA  | C3B-C4B-NB  | 4.71  | 114.73      | 110.53   |
| 11  | cB    | 820 | CLA  | O2D-CGD-CBD | 4.70  | 119.45      | 111.23   |
| 11  | aA    | 808 | CLA  | C3D-C2D-C1D | -4.70 | 99.41       | 105.83   |
| 11  | aB    | 805 | CLA  | C4A-NA-C1A  | -4.70 | 104.53      | 106.68   |
| 11  | bA    | 838 | CLA  | C2B-C1B-NB  | 4.70  | 115.20      | 110.33   |
| 11  | bA    | 834 | CLA  | C3B-C2B-C1B | -4.70 | 101.63      | 107.17   |
| 11  | bB    | 817 | CLA  | C3D-C2D-C1D | -4.70 | 99.41       | 105.83   |
| 11  | aL    | 205 | CLA  | C3B-C2B-C1B | -4.70 | 101.63      | 107.17   |
| 11  | aA    | 835 | CLA  | C2C-C1C-NC  | 4.70  | 114.92      | 109.98   |
| 11  | cA    | 842 | CLA  | C3D-C2D-C1D | -4.70 | 99.42       | 105.83   |
| 11  | aB    | 803 | CLA  | C3D-C2D-C1D | -4.70 | 99.42       | 105.83   |
| 11  | bB    | 808 | CLA  | C2B-C1B-NB  | 4.70  | 115.20      | 110.33   |
| 11  | aB    | 813 | CLA  | C3B-C2B-C1B | -4.70 | 101.63      | 107.17   |
| 11  | aA    | 838 | CLA  | C2B-C1B-NB  | 4.70  | 115.19      | 110.33   |
| 11  | cA    | 804 | CLA  | C2B-C1B-NB  | 4.70  | 115.19      | 110.33   |
| 11  | cB    | 830 | CLA  | C3B-C2B-C1B | -4.70 | 101.64      | 107.17   |
| 11  | cA    | 842 | CLA  | C2C-C1C-NC  | 4.69  | 114.91      | 109.98   |
| 11  | aB    | 836 | CLA  | O2D-CGD-CBD | 4.69  | 119.44      | 111.23   |
| 11  | aB    | 821 | CLA  | O2D-CGD-CBD | 4.69  | 119.44      | 111.23   |
| 11  | bA    | 815 | CLA  | C3B-C2B-C1B | -4.69 | 101.64      | 107.17   |
| 11  | cA    | 824 | CLA  | C2B-C1B-NB  | 4.69  | 115.19      | 110.33   |
| 11  | aA    | 841 | CLA  | C3D-C2D-C1D | -4.69 | 99.43       | 105.83   |
| 11  | bL    | 204 | CLA  | C3D-C2D-C1D | -4.69 | 99.43       | 105.83   |
| 11  | bA    | 835 | CLA  | C2B-C1B-NB  | 4.69  | 115.19      | 110.33   |
| 11  | aA    | 803 | CLA  | C3D-C2D-C1D | -4.69 | 99.43       | 105.83   |
| 11  | aA    | 824 | CLA  | C2B-C1B-NB  | 4.69  | 115.19      | 110.33   |
| 11  | aA    | 823 | CLA  | C2B-C1B-NB  | 4.69  | 115.19      | 110.33   |
| 11  | cA    | 838 | CLA  | C2B-C1B-NB  | 4.69  | 115.19      | 110.33   |
| 11  | cL    | 204 | CLA  | C3D-C2D-C1D | -4.69 | 99.44       | 105.83   |
| 11  | cA    | 833 | CLA  | C3D-C2D-C1D | -4.69 | 99.44       | 105.83   |
| 11  | cA    | 841 | CLA  | C3D-C2D-C1D | -4.69 | 99.44       | 105.83   |
| 11  | cA    | 806 | CLA  | O2D-CGD-CBD | 4.68  | 119.42      | 111.23   |
| 11  | aA    | 833 | CLA  | C3D-C2D-C1D | -4.68 | 99.44       | 105.83   |
| 11  | cK    | 103 | CLA  | O2D-CGD-CBD | 4.68  | 119.42      | 111.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bK    | 103 | CLA  | O2D-CGD-CBD | 4.68  | 119.42      | 111.23   |
| 11  | cB    | 808 | CLA  | C2B-C1B-NB  | 4.68  | 115.18      | 110.33   |
| 11  | aA    | 842 | CLA  | C2C-C1C-NC  | 4.68  | 114.90      | 109.98   |
| 11  | bB    | 831 | CLA  | C3D-C2D-C1D | -4.68 | 99.45       | 105.83   |
| 11  | aB    | 807 | CLA  | C3D-C2D-C1D | -4.68 | 99.45       | 105.83   |
| 11  | aL    | 204 | CLA  | C3D-C2D-C1D | -4.67 | 99.45       | 105.83   |
| 12  | aA    | 830 | F6C  | C3C-C4C-NC  | 4.67  | 115.44      | 110.32   |
| 11  | bA    | 803 | CLA  | C3D-C2D-C1D | -4.67 | 99.45       | 105.83   |
| 11  | aB    | 830 | CLA  | C3B-C2B-C1B | -4.67 | 101.66      | 107.17   |
| 11  | bL    | 206 | CLA  | O2D-CGD-CBD | 4.67  | 119.40      | 111.23   |
| 11  | cA    | 837 | CLA  | C3D-C2D-C1D | -4.67 | 99.45       | 105.83   |
| 11  | cL    | 206 | CLA  | O2D-CGD-CBD | 4.67  | 119.40      | 111.23   |
| 11  | bB    | 807 | CLA  | C3D-C2D-C1D | -4.67 | 99.46       | 105.83   |
| 11  | bA    | 806 | CLA  | O2D-CGD-CBD | 4.67  | 119.39      | 111.23   |
| 11  | cB    | 807 | CLA  | C3D-C2D-C1D | -4.67 | 99.46       | 105.83   |
| 11  | aL    | 206 | CLA  | O2D-CGD-CBD | 4.67  | 119.39      | 111.23   |
| 11  | bB    | 837 | CLA  | O2D-CGD-CBD | 4.67  | 119.39      | 111.23   |
| 11  | aB    | 812 | CLA  | C2B-C1B-NB  | 4.67  | 115.16      | 110.33   |
| 11  | cB    | 803 | CLA  | C3D-C2D-C1D | -4.67 | 99.46       | 105.83   |
| 11  | aA    | 839 | CLA  | C3D-C2D-C1D | -4.66 | 99.47       | 105.83   |
| 11  | aB    | 804 | CLA  | C3D-C2D-C1D | -4.66 | 99.47       | 105.83   |
| 11  | aB    | 836 | CLA  | C2C-C1C-NC  | 4.66  | 114.88      | 109.98   |
| 11  | bA    | 823 | CLA  | C2B-C1B-NB  | 4.66  | 115.16      | 110.33   |
| 11  | cA    | 803 | CLA  | C3D-C2D-C1D | -4.66 | 99.47       | 105.83   |
| 11  | aB    | 806 | CLA  | C2C-C1C-NC  | 4.66  | 114.88      | 109.98   |
| 11  | bA    | 837 | CLA  | C3D-C2D-C1D | -4.66 | 99.47       | 105.83   |
| 11  | aA    | 810 | CLA  | C3B-C2B-C1B | -4.66 | 101.67      | 107.17   |
| 11  | cA    | 810 | CLA  | C3B-C2B-C1B | -4.66 | 101.67      | 107.17   |
| 11  | bB    | 805 | CLA  | C3D-C2D-C1D | -4.66 | 99.47       | 105.83   |
| 12  | cA    | 826 | F6C  | CHD-C4C-C3C | -4.66 | 115.10      | 125.30   |
| 11  | aB    | 820 | CLA  | C2B-C1B-NB  | 4.66  | 115.16      | 110.33   |
| 11  | cB    | 837 | CLA  | C2B-C1B-NB  | 4.66  | 115.16      | 110.33   |
| 12  | cA    | 830 | F6C  | C3C-C4C-NC  | 4.66  | 115.42      | 110.32   |
| 11  | cA    | 840 | CLA  | C4A-NA-C1A  | -4.66 | 104.55      | 106.68   |
| 11  | aB    | 831 | CLA  | C3D-C2D-C1D | -4.66 | 99.48       | 105.83   |
| 11  | cA    | 804 | CLA  | C2C-C1C-NC  | 4.66  | 114.87      | 109.98   |
| 12  | bA    | 830 | F6C  | C3C-C4C-NC  | 4.66  | 115.42      | 110.32   |
| 11  | bA    | 833 | CLA  | C3D-C2D-C1D | -4.66 | 99.48       | 105.83   |
| 11  | aA    | 805 | CLA  | C3D-C2D-C1D | -4.66 | 99.48       | 105.83   |
| 11  | cA    | 815 | CLA  | C3B-C2B-C1B | -4.65 | 101.68      | 107.17   |
| 11  | cB    | 836 | CLA  | C2B-C1B-NB  | 4.65  | 115.15      | 110.33   |
| 11  | cB    | 837 | CLA  | O2D-CGD-CBD | 4.65  | 119.36      | 111.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bB    | 803 | CLA  | C3D-C2D-C1D | -4.65 | 99.48       | 105.83   |
| 11  | cA    | 802 | CLA  | C3B-C2B-C1B | -4.65 | 101.69      | 107.17   |
| 11  | cA    | 833 | CLA  | O2D-CGD-CBD | 4.65  | 119.36      | 111.23   |
| 11  | cB    | 833 | CLA  | C3D-C2D-C1D | -4.65 | 99.48       | 105.83   |
| 11  | aB    | 832 | CLA  | C2C-C1C-NC  | 4.65  | 114.87      | 109.98   |
| 11  | bL    | 205 | CLA  | C2B-C1B-NB  | 4.65  | 115.14      | 110.33   |
| 11  | bB    | 836 | CLA  | C2B-C1B-NB  | 4.65  | 115.14      | 110.33   |
| 11  | aA    | 809 | CLA  | C3D-C2D-C1D | -4.64 | 99.49       | 105.83   |
| 11  | aA    | 804 | CLA  | C2C-C1C-NC  | 4.64  | 114.86      | 109.98   |
| 11  | bB    | 836 | CLA  | C2C-C1C-NC  | 4.64  | 114.86      | 109.98   |
| 12  | aA    | 826 | F6C  | CHD-C4C-C3C | -4.64 | 115.13      | 125.30   |
| 11  | bA    | 842 | CLA  | C2C-C1C-NC  | 4.64  | 114.86      | 109.98   |
| 11  | bB    | 802 | CLA  | C2C-C1C-NC  | 4.64  | 114.86      | 109.98   |
| 11  | aB    | 837 | CLA  | O2D-CGD-CBD | 4.64  | 119.35      | 111.23   |
| 11  | aA    | 820 | CLA  | C4A-NA-C1A  | -4.64 | 104.56      | 106.68   |
| 11  | cA    | 823 | CLA  | C2B-C1B-NB  | 4.64  | 115.14      | 110.33   |
| 11  | bA    | 805 | CLA  | C3D-C2D-C1D | -4.64 | 99.50       | 105.83   |
| 11  | bA    | 839 | CLA  | C3D-C2D-C1D | -4.64 | 99.50       | 105.83   |
| 11  | aB    | 802 | CLA  | C2C-C1C-NC  | 4.64  | 114.86      | 109.98   |
| 11  | bA    | 833 | CLA  | O2D-CGD-CBD | 4.64  | 119.34      | 111.23   |
| 11  | cB    | 805 | CLA  | C3D-C2D-C1D | -4.64 | 99.50       | 105.83   |
| 11  | bB    | 804 | CLA  | C3D-C2D-C1D | -4.64 | 99.50       | 105.83   |
| 11  | cB    | 802 | CLA  | C2C-C1C-NC  | 4.64  | 114.85      | 109.98   |
| 11  | aB    | 805 | CLA  | C3D-C2D-C1D | -4.64 | 99.50       | 105.83   |
| 11  | aA    | 813 | CLA  | C2B-C1B-NB  | 4.64  | 115.14      | 110.33   |
| 11  | bB    | 833 | CLA  | C3D-C2D-C1D | -4.64 | 99.50       | 105.83   |
| 11  | aB    | 828 | CLA  | C3B-C4B-NB  | 4.64  | 114.67      | 110.53   |
| 11  | bA    | 802 | CLA  | C3B-C2B-C1B | -4.64 | 101.70      | 107.17   |
| 11  | cB    | 804 | CLA  | C3D-C2D-C1D | -4.64 | 99.51       | 105.83   |
| 11  | aB    | 827 | CLA  | C2B-C1B-NB  | 4.63  | 115.13      | 110.33   |
| 11  | aB    | 833 | CLA  | C3D-C2D-C1D | -4.63 | 99.51       | 105.83   |
| 12  | bA    | 826 | F6C  | CHD-C4C-C3C | -4.63 | 115.16      | 125.30   |
| 11  | bB    | 830 | CLA  | C3B-C2B-C1B | -4.63 | 101.71      | 107.17   |
| 11  | cB    | 832 | CLA  | C2C-C1C-NC  | 4.63  | 114.85      | 109.98   |
| 11  | aB    | 837 | CLA  | C2B-C1B-NB  | 4.63  | 115.13      | 110.33   |
| 11  | bA    | 813 | CLA  | C2B-C1B-NB  | 4.63  | 115.13      | 110.33   |
| 11  | cB    | 831 | CLA  | C3D-C2D-C1D | -4.63 | 99.51       | 105.83   |
| 11  | bA    | 802 | CLA  | C3B-C4B-NB  | 4.63  | 114.67      | 110.53   |
| 11  | cA    | 809 | CLA  | C3D-C2D-C1D | -4.63 | 99.51       | 105.83   |
| 11  | aA    | 815 | CLA  | C3B-C2B-C1B | -4.63 | 101.71      | 107.17   |
| 11  | aA    | 816 | CLA  | C3B-C2B-C1B | -4.63 | 101.71      | 107.17   |
| 11  | bB    | 827 | CLA  | C2B-C1B-NB  | 4.63  | 115.13      | 110.33   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cB    | 836 | CLA  | C2C-C1C-NC  | 4.63  | 114.84      | 109.98   |
| 11  | cA    | 805 | CLA  | C3D-C2D-C1D | -4.63 | 99.51       | 105.83   |
| 11  | cA    | 816 | CLA  | C3B-C2B-C1B | -4.63 | 101.71      | 107.17   |
| 11  | aB    | 836 | CLA  | C2B-C1B-NB  | 4.63  | 115.12      | 110.33   |
| 11  | bA    | 820 | CLA  | C4A-NA-C1A  | -4.63 | 104.57      | 106.68   |
| 11  | cA    | 839 | CLA  | C3D-C2D-C1D | -4.63 | 99.52       | 105.83   |
| 11  | cB    | 827 | CLA  | C2B-C1B-NB  | 4.63  | 115.12      | 110.33   |
| 11  | bB    | 821 | CLA  | C3B-C2B-C1B | -4.63 | 101.72      | 107.17   |
| 12  | cA    | 830 | F6C  | CMD-C2D-C1D | 4.63  | 132.26      | 125.03   |
| 11  | aB    | 825 | CLA  | C2B-C1B-NB  | 4.63  | 115.12      | 110.33   |
| 11  | aB    | 803 | CLA  | C2C-C1C-NC  | 4.63  | 114.84      | 109.98   |
| 11  | bA    | 804 | CLA  | C2C-C1C-NC  | 4.62  | 114.84      | 109.98   |
| 11  | bA    | 809 | CLA  | C3D-C2D-C1D | -4.62 | 99.52       | 105.83   |
| 11  | aL    | 205 | CLA  | C2B-C1B-NB  | 4.62  | 115.12      | 110.33   |
| 11  | bB    | 837 | CLA  | C2B-C1B-NB  | 4.62  | 115.12      | 110.33   |
| 11  | cB    | 828 | CLA  | C3B-C4B-NB  | 4.62  | 114.66      | 110.53   |
| 11  | aB    | 830 | CLA  | C3D-C2D-C1D | -4.62 | 99.52       | 105.83   |
| 11  | cB    | 812 | CLA  | C2B-C1B-NB  | 4.62  | 115.12      | 110.33   |
| 11  | bB    | 820 | CLA  | C2B-C1B-NB  | 4.62  | 115.12      | 110.33   |
| 11  | bB    | 806 | CLA  | C2C-C1C-NC  | 4.62  | 114.83      | 109.98   |
| 11  | bB    | 817 | CLA  | C3B-C2B-C1B | -4.62 | 101.72      | 107.17   |
| 11  | cB    | 838 | CLA  | C3B-C2B-C1B | -4.62 | 101.72      | 107.17   |
| 11  | aA    | 837 | CLA  | C3D-C2D-C1D | -4.62 | 99.53       | 105.83   |
| 12  | cA    | 832 | F6C  | C4A-C3A-C2A | -4.62 | 100.12      | 106.97   |
| 11  | bB    | 821 | CLA  | C3D-C2D-C1D | -4.62 | 99.53       | 105.83   |
| 11  | cA    | 813 | CLA  | C2B-C1B-NB  | 4.62  | 115.11      | 110.33   |
| 11  | bA    | 843 | CLA  | C3D-C2D-C1D | -4.62 | 99.53       | 105.83   |
| 11  | bA    | 810 | CLA  | C3B-C2B-C1B | -4.62 | 101.73      | 107.17   |
| 11  | cB    | 840 | CLA  | C3D-C2D-C1D | -4.61 | 99.53       | 105.83   |
| 12  | bL    | 202 | F6C  | C3D-C2D-C1D | -4.61 | 99.15       | 105.83   |
| 11  | bA    | 825 | CLA  | C2B-C1B-NB  | 4.61  | 115.11      | 110.33   |
| 11  | cL    | 205 | CLA  | C2B-C1B-NB  | 4.61  | 115.11      | 110.33   |
| 11  | cB    | 825 | CLA  | C2B-C1B-NB  | 4.61  | 115.11      | 110.33   |
| 11  | bB    | 825 | CLA  | C2B-C1B-NB  | 4.61  | 115.11      | 110.33   |
| 11  | bB    | 826 | CLA  | C2B-C1B-NB  | 4.61  | 115.11      | 110.33   |
| 11  | aB    | 808 | CLA  | C3B-C2B-C1B | -4.61 | 101.73      | 107.17   |
| 11  | cA    | 802 | CLA  | C3B-C4B-NB  | 4.61  | 114.65      | 110.53   |
| 12  | cA    | 827 | F6C  | C2B-C3B-C4B | -4.61 | 104.08      | 106.46   |
| 12  | aA    | 830 | F6C  | CMD-C2D-C1D | 4.61  | 132.24      | 125.03   |
| 11  | aA    | 833 | CLA  | O2D-CGD-CBD | 4.61  | 119.29      | 111.23   |
| 11  | bB    | 828 | CLA  | C3B-C4B-NB  | 4.61  | 114.64      | 110.53   |
| 11  | aB    | 817 | CLA  | C3B-C2B-C1B | -4.61 | 101.74      | 107.17   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bB    | 812 | CLA  | C2B-C1B-NB  | 4.61  | 115.10      | 110.33   |
| 11  | cB    | 817 | CLA  | C3B-C2B-C1B | -4.61 | 101.74      | 107.17   |
| 11  | bB    | 840 | CLA  | C3D-C2D-C1D | -4.61 | 99.54       | 105.83   |
| 11  | aA    | 802 | CLA  | C3B-C4B-NB  | 4.61  | 114.64      | 110.53   |
| 12  | cL    | 202 | F6C  | C3D-C2D-C1D | -4.61 | 99.16       | 105.83   |
| 11  | bB    | 803 | CLA  | C2C-C1C-NC  | 4.60  | 114.82      | 109.98   |
| 11  | cB    | 806 | CLA  | C2C-C1C-NC  | 4.60  | 114.82      | 109.98   |
| 11  | aB    | 840 | CLA  | C3D-C2D-C1D | -4.60 | 99.55       | 105.83   |
| 11  | aA    | 802 | CLA  | C3B-C2B-C1B | -4.60 | 101.75      | 107.17   |
| 12  | aA    | 832 | F6C  | C4A-C3A-C2A | -4.60 | 100.14      | 106.97   |
| 11  | bB    | 838 | CLA  | C3B-C2B-C1B | -4.60 | 101.75      | 107.17   |
| 11  | aB    | 831 | CLA  | C4A-NA-C1A  | -4.60 | 104.58      | 106.68   |
| 11  | bB    | 830 | CLA  | C3D-C2D-C1D | -4.60 | 99.55       | 105.83   |
| 12  | bA    | 832 | F6C  | C4A-C3A-C2A | -4.60 | 100.15      | 106.97   |
| 12  | bA    | 830 | F6C  | CMD-C2D-C1D | 4.60  | 132.22      | 125.03   |
| 12  | bA    | 827 | F6C  | C2B-C3B-C4B | -4.60 | 104.09      | 106.46   |
| 11  | cB    | 820 | CLA  | C2B-C1B-NB  | 4.60  | 115.09      | 110.33   |
| 11  | bB    | 805 | CLA  | C4A-NA-C1A  | -4.59 | 104.58      | 106.68   |
| 11  | bA    | 816 | CLA  | C3B-C2B-C1B | -4.59 | 101.76      | 107.17   |
| 12  | aL    | 202 | F6C  | C3D-C2D-C1D | -4.59 | 99.18       | 105.83   |
| 11  | cB    | 808 | CLA  | C3B-C2B-C1B | -4.59 | 101.76      | 107.17   |
| 11  | cB    | 821 | CLA  | C3B-C2B-C1B | -4.59 | 101.76      | 107.17   |
| 11  | aB    | 821 | CLA  | C3D-C2D-C1D | -4.59 | 99.57       | 105.83   |
| 11  | cA    | 843 | CLA  | C3D-C2D-C1D | -4.59 | 99.57       | 105.83   |
| 11  | aA    | 816 | CLA  | C2C-C1C-NC  | 4.59  | 114.80      | 109.98   |
| 11  | aB    | 821 | CLA  | C3B-C2B-C1B | -4.59 | 101.76      | 107.17   |
| 11  | aA    | 843 | CLA  | C3D-C2D-C1D | -4.59 | 99.57       | 105.83   |
| 11  | bB    | 808 | CLA  | C3B-C2B-C1B | -4.58 | 101.77      | 107.17   |
| 11  | cB    | 821 | CLA  | C3D-C2D-C1D | -4.58 | 99.58       | 105.83   |
| 11  | bB    | 832 | CLA  | C2C-C1C-NC  | 4.58  | 114.79      | 109.98   |
| 11  | cB    | 830 | CLA  | C3D-C2D-C1D | -4.58 | 99.58       | 105.83   |
| 11  | cA    | 824 | CLA  | O2D-CGD-CBD | 4.58  | 119.23      | 111.23   |
| 12  | aA    | 826 | F6C  | CHB-C4A-C3A | -4.58 | 115.97      | 125.49   |
| 11  | bB    | 817 | CLA  | C2B-C1B-NB  | 4.58  | 115.07      | 110.33   |
| 11  | cB    | 803 | CLA  | C2C-C1C-NC  | 4.57  | 114.79      | 109.98   |
| 11  | aA    | 829 | CLA  | C3D-C2D-C1D | -4.57 | 99.59       | 105.83   |
| 11  | aB    | 838 | CLA  | C3B-C2B-C1B | -4.57 | 101.78      | 107.17   |
| 11  | aB    | 819 | CLA  | C2B-C1B-NB  | 4.57  | 115.07      | 110.33   |
| 11  | bA    | 829 | CLA  | C3D-C2D-C1D | -4.57 | 99.59       | 105.83   |
| 11  | bA    | 804 | CLA  | C3D-C2D-C1D | -4.57 | 99.59       | 105.83   |
| 11  | cA    | 829 | CLA  | C3D-C2D-C1D | -4.57 | 99.59       | 105.83   |
| 11  | cB    | 826 | CLA  | C2B-C1B-NB  | 4.57  | 115.06      | 110.33   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12  | cA    | 826 | F6C  | CHB-C4A-C3A | -4.57 | 115.99      | 125.49   |
| 11  | aB    | 816 | CLA  | C3D-C2D-C1D | -4.57 | 99.60       | 105.83   |
| 11  | bB    | 816 | CLA  | C3D-C2D-C1D | -4.56 | 99.60       | 105.83   |
| 11  | aB    | 839 | CLA  | O2D-CGD-CBD | 4.56  | 119.21      | 111.23   |
| 11  | aB    | 826 | CLA  | C2B-C1B-NB  | 4.56  | 115.06      | 110.33   |
| 11  | aB    | 803 | CLA  | CAC-C3C-C4C | 4.56  | 130.73      | 124.79   |
| 11  | bK    | 101 | CLA  | C3D-C2D-C1D | -4.56 | 99.60       | 105.83   |
| 11  | cB    | 817 | CLA  | C2B-C1B-NB  | 4.56  | 115.06      | 110.33   |
| 12  | bA    | 844 | F6C  | C3D-C4D-ND  | 4.56  | 117.44      | 109.93   |
| 11  | bA    | 816 | CLA  | C2C-C1C-NC  | 4.56  | 114.77      | 109.98   |
| 11  | bB    | 826 | CLA  | C3B-C2B-C1B | -4.56 | 101.79      | 107.17   |
| 11  | aA    | 825 | CLA  | C2B-C1B-NB  | 4.56  | 115.05      | 110.33   |
| 11  | bA    | 838 | CLA  | C3D-C2D-C1D | -4.56 | 99.61       | 105.83   |
| 11  | cB    | 803 | CLA  | CAC-C3C-C4C | 4.56  | 130.72      | 124.79   |
| 11  | cA    | 820 | CLA  | C3D-C2D-C1D | -4.56 | 99.61       | 105.83   |
| 11  | cA    | 816 | CLA  | C2C-C1C-NC  | 4.56  | 114.77      | 109.98   |
| 11  | bA    | 807 | CLA  | C2B-C1B-NB  | 4.55  | 115.05      | 110.33   |
| 11  | cA    | 807 | CLA  | C2B-C1B-NB  | 4.55  | 115.05      | 110.33   |
| 12  | cA    | 844 | F6C  | C3D-C4D-ND  | 4.55  | 117.43      | 109.93   |
| 11  | aA    | 817 | CLA  | C2B-C1B-NB  | 4.55  | 115.05      | 110.33   |
| 11  | cA    | 825 | CLA  | C2B-C1B-NB  | 4.55  | 115.05      | 110.33   |
| 11  | cB    | 839 | CLA  | O2D-CGD-CBD | 4.55  | 119.19      | 111.23   |
| 11  | aA    | 838 | CLA  | C3D-C2D-C1D | -4.55 | 99.62       | 105.83   |
| 11  | aB    | 840 | CLA  | C1C-C2C-C3C | -4.55 | 102.19      | 106.98   |
| 11  | cB    | 816 | CLA  | C3D-C2D-C1D | -4.55 | 99.62       | 105.83   |
| 11  | cB    | 840 | CLA  | O2D-CGD-CBD | 4.55  | 119.19      | 111.23   |
| 11  | cK    | 101 | CLA  | C3D-C2D-C1D | -4.55 | 99.62       | 105.83   |
| 11  | aB    | 814 | CLA  | C3D-C2D-C1D | -4.55 | 99.62       | 105.83   |
| 11  | bB    | 821 | CLA  | C2B-C1B-NB  | 4.55  | 115.04      | 110.33   |
| 11  | cB    | 805 | CLA  | C4A-NA-C1A  | -4.55 | 104.60      | 106.68   |
| 11  | bA    | 824 | CLA  | O2D-CGD-CBD | 4.55  | 119.18      | 111.23   |
| 11  | bA    | 817 | CLA  | C2B-C1B-NB  | 4.55  | 115.04      | 110.33   |
| 11  | bB    | 839 | CLA  | O2D-CGD-CBD | 4.55  | 119.18      | 111.23   |
| 11  | bB    | 814 | CLA  | C3D-C2D-C1D | -4.55 | 99.63       | 105.83   |
| 11  | aA    | 820 | CLA  | C3D-C2D-C1D | -4.55 | 99.63       | 105.83   |
| 11  | aA    | 824 | CLA  | O2D-CGD-CBD | 4.55  | 119.18      | 111.23   |
| 11  | bB    | 840 | CLA  | O2D-CGD-CBD | 4.55  | 119.18      | 111.23   |
| 11  | bB    | 810 | CLA  | C3D-C2D-C1D | -4.55 | 99.63       | 105.83   |
| 11  | aA    | 804 | CLA  | C3D-C2D-C1D | -4.55 | 99.63       | 105.83   |
| 11  | aB    | 826 | CLA  | C3B-C2B-C1B | -4.54 | 101.81      | 107.17   |
| 11  | cB    | 821 | CLA  | C2B-C1B-NB  | 4.54  | 115.04      | 110.33   |
| 11  | cB    | 826 | CLA  | C3B-C2B-C1B | -4.54 | 101.81      | 107.17   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aB    | 840 | CLA  | O2D-CGD-CBD | 4.54  | 119.17      | 111.23   |
| 12  | bA    | 826 | F6C  | CHB-C4A-C3A | -4.54 | 116.04      | 125.49   |
| 11  | cB    | 818 | CLA  | C3D-C2D-C1D | -4.54 | 99.63       | 105.83   |
| 11  | cB    | 814 | CLA  | C3D-C2D-C1D | -4.54 | 99.63       | 105.83   |
| 11  | bB    | 840 | CLA  | C1C-C2C-C3C | -4.54 | 102.20      | 106.98   |
| 11  | cL    | 204 | CLA  | C2B-C1B-NB  | 4.54  | 115.04      | 110.33   |
| 11  | cA    | 838 | CLA  | C3D-C2D-C1D | -4.54 | 99.63       | 105.83   |
| 12  | aA    | 844 | F6C  | C3D-C4D-ND  | 4.54  | 117.41      | 109.93   |
| 11  | cA    | 804 | CLA  | C3D-C2D-C1D | -4.54 | 99.64       | 105.83   |
| 11  | cB    | 810 | CLA  | C3D-C2D-C1D | -4.54 | 99.64       | 105.83   |
| 11  | aA    | 813 | CLA  | C3D-C2D-C1D | -4.54 | 99.64       | 105.83   |
| 11  | cL    | 205 | CLA  | C3D-C2D-C1D | -4.54 | 99.64       | 105.83   |
| 11  | cB    | 819 | CLA  | C2B-C1B-NB  | 4.54  | 115.03      | 110.33   |
| 11  | aB    | 818 | CLA  | C3D-C2D-C1D | -4.54 | 99.64       | 105.83   |
| 11  | cB    | 837 | CLA  | C3D-C2D-C1D | -4.54 | 99.64       | 105.83   |
| 11  | aA    | 807 | CLA  | C2B-C1B-NB  | 4.53  | 115.03      | 110.33   |
| 11  | bB    | 818 | CLA  | C3D-C2D-C1D | -4.53 | 99.64       | 105.83   |
| 11  | bA    | 811 | CLA  | C4A-NA-C1A  | -4.53 | 104.61      | 106.68   |
| 11  | cA    | 813 | CLA  | C3D-C2D-C1D | -4.53 | 99.65       | 105.83   |
| 11  | aA    | 843 | CLA  | C2B-C1B-NB  | 4.53  | 115.03      | 110.33   |
| 11  | bB    | 832 | CLA  | C3D-C2D-C1D | -4.53 | 99.65       | 105.83   |
| 11  | cB    | 840 | CLA  | C1C-C2C-C3C | -4.53 | 102.21      | 106.98   |
| 11  | bB    | 837 | CLA  | C3D-C2D-C1D | -4.53 | 99.65       | 105.83   |
| 11  | bB    | 801 | CLA  | CMB-C2B-C1B | 4.53  | 132.32      | 125.42   |
| 11  | bL    | 205 | CLA  | C3D-C2D-C1D | -4.53 | 99.65       | 105.83   |
| 11  | bB    | 803 | CLA  | CAC-C3C-C4C | 4.53  | 130.68      | 124.79   |
| 11  | bA    | 824 | CLA  | C3B-C2B-C1B | -4.53 | 101.83      | 107.17   |
| 11  | bB    | 819 | CLA  | C2B-C1B-NB  | 4.53  | 115.02      | 110.33   |
| 11  | aA    | 842 | CLA  | C4A-NA-C1A  | -4.53 | 104.61      | 106.68   |
| 11  | cA    | 820 | CLA  | C4A-NA-C1A  | -4.53 | 104.61      | 106.68   |
| 11  | aB    | 821 | CLA  | C2B-C1B-NB  | 4.52  | 115.02      | 110.33   |
| 11  | bB    | 835 | CLA  | C3D-C2D-C1D | -4.52 | 99.66       | 105.83   |
| 11  | aB    | 801 | CLA  | CMB-C2B-C1B | 4.52  | 132.31      | 125.42   |
| 11  | aK    | 101 | CLA  | C3D-C2D-C1D | -4.52 | 99.66       | 105.83   |
| 11  | bA    | 820 | CLA  | C3D-C2D-C1D | -4.52 | 99.66       | 105.83   |
| 11  | bL    | 204 | CLA  | C2B-C1B-NB  | 4.52  | 115.01      | 110.33   |
| 11  | aB    | 809 | CLA  | C3D-C2D-C1D | -4.52 | 99.67       | 105.83   |
| 11  | bB    | 835 | CLA  | C3B-C2B-C1B | -4.52 | 101.84      | 107.17   |
| 11  | aB    | 835 | CLA  | C3B-C2B-C1B | -4.52 | 101.85      | 107.17   |
| 11  | aB    | 839 | CLA  | C3B-C2B-C1B | -4.52 | 101.85      | 107.17   |
| 11  | aB    | 810 | CLA  | C3D-C2D-C1D | -4.51 | 99.67       | 105.83   |
| 12  | aA    | 827 | F6C  | C3D-C4D-ND  | 4.51  | 117.37      | 109.93   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cB    | 835 | CLA  | C3B-C2B-C1B | -4.51 | 101.85      | 107.17   |
| 11  | cB    | 801 | CLA  | C3D-C2D-C1D | -4.51 | 99.67       | 105.83   |
| 11  | bB    | 801 | CLA  | C3D-C2D-C1D | -4.51 | 99.67       | 105.83   |
| 11  | bA    | 825 | CLA  | C3B-C2B-C1B | -4.51 | 101.85      | 107.17   |
| 11  | cA    | 824 | CLA  | C3B-C2B-C1B | -4.51 | 101.85      | 107.17   |
| 11  | aA    | 817 | CLA  | C3D-C2D-C1D | -4.51 | 99.68       | 105.83   |
| 11  | cA    | 817 | CLA  | C3D-C2D-C1D | -4.51 | 99.68       | 105.83   |
| 11  | cB    | 801 | CLA  | C2C-C1C-NC  | 4.51  | 114.72      | 109.98   |
| 12  | cA    | 827 | F6C  | C3D-C4D-ND  | 4.51  | 117.36      | 109.93   |
| 11  | bA    | 813 | CLA  | C3D-C2D-C1D | -4.51 | 99.68       | 105.83   |
| 11  | bA    | 817 | CLA  | C3D-C2D-C1D | -4.51 | 99.68       | 105.83   |
| 12  | bA    | 827 | F6C  | C3D-C4D-ND  | 4.51  | 117.35      | 109.93   |
| 11  | bB    | 809 | CLA  | C3D-C2D-C1D | -4.51 | 99.68       | 105.83   |
| 11  | aL    | 204 | CLA  | C2B-C1B-NB  | 4.51  | 115.00      | 110.33   |
| 11  | cB    | 829 | CLA  | CAC-C3C-C4C | 4.51  | 130.65      | 124.79   |
| 11  | cA    | 843 | CLA  | C2B-C1B-NB  | 4.50  | 115.00      | 110.33   |
| 11  | cB    | 835 | CLA  | C3D-C2D-C1D | -4.50 | 99.69       | 105.83   |
| 11  | aL    | 205 | CLA  | C3D-C2D-C1D | -4.50 | 99.69       | 105.83   |
| 11  | aB    | 817 | CLA  | C2B-C1B-NB  | 4.50  | 114.99      | 110.33   |
| 11  | cA    | 811 | CLA  | C4A-NA-C1A  | -4.50 | 104.63      | 106.68   |
| 11  | cA    | 816 | CLA  | C3D-C2D-C1D | -4.50 | 99.69       | 105.83   |
| 11  | bB    | 834 | CLA  | C3D-C2D-C1D | -4.50 | 99.70       | 105.83   |
| 11  | aA    | 824 | CLA  | C3B-C2B-C1B | -4.50 | 101.87      | 107.17   |
| 11  | cA    | 825 | CLA  | C3B-C2B-C1B | -4.50 | 101.87      | 107.17   |
| 11  | cB    | 839 | CLA  | C3B-C2B-C1B | -4.50 | 101.87      | 107.17   |
| 11  | aB    | 835 | CLA  | C3D-C2D-C1D | -4.50 | 99.70       | 105.83   |
| 11  | aA    | 815 | CLA  | C3D-C2D-C1D | -4.49 | 99.70       | 105.83   |
| 11  | aL    | 206 | CLA  | C3B-C2B-C1B | -4.49 | 101.87      | 107.17   |
| 11  | cA    | 811 | CLA  | C2B-C1B-NB  | 4.49  | 114.98      | 110.33   |
| 11  | cA    | 842 | CLA  | C4A-NA-C1A  | -4.49 | 104.63      | 106.68   |
| 11  | aB    | 801 | CLA  | C3D-C2D-C1D | -4.49 | 99.70       | 105.83   |
| 11  | aB    | 837 | CLA  | C3D-C2D-C1D | -4.49 | 99.70       | 105.83   |
| 12  | cL    | 202 | F6C  | C3C-C4C-NC  | 4.49  | 115.24      | 110.32   |
| 11  | bB    | 813 | CLA  | C2B-C1B-NB  | 4.49  | 114.98      | 110.33   |
| 11  | cB    | 809 | CLA  | C3D-C2D-C1D | -4.49 | 99.71       | 105.83   |
| 11  | cA    | 811 | CLA  | C3D-C2D-C1D | -4.49 | 99.71       | 105.83   |
| 12  | bL    | 202 | F6C  | C3C-C4C-NC  | 4.49  | 115.24      | 110.32   |
| 12  | cB    | 824 | F6C  | CHB-C4A-C3A | -4.49 | 116.16      | 125.49   |
| 11  | aB    | 832 | CLA  | C3D-C2D-C1D | -4.49 | 99.71       | 105.83   |
| 11  | aB    | 837 | CLA  | C2C-C1C-NC  | 4.49  | 114.69      | 109.98   |
| 11  | cB    | 832 | CLA  | C3D-C2D-C1D | -4.49 | 99.71       | 105.83   |
| 12  | aL    | 202 | F6C  | C3C-C4C-NC  | 4.48  | 115.23      | 110.32   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aA    | 825 | CLA  | C3B-C2B-C1B | -4.48 | 101.88      | 107.17   |
| 11  | cA    | 840 | CLA  | C3B-C2B-C1B | -4.48 | 101.88      | 107.17   |
| 11  | cA    | 815 | CLA  | C3D-C2D-C1D | -4.48 | 99.71       | 105.83   |
| 11  | bA    | 840 | CLA  | C3B-C2B-C1B | -4.48 | 101.89      | 107.17   |
| 11  | cB    | 806 | CLA  | C2B-C1B-NB  | 4.48  | 114.97      | 110.33   |
| 11  | bA    | 843 | CLA  | C2B-C1B-NB  | 4.48  | 114.97      | 110.33   |
| 11  | cA    | 817 | CLA  | C2B-C1B-NB  | 4.48  | 114.97      | 110.33   |
| 11  | aB    | 828 | CLA  | O2D-CGD-CBD | 4.48  | 119.06      | 111.23   |
| 11  | bA    | 815 | CLA  | C3D-C2D-C1D | -4.48 | 99.72       | 105.83   |
| 11  | bB    | 828 | CLA  | O2D-CGD-CBD | 4.48  | 119.06      | 111.23   |
| 11  | aB    | 834 | CLA  | C3D-C2D-C1D | -4.48 | 99.72       | 105.83   |
| 11  | aB    | 806 | CLA  | C2B-C1B-NB  | 4.48  | 114.97      | 110.33   |
| 11  | bB    | 829 | CLA  | CAC-C3C-C4C | 4.48  | 130.61      | 124.79   |
| 11  | aA    | 806 | CLA  | C2C-C1C-NC  | 4.47  | 114.68      | 109.98   |
| 11  | cA    | 812 | CLA  | C3D-C2D-C1D | -4.47 | 99.72       | 105.83   |
| 12  | aB    | 824 | F6C  | CHB-C4A-C3A | -4.47 | 116.18      | 125.49   |
| 11  | cA    | 802 | CLA  | C3D-C2D-C1D | -4.47 | 99.73       | 105.83   |
| 11  | cA    | 806 | CLA  | C2C-C1C-NC  | 4.47  | 114.68      | 109.98   |
| 11  | cB    | 801 | CLA  | CMB-C2B-C1B | 4.47  | 132.23      | 125.42   |
| 11  | aB    | 802 | CLA  | C3D-C2D-C1D | -4.47 | 99.73       | 105.83   |
| 11  | bB    | 835 | CLA  | C2B-C1B-NB  | 4.47  | 114.96      | 110.33   |
| 11  | cB    | 807 | CLA  | C3B-C2B-C1B | -4.47 | 101.90      | 107.17   |
| 11  | aB    | 807 | CLA  | C3B-C2B-C1B | -4.47 | 101.90      | 107.17   |
| 11  | aA    | 840 | CLA  | C3B-C2B-C1B | -4.47 | 101.90      | 107.17   |
| 11  | bB    | 839 | CLA  | C3B-C2B-C1B | -4.47 | 101.90      | 107.17   |
| 11  | aA    | 829 | CLA  | O2D-CGD-CBD | 4.47  | 119.04      | 111.23   |
| 12  | bB    | 824 | F6C  | CHB-C4A-C3A | -4.47 | 116.20      | 125.49   |
| 11  | cB    | 828 | CLA  | O2D-CGD-CBD | 4.47  | 119.04      | 111.23   |
| 11  | aB    | 829 | CLA  | CAC-C3C-C4C | 4.47  | 130.60      | 124.79   |
| 11  | bB    | 807 | CLA  | C3B-C2B-C1B | -4.47 | 101.91      | 107.17   |
| 11  | cB    | 813 | CLA  | C2B-C1B-NB  | 4.46  | 114.96      | 110.33   |
| 11  | bA    | 811 | CLA  | C3D-C2D-C1D | -4.46 | 99.74       | 105.83   |
| 11  | cA    | 806 | CLA  | CAC-C3C-C4C | 4.46  | 130.60      | 124.79   |
| 11  | bB    | 801 | CLA  | C2C-C1C-NC  | 4.46  | 114.67      | 109.98   |
| 11  | bL    | 206 | CLA  | C3D-C2D-C1D | -4.46 | 99.75       | 105.83   |
| 11  | cB    | 835 | CLA  | O2D-CGD-CBD | 4.46  | 119.02      | 111.23   |
| 11  | cB    | 834 | CLA  | C3D-C2D-C1D | -4.46 | 99.75       | 105.83   |
| 11  | bB    | 811 | CLA  | C3D-C2D-C1D | -4.46 | 99.75       | 105.83   |
| 11  | aA    | 811 | CLA  | C3D-C2D-C1D | -4.46 | 99.75       | 105.83   |
| 11  | bA    | 812 | CLA  | C3D-C2D-C1D | -4.45 | 99.75       | 105.83   |
| 12  | aA    | 827 | F6C  | C2C-C1C-NC  | 4.45  | 114.94      | 110.33   |
| 11  | bB    | 833 | CLA  | C2C-C1C-NC  | 4.45  | 114.66      | 109.98   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bB    | 835 | CLA  | O2D-CGD-CBD | 4.45  | 119.02      | 111.23   |
| 11  | cL    | 206 | CLA  | C3D-C2D-C1D | -4.45 | 99.75       | 105.83   |
| 12  | cA    | 827 | F6C  | C2C-C1C-NC  | 4.45  | 114.94      | 110.33   |
| 11  | cB    | 802 | CLA  | C3D-C2D-C1D | -4.45 | 99.76       | 105.83   |
| 12  | bA    | 844 | F6C  | CHB-C4A-C3A | -4.45 | 116.23      | 125.49   |
| 11  | aA    | 816 | CLA  | C3D-C2D-C1D | -4.45 | 99.76       | 105.83   |
| 12  | cA    | 844 | F6C  | CHB-C4A-C3A | -4.45 | 116.23      | 125.49   |
| 11  | cB    | 833 | CLA  | C2C-C1C-NC  | 4.45  | 114.66      | 109.98   |
| 11  | cB    | 811 | CLA  | C3D-C2D-C1D | -4.45 | 99.76       | 105.83   |
| 12  | bA    | 827 | F6C  | C2C-C1C-NC  | 4.45  | 114.94      | 110.33   |
| 11  | cA    | 829 | CLA  | O2D-CGD-CBD | 4.45  | 119.01      | 111.23   |
| 11  | bA    | 811 | CLA  | C2B-C1B-NB  | 4.45  | 114.94      | 110.33   |
| 11  | cA    | 814 | CLA  | C2C-C1C-NC  | 4.45  | 114.65      | 109.98   |
| 11  | cB    | 804 | CLA  | C2C-C1C-NC  | 4.45  | 114.65      | 109.98   |
| 11  | aA    | 814 | CLA  | C3D-C4D-ND  | 4.45  | 117.22      | 109.99   |
| 11  | aA    | 831 | CLA  | C3D-C2D-C1D | -4.45 | 99.76       | 105.83   |
| 11  | bB    | 801 | CLA  | CMA-C3A-C2A | -4.45 | 96.79       | 113.98   |
| 11  | cB    | 801 | CLA  | CMA-C3A-C2A | -4.44 | 96.80       | 113.98   |
| 11  | aB    | 801 | CLA  | CMA-C3A-C2A | -4.44 | 96.80       | 113.98   |
| 11  | aB    | 813 | CLA  | C2B-C1B-NB  | 4.44  | 114.93      | 110.33   |
| 11  | aA    | 802 | CLA  | C3D-C2D-C1D | -4.44 | 99.77       | 105.83   |
| 11  | aB    | 810 | CLA  | O2D-CGD-CBD | 4.44  | 119.00      | 111.23   |
| 11  | bA    | 820 | CLA  | O2D-CGD-CBD | 4.44  | 119.00      | 111.23   |
| 11  | bA    | 829 | CLA  | O2D-CGD-CBD | 4.44  | 119.00      | 111.23   |
| 11  | aA    | 812 | CLA  | C3D-C2D-C1D | -4.44 | 99.77       | 105.83   |
| 11  | aL    | 206 | CLA  | C3D-C2D-C1D | -4.44 | 99.77       | 105.83   |
| 11  | cA    | 820 | CLA  | O2D-CGD-CBD | 4.44  | 119.00      | 111.23   |
| 11  | bA    | 806 | CLA  | CAC-C3C-C4C | 4.44  | 130.57      | 124.79   |
| 11  | aB    | 835 | CLA  | C2B-C1B-NB  | 4.44  | 114.93      | 110.33   |
| 12  | aA    | 844 | F6C  | C2C-C1C-NC  | 4.44  | 114.93      | 110.33   |
| 11  | aA    | 828 | CLA  | C1D-CHD-C4C | -4.44 | 116.58      | 126.02   |
| 11  | aB    | 811 | CLA  | C3D-C2D-C1D | -4.44 | 99.77       | 105.83   |
| 11  | bA    | 816 | CLA  | C3D-C2D-C1D | -4.44 | 99.77       | 105.83   |
| 11  | bA    | 831 | CLA  | C3D-C2D-C1D | -4.44 | 99.77       | 105.83   |
| 11  | bB    | 822 | CLA  | C1D-CHD-C4C | -4.44 | 116.59      | 126.02   |
| 11  | bB    | 802 | CLA  | C3D-C2D-C1D | -4.44 | 99.78       | 105.83   |
| 11  | bA    | 820 | CLA  | C2B-C1B-NB  | 4.44  | 114.93      | 110.33   |
| 11  | aB    | 833 | CLA  | C2C-C1C-NC  | 4.44  | 114.64      | 109.98   |
| 11  | cL    | 206 | CLA  | C3B-C2B-C1B | -4.44 | 101.94      | 107.17   |
| 11  | bA    | 842 | CLA  | C4A-NA-C1A  | -4.43 | 104.66      | 106.68   |
| 11  | aA    | 811 | CLA  | C2B-C1B-NB  | 4.43  | 114.92      | 110.33   |
| 11  | bA    | 806 | CLA  | C3D-C2D-C1D | -4.43 | 99.78       | 105.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bA    | 834 | CLA  | C3D-C2D-C1D | -4.43 | 99.78       | 105.83   |
| 11  | aB    | 835 | CLA  | O2D-CGD-CBD | 4.43  | 118.98      | 111.23   |
| 11  | bL    | 206 | CLA  | C3B-C2B-C1B | -4.43 | 101.94      | 107.17   |
| 11  | aB    | 801 | CLA  | C2C-C1C-NC  | 4.43  | 114.64      | 109.98   |
| 11  | bA    | 828 | CLA  | C1D-CHD-C4C | -4.43 | 116.60      | 126.02   |
| 11  | aA    | 806 | CLA  | CAC-C3C-C4C | 4.43  | 130.55      | 124.79   |
| 11  | aA    | 820 | CLA  | C2B-C1B-NB  | 4.43  | 114.92      | 110.33   |
| 11  | cB    | 810 | CLA  | O2D-CGD-CBD | 4.43  | 118.97      | 111.23   |
| 12  | aB    | 824 | F6C  | OMB-CMB-C2B | -4.43 | 115.62      | 125.62   |
| 11  | bA    | 814 | CLA  | C2C-C1C-NC  | 4.43  | 114.63      | 109.98   |
| 11  | aA    | 806 | CLA  | C3D-C2D-C1D | -4.43 | 99.79       | 105.83   |
| 11  | bB    | 829 | CLA  | C3D-C2D-C1D | -4.43 | 99.79       | 105.83   |
| 11  | cA    | 828 | CLA  | C1D-CHD-C4C | -4.42 | 116.62      | 126.02   |
| 11  | bA    | 838 | CLA  | C4A-NA-C1A  | -4.42 | 104.66      | 106.68   |
| 11  | aA    | 831 | CLA  | C2B-C1B-NB  | 4.42  | 114.91      | 110.33   |
| 11  | bB    | 812 | CLA  | CAC-C3C-C4C | 4.42  | 130.54      | 124.79   |
| 12  | aA    | 844 | F6C  | CHB-C4A-C3A | -4.42 | 116.29      | 125.49   |
| 11  | cA    | 814 | CLA  | C3D-C4D-ND  | 4.42  | 117.18      | 109.99   |
| 11  | aA    | 820 | CLA  | O2D-CGD-CBD | 4.42  | 118.96      | 111.23   |
| 11  | aA    | 834 | CLA  | C3D-C2D-C1D | -4.42 | 99.80       | 105.83   |
| 11  | cB    | 822 | CLA  | C1D-CHD-C4C | -4.42 | 116.62      | 126.02   |
| 11  | cB    | 837 | CLA  | C2C-C1C-NC  | 4.42  | 114.62      | 109.98   |
| 11  | bA    | 802 | CLA  | C3D-C2D-C1D | -4.42 | 99.80       | 105.83   |
| 11  | cA    | 831 | CLA  | C3D-C2D-C1D | -4.42 | 99.80       | 105.83   |
| 11  | bA    | 831 | CLA  | C2B-C1B-NB  | 4.42  | 114.91      | 110.33   |
| 12  | cB    | 824 | F6C  | OMB-CMB-C2B | -4.42 | 115.65      | 125.62   |
| 11  | aB    | 822 | CLA  | C1D-CHD-C4C | -4.42 | 116.63      | 126.02   |
| 12  | cA    | 844 | F6C  | C2C-C1C-NC  | 4.42  | 114.91      | 110.33   |
| 11  | cA    | 820 | CLA  | C2B-C1B-NB  | 4.42  | 114.91      | 110.33   |
| 12  | bB    | 824 | F6C  | OMB-CMB-C2B | -4.41 | 115.66      | 125.62   |
| 11  | aB    | 812 | CLA  | CAC-C3C-C4C | 4.41  | 130.53      | 124.79   |
| 11  | bB    | 810 | CLA  | O2D-CGD-CBD | 4.41  | 118.94      | 111.23   |
| 11  | cA    | 834 | CLA  | C2B-C1B-NB  | 4.41  | 114.90      | 110.33   |
| 12  | aA    | 830 | F6C  | C3D-C4D-ND  | 4.41  | 117.20      | 109.93   |
| 11  | bA    | 814 | CLA  | C3D-C4D-ND  | 4.41  | 117.16      | 109.99   |
| 11  | cB    | 829 | CLA  | C3D-C2D-C1D | -4.41 | 99.82       | 105.83   |
| 11  | bA    | 806 | CLA  | C2C-C1C-NC  | 4.41  | 114.61      | 109.98   |
| 12  | bA    | 830 | F6C  | C3D-C4D-ND  | 4.41  | 117.19      | 109.93   |
| 11  | cA    | 824 | CLA  | C3D-C2D-C1D | -4.41 | 99.82       | 105.83   |
| 11  | aA    | 834 | CLA  | C2B-C1B-NB  | 4.41  | 114.89      | 110.33   |
| 11  | aB    | 810 | CLA  | C4A-NA-C1A  | -4.41 | 104.67      | 106.68   |
| 11  | bB    | 804 | CLA  | C2C-C1C-NC  | 4.41  | 114.61      | 109.98   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cB    | 839 | CLA  | C2C-C1C-NC  | 4.41  | 114.61      | 109.98   |
| 11  | aA    | 824 | CLA  | C3D-C2D-C1D | -4.40 | 99.82       | 105.83   |
| 11  | aB    | 818 | CLA  | C2B-C1B-NB  | 4.40  | 114.89      | 110.33   |
| 11  | cA    | 834 | CLA  | C3D-C2D-C1D | -4.40 | 99.82       | 105.83   |
| 11  | bB    | 806 | CLA  | C2B-C1B-NB  | 4.40  | 114.89      | 110.33   |
| 11  | cA    | 831 | CLA  | C2B-C1B-NB  | 4.40  | 114.89      | 110.33   |
| 11  | bB    | 837 | CLA  | C2C-C1C-NC  | 4.40  | 114.61      | 109.98   |
| 11  | aA    | 819 | CLA  | C4A-NA-C1A  | -4.40 | 104.67      | 106.68   |
| 11  | aB    | 812 | CLA  | C4A-NA-C1A  | -4.40 | 104.67      | 106.68   |
| 11  | cB    | 829 | CLA  | CHD-C4C-C3C | -4.40 | 118.36      | 124.77   |
| 11  | cA    | 811 | CLA  | C3B-C2B-C1B | -4.40 | 101.98      | 107.17   |
| 11  | aB    | 829 | CLA  | C3D-C2D-C1D | -4.40 | 99.83       | 105.83   |
| 11  | cA    | 806 | CLA  | C3D-C2D-C1D | -4.40 | 99.83       | 105.83   |
| 11  | aL    | 206 | CLA  | C3D-C4D-ND  | 4.40  | 117.14      | 109.99   |
| 11  | bB    | 829 | CLA  | CHD-C4C-C3C | -4.40 | 118.36      | 124.77   |
| 11  | cB    | 835 | CLA  | C2B-C1B-NB  | 4.39  | 114.88      | 110.33   |
| 11  | aA    | 843 | CLA  | C3B-C2B-C1B | -4.39 | 101.99      | 107.17   |
| 11  | aB    | 839 | CLA  | C2B-C1B-NB  | 4.39  | 114.88      | 110.33   |
| 11  | cB    | 828 | CLA  | C4B-C3B-C2B | -4.39 | 101.84      | 107.30   |
| 11  | bL    | 206 | CLA  | C3D-C4D-ND  | 4.39  | 117.12      | 109.99   |
| 12  | cA    | 830 | F6C  | C3D-C4D-ND  | 4.39  | 117.16      | 109.93   |
| 12  | aA    | 830 | F6C  | O2D-CGD-CBD | 4.39  | 118.90      | 111.23   |
| 12  | bA    | 844 | F6C  | C2C-C1C-NC  | 4.39  | 114.88      | 110.33   |
| 12  | cA    | 832 | F6C  | CHB-C4A-C3A | -4.39 | 116.36      | 125.49   |
| 11  | aB    | 828 | CLA  | C4B-C3B-C2B | -4.39 | 101.85      | 107.30   |
| 11  | bB    | 839 | CLA  | C2B-C1B-NB  | 4.39  | 114.88      | 110.33   |
| 11  | cB    | 839 | CLA  | C2B-C1B-NB  | 4.39  | 114.88      | 110.33   |
| 11  | aB    | 828 | CLA  | C2D-C1D-ND  | 4.39  | 114.47      | 110.13   |
| 12  | bB    | 824 | F6C  | C3D-C4D-ND  | 4.38  | 117.15      | 109.93   |
| 11  | cL    | 206 | CLA  | C3D-C4D-ND  | 4.38  | 117.11      | 109.99   |
| 11  | aB    | 815 | CLA  | C2C-C1C-NC  | 4.38  | 114.58      | 109.98   |
| 11  | aB    | 829 | CLA  | CHD-C4C-C3C | -4.38 | 118.39      | 124.77   |
| 11  | cB    | 812 | CLA  | CAC-C3C-C4C | 4.38  | 130.49      | 124.79   |
| 11  | aA    | 814 | CLA  | C2C-C1C-NC  | 4.38  | 114.58      | 109.98   |
| 16  | aA    | 852 | LHG  | O4-P-O5     | 4.38  | 132.82      | 112.44   |
| 16  | cA    | 852 | LHG  | O4-P-O5     | 4.38  | 132.82      | 112.44   |
| 12  | bA    | 832 | F6C  | CHB-C4A-C3A | -4.38 | 116.38      | 125.49   |
| 11  | cB    | 812 | CLA  | C4A-NA-C1A  | -4.38 | 104.68      | 106.68   |
| 11  | aB    | 804 | CLA  | C2C-C1C-NC  | 4.38  | 114.58      | 109.98   |
| 11  | aA    | 817 | CLA  | C3B-C2B-C1B | -4.38 | 102.01      | 107.17   |
| 11  | bA    | 824 | CLA  | C3D-C2D-C1D | -4.38 | 99.86       | 105.83   |
| 11  | bB    | 828 | CLA  | C2D-C1D-ND  | 4.38  | 114.46      | 110.13   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 16  | bA    | 852 | LHG  | O4-P-O5     | 4.38  | 132.81      | 112.44   |
| 11  | aA    | 811 | CLA  | C4A-NA-C1A  | -4.38 | 104.68      | 106.68   |
| 11  | cB    | 803 | CLA  | CHD-C4C-C3C | -4.37 | 118.40      | 124.77   |
| 11  | cB    | 837 | CLA  | C4A-NA-C1A  | -4.37 | 104.68      | 106.68   |
| 12  | cB    | 824 | F6C  | C3D-C4D-ND  | 4.37  | 117.13      | 109.93   |
| 11  | aB    | 801 | CLA  | C1D-CHD-C4C | -4.37 | 116.73      | 126.02   |
| 11  | cB    | 828 | CLA  | C2D-C1D-ND  | 4.37  | 114.45      | 110.13   |
| 11  | cA    | 843 | CLA  | C3B-C2B-C1B | -4.37 | 102.02      | 107.17   |
| 12  | cA    | 830 | F6C  | C1-C2-C3    | -4.37 | 119.04      | 126.20   |
| 12  | aB    | 824 | F6C  | C3D-C4D-ND  | 4.37  | 117.13      | 109.93   |
| 11  | bA    | 810 | CLA  | O2D-CGD-CBD | 4.37  | 118.86      | 111.23   |
| 11  | bB    | 816 | CLA  | C2C-C1C-NC  | 4.37  | 114.57      | 109.98   |
| 12  | cA    | 830 | F6C  | O2D-CGD-CBD | 4.37  | 118.86      | 111.23   |
| 17  | aA    | 853 | LMT  | C6B-C5B-C4B | -4.36 | 102.30      | 113.02   |
| 11  | cB    | 801 | CLA  | C1D-CHD-C4C | -4.36 | 116.74      | 126.02   |
| 11  | cB    | 815 | CLA  | C2C-C1C-NC  | 4.36  | 114.57      | 109.98   |
| 17  | cA    | 853 | LMT  | C6B-C5B-C4B | -4.36 | 102.31      | 113.02   |
| 11  | bB    | 828 | CLA  | C4B-C3B-C2B | -4.36 | 101.88      | 107.30   |
| 12  | aL    | 202 | F6C  | C4C-CHD-C1D | -4.36 | 115.99      | 126.25   |
| 11  | aB    | 812 | CLA  | C3D-C2D-C1D | -4.36 | 99.88       | 105.83   |
| 11  | bB    | 801 | CLA  | C1D-CHD-C4C | -4.36 | 116.75      | 126.02   |
| 11  | aB    | 803 | CLA  | CHD-C4C-C3C | -4.36 | 118.42      | 124.77   |
| 12  | aA    | 832 | F6C  | CHB-C4A-C3A | -4.36 | 116.42      | 125.49   |
| 11  | cA    | 808 | CLA  | C3D-C4D-ND  | 4.36  | 117.07      | 109.99   |
| 11  | bB    | 803 | CLA  | CHD-C4C-C3C | -4.36 | 118.42      | 124.77   |
| 11  | aB    | 816 | CLA  | C2C-C1C-NC  | 4.36  | 114.56      | 109.98   |
| 11  | aA    | 808 | CLA  | C3D-C4D-ND  | 4.36  | 117.07      | 109.99   |
| 12  | cL    | 202 | F6C  | C4C-CHD-C1D | -4.36 | 116.00      | 126.25   |
| 11  | bA    | 843 | CLA  | C3B-C2B-C1B | -4.36 | 102.03      | 107.17   |
| 11  | bB    | 839 | CLA  | C2C-C1C-NC  | 4.35  | 114.56      | 109.98   |
| 11  | bA    | 811 | CLA  | C3B-C2B-C1B | -4.35 | 102.04      | 107.17   |
| 11  | aB    | 808 | CLA  | C1D-CHD-C4C | -4.35 | 116.77      | 126.02   |
| 11  | cB    | 808 | CLA  | C1D-CHD-C4C | -4.35 | 116.77      | 126.02   |
| 11  | bA    | 825 | CLA  | C3D-C2D-C1D | -4.35 | 99.89       | 105.83   |
| 11  | aA    | 831 | CLA  | C4B-C3B-C2B | -4.35 | 101.89      | 107.30   |
| 11  | bB    | 815 | CLA  | C2C-C1C-NC  | 4.35  | 114.55      | 109.98   |
| 12  | aA    | 830 | F6C  | C1-C2-C3    | -4.35 | 119.07      | 126.20   |
| 11  | bB    | 837 | CLA  | C4A-NA-C1A  | -4.35 | 104.69      | 106.68   |
| 11  | aA    | 810 | CLA  | O2D-CGD-CBD | 4.35  | 118.83      | 111.23   |
| 11  | aB    | 839 | CLA  | C2C-C1C-NC  | 4.35  | 114.55      | 109.98   |
| 12  | bA    | 830 | F6C  | O2D-CGD-CBD | 4.35  | 118.83      | 111.23   |
| 17  | bA    | 853 | LMT  | C6B-C5B-C4B | -4.35 | 102.35      | 113.02   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cA    | 817 | CLA  | C3B-C2B-C1B | -4.35 | 102.05      | 107.17   |
| 12  | bL    | 202 | F6C  | C4C-CHD-C1D | -4.35 | 116.03      | 126.25   |
| 11  | bA    | 822 | CLA  | C3D-C2D-C1D | -4.34 | 99.90       | 105.83   |
| 12  | bA    | 826 | F6C  | C3D-C2D-C1D | -4.34 | 99.54       | 105.83   |
| 11  | aA    | 821 | CLA  | C3B-C2B-C1B | -4.34 | 102.05      | 107.17   |
| 11  | bA    | 817 | CLA  | C3B-C2B-C1B | -4.34 | 102.05      | 107.17   |
| 11  | bB    | 808 | CLA  | C1D-CHD-C4C | -4.34 | 116.79      | 126.02   |
| 11  | cA    | 810 | CLA  | O2D-CGD-CBD | 4.34  | 118.82      | 111.23   |
| 11  | cA    | 822 | CLA  | C3D-C2D-C1D | -4.34 | 99.91       | 105.83   |
| 12  | cA    | 826 | F6C  | C3D-C2D-C1D | -4.34 | 99.55       | 105.83   |
| 11  | aA    | 811 | CLA  | C3B-C2B-C1B | -4.34 | 102.05      | 107.17   |
| 12  | bA    | 830 | F6C  | C1-C2-C3    | -4.34 | 119.09      | 126.20   |
| 11  | cA    | 831 | CLA  | C4B-C3B-C2B | -4.34 | 101.91      | 107.30   |
| 11  | bA    | 834 | CLA  | C2B-C1B-NB  | 4.33  | 114.82      | 110.33   |
| 11  | aA    | 822 | CLA  | C3D-C2D-C1D | -4.33 | 99.92       | 105.83   |
| 12  | cA    | 827 | F6C  | C3D-C2D-C1D | -4.33 | 99.56       | 105.83   |
| 11  | cB    | 818 | CLA  | C2B-C1B-NB  | 4.33  | 114.81      | 110.33   |
| 11  | cB    | 829 | CLA  | C3B-C4B-NB  | 4.33  | 114.39      | 110.53   |
| 11  | cB    | 820 | CLA  | C1C-C2C-C3C | -4.33 | 102.43      | 106.98   |
| 11  | cB    | 812 | CLA  | C3D-C2D-C1D | -4.33 | 99.93       | 105.83   |
| 11  | cB    | 816 | CLA  | C2C-C1C-NC  | 4.33  | 114.53      | 109.98   |
| 11  | cA    | 806 | CLA  | C3D-C4D-ND  | 4.33  | 117.02      | 109.99   |
| 11  | aA    | 838 | CLA  | C4A-NA-C1A  | -4.32 | 104.71      | 106.68   |
| 11  | bA    | 839 | CLA  | C4A-NA-C1A  | -4.32 | 104.71      | 106.68   |
| 11  | bA    | 821 | CLA  | C3B-C2B-C1B | -4.32 | 102.07      | 107.17   |
| 11  | bB    | 818 | CLA  | C2B-C1B-NB  | 4.32  | 114.81      | 110.33   |
| 12  | aA    | 832 | F6C  | C3D-C4D-ND  | 4.32  | 117.05      | 109.93   |
| 11  | bA    | 819 | CLA  | O2D-CGD-CBD | 4.32  | 118.79      | 111.23   |
| 11  | bA    | 808 | CLA  | C3D-C4D-ND  | 4.32  | 117.01      | 109.99   |
| 11  | cB    | 818 | CLA  | C3D-C4D-ND  | 4.32  | 117.01      | 109.99   |
| 12  | bA    | 832 | F6C  | C3D-C4D-ND  | 4.32  | 117.04      | 109.93   |
| 12  | cA    | 832 | F6C  | C3D-C4D-ND  | 4.32  | 117.04      | 109.93   |
| 11  | cA    | 821 | CLA  | C3B-C2B-C1B | -4.32 | 102.08      | 107.17   |
| 11  | bB    | 812 | CLA  | C3D-C2D-C1D | -4.31 | 99.95       | 105.83   |
| 11  | aA    | 840 | CLA  | C3D-C4D-ND  | 4.31  | 117.00      | 109.99   |
| 11  | bB    | 818 | CLA  | C3D-C4D-ND  | 4.31  | 117.00      | 109.99   |
| 11  | aA    | 819 | CLA  | O2D-CGD-CBD | 4.31  | 118.77      | 111.23   |
| 12  | aA    | 827 | F6C  | C3D-C2D-C1D | -4.31 | 99.59       | 105.83   |
| 12  | aA    | 826 | F6C  | C3D-C2D-C1D | -4.31 | 99.59       | 105.83   |
| 11  | aB    | 818 | CLA  | C3D-C4D-ND  | 4.31  | 116.99      | 109.99   |
| 11  | bA    | 831 | CLA  | C4B-C3B-C2B | -4.31 | 101.94      | 107.30   |
| 11  | aA    | 825 | CLA  | C3D-C2D-C1D | -4.31 | 99.95       | 105.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12  | bA    | 827 | F6C  | C3D-C2D-C1D | -4.31 | 99.59       | 105.83   |
| 11  | bA    | 810 | CLA  | C3D-C2D-C1D | -4.31 | 99.95       | 105.83   |
| 11  | bB    | 809 | CLA  | C3D-C4D-ND  | 4.30  | 116.98      | 109.99   |
| 11  | bB    | 820 | CLA  | C1C-C2C-C3C | -4.30 | 102.45      | 106.98   |
| 11  | cA    | 819 | CLA  | C4A-NA-C1A  | -4.30 | 104.72      | 106.68   |
| 11  | cB    | 838 | CLA  | C3D-C4D-ND  | 4.30  | 116.98      | 109.99   |
| 11  | aB    | 829 | CLA  | C3B-C4B-NB  | 4.30  | 114.37      | 110.53   |
| 11  | bB    | 838 | CLA  | C3D-C4D-ND  | 4.30  | 116.98      | 109.99   |
| 11  | bA    | 836 | CLA  | C3D-C2D-C1D | -4.30 | 99.96       | 105.83   |
| 11  | aB    | 809 | CLA  | C3D-C4D-ND  | 4.30  | 116.97      | 109.99   |
| 11  | cA    | 836 | CLA  | C3D-C2D-C1D | -4.30 | 99.97       | 105.83   |
| 11  | cB    | 810 | CLA  | C4A-NA-C1A  | -4.30 | 104.72      | 106.68   |
| 11  | aL    | 205 | CLA  | C3D-C4D-ND  | 4.30  | 116.97      | 109.99   |
| 11  | cA    | 825 | CLA  | C3D-C2D-C1D | -4.29 | 99.97       | 105.83   |
| 11  | cB    | 827 | CLA  | C4A-NA-C1A  | -4.29 | 104.72      | 106.68   |
| 12  | aA    | 827 | F6C  | CHB-C4A-C3A | -4.29 | 116.56      | 125.49   |
| 11  | aA    | 839 | CLA  | C4A-NA-C1A  | -4.29 | 104.72      | 106.68   |
| 11  | aA    | 836 | CLA  | C3D-C2D-C1D | -4.29 | 99.98       | 105.83   |
| 11  | bA    | 840 | CLA  | C3D-C4D-ND  | 4.29  | 116.96      | 109.99   |
| 11  | cB    | 813 | CLA  | C3D-C2D-C1D | -4.29 | 99.98       | 105.83   |
| 11  | cA    | 840 | CLA  | C3D-C4D-ND  | 4.28  | 116.95      | 109.99   |
| 11  | bA    | 806 | CLA  | C3D-C4D-ND  | 4.28  | 116.95      | 109.99   |
| 11  | bB    | 810 | CLA  | C4A-NA-C1A  | -4.28 | 104.72      | 106.68   |
| 12  | bA    | 827 | F6C  | CHB-C4A-C3A | -4.28 | 116.58      | 125.49   |
| 11  | cA    | 819 | CLA  | O2D-CGD-CBD | 4.28  | 118.71      | 111.23   |
| 11  | cB    | 809 | CLA  | O2D-CGD-CBD | 4.28  | 118.71      | 111.23   |
| 11  | bB    | 809 | CLA  | O2D-CGD-CBD | 4.28  | 118.71      | 111.23   |
| 11  | aB    | 838 | CLA  | C3D-C4D-ND  | 4.28  | 116.94      | 109.99   |
| 11  | aA    | 806 | CLA  | C3D-C4D-ND  | 4.28  | 116.94      | 109.99   |
| 11  | cB    | 834 | CLA  | O2D-CGD-CBD | 4.28  | 118.70      | 111.23   |
| 11  | bL    | 205 | CLA  | C3D-C4D-ND  | 4.28  | 116.94      | 109.99   |
| 11  | cA    | 821 | CLA  | C3D-C2D-C1D | -4.27 | 100.00      | 105.83   |
| 11  | bB    | 829 | CLA  | C3B-C4B-NB  | 4.27  | 114.34      | 110.53   |
| 11  | cA    | 814 | CLA  | C3D-C2D-C1D | -4.27 | 100.00      | 105.83   |
| 11  | bA    | 821 | CLA  | C3D-C2D-C1D | -4.27 | 100.00      | 105.83   |
| 11  | aB    | 820 | CLA  | C1C-C2C-C3C | -4.27 | 102.49      | 106.98   |
| 11  | bB    | 812 | CLA  | C4A-NA-C1A  | -4.27 | 104.73      | 106.68   |
| 11  | cA    | 838 | CLA  | C4A-NA-C1A  | -4.27 | 104.73      | 106.68   |
| 11  | cB    | 809 | CLA  | C3D-C4D-ND  | 4.27  | 116.93      | 109.99   |
| 11  | aA    | 837 | CLA  | C3D-C4D-ND  | 4.27  | 116.92      | 109.99   |
| 11  | cL    | 205 | CLA  | C3D-C4D-ND  | 4.27  | 116.92      | 109.99   |
| 11  | aB    | 809 | CLA  | O2D-CGD-CBD | 4.26  | 118.68      | 111.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bA    | 814 | CLA  | C3D-C2D-C1D | -4.26 | 100.01      | 105.83   |
| 11  | aA    | 821 | CLA  | C3D-C2D-C1D | -4.26 | 100.02      | 105.83   |
| 11  | aB    | 813 | CLA  | C3D-C2D-C1D | -4.26 | 100.02      | 105.83   |
| 11  | cB    | 829 | CLA  | CMB-C2B-C1B | 4.26  | 131.91      | 125.42   |
| 11  | cA    | 810 | CLA  | C3D-C2D-C1D | -4.26 | 100.02      | 105.83   |
| 11  | aA    | 843 | CLA  | C4A-NA-C1A  | -4.26 | 104.74      | 106.68   |
| 11  | bA    | 819 | CLA  | C4A-NA-C1A  | -4.26 | 104.74      | 106.68   |
| 11  | bA    | 843 | CLA  | C4A-NA-C1A  | -4.26 | 104.74      | 106.68   |
| 11  | aA    | 810 | CLA  | C3D-C2D-C1D | -4.26 | 100.02      | 105.83   |
| 11  | cA    | 815 | CLA  | C3B-C4B-NB  | 4.26  | 114.33      | 110.53   |
| 12  | bA    | 827 | F6C  | CHA-C1A-C2A | -4.25 | 118.97      | 130.41   |
| 11  | bB    | 818 | CLA  | C2C-C1C-NC  | 4.25  | 114.45      | 109.98   |
| 12  | aA    | 827 | F6C  | CHA-C1A-C2A | -4.25 | 118.97      | 130.41   |
| 11  | cB    | 818 | CLA  | C2C-C1C-NC  | 4.25  | 114.45      | 109.98   |
| 11  | bB    | 834 | CLA  | O2D-CGD-CBD | 4.25  | 118.66      | 111.23   |
| 11  | cA    | 843 | CLA  | C4A-NA-C1A  | -4.25 | 104.74      | 106.68   |
| 11  | bB    | 813 | CLA  | C3D-C2D-C1D | -4.25 | 100.03      | 105.83   |
| 12  | cA    | 827 | F6C  | CHB-C4A-C3A | -4.25 | 116.65      | 125.49   |
| 11  | cA    | 813 | CLA  | O2D-CGD-CBD | 4.25  | 118.66      | 111.23   |
| 11  | bA    | 815 | CLA  | C3B-C4B-NB  | 4.25  | 114.32      | 110.53   |
| 11  | aA    | 821 | CLA  | C2B-C1B-NB  | 4.25  | 114.73      | 110.33   |
| 11  | bB    | 806 | CLA  | C4A-NA-C1A  | -4.25 | 104.74      | 106.68   |
| 11  | aA    | 814 | CLA  | C3D-C2D-C1D | -4.24 | 100.04      | 105.83   |
| 11  | bB    | 822 | CLA  | C3D-C4D-ND  | 4.24  | 116.89      | 109.99   |
| 11  | cA    | 837 | CLA  | C3D-C4D-ND  | 4.24  | 116.88      | 109.99   |
| 12  | bA    | 832 | F6C  | C3D-C2D-C1D | -4.24 | 99.69       | 105.83   |
| 12  | cA    | 827 | F6C  | CHA-C1A-C2A | -4.24 | 119.01      | 130.41   |
| 11  | aA    | 815 | CLA  | C3B-C4B-NB  | 4.24  | 114.31      | 110.53   |
| 11  | aB    | 834 | CLA  | O2D-CGD-CBD | 4.24  | 118.64      | 111.23   |
| 11  | aA    | 807 | CLA  | C1C-C2C-C3C | -4.24 | 102.52      | 106.98   |
| 11  | bA    | 821 | CLA  | C2B-C1B-NB  | 4.24  | 114.72      | 110.33   |
| 11  | bA    | 837 | CLA  | C3D-C4D-ND  | 4.23  | 116.87      | 109.99   |
| 11  | aB    | 829 | CLA  | CMB-C2B-C1B | 4.23  | 131.87      | 125.42   |
| 11  | cA    | 839 | CLA  | C3D-C4D-ND  | 4.23  | 116.87      | 109.99   |
| 11  | aB    | 818 | CLA  | C2C-C1C-NC  | 4.23  | 114.43      | 109.98   |
| 12  | bA    | 827 | F6C  | C3C-C4C-NC  | 4.23  | 114.96      | 110.32   |
| 11  | cB    | 833 | CLA  | C3D-C4D-ND  | 4.23  | 116.87      | 109.99   |
| 11  | aB    | 822 | CLA  | C3D-C4D-ND  | 4.23  | 116.87      | 109.99   |
| 11  | bA    | 813 | CLA  | O2D-CGD-CBD | 4.23  | 118.63      | 111.23   |
| 11  | bB    | 829 | CLA  | CMB-C2B-C1B | 4.23  | 131.86      | 125.42   |
| 11  | cA    | 821 | CLA  | C2B-C1B-NB  | 4.23  | 114.71      | 110.33   |
| 11  | cB    | 833 | CLA  | O2D-CGD-CBD | 4.23  | 118.62      | 111.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cB    | 822 | CLA  | C3D-C4D-ND  | 4.23  | 116.86      | 109.99   |
| 11  | bB    | 826 | CLA  | C3C-C4C-NC  | 4.23  | 115.85      | 110.43   |
| 12  | cA    | 827 | F6C  | C3C-C4C-NC  | 4.23  | 114.95      | 110.32   |
| 11  | aB    | 837 | CLA  | C3D-C4D-ND  | 4.23  | 116.86      | 109.99   |
| 12  | aA    | 832 | F6C  | C3D-C2D-C1D | -4.23 | 99.71       | 105.83   |
| 11  | aA    | 813 | CLA  | O2D-CGD-CBD | 4.22  | 118.62      | 111.23   |
| 11  | bA    | 839 | CLA  | C3D-C4D-ND  | 4.22  | 116.85      | 109.99   |
| 11  | bB    | 827 | CLA  | C4A-NA-C1A  | -4.22 | 104.75      | 106.68   |
| 11  | aA    | 802 | CLA  | CHD-C1D-ND  | -4.22 | 118.86      | 124.80   |
| 11  | bK    | 101 | CLA  | C3D-C4D-ND  | 4.22  | 116.85      | 109.99   |
| 11  | cK    | 101 | CLA  | C3D-C4D-ND  | 4.22  | 116.85      | 109.99   |
| 11  | cA    | 839 | CLA  | C4A-NA-C1A  | -4.22 | 104.75      | 106.68   |
| 11  | aA    | 839 | CLA  | C3D-C4D-ND  | 4.22  | 116.84      | 109.99   |
| 11  | bB    | 837 | CLA  | C3D-C4D-ND  | 4.22  | 116.84      | 109.99   |
| 11  | bB    | 833 | CLA  | C3D-C4D-ND  | 4.22  | 116.84      | 109.99   |
| 11  | aB    | 833 | CLA  | O2D-CGD-CBD | 4.21  | 118.60      | 111.23   |
| 11  | bB    | 833 | CLA  | O2D-CGD-CBD | 4.21  | 118.59      | 111.23   |
| 12  | cA    | 844 | F6C  | O2D-CGD-CBD | 4.21  | 118.59      | 111.23   |
| 11  | cB    | 826 | CLA  | C3C-C4C-NC  | 4.21  | 115.82      | 110.43   |
| 11  | aK    | 101 | CLA  | C3D-C4D-ND  | 4.21  | 116.83      | 109.99   |
| 12  | cA    | 832 | F6C  | C3D-C2D-C1D | -4.21 | 99.74       | 105.83   |
| 11  | cA    | 820 | CLA  | C3B-C2B-C1B | -4.21 | 102.21      | 107.17   |
| 11  | aA    | 841 | CLA  | C3D-C4D-ND  | 4.21  | 116.82      | 109.99   |
| 12  | cA    | 830 | F6C  | CHD-C4C-C3C | -4.20 | 116.10      | 125.30   |
| 11  | bA    | 841 | CLA  | C3D-C4D-ND  | 4.20  | 116.82      | 109.99   |
| 11  | bA    | 807 | CLA  | C1C-C2C-C3C | -4.20 | 102.56      | 106.98   |
| 12  | cA    | 830 | F6C  | CHB-C4A-C3A | -4.20 | 116.75      | 125.49   |
| 12  | aA    | 830 | F6C  | CHD-C4C-C3C | -4.20 | 116.11      | 125.30   |
| 11  | bA    | 805 | CLA  | C2C-C1C-NC  | 4.20  | 114.39      | 109.98   |
| 11  | aB    | 805 | CLA  | C3D-C4D-ND  | 4.20  | 116.81      | 109.99   |
| 12  | bA    | 844 | F6C  | O2D-CGD-CBD | 4.20  | 118.57      | 111.23   |
| 11  | aB    | 833 | CLA  | C3D-C4D-ND  | 4.20  | 116.81      | 109.99   |
| 11  | aB    | 837 | CLA  | C4A-NA-C1A  | -4.20 | 104.76      | 106.68   |
| 11  | aA    | 802 | CLA  | C3D-C4D-ND  | 4.19  | 116.81      | 109.99   |
| 11  | bB    | 839 | CLA  | C3D-C4D-ND  | 4.19  | 116.81      | 109.99   |
| 11  | cB    | 810 | CLA  | C3B-C2B-C1B | -4.19 | 102.23      | 107.17   |
| 11  | cA    | 802 | CLA  | CHD-C1D-ND  | -4.19 | 118.90      | 124.80   |
| 11  | cB    | 806 | CLA  | C4A-NA-C1A  | -4.19 | 104.77      | 106.68   |
| 11  | aA    | 820 | CLA  | C3B-C2B-C1B | -4.19 | 102.23      | 107.17   |
| 11  | aB    | 810 | CLA  | C2B-C1B-NB  | 4.19  | 114.67      | 110.33   |
| 11  | aB    | 826 | CLA  | C3C-C4C-NC  | 4.19  | 115.80      | 110.43   |
| 11  | cB    | 837 | CLA  | C3D-C4D-ND  | 4.19  | 116.80      | 109.99   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bA    | 804 | CLA  | C3D-C4D-ND  | 4.19  | 116.80      | 109.99   |
| 12  | aA    | 830 | F6C  | CHB-C4A-C3A | -4.19 | 116.77      | 125.49   |
| 11  | aL    | 206 | CLA  | C2B-C1B-NB  | 4.19  | 114.67      | 110.33   |
| 11  | bA    | 802 | CLA  | CHD-C1D-ND  | -4.19 | 118.91      | 124.80   |
| 11  | cB    | 817 | CLA  | C3D-C4D-ND  | 4.19  | 116.80      | 109.99   |
| 11  | bA    | 820 | CLA  | C3B-C2B-C1B | -4.19 | 102.23      | 107.17   |
| 11  | aA    | 823 | CLA  | C1C-C2C-C3C | -4.19 | 102.57      | 106.98   |
| 12  | bA    | 830 | F6C  | CHD-C4C-C3C | -4.19 | 116.13      | 125.30   |
| 11  | aB    | 820 | CLA  | C3D-C4D-ND  | 4.19  | 116.80      | 109.99   |
| 11  | cA    | 841 | CLA  | C3D-C4D-ND  | 4.19  | 116.80      | 109.99   |
| 11  | cA    | 802 | CLA  | C1C-C2C-C3C | -4.19 | 102.58      | 106.98   |
| 11  | aA    | 804 | CLA  | C3D-C4D-ND  | 4.19  | 116.79      | 109.99   |
| 11  | aB    | 816 | CLA  | C3D-C4D-ND  | 4.19  | 116.79      | 109.99   |
| 11  | bB    | 805 | CLA  | C3D-C4D-ND  | 4.19  | 116.79      | 109.99   |
| 11  | cA    | 807 | CLA  | C1C-C2C-C3C | -4.19 | 102.58      | 106.98   |
| 11  | cB    | 822 | CLA  | C3C-C4C-NC  | 4.19  | 115.79      | 110.43   |
| 11  | bB    | 817 | CLA  | C3D-C4D-ND  | 4.19  | 116.79      | 109.99   |
| 11  | aB    | 822 | CLA  | C3C-C4C-NC  | 4.18  | 115.79      | 110.43   |
| 11  | bB    | 833 | CLA  | CHD-C1D-ND  | -4.18 | 118.92      | 124.80   |
| 11  | aB    | 839 | CLA  | C3D-C4D-ND  | 4.18  | 116.79      | 109.99   |
| 11  | bB    | 822 | CLA  | C3C-C4C-NC  | 4.18  | 115.79      | 110.43   |
| 12  | bA    | 830 | F6C  | CHB-C4A-C3A | -4.18 | 116.79      | 125.49   |
| 11  | aB    | 833 | CLA  | CHD-C1D-ND  | -4.18 | 118.92      | 124.80   |
| 12  | aA    | 844 | F6C  | O2D-CGD-CBD | 4.18  | 118.54      | 111.23   |
| 12  | aA    | 827 | F6C  | C3C-C4C-NC  | 4.18  | 114.90      | 110.32   |
| 11  | cA    | 802 | CLA  | C3D-C4D-ND  | 4.18  | 116.78      | 109.99   |
| 11  | cB    | 834 | CLA  | C2B-C1B-NB  | 4.18  | 114.66      | 110.33   |
| 11  | cA    | 823 | CLA  | C1C-C2C-C3C | -4.18 | 102.59      | 106.98   |
| 11  | aA    | 811 | CLA  | C3D-C4D-ND  | 4.18  | 116.78      | 109.99   |
| 11  | aA    | 824 | CLA  | C3D-C4D-ND  | 4.18  | 116.78      | 109.99   |
| 11  | cB    | 839 | CLA  | C3D-C4D-ND  | 4.18  | 116.78      | 109.99   |
| 11  | bA    | 823 | CLA  | C1C-C2C-C3C | -4.18 | 102.59      | 106.98   |
| 11  | aB    | 827 | CLA  | C4A-NA-C1A  | -4.18 | 104.77      | 106.68   |
| 11  | cB    | 819 | CLA  | C3D-C2D-C1D | -4.17 | 100.14      | 105.83   |
| 11  | cB    | 833 | CLA  | CHD-C1D-ND  | -4.17 | 118.93      | 124.80   |
| 11  | aA    | 817 | CLA  | C1C-C2C-C3C | -4.17 | 102.59      | 106.98   |
| 11  | bA    | 804 | CLA  | O2D-CGD-CBD | 4.17  | 118.53      | 111.23   |
| 11  | bA    | 802 | CLA  | C3D-C4D-ND  | 4.17  | 116.77      | 109.99   |
| 11  | cA    | 811 | CLA  | C3D-C4D-ND  | 4.17  | 116.77      | 109.99   |
| 11  | cB    | 820 | CLA  | C3D-C4D-ND  | 4.17  | 116.77      | 109.99   |
| 11  | cB    | 805 | CLA  | C3D-C4D-ND  | 4.17  | 116.77      | 109.99   |
| 11  | bB    | 820 | CLA  | C3D-C4D-ND  | 4.17  | 116.76      | 109.99   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aB    | 817 | CLA  | C3D-C4D-ND  | 4.17  | 116.76      | 109.99   |
| 11  | aB    | 819 | CLA  | C3D-C2D-C1D | -4.17 | 100.15      | 105.83   |
| 11  | bA    | 824 | CLA  | C3D-C4D-ND  | 4.16  | 116.76      | 109.99   |
| 11  | aA    | 833 | CLA  | C3D-C4D-ND  | 4.16  | 116.75      | 109.99   |
| 11  | bA    | 839 | CLA  | C3B-C2B-C1B | -4.16 | 102.26      | 107.17   |
| 11  | bA    | 811 | CLA  | C3D-C4D-ND  | 4.16  | 116.75      | 109.99   |
| 11  | cA    | 804 | CLA  | O2D-CGD-CBD | 4.16  | 118.50      | 111.23   |
| 11  | cA    | 839 | CLA  | C3B-C2B-C1B | -4.16 | 102.27      | 107.17   |
| 11  | aA    | 802 | CLA  | C1C-C2C-C3C | -4.16 | 102.61      | 106.98   |
| 11  | bA    | 829 | CLA  | C3B-C4B-NB  | 4.16  | 114.24      | 110.53   |
| 11  | aB    | 834 | CLA  | C2B-C1B-NB  | 4.16  | 114.64      | 110.33   |
| 11  | aB    | 810 | CLA  | C3B-C2B-C1B | -4.16 | 102.27      | 107.17   |
| 12  | cA    | 844 | F6C  | C3D-C2D-C1D | -4.16 | 99.81       | 105.83   |
| 11  | cA    | 804 | CLA  | C3D-C4D-ND  | 4.16  | 116.75      | 109.99   |
| 11  | cA    | 805 | CLA  | C2C-C1C-NC  | 4.16  | 114.35      | 109.98   |
| 11  | bA    | 835 | CLA  | C3D-C4D-ND  | 4.16  | 116.74      | 109.99   |
| 11  | cB    | 816 | CLA  | C3D-C4D-ND  | 4.16  | 116.74      | 109.99   |
| 11  | bB    | 802 | CLA  | C3C-C4C-NC  | 4.16  | 115.75      | 110.43   |
| 11  | cB    | 810 | CLA  | C2B-C1B-NB  | 4.16  | 114.64      | 110.33   |
| 11  | aA    | 829 | CLA  | C3B-C4B-NB  | 4.15  | 114.24      | 110.53   |
| 11  | cB    | 835 | CLA  | C3D-C4D-ND  | 4.15  | 116.74      | 109.99   |
| 11  | aB    | 823 | CLA  | C3D-C2D-C1D | -4.15 | 100.16      | 105.83   |
| 11  | bB    | 839 | CLA  | C4A-NA-C1A  | -4.15 | 104.78      | 106.68   |
| 11  | bB    | 817 | CLA  | CHD-C1D-ND  | -4.15 | 118.96      | 124.80   |
| 11  | cB    | 829 | CLA  | C3B-C2B-C1B | -4.15 | 102.28      | 107.17   |
| 11  | aA    | 804 | CLA  | O2D-CGD-CBD | 4.15  | 118.48      | 111.23   |
| 11  | aA    | 839 | CLA  | C3B-C2B-C1B | -4.15 | 102.28      | 107.17   |
| 11  | cA    | 833 | CLA  | C3D-C4D-ND  | 4.15  | 116.72      | 109.99   |
| 11  | cA    | 824 | CLA  | C3D-C4D-ND  | 4.14  | 116.72      | 109.99   |
| 15  | bA    | 847 | BCR  | C2-C1-C6    | 4.14  | 116.46      | 110.44   |
| 11  | bB    | 823 | CLA  | C3D-C2D-C1D | -4.14 | 100.18      | 105.83   |
| 11  | bB    | 810 | CLA  | C3B-C2B-C1B | -4.14 | 102.29      | 107.17   |
| 11  | bB    | 819 | CLA  | C3D-C2D-C1D | -4.14 | 100.18      | 105.83   |
| 11  | cB    | 802 | CLA  | C3C-C4C-NC  | 4.14  | 115.73      | 110.43   |
| 11  | bA    | 816 | CLA  | C3D-C4D-ND  | 4.14  | 116.72      | 109.99   |
| 11  | bB    | 816 | CLA  | C3D-C4D-ND  | 4.14  | 116.72      | 109.99   |
| 11  | aB    | 829 | CLA  | C3B-C2B-C1B | -4.14 | 102.29      | 107.17   |
| 12  | bA    | 844 | F6C  | C3D-C2D-C1D | -4.14 | 99.84       | 105.83   |
| 11  | cL    | 206 | CLA  | C2B-C1B-NB  | 4.14  | 114.62      | 110.33   |
| 11  | bB    | 829 | CLA  | C3B-C2B-C1B | -4.14 | 102.29      | 107.17   |
| 11  | cA    | 835 | CLA  | C3D-C4D-ND  | 4.14  | 116.71      | 109.99   |
| 11  | cA    | 829 | CLA  | C3B-C4B-NB  | 4.14  | 114.22      | 110.53   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bB    | 810 | CLA  | C2B-C1B-NB  | 4.13  | 114.61      | 110.33   |
| 11  | bL    | 206 | CLA  | C2B-C1B-NB  | 4.13  | 114.61      | 110.33   |
| 11  | bB    | 807 | CLA  | C3D-C4D-ND  | 4.13  | 116.71      | 109.99   |
| 11  | cB    | 828 | CLA  | C2B-C1B-NB  | 4.13  | 114.61      | 110.33   |
| 12  | aA    | 844 | F6C  | C3D-C2D-C1D | -4.13 | 99.84       | 105.83   |
| 11  | cA    | 817 | CLA  | C1C-C2C-C3C | -4.13 | 102.64      | 106.98   |
| 11  | bA    | 833 | CLA  | C3D-C4D-ND  | 4.13  | 116.70      | 109.99   |
| 11  | bB    | 834 | CLA  | C2B-C1B-NB  | 4.13  | 114.61      | 110.33   |
| 11  | bB    | 816 | CLA  | O2D-CGD-CBD | 4.13  | 118.45      | 111.23   |
| 15  | cA    | 847 | BCR  | C2-C1-C6    | 4.13  | 116.44      | 110.44   |
| 11  | bA    | 817 | CLA  | C1C-C2C-C3C | -4.13 | 102.64      | 106.98   |
| 11  | aB    | 817 | CLA  | C1C-C2C-C3C | -4.13 | 102.64      | 106.98   |
| 11  | aB    | 802 | CLA  | C3C-C4C-NC  | 4.13  | 115.72      | 110.43   |
| 11  | aA    | 805 | CLA  | C2C-C1C-NC  | 4.13  | 114.31      | 109.98   |
| 11  | cA    | 816 | CLA  | C3D-C4D-ND  | 4.13  | 116.69      | 109.99   |
| 11  | aB    | 816 | CLA  | O2D-CGD-CBD | 4.12  | 118.44      | 111.23   |
| 11  | aB    | 807 | CLA  | C2B-C1B-NB  | 4.12  | 114.60      | 110.33   |
| 11  | bA    | 837 | CLA  | O2D-CGD-CBD | 4.12  | 118.44      | 111.23   |
| 11  | aB    | 801 | CLA  | C2B-C1B-NB  | 4.12  | 114.60      | 110.33   |
| 11  | cB    | 823 | CLA  | C3D-C2D-C1D | -4.12 | 100.20      | 105.83   |
| 11  | cB    | 839 | CLA  | C4A-NA-C1A  | -4.12 | 104.80      | 106.68   |
| 11  | cB    | 817 | CLA  | C1C-C2C-C3C | -4.12 | 102.64      | 106.98   |
| 11  | bB    | 811 | CLA  | O2D-CGD-CBD | 4.12  | 118.44      | 111.23   |
| 11  | cB    | 807 | CLA  | C2B-C1B-NB  | 4.12  | 114.60      | 110.33   |
| 11  | aB    | 817 | CLA  | CHD-C1D-ND  | -4.12 | 119.00      | 124.80   |
| 11  | cB    | 816 | CLA  | O2D-CGD-CBD | 4.12  | 118.43      | 111.23   |
| 15  | aA    | 847 | BCR  | C2-C1-C6    | 4.12  | 116.42      | 110.44   |
| 11  | cB    | 817 | CLA  | CHD-C1D-ND  | -4.12 | 119.00      | 124.80   |
| 11  | bA    | 834 | CLA  | C3D-C4D-ND  | 4.12  | 116.68      | 109.99   |
| 11  | cA    | 834 | CLA  | C3D-C4D-ND  | 4.12  | 116.68      | 109.99   |
| 11  | cA    | 837 | CLA  | O2D-CGD-CBD | 4.12  | 118.43      | 111.23   |
| 11  | aB    | 804 | CLA  | C3D-C4D-ND  | 4.12  | 116.68      | 109.99   |
| 11  | aB    | 810 | CLA  | C3D-C4D-ND  | 4.12  | 116.68      | 109.99   |
| 11  | aB    | 835 | CLA  | C3D-C4D-ND  | 4.12  | 116.68      | 109.99   |
| 11  | bA    | 818 | CLA  | C3D-C4D-ND  | 4.12  | 116.68      | 109.99   |
| 11  | bA    | 802 | CLA  | C1C-C2C-C3C | -4.11 | 102.65      | 106.98   |
| 11  | bB    | 828 | CLA  | C1C-C2C-C3C | -4.11 | 102.65      | 106.98   |
| 11  | bB    | 835 | CLA  | C3D-C4D-ND  | 4.11  | 116.68      | 109.99   |
| 11  | cB    | 832 | CLA  | C3D-C4D-ND  | 4.11  | 116.68      | 109.99   |
| 11  | cB    | 827 | CLA  | C3C-C4C-NC  | 4.11  | 115.70      | 110.43   |
| 11  | aA    | 835 | CLA  | C3D-C4D-ND  | 4.11  | 116.67      | 109.99   |
| 11  | aB    | 807 | CLA  | C3D-C4D-ND  | 4.11  | 116.67      | 109.99   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bB    | 817 | CLA  | C1C-C2C-C3C | -4.11 | 102.65      | 106.98   |
| 12  | cA    | 827 | F6C  | CHD-C4C-C3C | -4.11 | 116.30      | 125.30   |
| 11  | aA    | 816 | CLA  | C3D-C4D-ND  | 4.11  | 116.67      | 109.99   |
| 11  | aB    | 839 | CLA  | C4A-NA-C1A  | -4.11 | 104.80      | 106.68   |
| 11  | cB    | 804 | CLA  | C3D-C4D-ND  | 4.11  | 116.67      | 109.99   |
| 11  | aA    | 834 | CLA  | C3D-C4D-ND  | 4.11  | 116.67      | 109.99   |
| 11  | aA    | 810 | CLA  | C2B-C1B-NB  | 4.11  | 114.59      | 110.33   |
| 11  | aB    | 811 | CLA  | O2D-CGD-CBD | 4.11  | 118.41      | 111.23   |
| 11  | bB    | 832 | CLA  | C3D-C4D-ND  | 4.11  | 116.66      | 109.99   |
| 11  | bA    | 808 | CLA  | CHD-C1D-ND  | -4.11 | 119.02      | 124.80   |
| 11  | cB    | 828 | CLA  | C1C-C2C-C3C | -4.11 | 102.66      | 106.98   |
| 11  | cB    | 807 | CLA  | C3D-C4D-ND  | 4.11  | 116.66      | 109.99   |
| 11  | bB    | 807 | CLA  | C2B-C1B-NB  | 4.10  | 114.58      | 110.33   |
| 11  | cA    | 836 | CLA  | C3C-C4C-NC  | 4.10  | 115.69      | 110.43   |
| 12  | bA    | 827 | F6C  | CHD-C4C-C3C | -4.10 | 116.32      | 125.30   |
| 11  | aA    | 837 | CLA  | O2D-CGD-CBD | 4.10  | 118.40      | 111.23   |
| 11  | aA    | 836 | CLA  | C3C-C4C-NC  | 4.10  | 115.69      | 110.43   |
| 11  | bB    | 828 | CLA  | C2B-C1B-NB  | 4.10  | 114.58      | 110.33   |
| 11  | aA    | 822 | CLA  | C3D-C4D-ND  | 4.10  | 116.65      | 109.99   |
| 11  | bB    | 804 | CLA  | C3D-C4D-ND  | 4.10  | 116.65      | 109.99   |
| 11  | cB    | 813 | CLA  | C3D-C4D-ND  | 4.10  | 116.65      | 109.99   |
| 12  | aA    | 827 | F6C  | CHD-C4C-C3C | -4.10 | 116.32      | 125.30   |
| 11  | cA    | 822 | CLA  | C3D-C4D-ND  | 4.10  | 116.65      | 109.99   |
| 11  | cA    | 813 | CLA  | C3D-C4D-ND  | 4.10  | 116.65      | 109.99   |
| 11  | cA    | 818 | CLA  | C3D-C4D-ND  | 4.10  | 116.65      | 109.99   |
| 11  | cB    | 810 | CLA  | C3D-C4D-ND  | 4.10  | 116.65      | 109.99   |
| 11  | cA    | 808 | CLA  | CHD-C1D-ND  | -4.10 | 119.04      | 124.80   |
| 11  | cA    | 803 | CLA  | C3D-C4D-ND  | 4.10  | 116.64      | 109.99   |
| 11  | bB    | 805 | CLA  | C3B-C4B-NB  | 4.10  | 114.19      | 110.53   |
| 11  | bB    | 810 | CLA  | C3D-C4D-ND  | 4.10  | 116.64      | 109.99   |
| 11  | aB    | 806 | CLA  | C4A-NA-C1A  | -4.09 | 104.81      | 106.68   |
| 11  | bA    | 812 | CLA  | C4A-NA-C1A  | -4.09 | 104.81      | 106.68   |
| 11  | bA    | 822 | CLA  | C3D-C4D-ND  | 4.09  | 116.64      | 109.99   |
| 11  | bA    | 820 | CLA  | C1C-C2C-C3C | -4.09 | 102.67      | 106.98   |
| 11  | aA    | 808 | CLA  | CHD-C1D-ND  | -4.09 | 119.04      | 124.80   |
| 11  | cB    | 811 | CLA  | O2D-CGD-CBD | 4.09  | 118.38      | 111.23   |
| 11  | aB    | 807 | CLA  | C1C-C2C-C3C | -4.09 | 102.68      | 106.98   |
| 11  | bA    | 836 | CLA  | C3C-C4C-NC  | 4.09  | 115.67      | 110.43   |
| 11  | bB    | 828 | CLA  | C4A-NA-C1A  | -4.09 | 104.81      | 106.68   |
| 11  | aB    | 832 | CLA  | C3D-C4D-ND  | 4.09  | 116.64      | 109.99   |
| 11  | bA    | 803 | CLA  | CMD-C2D-C1D | 4.09  | 131.93      | 124.73   |
| 11  | bB    | 823 | CLA  | C3C-C4C-NC  | 4.09  | 115.67      | 110.43   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bB    | 827 | CLA  | C3C-C4C-NC  | 4.09  | 115.67      | 110.43   |
| 11  | bA    | 841 | CLA  | O2D-CGD-CBD | 4.09  | 118.38      | 111.23   |
| 12  | bA    | 826 | F6C  | C3D-C4D-ND  | 4.09  | 116.67      | 109.93   |
| 12  | aA    | 826 | F6C  | C3D-C4D-ND  | 4.09  | 116.66      | 109.93   |
| 11  | aA    | 841 | CLA  | O2D-CGD-CBD | 4.09  | 118.38      | 111.23   |
| 11  | aA    | 803 | CLA  | C3D-C4D-ND  | 4.09  | 116.63      | 109.99   |
| 11  | aA    | 818 | CLA  | C3D-C4D-ND  | 4.09  | 116.63      | 109.99   |
| 11  | bA    | 810 | CLA  | C3D-C4D-ND  | 4.08  | 116.63      | 109.99   |
| 11  | cA    | 839 | CLA  | C2B-C1B-NB  | 4.08  | 114.56      | 110.33   |
| 11  | aB    | 839 | CLA  | C1D-CHD-C4C | -4.08 | 117.34      | 126.02   |
| 11  | bA    | 803 | CLA  | C3D-C4D-ND  | 4.08  | 116.62      | 109.99   |
| 11  | cA    | 842 | CLA  | C3D-C4D-ND  | 4.08  | 116.62      | 109.99   |
| 11  | bB    | 839 | CLA  | C1D-CHD-C4C | -4.08 | 117.34      | 126.02   |
| 11  | cA    | 828 | CLA  | C3C-C4C-NC  | 4.08  | 115.66      | 110.43   |
| 11  | bB    | 827 | CLA  | C1D-CHD-C4C | -4.08 | 117.35      | 126.02   |
| 11  | bA    | 810 | CLA  | C2B-C1B-NB  | 4.08  | 114.56      | 110.33   |
| 11  | bA    | 813 | CLA  | C3B-C2B-C1B | -4.08 | 102.36      | 107.17   |
| 11  | aB    | 813 | CLA  | C3D-C4D-ND  | 4.08  | 116.62      | 109.99   |
| 11  | cB    | 827 | CLA  | C1D-CHD-C4C | -4.08 | 117.35      | 126.02   |
| 11  | cA    | 841 | CLA  | O2D-CGD-CBD | 4.08  | 118.36      | 111.23   |
| 11  | aA    | 803 | CLA  | CMD-C2D-C1D | 4.08  | 131.91      | 124.73   |
| 11  | bA    | 818 | CLA  | C2C-C1C-NC  | 4.08  | 114.26      | 109.98   |
| 11  | cB    | 816 | CLA  | CHD-C1D-ND  | -4.08 | 119.06      | 124.80   |
| 11  | cB    | 839 | CLA  | C1D-CHD-C4C | -4.08 | 117.36      | 126.02   |
| 11  | cA    | 810 | CLA  | C3D-C4D-ND  | 4.07  | 116.61      | 109.99   |
| 11  | aA    | 813 | CLA  | C3D-C4D-ND  | 4.07  | 116.61      | 109.99   |
| 12  | cA    | 826 | F6C  | C3D-C4D-ND  | 4.07  | 116.64      | 109.93   |
| 11  | aA    | 810 | CLA  | C3D-C4D-ND  | 4.07  | 116.61      | 109.99   |
| 11  | aB    | 827 | CLA  | C3D-C4D-ND  | 4.07  | 116.61      | 109.99   |
| 11  | aB    | 827 | CLA  | C3C-C4C-NC  | 4.07  | 115.65      | 110.43   |
| 11  | cA    | 810 | CLA  | C2B-C1B-NB  | 4.07  | 114.55      | 110.33   |
| 11  | bB    | 813 | CLA  | C3D-C4D-ND  | 4.07  | 116.61      | 109.99   |
| 11  | bB    | 827 | CLA  | C3D-C4D-ND  | 4.07  | 116.61      | 109.99   |
| 11  | bA    | 839 | CLA  | C2B-C1B-NB  | 4.07  | 114.55      | 110.33   |
| 11  | cB    | 801 | CLA  | C2B-C1B-NB  | 4.07  | 114.55      | 110.33   |
| 11  | aB    | 814 | CLA  | C3D-C4D-ND  | 4.07  | 116.60      | 109.99   |
| 11  | aA    | 820 | CLA  | C1C-C2C-C3C | -4.07 | 102.70      | 106.98   |
| 11  | aB    | 803 | CLA  | CHD-C1D-ND  | -4.07 | 119.08      | 124.80   |
| 11  | bB    | 803 | CLA  | CAA-C2A-C3A | -4.07 | 102.01      | 113.00   |
| 11  | aB    | 803 | CLA  | CAA-C2A-C3A | -4.07 | 102.01      | 113.00   |
| 11  | aB    | 805 | CLA  | C3B-C4B-NB  | 4.07  | 114.16      | 110.53   |
| 11  | bB    | 803 | CLA  | CHD-C1D-ND  | -4.07 | 119.08      | 124.80   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bB    | 818 | CLA  | O2D-CGD-CBD | 4.07  | 118.34      | 111.23   |
| 11  | bK    | 103 | CLA  | C3D-C4D-ND  | 4.06  | 116.59      | 109.99   |
| 11  | bA    | 836 | CLA  | C3D-C4D-ND  | 4.06  | 116.59      | 109.99   |
| 11  | cL    | 204 | CLA  | C3D-C4D-ND  | 4.06  | 116.59      | 109.99   |
| 11  | bA    | 812 | CLA  | C3D-C4D-ND  | 4.06  | 116.59      | 109.99   |
| 11  | bL    | 204 | CLA  | C3D-C4D-ND  | 4.06  | 116.59      | 109.99   |
| 11  | aA    | 818 | CLA  | C3C-C4C-NC  | 4.06  | 115.63      | 110.43   |
| 11  | cB    | 803 | CLA  | CAA-C2A-C3A | -4.06 | 102.02      | 113.00   |
| 11  | aB    | 828 | CLA  | C1C-C2C-C3C | -4.06 | 102.71      | 106.98   |
| 11  | cA    | 812 | CLA  | C4A-NA-C1A  | -4.06 | 104.83      | 106.68   |
| 11  | cA    | 820 | CLA  | C1C-C2C-C3C | -4.06 | 102.71      | 106.98   |
| 11  | bB    | 816 | CLA  | CHD-C1D-ND  | -4.06 | 119.09      | 124.80   |
| 10  | cA    | 801 | CL0  | CBC-CAC-C3C | -4.06 | 107.06      | 112.87   |
| 11  | aK    | 103 | CLA  | C3D-C4D-ND  | 4.06  | 116.58      | 109.99   |
| 11  | aB    | 813 | CLA  | C3B-C4B-NB  | 4.06  | 114.15      | 110.53   |
| 11  | cB    | 813 | CLA  | C1D-CHD-C4C | -4.06 | 117.40      | 126.02   |
| 11  | aB    | 822 | CLA  | CHD-C1D-ND  | -4.06 | 119.09      | 124.80   |
| 11  | bA    | 814 | CLA  | C4A-NA-C1A  | -4.06 | 104.83      | 106.68   |
| 11  | bB    | 801 | CLA  | C2B-C1B-NB  | 4.05  | 114.53      | 110.33   |
| 11  | aB    | 811 | CLA  | C3D-C4D-ND  | 4.05  | 116.58      | 109.99   |
| 11  | bB    | 807 | CLA  | C1C-C2C-C3C | -4.05 | 102.72      | 106.98   |
| 11  | aB    | 827 | CLA  | C1D-CHD-C4C | -4.05 | 117.40      | 126.02   |
| 11  | aB    | 839 | CLA  | C3C-C4C-NC  | 4.05  | 115.62      | 110.43   |
| 11  | cA    | 803 | CLA  | CMD-C2D-C1D | 4.05  | 131.86      | 124.73   |
| 11  | bB    | 811 | CLA  | C3D-C4D-ND  | 4.05  | 116.57      | 109.99   |
| 11  | cB    | 840 | CLA  | C3D-C4D-ND  | 4.05  | 116.57      | 109.99   |
| 11  | aA    | 828 | CLA  | C3C-C4C-NC  | 4.05  | 115.62      | 110.43   |
| 11  | cB    | 811 | CLA  | C3D-C4D-ND  | 4.05  | 116.57      | 109.99   |
| 11  | aB    | 828 | CLA  | C2B-C1B-NB  | 4.05  | 114.53      | 110.33   |
| 11  | cB    | 803 | CLA  | CHD-C1D-ND  | -4.05 | 119.10      | 124.80   |
| 11  | cA    | 812 | CLA  | C3D-C4D-ND  | 4.05  | 116.57      | 109.99   |
| 11  | aB    | 813 | CLA  | C1D-CHD-C4C | -4.05 | 117.41      | 126.02   |
| 11  | aB    | 818 | CLA  | O2D-CGD-CBD | 4.05  | 118.31      | 111.23   |
| 11  | cB    | 827 | CLA  | C3D-C4D-ND  | 4.05  | 116.57      | 109.99   |
| 11  | aA    | 812 | CLA  | C3D-C4D-ND  | 4.05  | 116.57      | 109.99   |
| 11  | bA    | 813 | CLA  | C3D-C4D-ND  | 4.05  | 116.56      | 109.99   |
| 11  | cB    | 805 | CLA  | C3B-C4B-NB  | 4.05  | 114.14      | 110.53   |
| 10  | bA    | 801 | CL0  | CBC-CAC-C3C | -4.05 | 107.08      | 112.87   |
| 11  | aA    | 813 | CLA  | C3B-C2B-C1B | -4.05 | 102.40      | 107.17   |
| 11  | aA    | 842 | CLA  | C3D-C4D-ND  | 4.04  | 116.56      | 109.99   |
| 11  | cB    | 823 | CLA  | C3C-C4C-NC  | 4.04  | 115.61      | 110.43   |
| 11  | bB    | 801 | CLA  | CAA-C2A-C3A | -4.04 | 102.07      | 113.00   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aA    | 819 | CLA  | C2C-C1C-NC  | 4.04  | 114.23      | 109.98   |
| 11  | aA    | 839 | CLA  | C2B-C1B-NB  | 4.04  | 114.52      | 110.33   |
| 12  | aA    | 844 | F6C  | CHA-C1A-C2A | -4.04 | 119.54      | 130.41   |
| 12  | bA    | 832 | F6C  | C3C-C4C-NC  | 4.04  | 114.75      | 110.32   |
| 11  | bB    | 840 | CLA  | C3D-C4D-ND  | 4.04  | 116.56      | 109.99   |
| 11  | aA    | 806 | CLA  | CHD-C1D-ND  | -4.04 | 119.11      | 124.80   |
| 11  | bB    | 822 | CLA  | CHD-C1D-ND  | -4.04 | 119.11      | 124.80   |
| 11  | bB    | 801 | CLA  | C3C-C4C-NC  | 4.04  | 115.61      | 110.43   |
| 11  | cB    | 818 | CLA  | O2D-CGD-CBD | 4.04  | 118.29      | 111.23   |
| 11  | cB    | 814 | CLA  | C3D-C4D-ND  | 4.04  | 116.55      | 109.99   |
| 12  | bB    | 824 | F6C  | C3D-C2D-C1D | -4.04 | 99.98       | 105.83   |
| 11  | aB    | 807 | CLA  | C4A-NA-C1A  | -4.04 | 104.84      | 106.68   |
| 11  | cA    | 836 | CLA  | C3D-C4D-ND  | 4.04  | 116.55      | 109.99   |
| 11  | cB    | 801 | CLA  | C3C-C4C-NC  | 4.04  | 115.60      | 110.43   |
| 11  | aB    | 801 | CLA  | CAA-C2A-C3A | -4.04 | 102.09      | 113.00   |
| 11  | aB    | 840 | CLA  | C3D-C4D-ND  | 4.04  | 116.55      | 109.99   |
| 11  | aB    | 823 | CLA  | C3C-C4C-NC  | 4.03  | 115.60      | 110.43   |
| 11  | cA    | 813 | CLA  | C3B-C2B-C1B | -4.03 | 102.41      | 107.17   |
| 11  | aB    | 816 | CLA  | CHD-C1D-ND  | -4.03 | 119.12      | 124.80   |
| 11  | cB    | 801 | CLA  | CAA-C2A-C3A | -4.03 | 102.10      | 113.00   |
| 11  | aA    | 812 | CLA  | C4A-NA-C1A  | -4.03 | 104.84      | 106.68   |
| 11  | aL    | 204 | CLA  | C3D-C4D-ND  | 4.03  | 116.54      | 109.99   |
| 11  | cB    | 807 | CLA  | C1C-C2C-C3C | -4.03 | 102.74      | 106.98   |
| 12  | aB    | 824 | F6C  | C3D-C2D-C1D | -4.03 | 99.99       | 105.83   |
| 12  | cA    | 844 | F6C  | CHA-C1A-C2A | -4.03 | 119.57      | 130.41   |
| 11  | bB    | 814 | CLA  | C3D-C4D-ND  | 4.03  | 116.54      | 109.99   |
| 11  | bA    | 828 | CLA  | C3C-C4C-NC  | 4.03  | 115.59      | 110.43   |
| 11  | aA    | 836 | CLA  | C3D-C4D-ND  | 4.03  | 116.54      | 109.99   |
| 11  | bA    | 842 | CLA  | C3D-C4D-ND  | 4.03  | 116.54      | 109.99   |
| 11  | bB    | 834 | CLA  | C1C-C2C-C3C | -4.03 | 102.74      | 106.98   |
| 11  | bB    | 809 | CLA  | C3B-C2B-C1B | -4.03 | 102.42      | 107.17   |
| 11  | aB    | 808 | CLA  | C3D-C4D-ND  | 4.03  | 116.54      | 109.99   |
| 11  | aB    | 828 | CLA  | C4A-NA-C1A  | -4.03 | 104.84      | 106.68   |
| 11  | bA    | 818 | CLA  | C3C-C4C-NC  | 4.03  | 115.59      | 110.43   |
| 11  | cB    | 822 | CLA  | CHD-C1D-ND  | -4.03 | 119.14      | 124.80   |
| 11  | bA    | 806 | CLA  | CHD-C1D-ND  | -4.03 | 119.14      | 124.80   |
| 11  | aB    | 834 | CLA  | C1C-C2C-C3C | -4.03 | 102.75      | 106.98   |
| 11  | bB    | 839 | CLA  | C3C-C4C-NC  | 4.02  | 115.59      | 110.43   |
| 12  | cA    | 832 | F6C  | C3C-C4C-NC  | 4.02  | 114.73      | 110.32   |
| 12  | cB    | 824 | F6C  | C3D-C2D-C1D | -4.02 | 100.00      | 105.83   |
| 11  | cK    | 103 | CLA  | C3D-C4D-ND  | 4.02  | 116.52      | 109.99   |
| 11  | aB    | 820 | CLA  | CHD-C1D-ND  | -4.02 | 119.15      | 124.80   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cB    | 834 | CLA  | C1C-C2C-C3C | -4.02 | 102.75      | 106.98   |
| 11  | cA    | 807 | CLA  | C3D-C4D-ND  | 4.02  | 116.52      | 109.99   |
| 11  | cB    | 831 | CLA  | C3D-C4D-ND  | 4.02  | 116.52      | 109.99   |
| 11  | bB    | 808 | CLA  | C3D-C4D-ND  | 4.02  | 116.52      | 109.99   |
| 11  | aA    | 840 | CLA  | CHD-C1D-ND  | -4.02 | 119.15      | 124.80   |
| 12  | bA    | 844 | F6C  | CHA-C1A-C2A | -4.01 | 119.61      | 130.41   |
| 11  | aB    | 801 | CLA  | C3D-C4D-ND  | 4.01  | 116.51      | 109.99   |
| 10  | aA    | 801 | CL0  | CBC-CAC-C3C | -4.01 | 107.13      | 112.87   |
| 11  | cA    | 818 | CLA  | C3C-C4C-NC  | 4.01  | 115.57      | 110.43   |
| 11  | bA    | 822 | CLA  | C3B-C2B-C1B | -4.01 | 102.44      | 107.17   |
| 11  | cA    | 831 | CLA  | C1D-CHD-C4C | -4.01 | 117.49      | 126.02   |
| 11  | bA    | 840 | CLA  | CHD-C1D-ND  | -4.01 | 119.15      | 124.80   |
| 11  | cA    | 803 | CLA  | O2D-CGD-CBD | 4.01  | 118.25      | 111.23   |
| 11  | aA    | 838 | CLA  | C1C-C2C-C3C | -4.01 | 102.76      | 106.98   |
| 11  | aA    | 822 | CLA  | C3B-C2B-C1B | -4.01 | 102.44      | 107.17   |
| 11  | cA    | 822 | CLA  | C3B-C2B-C1B | -4.01 | 102.44      | 107.17   |
| 11  | cB    | 808 | CLA  | C3D-C4D-ND  | 4.01  | 116.51      | 109.99   |
| 11  | aB    | 803 | CLA  | C3D-C4D-ND  | 4.01  | 116.51      | 109.99   |
| 11  | cB    | 804 | CLA  | C1D-CHD-C4C | -4.01 | 117.50      | 126.02   |
| 11  | aB    | 801 | CLA  | C3C-C4C-NC  | 4.01  | 115.57      | 110.43   |
| 11  | cA    | 840 | CLA  | CHD-C1D-ND  | -4.01 | 119.16      | 124.80   |
| 11  | bB    | 813 | CLA  | C1D-CHD-C4C | -4.01 | 117.50      | 126.02   |
| 11  | bB    | 804 | CLA  | C3C-C4C-NC  | 4.01  | 115.56      | 110.43   |
| 11  | aA    | 828 | CLA  | C2C-C1C-NC  | 4.01  | 114.19      | 109.98   |
| 11  | bA    | 819 | CLA  | C1D-CHD-C4C | -4.00 | 117.51      | 126.02   |
| 11  | bB    | 804 | CLA  | C1D-CHD-C4C | -4.00 | 117.51      | 126.02   |
| 11  | cA    | 828 | CLA  | C2C-C1C-NC  | 4.00  | 114.19      | 109.98   |
| 11  | bA    | 803 | CLA  | O2D-CGD-CBD | 4.00  | 118.23      | 111.23   |
| 11  | aA    | 831 | CLA  | C1D-CHD-C4C | -4.00 | 117.51      | 126.02   |
| 11  | aB    | 801 | CLA  | O2D-CGD-CBD | 4.00  | 118.23      | 111.23   |
| 11  | cB    | 820 | CLA  | CHD-C1D-ND  | -4.00 | 119.17      | 124.80   |
| 11  | cA    | 809 | CLA  | C3D-C4D-ND  | 4.00  | 116.49      | 109.99   |
| 11  | aB    | 809 | CLA  | C3B-C2B-C1B | -4.00 | 102.45      | 107.17   |
| 11  | aA    | 803 | CLA  | O2D-CGD-CBD | 4.00  | 118.22      | 111.23   |
| 11  | cB    | 839 | CLA  | C3C-C4C-NC  | 4.00  | 115.55      | 110.43   |
| 11  | cA    | 818 | CLA  | C2C-C1C-NC  | 4.00  | 114.18      | 109.98   |
| 11  | bB    | 808 | CLA  | C3C-C4C-NC  | 4.00  | 115.55      | 110.43   |
| 11  | bB    | 801 | CLA  | O2D-CGD-CBD | 4.00  | 118.22      | 111.23   |
| 11  | bB    | 836 | CLA  | C3C-C4C-NC  | 4.00  | 115.55      | 110.43   |
| 11  | cB    | 828 | CLA  | C4A-NA-C1A  | -4.00 | 104.86      | 106.68   |
| 11  | aB    | 821 | CLA  | C3D-C4D-ND  | 4.00  | 116.48      | 109.99   |
| 11  | cB    | 803 | CLA  | C3D-C4D-ND  | 4.00  | 116.48      | 109.99   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aA    | 803 | CLA  | C2C-C1C-NC  | 3.99  | 114.18      | 109.98   |
| 11  | bA    | 828 | CLA  | C2C-C1C-NC  | 3.99  | 114.18      | 109.98   |
| 11  | bB    | 831 | CLA  | C3D-C4D-ND  | 3.99  | 116.48      | 109.99   |
| 11  | cA    | 806 | CLA  | CHD-C1D-ND  | -3.99 | 119.18      | 124.80   |
| 12  | aA    | 832 | F6C  | C3C-C4C-NC  | 3.99  | 114.69      | 110.32   |
| 11  | cB    | 804 | CLA  | C3C-C4C-NC  | 3.99  | 115.54      | 110.43   |
| 11  | aA    | 818 | CLA  | C2C-C1C-NC  | 3.99  | 114.17      | 109.98   |
| 11  | bA    | 807 | CLA  | C3D-C4D-ND  | 3.99  | 116.47      | 109.99   |
| 11  | bB    | 803 | CLA  | C3D-C4D-ND  | 3.99  | 116.47      | 109.99   |
| 11  | aB    | 804 | CLA  | C1D-CHD-C4C | -3.99 | 117.54      | 126.02   |
| 11  | bB    | 801 | CLA  | C3D-C4D-ND  | 3.99  | 116.47      | 109.99   |
| 11  | aB    | 808 | CLA  | C3C-C4C-NC  | 3.99  | 115.54      | 110.43   |
| 11  | bA    | 831 | CLA  | C1D-CHD-C4C | -3.99 | 117.54      | 126.02   |
| 12  | aA    | 832 | F6C  | CHA-C1A-C2A | -3.99 | 119.68      | 130.41   |
| 11  | aA    | 809 | CLA  | C3D-C4D-ND  | 3.99  | 116.47      | 109.99   |
| 11  | bA    | 829 | CLA  | C3D-C4D-ND  | 3.99  | 116.47      | 109.99   |
| 12  | cA    | 832 | F6C  | CHA-C1A-C2A | -3.99 | 119.68      | 130.41   |
| 11  | bB    | 813 | CLA  | C3B-C4B-NB  | 3.99  | 114.09      | 110.53   |
| 11  | aA    | 807 | CLA  | C3D-C4D-ND  | 3.99  | 116.47      | 109.99   |
| 12  | bL    | 202 | F6C  | O2A-CGA-CBA | 3.99  | 123.99      | 111.83   |
| 11  | cB    | 808 | CLA  | C3C-C4C-NC  | 3.99  | 115.54      | 110.43   |
| 11  | aA    | 819 | CLA  | C1D-CHD-C4C | -3.99 | 117.55      | 126.02   |
| 11  | aA    | 817 | CLA  | O2D-CGD-CBD | 3.99  | 118.20      | 111.23   |
| 11  | aB    | 812 | CLA  | C3D-C4D-ND  | 3.99  | 116.47      | 109.99   |
| 11  | cB    | 827 | CLA  | O2D-CGD-CBD | 3.98  | 118.20      | 111.23   |
| 11  | cB    | 813 | CLA  | C3B-C4B-NB  | 3.98  | 114.09      | 110.53   |
| 11  | aA    | 829 | CLA  | C3D-C4D-ND  | 3.98  | 116.46      | 109.99   |
| 12  | bA    | 832 | F6C  | CHA-C1A-C2A | -3.98 | 119.70      | 130.41   |
| 11  | cB    | 801 | CLA  | C3D-C4D-ND  | 3.98  | 116.46      | 109.99   |
| 11  | aA    | 838 | CLA  | C3D-C4D-ND  | 3.98  | 116.46      | 109.99   |
| 11  | cA    | 803 | CLA  | C2C-C1C-NC  | 3.98  | 114.16      | 109.98   |
| 11  | cB    | 809 | CLA  | C3B-C2B-C1B | -3.98 | 102.48      | 107.17   |
| 11  | cA    | 819 | CLA  | C2C-C1C-NC  | 3.98  | 114.16      | 109.98   |
| 11  | aB    | 804 | CLA  | C3C-C4C-NC  | 3.98  | 115.53      | 110.43   |
| 11  | bB    | 812 | CLA  | C3D-C4D-ND  | 3.98  | 116.45      | 109.99   |
| 12  | cL    | 202 | F6C  | O2A-CGA-CBA | 3.98  | 123.96      | 111.83   |
| 11  | cB    | 821 | CLA  | C3D-C4D-ND  | 3.98  | 116.45      | 109.99   |
| 11  | cB    | 835 | CLA  | C1C-C2C-C3C | -3.98 | 102.80      | 106.98   |
| 11  | bA    | 819 | CLA  | C2C-C1C-NC  | 3.98  | 114.16      | 109.98   |
| 11  | cA    | 819 | CLA  | C1D-CHD-C4C | -3.98 | 117.57      | 126.02   |
| 11  | bB    | 820 | CLA  | CHD-C1D-ND  | -3.98 | 119.21      | 124.80   |
| 12  | bB    | 824 | F6C  | CHA-C1A-C2A | -3.98 | 119.72      | 130.41   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12  | aB    | 824 | F6C  | CHA-C1A-C2A | -3.97 | 119.72      | 130.41   |
| 11  | aB    | 802 | CLA  | C3D-C4D-ND  | 3.97  | 116.45      | 109.99   |
| 11  | bA    | 809 | CLA  | C3D-C4D-ND  | 3.97  | 116.45      | 109.99   |
| 11  | aL    | 204 | CLA  | C1C-C2C-C3C | -3.97 | 102.80      | 106.98   |
| 11  | cB    | 809 | CLA  | C1D-CHD-C4C | -3.97 | 117.58      | 126.02   |
| 11  | cB    | 815 | CLA  | C1D-CHD-C4C | -3.97 | 117.58      | 126.02   |
| 11  | aB    | 818 | CLA  | C3B-C2B-C1B | -3.97 | 102.49      | 107.17   |
| 11  | cB    | 801 | CLA  | O2D-CGD-CBD | 3.97  | 118.17      | 111.23   |
| 12  | cB    | 824 | F6C  | CHA-C1A-C2A | -3.97 | 119.73      | 130.41   |
| 11  | bB    | 827 | CLA  | O2D-CGD-CBD | 3.97  | 118.17      | 111.23   |
| 11  | cB    | 806 | CLA  | C1D-CHD-C4C | -3.97 | 117.58      | 126.02   |
| 11  | bB    | 835 | CLA  | C1C-C2C-C3C | -3.97 | 102.81      | 106.98   |
| 11  | cA    | 819 | CLA  | C3D-C4D-ND  | 3.97  | 116.44      | 109.99   |
| 11  | bB    | 806 | CLA  | C1D-CHD-C4C | -3.97 | 117.59      | 126.02   |
| 11  | bL    | 204 | CLA  | C1C-C2C-C3C | -3.97 | 102.81      | 106.98   |
| 11  | aB    | 827 | CLA  | O2D-CGD-CBD | 3.97  | 118.17      | 111.23   |
| 11  | aA    | 819 | CLA  | C3D-C4D-ND  | 3.97  | 116.44      | 109.99   |
| 12  | aL    | 202 | F6C  | O2A-CGA-CBA | 3.97  | 123.93      | 111.83   |
| 11  | cA    | 814 | CLA  | C4A-NA-C1A  | -3.97 | 104.87      | 106.68   |
| 11  | cB    | 807 | CLA  | C4A-NA-C1A  | -3.97 | 104.87      | 106.68   |
| 12  | aA    | 830 | F6C  | CHA-C1A-C2A | -3.97 | 119.75      | 130.41   |
| 11  | aA    | 825 | CLA  | C3D-C4D-ND  | 3.96  | 116.43      | 109.99   |
| 11  | aA    | 836 | CLA  | C1C-C2C-C3C | -3.96 | 102.81      | 106.98   |
| 11  | bA    | 810 | CLA  | C3C-C4C-NC  | 3.96  | 115.51      | 110.43   |
| 11  | cA    | 829 | CLA  | CHD-C1D-ND  | -3.96 | 119.22      | 124.80   |
| 11  | cA    | 838 | CLA  | C1C-C2C-C3C | -3.96 | 102.81      | 106.98   |
| 11  | aA    | 824 | CLA  | C1D-CHD-C4C | -3.96 | 117.59      | 126.02   |
| 12  | bA    | 830 | F6C  | CHA-C1A-C2A | -3.96 | 119.75      | 130.41   |
| 11  | bA    | 805 | CLA  | C3D-C4D-ND  | 3.96  | 116.43      | 109.99   |
| 11  | cB    | 812 | CLA  | C3D-C4D-ND  | 3.96  | 116.43      | 109.99   |
| 11  | cB    | 836 | CLA  | C3C-C4C-NC  | 3.96  | 115.51      | 110.43   |
| 12  | bL    | 202 | F6C  | C1A-C2A-C3A | -3.96 | 102.80      | 106.97   |
| 11  | bA    | 838 | CLA  | C1C-C2C-C3C | -3.96 | 102.81      | 106.98   |
| 11  | aB    | 836 | CLA  | C3C-C4C-NC  | 3.96  | 115.50      | 110.43   |
| 11  | bA    | 818 | CLA  | C1D-CHD-C4C | -3.96 | 117.60      | 126.02   |
| 11  | bA    | 819 | CLA  | C3D-C4D-ND  | 3.96  | 116.42      | 109.99   |
| 12  | cA    | 826 | F6C  | CAC-C3C-C2C | 3.96  | 133.16      | 126.89   |
| 11  | aB    | 814 | CLA  | C1D-CHD-C4C | -3.96 | 117.60      | 126.02   |
| 11  | cA    | 838 | CLA  | C3D-C4D-ND  | 3.96  | 116.42      | 109.99   |
| 11  | aB    | 815 | CLA  | C1D-CHD-C4C | -3.96 | 117.61      | 126.02   |
| 11  | bB    | 815 | CLA  | C1D-CHD-C4C | -3.96 | 117.61      | 126.02   |
| 11  | aA    | 817 | CLA  | C3D-C4D-ND  | 3.96  | 116.42      | 109.99   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aA    | 810 | CLA  | C3C-C4C-NC  | 3.96  | 115.50      | 110.43   |
| 11  | aB    | 806 | CLA  | C1D-CHD-C4C | -3.96 | 117.61      | 126.02   |
| 11  | aB    | 829 | CLA  | CHC-C1C-C2C | -3.96 | 115.70      | 126.95   |
| 11  | cA    | 843 | CLA  | C1D-CHD-C4C | -3.96 | 117.61      | 126.02   |
| 11  | cA    | 829 | CLA  | C3D-C4D-ND  | 3.96  | 116.42      | 109.99   |
| 11  | aA    | 818 | CLA  | C1D-CHD-C4C | -3.96 | 117.61      | 126.02   |
| 11  | bB    | 809 | CLA  | C1D-CHD-C4C | -3.96 | 117.61      | 126.02   |
| 11  | cA    | 825 | CLA  | C3D-C4D-ND  | 3.96  | 116.42      | 109.99   |
| 11  | bA    | 843 | CLA  | C1D-CHD-C4C | -3.96 | 117.61      | 126.02   |
| 11  | bB    | 810 | CLA  | CHD-C1D-ND  | -3.96 | 119.24      | 124.80   |
| 11  | aA    | 805 | CLA  | C3D-C4D-ND  | 3.96  | 116.42      | 109.99   |
| 11  | bA    | 825 | CLA  | C3D-C4D-ND  | 3.96  | 116.42      | 109.99   |
| 11  | cB    | 802 | CLA  | C3D-C4D-ND  | 3.96  | 116.42      | 109.99   |
| 11  | cA    | 810 | CLA  | C1D-CHD-C4C | -3.95 | 117.61      | 126.02   |
| 11  | aB    | 828 | CLA  | C3D-C4D-ND  | 3.95  | 116.42      | 109.99   |
| 11  | bA    | 810 | CLA  | C1D-CHD-C4C | -3.95 | 117.62      | 126.02   |
| 11  | aB    | 835 | CLA  | C1C-C2C-C3C | -3.95 | 102.82      | 106.98   |
| 11  | aA    | 812 | CLA  | O2D-CGD-CBD | 3.95  | 118.14      | 111.23   |
| 11  | cL    | 204 | CLA  | C1C-C2C-C3C | -3.95 | 102.82      | 106.98   |
| 11  | cA    | 810 | CLA  | C3C-C4C-NC  | 3.95  | 115.49      | 110.43   |
| 12  | cA    | 830 | F6C  | CHA-C1A-C2A | -3.95 | 119.78      | 130.41   |
| 11  | bB    | 821 | CLA  | C3D-C4D-ND  | 3.95  | 116.41      | 109.99   |
| 11  | bA    | 803 | CLA  | C2C-C1C-NC  | 3.95  | 114.13      | 109.98   |
| 11  | cA    | 802 | CLA  | C1D-CHD-C4C | -3.95 | 117.62      | 126.02   |
| 12  | cL    | 202 | F6C  | C1A-C2A-C3A | -3.95 | 102.81      | 106.97   |
| 11  | bB    | 802 | CLA  | C3D-C4D-ND  | 3.95  | 116.41      | 109.99   |
| 11  | cB    | 829 | CLA  | C2B-C1B-NB  | 3.95  | 114.42      | 110.33   |
| 11  | bB    | 821 | CLA  | C1C-C2C-C3C | -3.95 | 102.83      | 106.98   |
| 11  | bA    | 836 | CLA  | C1D-CHD-C4C | -3.95 | 117.62      | 126.02   |
| 11  | aB    | 810 | CLA  | C1C-C2C-C3C | -3.95 | 102.83      | 106.98   |
| 12  | bA    | 826 | F6C  | CAC-C3C-C2C | 3.95  | 133.14      | 126.89   |
| 11  | aB    | 831 | CLA  | C3D-C4D-ND  | 3.95  | 116.40      | 109.99   |
| 11  | bA    | 817 | CLA  | C3D-C4D-ND  | 3.95  | 116.40      | 109.99   |
| 11  | aA    | 843 | CLA  | C1D-CHD-C4C | -3.95 | 117.63      | 126.02   |
| 11  | aA    | 836 | CLA  | C3B-C2B-C1B | -3.95 | 102.52      | 107.17   |
| 11  | bA    | 824 | CLA  | C1D-CHD-C4C | -3.95 | 117.63      | 126.02   |
| 11  | cA    | 817 | CLA  | C3B-C4B-NB  | 3.95  | 114.05      | 110.53   |
| 11  | bA    | 820 | CLA  | CHD-C1D-ND  | -3.95 | 119.25      | 124.80   |
| 11  | bA    | 829 | CLA  | CHD-C1D-ND  | -3.95 | 119.25      | 124.80   |
| 11  | bA    | 812 | CLA  | O2D-CGD-CBD | 3.95  | 118.13      | 111.23   |
| 11  | cB    | 829 | CLA  | CHC-C1C-C2C | -3.95 | 115.74      | 126.95   |
| 11  | aA    | 843 | CLA  | C3D-C4D-ND  | 3.94  | 116.40      | 109.99   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bA    | 820 | CLA  | C3D-C4D-ND  | 3.94  | 116.40      | 109.99   |
| 11  | cB    | 819 | CLA  | C3D-C4D-ND  | 3.94  | 116.40      | 109.99   |
| 11  | cA    | 824 | CLA  | C1D-CHD-C4C | -3.94 | 117.64      | 126.02   |
| 11  | cA    | 836 | CLA  | C1D-CHD-C4C | -3.94 | 117.64      | 126.02   |
| 11  | bA    | 817 | CLA  | O2D-CGD-CBD | 3.94  | 118.12      | 111.23   |
| 11  | bA    | 834 | CLA  | O2D-CGD-CBD | 3.94  | 118.12      | 111.23   |
| 11  | aA    | 814 | CLA  | CHD-C1D-ND  | -3.94 | 119.25      | 124.80   |
| 11  | bA    | 815 | CLA  | C1D-CHD-C4C | -3.94 | 117.64      | 126.02   |
| 11  | aB    | 805 | CLA  | CHD-C1D-ND  | -3.94 | 119.25      | 124.80   |
| 11  | aB    | 829 | CLA  | C2B-C1B-NB  | 3.94  | 114.41      | 110.33   |
| 11  | aA    | 834 | CLA  | C1C-C2C-C3C | -3.94 | 102.83      | 106.98   |
| 11  | aK    | 101 | CLA  | CHD-C1D-ND  | -3.94 | 119.26      | 124.80   |
| 11  | cA    | 829 | CLA  | C1-C2-C3    | -3.94 | 119.74      | 126.20   |
| 11  | cB    | 818 | CLA  | C3B-C2B-C1B | -3.94 | 102.53      | 107.17   |
| 11  | cB    | 831 | CLA  | CHD-C1D-ND  | -3.94 | 119.26      | 124.80   |
| 11  | cA    | 818 | CLA  | C1D-CHD-C4C | -3.94 | 117.65      | 126.02   |
| 11  | bA    | 833 | CLA  | C1C-C2C-C3C | -3.94 | 102.84      | 106.98   |
| 11  | bB    | 823 | CLA  | C4A-NA-C1A  | -3.94 | 104.88      | 106.68   |
| 11  | bA    | 831 | CLA  | C3D-C4D-ND  | 3.94  | 116.39      | 109.99   |
| 12  | aL    | 202 | F6C  | C1A-C2A-C3A | -3.94 | 102.82      | 106.97   |
| 11  | cA    | 833 | CLA  | CHD-C1D-ND  | -3.94 | 119.26      | 124.80   |
| 11  | bB    | 829 | CLA  | CHC-C1C-C2C | -3.94 | 115.76      | 126.95   |
| 11  | aA    | 814 | CLA  | C4A-NA-C1A  | -3.94 | 104.88      | 106.68   |
| 11  | bA    | 838 | CLA  | C3D-C4D-ND  | 3.94  | 116.39      | 109.99   |
| 11  | bB    | 819 | CLA  | C3D-C4D-ND  | 3.94  | 116.39      | 109.99   |
| 12  | aA    | 826 | F6C  | CAC-C3C-C2C | 3.94  | 133.12      | 126.89   |
| 11  | bB    | 818 | CLA  | C3B-C2B-C1B | -3.93 | 102.53      | 107.17   |
| 11  | aB    | 823 | CLA  | C4A-NA-C1A  | -3.93 | 104.88      | 106.68   |
| 11  | bB    | 807 | CLA  | C4A-NA-C1A  | -3.93 | 104.88      | 106.68   |
| 11  | cB    | 814 | CLA  | C1D-CHD-C4C | -3.93 | 117.66      | 126.02   |
| 11  | cA    | 821 | CLA  | C3D-C4D-ND  | 3.93  | 116.38      | 109.99   |
| 11  | bB    | 828 | CLA  | C3D-C4D-ND  | 3.93  | 116.38      | 109.99   |
| 11  | bA    | 831 | CLA  | C1C-C2C-C3C | -3.93 | 102.84      | 106.98   |
| 11  | aB    | 809 | CLA  | C1D-CHD-C4C | -3.93 | 117.66      | 126.02   |
| 11  | cA    | 819 | CLA  | C3C-C4C-NC  | 3.93  | 115.47      | 110.43   |
| 11  | aB    | 819 | CLA  | C3D-C4D-ND  | 3.93  | 116.38      | 109.99   |
| 11  | cA    | 817 | CLA  | O2D-CGD-CBD | 3.93  | 118.10      | 111.23   |
| 11  | aA    | 810 | CLA  | C1D-CHD-C4C | -3.93 | 117.66      | 126.02   |
| 11  | cA    | 842 | CLA  | CHD-C1D-ND  | -3.93 | 119.27      | 124.80   |
| 11  | cA    | 836 | CLA  | C1C-C2C-C3C | -3.93 | 102.84      | 106.98   |
| 11  | bA    | 836 | CLA  | C3B-C2B-C1B | -3.93 | 102.53      | 107.17   |
| 11  | cA    | 811 | CLA  | CHD-C1D-ND  | -3.93 | 119.27      | 124.80   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aA    | 820 | CLA  | C3D-C4D-ND  | 3.93  | 116.38      | 109.99   |
| 11  | cA    | 834 | CLA  | O2D-CGD-CBD | 3.93  | 118.10      | 111.23   |
| 11  | aA    | 836 | CLA  | C1D-CHD-C4C | -3.93 | 117.67      | 126.02   |
| 11  | bB    | 829 | CLA  | C2B-C1B-NB  | 3.93  | 114.40      | 110.33   |
| 11  | cA    | 805 | CLA  | C3D-C4D-ND  | 3.93  | 116.38      | 109.99   |
| 11  | bA    | 802 | CLA  | C1D-CHD-C4C | -3.93 | 117.67      | 126.02   |
| 11  | aA    | 834 | CLA  | O2D-CGD-CBD | 3.93  | 118.10      | 111.23   |
| 11  | bB    | 831 | CLA  | CHD-C1D-ND  | -3.93 | 119.27      | 124.80   |
| 11  | aA    | 821 | CLA  | C3D-C4D-ND  | 3.93  | 116.37      | 109.99   |
| 11  | bB    | 814 | CLA  | C1D-CHD-C4C | -3.93 | 117.67      | 126.02   |
| 11  | aA    | 829 | CLA  | C1-C2-C3    | -3.93 | 119.76      | 126.20   |
| 11  | cB    | 810 | CLA  | C1C-C2C-C3C | -3.93 | 102.85      | 106.98   |
| 11  | cA    | 820 | CLA  | CHD-C1D-ND  | -3.93 | 119.28      | 124.80   |
| 11  | bA    | 843 | CLA  | C3D-C4D-ND  | 3.93  | 116.37      | 109.99   |
| 11  | bB    | 806 | CLA  | C3D-C4D-ND  | 3.93  | 116.37      | 109.99   |
| 11  | cB    | 821 | CLA  | C1C-C2C-C3C | -3.93 | 102.85      | 106.98   |
| 11  | aA    | 837 | CLA  | CHD-C1D-ND  | -3.93 | 119.28      | 124.80   |
| 11  | aA    | 831 | CLA  | C1C-C2C-C3C | -3.92 | 102.85      | 106.98   |
| 11  | cB    | 828 | CLA  | C3D-C4D-ND  | 3.92  | 116.36      | 109.99   |
| 11  | bB    | 816 | CLA  | C4A-NA-C1A  | -3.92 | 104.89      | 106.68   |
| 11  | bB    | 826 | CLA  | C4A-NA-C1A  | -3.92 | 104.89      | 106.68   |
| 11  | bA    | 833 | CLA  | CHD-C1D-ND  | -3.92 | 119.28      | 124.80   |
| 11  | cA    | 843 | CLA  | C3D-C4D-ND  | 3.92  | 116.36      | 109.99   |
| 11  | cB    | 806 | CLA  | C3D-C4D-ND  | 3.92  | 116.36      | 109.99   |
| 11  | aA    | 833 | CLA  | C1C-C2C-C3C | -3.92 | 102.86      | 106.98   |
| 11  | aB    | 831 | CLA  | CHD-C1D-ND  | -3.92 | 119.28      | 124.80   |
| 11  | cB    | 823 | CLA  | C4A-NA-C1A  | -3.92 | 104.89      | 106.68   |
| 11  | aA    | 842 | CLA  | CHD-C1D-ND  | -3.92 | 119.28      | 124.80   |
| 11  | aA    | 831 | CLA  | C3D-C4D-ND  | 3.92  | 116.36      | 109.99   |
| 11  | cA    | 836 | CLA  | C3B-C2B-C1B | -3.92 | 102.55      | 107.17   |
| 11  | cB    | 819 | CLA  | C1D-CHD-C4C | -3.92 | 117.69      | 126.02   |
| 11  | bB    | 825 | CLA  | C3C-C4C-NC  | 3.92  | 115.45      | 110.43   |
| 11  | cA    | 831 | CLA  | C3D-C4D-ND  | 3.92  | 116.36      | 109.99   |
| 11  | bA    | 836 | CLA  | C1C-C2C-C3C | -3.92 | 102.86      | 106.98   |
| 11  | cA    | 812 | CLA  | O2D-CGD-CBD | 3.92  | 118.08      | 111.23   |
| 11  | bA    | 819 | CLA  | C3C-C4C-NC  | 3.92  | 115.45      | 110.43   |
| 11  | aB    | 826 | CLA  | C4A-NA-C1A  | -3.92 | 104.89      | 106.68   |
| 11  | cB    | 816 | CLA  | C4A-NA-C1A  | -3.92 | 104.89      | 106.68   |
| 11  | cA    | 820 | CLA  | C3D-C4D-ND  | 3.92  | 116.35      | 109.99   |
| 11  | bA    | 811 | CLA  | CHD-C1D-ND  | -3.92 | 119.29      | 124.80   |
| 11  | bA    | 842 | CLA  | CHD-C1D-ND  | -3.92 | 119.29      | 124.80   |
| 11  | cA    | 822 | CLA  | O2D-CGD-CBD | 3.91  | 118.07      | 111.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aA    | 820 | CLA  | CHD-C1D-ND  | -3.91 | 119.29      | 124.80   |
| 11  | bA    | 814 | CLA  | CHD-C1D-ND  | -3.91 | 119.29      | 124.80   |
| 11  | aA    | 822 | CLA  | O2D-CGD-CBD | 3.91  | 118.07      | 111.23   |
| 11  | aA    | 829 | CLA  | CHD-C1D-ND  | -3.91 | 119.29      | 124.80   |
| 11  | bA    | 835 | CLA  | CHD-C1D-ND  | -3.91 | 119.29      | 124.80   |
| 11  | cA    | 837 | CLA  | CHD-C1D-ND  | -3.91 | 119.29      | 124.80   |
| 11  | aB    | 821 | CLA  | C1C-C2C-C3C | -3.91 | 102.86      | 106.98   |
| 11  | bB    | 819 | CLA  | C1D-CHD-C4C | -3.91 | 117.70      | 126.02   |
| 11  | aA    | 835 | CLA  | CHD-C1D-ND  | -3.91 | 119.30      | 124.80   |
| 11  | cA    | 814 | CLA  | CHD-C1D-ND  | -3.91 | 119.30      | 124.80   |
| 11  | aB    | 819 | CLA  | C1D-CHD-C4C | -3.91 | 117.70      | 126.02   |
| 11  | aB    | 825 | CLA  | C3C-C4C-NC  | 3.91  | 115.44      | 110.43   |
| 11  | cA    | 817 | CLA  | C3D-C4D-ND  | 3.91  | 116.34      | 109.99   |
| 11  | bA    | 823 | CLA  | C1D-CHD-C4C | -3.91 | 117.71      | 126.02   |
| 11  | cA    | 815 | CLA  | C1D-CHD-C4C | -3.91 | 117.71      | 126.02   |
| 11  | bB    | 805 | CLA  | CHD-C1D-ND  | -3.91 | 119.30      | 124.80   |
| 11  | bA    | 821 | CLA  | C3D-C4D-ND  | 3.91  | 116.34      | 109.99   |
| 11  | aA    | 802 | CLA  | C1D-CHD-C4C | -3.91 | 117.71      | 126.02   |
| 11  | aA    | 819 | CLA  | C3C-C4C-NC  | 3.91  | 115.44      | 110.43   |
| 11  | bB    | 818 | CLA  | C1D-CHD-C4C | -3.91 | 117.72      | 126.02   |
| 11  | bK    | 101 | CLA  | CHD-C1D-ND  | -3.91 | 119.30      | 124.80   |
| 12  | cA    | 832 | F6C  | CHD-C4C-C3C | -3.91 | 116.75      | 125.30   |
| 11  | cK    | 101 | CLA  | CHD-C1D-ND  | -3.91 | 119.31      | 124.80   |
| 11  | aA    | 815 | CLA  | C1D-CHD-C4C | -3.91 | 117.72      | 126.02   |
| 11  | cA    | 835 | CLA  | CHD-C1D-ND  | -3.90 | 119.31      | 124.80   |
| 11  | aB    | 815 | CLA  | C3D-C4D-ND  | 3.90  | 116.33      | 109.99   |
| 11  | bA    | 834 | CLA  | C1C-C2C-C3C | -3.90 | 102.87      | 106.98   |
| 11  | bA    | 817 | CLA  | C3B-C4B-NB  | 3.90  | 114.01      | 110.53   |
| 11  | bA    | 829 | CLA  | C1-C2-C3    | -3.90 | 119.80      | 126.20   |
| 11  | aB    | 810 | CLA  | CHD-C1D-ND  | -3.90 | 119.31      | 124.80   |
| 11  | bB    | 815 | CLA  | O2D-CGD-CBD | 3.90  | 118.05      | 111.23   |
| 11  | cB    | 823 | CLA  | C1D-CHD-C4C | -3.90 | 117.73      | 126.02   |
| 12  | bA    | 832 | F6C  | CHD-C4C-C3C | -3.90 | 116.76      | 125.30   |
| 11  | cB    | 810 | CLA  | CHD-C1D-ND  | -3.90 | 119.31      | 124.80   |
| 11  | aA    | 823 | CLA  | C1D-CHD-C4C | -3.90 | 117.73      | 126.02   |
| 11  | cB    | 838 | CLA  | C4A-NA-C1A  | -3.90 | 104.90      | 106.68   |
| 12  | bA    | 844 | F6C  | C3C-C4C-NC  | 3.90  | 114.59      | 110.32   |
| 11  | aB    | 836 | CLA  | C3D-C4D-ND  | 3.90  | 116.32      | 109.99   |
| 12  | aA    | 832 | F6C  | CHD-C4C-C3C | -3.90 | 116.77      | 125.30   |
| 11  | bB    | 836 | CLA  | C1D-CHD-C4C | -3.90 | 117.73      | 126.02   |
| 11  | cB    | 823 | CLA  | C1C-C2C-C3C | -3.90 | 102.88      | 106.98   |
| 11  | bA    | 807 | CLA  | CHD-C1D-ND  | -3.90 | 119.32      | 124.80   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aB    | 808 | CLA  | C3D-C2D-C1D | -3.90 | 100.51      | 105.83   |
| 11  | cB    | 818 | CLA  | C1D-CHD-C4C | -3.90 | 117.74      | 126.02   |
| 11  | aA    | 811 | CLA  | CHD-C1D-ND  | -3.90 | 119.32      | 124.80   |
| 11  | aB    | 806 | CLA  | C3D-C4D-ND  | 3.90  | 116.32      | 109.99   |
| 11  | cB    | 808 | CLA  | C3D-C2D-C1D | -3.89 | 100.52      | 105.83   |
| 11  | bA    | 809 | CLA  | C1C-C2C-C3C | -3.89 | 102.89      | 106.98   |
| 11  | bA    | 804 | CLA  | CHD-C1D-ND  | -3.89 | 119.32      | 124.80   |
| 11  | aB    | 834 | CLA  | C3D-C4D-ND  | 3.89  | 116.31      | 109.99   |
| 11  | aA    | 833 | CLA  | CHD-C1D-ND  | -3.89 | 119.33      | 124.80   |
| 11  | cA    | 804 | CLA  | CHD-C1D-ND  | -3.89 | 119.33      | 124.80   |
| 11  | cB    | 805 | CLA  | CHD-C1D-ND  | -3.89 | 119.33      | 124.80   |
| 12  | aA    | 827 | F6C  | C1-C2-C3    | -3.89 | 119.82      | 126.20   |
| 11  | bA    | 821 | CLA  | C3C-C4C-NC  | 3.89  | 115.41      | 110.43   |
| 11  | aB    | 823 | CLA  | C1C-C2C-C3C | -3.89 | 102.89      | 106.98   |
| 11  | cA    | 823 | CLA  | C1D-CHD-C4C | -3.89 | 117.75      | 126.02   |
| 11  | cB    | 826 | CLA  | C1D-CHD-C4C | -3.89 | 117.75      | 126.02   |
| 11  | bB    | 823 | CLA  | C1D-CHD-C4C | -3.89 | 117.76      | 126.02   |
| 11  | cB    | 815 | CLA  | C3D-C4D-ND  | 3.89  | 116.31      | 109.99   |
| 11  | aA    | 804 | CLA  | CHD-C1D-ND  | -3.89 | 119.33      | 124.80   |
| 11  | bA    | 812 | CLA  | CHD-C1D-ND  | -3.89 | 119.33      | 124.80   |
| 11  | aB    | 818 | CLA  | C1D-CHD-C4C | -3.89 | 117.76      | 126.02   |
| 11  | cA    | 831 | CLA  | C1C-C2C-C3C | -3.89 | 102.89      | 106.98   |
| 11  | bB    | 826 | CLA  | C3D-C4D-ND  | 3.89  | 116.30      | 109.99   |
| 11  | cA    | 815 | CLA  | C1C-C2C-C3C | -3.89 | 102.89      | 106.98   |
| 11  | bB    | 815 | CLA  | C3D-C4D-ND  | 3.88  | 116.30      | 109.99   |
| 11  | bB    | 826 | CLA  | C1D-CHD-C4C | -3.88 | 117.76      | 126.02   |
| 11  | cA    | 834 | CLA  | C1D-CHD-C4C | -3.88 | 117.76      | 126.02   |
| 11  | bA    | 837 | CLA  | CHD-C1D-ND  | -3.88 | 119.34      | 124.80   |
| 11  | cB    | 826 | CLA  | C4A-NA-C1A  | -3.88 | 104.91      | 106.68   |
| 11  | cA    | 834 | CLA  | C1C-C2C-C3C | -3.88 | 102.89      | 106.98   |
| 11  | aB    | 823 | CLA  | C1D-CHD-C4C | -3.88 | 117.77      | 126.02   |
| 12  | bA    | 827 | F6C  | C1-C2-C3    | -3.88 | 119.84      | 126.20   |
| 11  | bB    | 836 | CLA  | C3D-C4D-ND  | 3.88  | 116.30      | 109.99   |
| 11  | cB    | 840 | CLA  | C3B-C2B-C1B | -3.88 | 102.59      | 107.17   |
| 11  | cA    | 806 | CLA  | CHB-C4A-NA  | 3.88  | 130.00      | 124.40   |
| 11  | cB    | 835 | CLA  | C4A-NA-C1A  | -3.88 | 104.91      | 106.68   |
| 11  | cB    | 838 | CLA  | CHD-C1D-ND  | -3.88 | 119.34      | 124.80   |
| 11  | bA    | 823 | CLA  | C3D-C4D-ND  | 3.88  | 116.30      | 109.99   |
| 11  | aA    | 817 | CLA  | C3B-C4B-NB  | 3.88  | 113.99      | 110.53   |
| 11  | bA    | 822 | CLA  | C4A-NA-C1A  | -3.88 | 104.91      | 106.68   |
| 11  | bA    | 822 | CLA  | O2D-CGD-CBD | 3.88  | 118.01      | 111.23   |
| 11  | cA    | 833 | CLA  | C1C-C2C-C3C | -3.88 | 102.90      | 106.98   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aA    | 823 | CLA  | C3D-C4D-ND  | 3.88  | 116.29      | 109.99   |
| 11  | cB    | 836 | CLA  | C1D-CHD-C4C | -3.88 | 117.78      | 126.02   |
| 11  | bB    | 822 | CLA  | C4C-C3C-C2C | -3.88 | 101.25      | 106.89   |
| 11  | bB    | 834 | CLA  | C3D-C4D-ND  | 3.88  | 116.29      | 109.99   |
| 11  | cB    | 834 | CLA  | C3D-C4D-ND  | 3.88  | 116.29      | 109.99   |
| 11  | aB    | 836 | CLA  | C1D-CHD-C4C | -3.88 | 117.78      | 126.02   |
| 11  | bA    | 806 | CLA  | CHB-C4A-NA  | 3.88  | 129.99      | 124.40   |
| 11  | bA    | 834 | CLA  | C1D-CHD-C4C | -3.88 | 117.78      | 126.02   |
| 11  | aA    | 834 | CLA  | C1D-CHD-C4C | -3.88 | 117.78      | 126.02   |
| 12  | cA    | 827 | F6C  | C1-C2-C3    | -3.88 | 119.85      | 126.20   |
| 11  | cB    | 825 | CLA  | C3D-C4D-ND  | 3.88  | 116.29      | 109.99   |
| 11  | cA    | 823 | CLA  | C3D-C4D-ND  | 3.87  | 116.28      | 109.99   |
| 11  | bB    | 838 | CLA  | CHD-C1D-ND  | -3.87 | 119.35      | 124.80   |
| 11  | aB    | 826 | CLA  | C1D-CHD-C4C | -3.87 | 117.79      | 126.02   |
| 11  | cA    | 839 | CLA  | CHD-C1D-ND  | -3.87 | 119.35      | 124.80   |
| 11  | aA    | 809 | CLA  | C1C-C2C-C3C | -3.87 | 102.91      | 106.98   |
| 11  | bB    | 823 | CLA  | C1C-C2C-C3C | -3.87 | 102.91      | 106.98   |
| 11  | cB    | 822 | CLA  | C4C-C3C-C2C | -3.87 | 101.26      | 106.89   |
| 11  | cB    | 826 | CLA  | C3D-C4D-ND  | 3.87  | 116.28      | 109.99   |
| 11  | bB    | 823 | CLA  | C3D-C4D-ND  | 3.87  | 116.28      | 109.99   |
| 11  | bB    | 810 | CLA  | C1C-C2C-C3C | -3.87 | 102.91      | 106.98   |
| 11  | bB    | 802 | CLA  | C1D-CHD-C4C | -3.87 | 117.79      | 126.02   |
| 12  | cA    | 844 | F6C  | C3C-C4C-NC  | 3.87  | 114.56      | 110.32   |
| 11  | bA    | 840 | CLA  | C1C-C2C-C3C | -3.87 | 102.91      | 106.98   |
| 11  | cA    | 840 | CLA  | C1C-C2C-C3C | -3.87 | 102.91      | 106.98   |
| 11  | bA    | 839 | CLA  | CHD-C1D-ND  | -3.87 | 119.36      | 124.80   |
| 11  | cB    | 830 | CLA  | C3D-C4D-ND  | 3.87  | 116.27      | 109.99   |
| 11  | cB    | 836 | CLA  | C3D-C4D-ND  | 3.87  | 116.27      | 109.99   |
| 11  | aB    | 822 | CLA  | C4C-C3C-C2C | -3.87 | 101.26      | 106.89   |
| 11  | bB    | 808 | CLA  | C3D-C2D-C1D | -3.87 | 100.56      | 105.83   |
| 11  | cB    | 802 | CLA  | C1D-CHD-C4C | -3.87 | 117.80      | 126.02   |
| 11  | cA    | 821 | CLA  | C3C-C4C-NC  | 3.87  | 115.38      | 110.43   |
| 11  | cB    | 815 | CLA  | O2D-CGD-CBD | 3.87  | 117.99      | 111.23   |
| 11  | bB    | 815 | CLA  | C3C-C4C-NC  | 3.86  | 115.38      | 110.43   |
| 12  | bB    | 824 | F6C  | C3C-C4C-NC  | 3.86  | 114.55      | 110.32   |
| 11  | aB    | 830 | CLA  | C3D-C4D-ND  | 3.86  | 116.27      | 109.99   |
| 11  | aB    | 838 | CLA  | CHD-C1D-ND  | -3.86 | 119.37      | 124.80   |
| 12  | aB    | 824 | F6C  | C3C-C4C-NC  | 3.86  | 114.55      | 110.32   |
| 11  | bA    | 825 | CLA  | C1D-CHD-C4C | -3.86 | 117.81      | 126.02   |
| 11  | aA    | 839 | CLA  | CHD-C1D-ND  | -3.86 | 119.37      | 124.80   |
| 11  | bB    | 837 | CLA  | CHD-C1D-ND  | -3.86 | 119.37      | 124.80   |
| 11  | aB    | 826 | CLA  | C3D-C4D-ND  | 3.86  | 116.26      | 109.99   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aB    | 834 | CLA  | C3B-C2B-C1B | -3.86 | 102.62      | 107.17   |
| 11  | aA    | 815 | CLA  | C1C-C2C-C3C | -3.86 | 102.92      | 106.98   |
| 11  | aA    | 809 | CLA  | CHD-C1D-ND  | -3.86 | 119.37      | 124.80   |
| 11  | aB    | 815 | CLA  | C3C-C4C-NC  | 3.86  | 115.37      | 110.43   |
| 11  | bB    | 840 | CLA  | C3B-C2B-C1B | -3.86 | 102.62      | 107.17   |
| 11  | cB    | 823 | CLA  | C3D-C4D-ND  | 3.86  | 116.26      | 109.99   |
| 11  | bK    | 101 | CLA  | C4A-NA-C1A  | -3.86 | 104.92      | 106.68   |
| 11  | aA    | 806 | CLA  | CHB-C4A-NA  | 3.86  | 129.97      | 124.40   |
| 11  | bB    | 835 | CLA  | CHD-C1D-ND  | -3.86 | 119.38      | 124.80   |
| 11  | aB    | 815 | CLA  | O2D-CGD-CBD | 3.86  | 117.97      | 111.23   |
| 11  | aB    | 802 | CLA  | C1D-CHD-C4C | -3.86 | 117.83      | 126.02   |
| 11  | aB    | 832 | CLA  | CHD-C1D-ND  | -3.85 | 119.38      | 124.80   |
| 11  | aA    | 828 | CLA  | C3D-C4D-ND  | 3.85  | 116.25      | 109.99   |
| 11  | aA    | 821 | CLA  | C1D-CHD-C4C | -3.85 | 117.83      | 126.02   |
| 11  | bB    | 828 | CLA  | C1D-CHD-C4C | -3.85 | 117.83      | 126.02   |
| 11  | cB    | 831 | CLA  | C1C-C2C-C3C | -3.85 | 102.93      | 106.98   |
| 11  | bB    | 809 | CLA  | C2B-C1B-NB  | 3.85  | 114.32      | 110.33   |
| 11  | aB    | 802 | CLA  | CHD-C1D-ND  | -3.85 | 119.38      | 124.80   |
| 11  | aB    | 825 | CLA  | C3D-C4D-ND  | 3.85  | 116.25      | 109.99   |
| 11  | cA    | 809 | CLA  | CHD-C1D-ND  | -3.85 | 119.38      | 124.80   |
| 11  | aB    | 818 | CLA  | C3C-C4C-NC  | 3.85  | 115.36      | 110.43   |
| 11  | bB    | 819 | CLA  | C1C-C2C-C3C | -3.85 | 102.93      | 106.98   |
| 11  | aA    | 807 | CLA  | CHD-C1D-ND  | -3.85 | 119.38      | 124.80   |
| 11  | cA    | 821 | CLA  | C1D-CHD-C4C | -3.85 | 117.84      | 126.02   |
| 11  | aB    | 823 | CLA  | C3D-C4D-ND  | 3.85  | 116.25      | 109.99   |
| 11  | bA    | 839 | CLA  | C1C-C2C-C3C | -3.85 | 102.93      | 106.98   |
| 11  | cA    | 825 | CLA  | C1D-CHD-C4C | -3.85 | 117.84      | 126.02   |
| 11  | cB    | 829 | CLA  | CHD-C1D-ND  | -3.85 | 119.39      | 124.80   |
| 12  | aL    | 202 | F6C  | CHD-C4C-C3C | -3.85 | 116.87      | 125.30   |
| 11  | aA    | 822 | CLA  | C4A-NA-C1A  | -3.85 | 104.92      | 106.68   |
| 11  | cA    | 837 | CLA  | C1D-CHD-C4C | -3.85 | 117.84      | 126.02   |
| 11  | aK    | 103 | CLA  | C1D-CHD-C4C | -3.85 | 117.84      | 126.02   |
| 11  | cB    | 825 | CLA  | C3C-C4C-NC  | 3.85  | 115.36      | 110.43   |
| 11  | aL    | 204 | CLA  | C3B-C4B-NB  | 3.85  | 113.97      | 110.53   |
| 11  | aA    | 812 | CLA  | C1D-CHD-C4C | -3.85 | 117.84      | 126.02   |
| 11  | bK    | 103 | CLA  | C1D-CHD-C4C | -3.85 | 117.84      | 126.02   |
| 11  | cA    | 807 | CLA  | CHD-C1D-ND  | -3.85 | 119.39      | 124.80   |
| 11  | bA    | 828 | CLA  | C3D-C4D-ND  | 3.85  | 116.24      | 109.99   |
| 12  | bL    | 202 | F6C  | CHD-C4C-C3C | -3.85 | 116.88      | 125.30   |
| 11  | bA    | 837 | CLA  | C1D-CHD-C4C | -3.85 | 117.84      | 126.02   |
| 11  | cB    | 828 | CLA  | C1D-CHD-C4C | -3.85 | 117.84      | 126.02   |
| 11  | cA    | 809 | CLA  | C1C-C2C-C3C | -3.85 | 102.94      | 106.98   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aA    | 812 | CLA  | CHD-C1D-ND  | -3.85 | 119.39      | 124.80   |
| 11  | bB    | 834 | CLA  | C3B-C2B-C1B | -3.84 | 102.64      | 107.17   |
| 11  | bA    | 809 | CLA  | CHD-C1D-ND  | -3.84 | 119.39      | 124.80   |
| 11  | bB    | 829 | CLA  | CHD-C1D-ND  | -3.84 | 119.39      | 124.80   |
| 11  | cA    | 822 | CLA  | C2B-C1B-NB  | 3.84  | 114.31      | 110.33   |
| 11  | aB    | 835 | CLA  | CHD-C1D-ND  | -3.84 | 119.40      | 124.80   |
| 11  | cB    | 835 | CLA  | CHD-C1D-ND  | -3.84 | 119.40      | 124.80   |
| 11  | aA    | 825 | CLA  | C1D-CHD-C4C | -3.84 | 117.86      | 126.02   |
| 12  | cL    | 202 | F6C  | CHD-C4C-C3C | -3.84 | 116.89      | 125.30   |
| 11  | bB    | 830 | CLA  | C3D-C4D-ND  | 3.84  | 116.23      | 109.99   |
| 11  | aB    | 825 | CLA  | C1D-CHD-C4C | -3.84 | 117.86      | 126.02   |
| 11  | bA    | 813 | CLA  | C1D-CHD-C4C | -3.84 | 117.86      | 126.02   |
| 11  | bB    | 839 | CLA  | C3D-C2D-C1D | -3.84 | 100.59      | 105.83   |
| 11  | aB    | 838 | CLA  | C4A-NA-C1A  | -3.84 | 104.93      | 106.68   |
| 11  | aB    | 809 | CLA  | CHD-C1D-ND  | -3.84 | 119.40      | 124.80   |
| 11  | bB    | 825 | CLA  | C3D-C4D-ND  | 3.84  | 116.22      | 109.99   |
| 11  | aA    | 840 | CLA  | C1C-C2C-C3C | -3.84 | 102.94      | 106.98   |
| 11  | bB    | 831 | CLA  | C1C-C2C-C3C | -3.84 | 102.94      | 106.98   |
| 11  | cB    | 834 | CLA  | C3B-C2B-C1B | -3.84 | 102.65      | 107.17   |
| 11  | cB    | 802 | CLA  | CHD-C1D-ND  | -3.84 | 119.40      | 124.80   |
| 12  | aA    | 844 | F6C  | C3C-C4C-NC  | 3.84  | 114.52      | 110.32   |
| 12  | cB    | 824 | F6C  | C3C-C4C-NC  | 3.84  | 114.52      | 110.32   |
| 11  | cB    | 832 | CLA  | CHD-C1D-ND  | -3.84 | 119.40      | 124.80   |
| 11  | bB    | 838 | CLA  | C1C-C2C-C3C | -3.84 | 102.94      | 106.98   |
| 11  | aB    | 829 | CLA  | CHD-C1D-ND  | -3.84 | 119.40      | 124.80   |
| 11  | aB    | 837 | CLA  | CHD-C1D-ND  | -3.84 | 119.40      | 124.80   |
| 11  | aA    | 839 | CLA  | C1C-C2C-C3C | -3.84 | 102.95      | 106.98   |
| 11  | cB    | 801 | CLA  | CMA-C3A-C4A | -3.84 | 101.47      | 111.77   |
| 11  | cA    | 828 | CLA  | C3D-C4D-ND  | 3.84  | 116.22      | 109.99   |
| 11  | cB    | 829 | CLA  | C3D-C4D-ND  | 3.84  | 116.22      | 109.99   |
| 11  | aB    | 809 | CLA  | C2B-C1B-NB  | 3.83  | 114.30      | 110.33   |
| 11  | bB    | 829 | CLA  | C3D-C4D-ND  | 3.83  | 116.22      | 109.99   |
| 11  | aB    | 828 | CLA  | C1D-CHD-C4C | -3.83 | 117.87      | 126.02   |
| 11  | bB    | 825 | CLA  | C1D-CHD-C4C | -3.83 | 117.87      | 126.02   |
| 11  | aA    | 813 | CLA  | C1D-CHD-C4C | -3.83 | 117.87      | 126.02   |
| 11  | cB    | 840 | CLA  | C2B-C1B-NB  | 3.83  | 114.30      | 110.33   |
| 11  | aA    | 821 | CLA  | C3C-C4C-NC  | 3.83  | 115.34      | 110.43   |
| 11  | cK    | 103 | CLA  | C1D-CHD-C4C | -3.83 | 117.88      | 126.02   |
| 11  | aB    | 819 | CLA  | C1C-C2C-C3C | -3.83 | 102.95      | 106.98   |
| 11  | cA    | 812 | CLA  | C1D-CHD-C4C | -3.83 | 117.88      | 126.02   |
| 11  | cB    | 815 | CLA  | C3C-C4C-NC  | 3.83  | 115.34      | 110.43   |
| 11  | aB    | 806 | CLA  | CHD-C1D-ND  | -3.83 | 119.41      | 124.80   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bB    | 809 | CLA  | CHD-C1D-ND  | -3.83 | 119.41      | 124.80   |
| 12  | bA    | 844 | F6C  | CHD-C4C-C3C | -3.83 | 116.92      | 125.30   |
| 11  | aB    | 816 | CLA  | C4A-NA-C1A  | -3.83 | 104.93      | 106.68   |
| 11  | bB    | 819 | CLA  | C3C-C4C-NC  | 3.83  | 115.33      | 110.43   |
| 11  | aB    | 840 | CLA  | C3B-C2B-C1B | -3.83 | 102.66      | 107.17   |
| 11  | bB    | 811 | CLA  | C1D-CHD-C4C | -3.83 | 117.88      | 126.02   |
| 11  | bA    | 822 | CLA  | C2B-C1B-NB  | 3.83  | 114.29      | 110.33   |
| 11  | bA    | 815 | CLA  | C1C-C2C-C3C | -3.83 | 102.96      | 106.98   |
| 11  | bB    | 832 | CLA  | CHD-C1D-ND  | -3.83 | 119.42      | 124.80   |
| 11  | bB    | 836 | CLA  | CAC-C3C-C4C | 3.83  | 129.77      | 124.79   |
| 11  | cA    | 821 | CLA  | C1C-C2C-C3C | -3.82 | 102.96      | 106.98   |
| 11  | cB    | 825 | CLA  | C1D-CHD-C4C | -3.82 | 117.89      | 126.02   |
| 11  | aB    | 839 | CLA  | C3D-C2D-C1D | -3.82 | 100.61      | 105.83   |
| 11  | bA    | 821 | CLA  | C1D-CHD-C4C | -3.82 | 117.89      | 126.02   |
| 11  | cL    | 206 | CLA  | C1D-CHD-C4C | -3.82 | 117.89      | 126.02   |
| 11  | cA    | 812 | CLA  | CHD-C1D-ND  | -3.82 | 119.42      | 124.80   |
| 11  | cB    | 837 | CLA  | CHD-C1D-ND  | -3.82 | 119.42      | 124.80   |
| 11  | bA    | 812 | CLA  | C1D-CHD-C4C | -3.82 | 117.90      | 126.02   |
| 11  | aA    | 821 | CLA  | C1C-C2C-C3C | -3.82 | 102.96      | 106.98   |
| 11  | aB    | 840 | CLA  | C2B-C1B-NB  | 3.82  | 114.29      | 110.33   |
| 11  | bB    | 801 | CLA  | CMA-C3A-C4A | -3.82 | 101.50      | 111.77   |
| 12  | cA    | 844 | F6C  | CHD-C4C-C3C | -3.82 | 116.94      | 125.30   |
| 11  | bB    | 840 | CLA  | C2B-C1B-NB  | 3.82  | 114.29      | 110.33   |
| 12  | cL    | 202 | F6C  | CMA-C3A-C2A | -3.82 | 115.82      | 126.15   |
| 12  | cL    | 202 | F6C  | C3D-C4D-ND  | 3.82  | 116.22      | 109.93   |
| 12  | aL    | 202 | F6C  | CMA-C3A-C2A | -3.82 | 115.82      | 126.15   |
| 11  | aB    | 801 | CLA  | CMA-C3A-C4A | -3.82 | 101.51      | 111.77   |
| 11  | aB    | 806 | CLA  | C1C-C2C-C3C | -3.82 | 102.97      | 106.98   |
| 11  | bA    | 821 | CLA  | C1C-C2C-C3C | -3.82 | 102.97      | 106.98   |
| 11  | cB    | 838 | CLA  | C1C-C2C-C3C | -3.82 | 102.97      | 106.98   |
| 11  | aB    | 829 | CLA  | C3D-C4D-ND  | 3.82  | 116.19      | 109.99   |
| 11  | aA    | 842 | CLA  | C1C-C2C-C3C | -3.82 | 102.97      | 106.98   |
| 11  | aK    | 101 | CLA  | C4A-NA-C1A  | -3.82 | 104.94      | 106.68   |
| 11  | aA    | 837 | CLA  | C1D-CHD-C4C | -3.82 | 117.91      | 126.02   |
| 11  | aL    | 206 | CLA  | C1D-CHD-C4C | -3.82 | 117.91      | 126.02   |
| 11  | bB    | 806 | CLA  | C1C-C2C-C3C | -3.82 | 102.97      | 106.98   |
| 11  | cB    | 840 | CLA  | CHD-C1D-ND  | -3.82 | 119.43      | 124.80   |
| 11  | cA    | 813 | CLA  | C1D-CHD-C4C | -3.81 | 117.91      | 126.02   |
| 11  | aB    | 838 | CLA  | C1C-C2C-C3C | -3.81 | 102.97      | 106.98   |
| 11  | cK    | 101 | CLA  | C4A-NA-C1A  | -3.81 | 104.94      | 106.68   |
| 11  | bB    | 840 | CLA  | CHD-C1D-ND  | -3.81 | 119.44      | 124.80   |
| 11  | cA    | 805 | CLA  | CHD-C1D-ND  | -3.81 | 119.44      | 124.80   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aB    | 813 | CLA  | C1C-C2C-C3C | -3.81 | 102.97      | 106.98   |
| 11  | aB    | 804 | CLA  | CHD-C1D-ND  | -3.81 | 119.44      | 124.80   |
| 11  | cB    | 809 | CLA  | CHD-C1D-ND  | -3.81 | 119.44      | 124.80   |
| 11  | cA    | 811 | CLA  | C1C-C2C-C3C | -3.81 | 102.97      | 106.98   |
| 11  | aA    | 839 | CLA  | C1D-CHD-C4C | -3.81 | 117.92      | 126.02   |
| 11  | bL    | 204 | CLA  | C3B-C4B-NB  | 3.81  | 113.93      | 110.53   |
| 11  | cB    | 806 | CLA  | C1C-C2C-C3C | -3.81 | 102.97      | 106.98   |
| 12  | bL    | 202 | F6C  | CMA-C3A-C2A | -3.81 | 115.84      | 126.15   |
| 11  | cA    | 839 | CLA  | C1C-C2C-C3C | -3.81 | 102.97      | 106.98   |
| 11  | cB    | 819 | CLA  | C3C-C4C-NC  | 3.81  | 115.31      | 110.43   |
| 11  | cB    | 839 | CLA  | C3D-C2D-C1D | -3.81 | 100.64      | 105.83   |
| 12  | aA    | 844 | F6C  | CHD-C4C-C3C | -3.81 | 116.97      | 125.30   |
| 12  | aL    | 202 | F6C  | C3D-C4D-ND  | 3.81  | 116.20      | 109.93   |
| 11  | aA    | 811 | CLA  | C1C-C2C-C3C | -3.81 | 102.98      | 106.98   |
| 11  | aB    | 811 | CLA  | C3C-C4C-NC  | 3.81  | 115.31      | 110.43   |
| 11  | cA    | 822 | CLA  | C1C-C2C-C3C | -3.81 | 102.98      | 106.98   |
| 11  | cB    | 819 | CLA  | C1C-C2C-C3C | -3.81 | 102.98      | 106.98   |
| 11  | aA    | 838 | CLA  | C1D-CHD-C4C | -3.80 | 117.93      | 126.02   |
| 11  | bB    | 807 | CLA  | C3C-C4C-NC  | 3.80  | 115.30      | 110.43   |
| 11  | aB    | 831 | CLA  | C1C-C2C-C3C | -3.80 | 102.98      | 106.98   |
| 11  | bA    | 842 | CLA  | C1C-C2C-C3C | -3.80 | 102.98      | 106.98   |
| 11  | bA    | 814 | CLA  | C1-C2-C3    | -3.80 | 119.97      | 126.20   |
| 11  | aA    | 818 | CLA  | O2D-CGD-O1D | -3.80 | 116.45      | 123.85   |
| 11  | cB    | 818 | CLA  | C3C-C4C-NC  | 3.80  | 115.30      | 110.43   |
| 11  | aB    | 811 | CLA  | C1D-CHD-C4C | -3.80 | 117.94      | 126.02   |
| 11  | cB    | 813 | CLA  | C1C-C2C-C3C | -3.80 | 102.98      | 106.98   |
| 11  | bA    | 818 | CLA  | O2D-CGD-O1D | -3.80 | 116.45      | 123.85   |
| 11  | bA    | 838 | CLA  | C1D-CHD-C4C | -3.80 | 117.94      | 126.02   |
| 11  | bA    | 805 | CLA  | CHD-C1D-ND  | -3.80 | 119.45      | 124.80   |
| 12  | bL    | 202 | F6C  | C3D-C4D-ND  | 3.80  | 116.19      | 109.93   |
| 11  | cA    | 818 | CLA  | O2D-CGD-O1D | -3.80 | 116.45      | 123.85   |
| 11  | aB    | 840 | CLA  | CHD-C1D-ND  | -3.80 | 119.45      | 124.80   |
| 11  | bL    | 206 | CLA  | C1D-CHD-C4C | -3.80 | 117.94      | 126.02   |
| 11  | cB    | 811 | CLA  | C1D-CHD-C4C | -3.80 | 117.95      | 126.02   |
| 11  | bA    | 831 | CLA  | C3B-C2B-C1B | -3.80 | 102.69      | 107.17   |
| 11  | cB    | 840 | CLA  | C1D-CHD-C4C | -3.80 | 117.95      | 126.02   |
| 11  | bB    | 818 | CLA  | C3C-C4C-NC  | 3.80  | 115.29      | 110.43   |
| 11  | bB    | 802 | CLA  | CHD-C1D-ND  | -3.80 | 119.46      | 124.80   |
| 11  | aA    | 822 | CLA  | C2B-C1B-NB  | 3.80  | 114.26      | 110.33   |
| 11  | bA    | 822 | CLA  | C1D-CHD-C4C | -3.80 | 117.95      | 126.02   |
| 11  | cA    | 807 | CLA  | C1D-CHD-C4C | -3.80 | 117.95      | 126.02   |
| 11  | aA    | 822 | CLA  | C1C-C2C-C3C | -3.79 | 102.99      | 106.98   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aA    | 824 | CLA  | C1C-C2C-C3C | -3.79 | 102.99      | 106.98   |
| 11  | bA    | 839 | CLA  | C1D-CHD-C4C | -3.79 | 117.95      | 126.02   |
| 11  | bB    | 840 | CLA  | C1D-CHD-C4C | -3.79 | 117.96      | 126.02   |
| 11  | bA    | 822 | CLA  | C1C-C2C-C3C | -3.79 | 102.99      | 106.98   |
| 11  | bA    | 824 | CLA  | C1C-C2C-C3C | -3.79 | 102.99      | 106.98   |
| 11  | aA    | 802 | CLA  | C3C-C4C-NC  | 3.79  | 115.29      | 110.43   |
| 11  | cA    | 822 | CLA  | C3C-C4C-NC  | 3.79  | 115.29      | 110.43   |
| 11  | bA    | 817 | CLA  | CHD-C1D-ND  | -3.79 | 119.47      | 124.80   |
| 11  | bA    | 815 | CLA  | C3D-C4D-ND  | 3.79  | 116.15      | 109.99   |
| 11  | cA    | 838 | CLA  | C1D-CHD-C4C | -3.79 | 117.97      | 126.02   |
| 11  | aB    | 840 | CLA  | C1D-CHD-C4C | -3.79 | 117.97      | 126.02   |
| 11  | aB    | 836 | CLA  | CAC-C3C-C4C | 3.79  | 129.72      | 124.79   |
| 11  | cA    | 824 | CLA  | C1C-C2C-C3C | -3.79 | 103.00      | 106.98   |
| 11  | bB    | 838 | CLA  | C4A-NA-C1A  | -3.79 | 104.95      | 106.68   |
| 11  | cB    | 830 | CLA  | C4A-NA-C1A  | -3.79 | 104.95      | 106.68   |
| 11  | aA    | 835 | CLA  | C1D-CHD-C4C | -3.79 | 117.97      | 126.02   |
| 11  | bA    | 835 | CLA  | C1D-CHD-C4C | -3.79 | 117.97      | 126.02   |
| 11  | cA    | 810 | CLA  | C1C-C2C-C3C | -3.79 | 103.00      | 106.98   |
| 11  | cB    | 836 | CLA  | CAC-C3C-C4C | 3.79  | 129.72      | 124.79   |
| 11  | aA    | 822 | CLA  | C1D-CHD-C4C | -3.79 | 117.97      | 126.02   |
| 11  | aL    | 206 | CLA  | C3C-C4C-NC  | 3.79  | 115.28      | 110.43   |
| 11  | cL    | 206 | CLA  | C3C-C4C-NC  | 3.79  | 115.28      | 110.43   |
| 11  | aA    | 805 | CLA  | C4A-NA-C1A  | -3.79 | 104.95      | 106.68   |
| 11  | aA    | 822 | CLA  | C3C-C4C-NC  | 3.79  | 115.28      | 110.43   |
| 11  | cA    | 816 | CLA  | C1D-CHD-C4C | -3.78 | 117.97      | 126.02   |
| 11  | aB    | 819 | CLA  | C3C-C4C-NC  | 3.78  | 115.28      | 110.43   |
| 11  | bL    | 206 | CLA  | C3C-C4C-NC  | 3.78  | 115.28      | 110.43   |
| 11  | aB    | 831 | CLA  | C1D-CHD-C4C | -3.78 | 117.98      | 126.02   |
| 11  | bB    | 806 | CLA  | CHD-C1D-ND  | -3.78 | 119.48      | 124.80   |
| 11  | bA    | 811 | CLA  | C1C-C2C-C3C | -3.78 | 103.00      | 106.98   |
| 11  | cA    | 842 | CLA  | C1C-C2C-C3C | -3.78 | 103.00      | 106.98   |
| 11  | cA    | 835 | CLA  | C1D-CHD-C4C | -3.78 | 117.98      | 126.02   |
| 11  | aB    | 807 | CLA  | C3C-C4C-NC  | 3.78  | 115.28      | 110.43   |
| 11  | cA    | 839 | CLA  | C1D-CHD-C4C | -3.78 | 117.98      | 126.02   |
| 11  | aA    | 820 | CLA  | C1D-CHD-C4C | -3.78 | 117.98      | 126.02   |
| 11  | aA    | 843 | CLA  | C3C-C4C-NC  | 3.78  | 115.27      | 110.43   |
| 11  | aA    | 816 | CLA  | C1D-CHD-C4C | -3.78 | 117.98      | 126.02   |
| 11  | cB    | 833 | CLA  | CMA-C3A-C4A | -3.78 | 101.61      | 111.77   |
| 11  | aA    | 817 | CLA  | CHD-C1D-ND  | -3.78 | 119.48      | 124.80   |
| 11  | cA    | 824 | CLA  | CHD-C1D-ND  | -3.78 | 119.48      | 124.80   |
| 11  | bB    | 831 | CLA  | C1D-CHD-C4C | -3.78 | 117.99      | 126.02   |
| 11  | cA    | 802 | CLA  | C3C-C4C-NC  | 3.78  | 115.27      | 110.43   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bB    | 809 | CLA  | C4A-NA-C1A  | -3.78 | 104.95      | 106.68   |
| 11  | cA    | 833 | CLA  | C4A-NA-C1A  | -3.78 | 104.95      | 106.68   |
| 11  | bB    | 833 | CLA  | CMA-C3A-C4A | -3.78 | 101.62      | 111.77   |
| 11  | cB    | 807 | CLA  | C3C-C4C-NC  | 3.78  | 115.27      | 110.43   |
| 11  | bA    | 824 | CLA  | CHD-C1D-ND  | -3.78 | 119.49      | 124.80   |
| 11  | cA    | 819 | CLA  | CHD-C1D-ND  | -3.78 | 119.49      | 124.80   |
| 11  | cA    | 817 | CLA  | CHD-C1D-ND  | -3.78 | 119.49      | 124.80   |
| 11  | aA    | 815 | CLA  | C3D-C4D-ND  | 3.78  | 116.13      | 109.99   |
| 11  | cA    | 822 | CLA  | C1D-CHD-C4C | -3.78 | 117.99      | 126.02   |
| 11  | cL    | 204 | CLA  | C3B-C4B-NB  | 3.78  | 113.90      | 110.53   |
| 11  | aA    | 805 | CLA  | CHD-C1D-ND  | -3.78 | 119.49      | 124.80   |
| 11  | cA    | 843 | CLA  | C3C-C4C-NC  | 3.78  | 115.27      | 110.43   |
| 11  | aA    | 814 | CLA  | C1-C2-C3    | -3.78 | 120.01      | 126.20   |
| 11  | cB    | 821 | CLA  | C1D-CHD-C4C | -3.78 | 118.00      | 126.02   |
| 11  | cB    | 831 | CLA  | C1D-CHD-C4C | -3.78 | 118.00      | 126.02   |
| 11  | aB    | 803 | CLA  | C3B-C4B-NB  | 3.77  | 113.90      | 110.53   |
| 15  | bL    | 207 | BCR  | C3-C4-C5    | -3.77 | 107.33      | 114.06   |
| 11  | aB    | 833 | CLA  | CMA-C3A-C4A | -3.77 | 101.63      | 111.77   |
| 11  | aA    | 807 | CLA  | C1D-CHD-C4C | -3.77 | 118.00      | 126.02   |
| 11  | bA    | 816 | CLA  | C1D-CHD-C4C | -3.77 | 118.00      | 126.02   |
| 11  | bB    | 821 | CLA  | C1D-CHD-C4C | -3.77 | 118.00      | 126.02   |
| 11  | aA    | 810 | CLA  | C1C-C2C-C3C | -3.77 | 103.01      | 106.98   |
| 11  | aA    | 833 | CLA  | C4A-NA-C1A  | -3.77 | 104.96      | 106.68   |
| 15  | aL    | 207 | BCR  | C3-C4-C5    | -3.77 | 107.33      | 114.06   |
| 11  | cL    | 204 | CLA  | C1D-CHD-C4C | -3.77 | 118.01      | 126.02   |
| 11  | bA    | 843 | CLA  | C3C-C4C-NC  | 3.77  | 115.26      | 110.43   |
| 11  | cA    | 831 | CLA  | C3B-C2B-C1B | -3.77 | 102.73      | 107.17   |
| 11  | cB    | 803 | CLA  | C3B-C4B-NB  | 3.77  | 113.89      | 110.53   |
| 11  | cB    | 810 | CLA  | C1D-CHD-C4C | -3.77 | 118.01      | 126.02   |
| 15  | aI    | 101 | BCR  | C2-C1-C6    | 3.77  | 115.91      | 110.44   |
| 11  | cA    | 829 | CLA  | C1C-C2C-C3C | -3.77 | 103.02      | 106.98   |
| 11  | bB    | 804 | CLA  | CHD-C1D-ND  | -3.77 | 119.50      | 124.80   |
| 11  | aA    | 831 | CLA  | C3B-C2B-C1B | -3.77 | 102.73      | 107.17   |
| 11  | cA    | 814 | CLA  | C1-C2-C3    | -3.77 | 120.03      | 126.20   |
| 11  | bB    | 835 | CLA  | C4A-NA-C1A  | -3.77 | 104.96      | 106.68   |
| 11  | aA    | 824 | CLA  | CHD-C1D-ND  | -3.77 | 119.50      | 124.80   |
| 11  | aB    | 810 | CLA  | C1D-CHD-C4C | -3.77 | 118.02      | 126.02   |
| 11  | cB    | 806 | CLA  | CHD-C1D-ND  | -3.76 | 119.50      | 124.80   |
| 11  | cA    | 820 | CLA  | C1D-CHD-C4C | -3.76 | 118.02      | 126.02   |
| 11  | aA    | 808 | CLA  | C1C-C2C-C3C | -3.76 | 103.02      | 106.98   |
| 11  | bA    | 837 | CLA  | C3C-C4C-NC  | 3.76  | 115.25      | 110.43   |
| 11  | cB    | 804 | CLA  | CHD-C1D-ND  | -3.76 | 119.51      | 124.80   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bA    | 807 | CLA  | C1D-CHD-C4C | -3.76 | 118.03      | 126.02   |
| 11  | cA    | 815 | CLA  | C3D-C4D-ND  | 3.76  | 116.10      | 109.99   |
| 11  | bA    | 802 | CLA  | C3C-C4C-NC  | 3.76  | 115.25      | 110.43   |
| 11  | cB    | 809 | CLA  | C2B-C1B-NB  | 3.76  | 114.22      | 110.33   |
| 11  | aB    | 821 | CLA  | C1D-CHD-C4C | -3.76 | 118.03      | 126.02   |
| 11  | cA    | 803 | CLA  | C3C-C4C-NC  | 3.76  | 115.25      | 110.43   |
| 11  | cB    | 811 | CLA  | C3C-C4C-NC  | 3.76  | 115.25      | 110.43   |
| 11  | aA    | 840 | CLA  | C1D-CHD-C4C | -3.76 | 118.03      | 126.02   |
| 11  | bA    | 841 | CLA  | CHD-C1D-ND  | -3.76 | 119.51      | 124.80   |
| 11  | bA    | 820 | CLA  | C1D-CHD-C4C | -3.76 | 118.03      | 126.02   |
| 11  | cB    | 805 | CLA  | C1D-CHD-C4C | -3.76 | 118.03      | 126.02   |
| 11  | bB    | 811 | CLA  | C3C-C4C-NC  | 3.76  | 115.24      | 110.43   |
| 11  | bL    | 204 | CLA  | C1D-CHD-C4C | -3.76 | 118.04      | 126.02   |
| 11  | bB    | 821 | CLA  | C3C-C4C-NC  | 3.76  | 115.24      | 110.43   |
| 11  | aB    | 803 | CLA  | C4C-C3C-C2C | -3.76 | 101.42      | 106.89   |
| 11  | bA    | 840 | CLA  | C1D-CHD-C4C | -3.76 | 118.04      | 126.02   |
| 11  | bB    | 813 | CLA  | C1C-C2C-C3C | -3.75 | 103.03      | 106.98   |
| 15  | cL    | 207 | BCR  | C3-C4-C5    | -3.75 | 107.36      | 114.06   |
| 11  | cA    | 817 | CLA  | C1D-CHD-C4C | -3.75 | 118.04      | 126.02   |
| 11  | aB    | 805 | CLA  | C1D-CHD-C4C | -3.75 | 118.04      | 126.02   |
| 11  | bA    | 829 | CLA  | C1C-C2C-C3C | -3.75 | 103.03      | 106.98   |
| 11  | cB    | 803 | CLA  | C4C-C3C-C2C | -3.75 | 101.43      | 106.89   |
| 11  | aL    | 204 | CLA  | C1D-CHD-C4C | -3.75 | 118.05      | 126.02   |
| 11  | bB    | 805 | CLA  | C1D-CHD-C4C | -3.75 | 118.05      | 126.02   |
| 11  | bA    | 825 | CLA  | C1C-C2C-C3C | -3.75 | 103.03      | 106.98   |
| 11  | cA    | 840 | CLA  | C1D-CHD-C4C | -3.75 | 118.05      | 126.02   |
| 11  | bA    | 822 | CLA  | C3C-C4C-NC  | 3.75  | 115.23      | 110.43   |
| 11  | cA    | 841 | CLA  | CHD-C1D-ND  | -3.75 | 119.53      | 124.80   |
| 11  | aA    | 817 | CLA  | C1D-CHD-C4C | -3.75 | 118.05      | 126.02   |
| 11  | cA    | 842 | CLA  | C1D-CHD-C4C | -3.75 | 118.05      | 126.02   |
| 11  | cK    | 103 | CLA  | CHD-C1D-ND  | -3.75 | 119.53      | 124.80   |
| 11  | aA    | 817 | CLA  | C4A-NA-C1A  | -3.75 | 104.97      | 106.68   |
| 11  | bA    | 805 | CLA  | C4A-NA-C1A  | -3.75 | 104.97      | 106.68   |
| 11  | bA    | 841 | CLA  | C1C-C2C-C3C | -3.75 | 103.04      | 106.98   |
| 11  | cA    | 825 | CLA  | C1C-C2C-C3C | -3.75 | 103.04      | 106.98   |
| 11  | cB    | 821 | CLA  | C3C-C4C-NC  | 3.75  | 115.23      | 110.43   |
| 11  | bA    | 817 | CLA  | C1D-CHD-C4C | -3.75 | 118.06      | 126.02   |
| 11  | bB    | 815 | CLA  | C4A-NA-C1A  | -3.75 | 104.97      | 106.68   |
| 11  | bA    | 804 | CLA  | C1D-CHD-C4C | -3.75 | 118.06      | 126.02   |
| 11  | bB    | 810 | CLA  | C1D-CHD-C4C | -3.75 | 118.06      | 126.02   |
| 11  | cK    | 101 | CLA  | C1D-CHD-C4C | -3.75 | 118.06      | 126.02   |
| 11  | cA    | 804 | CLA  | C1C-C2C-C3C | -3.75 | 103.04      | 106.98   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aA    | 819 | CLA  | CHD-C1D-ND  | -3.74 | 119.53      | 124.80   |
| 11  | aA    | 841 | CLA  | CHD-C1D-ND  | -3.74 | 119.53      | 124.80   |
| 11  | cA    | 822 | CLA  | C4A-NA-C1A  | -3.74 | 104.97      | 106.68   |
| 11  | cA    | 828 | CLA  | C4C-C3C-C2C | -3.74 | 101.44      | 106.89   |
| 15  | cI    | 103 | BCR  | C2-C1-C6    | 3.74  | 115.88      | 110.44   |
| 11  | cB    | 829 | CLA  | C1D-CHD-C4C | -3.74 | 118.06      | 126.02   |
| 11  | cA    | 841 | CLA  | C1C-C2C-C3C | -3.74 | 103.04      | 106.98   |
| 11  | cA    | 804 | CLA  | C1D-CHD-C4C | -3.74 | 118.06      | 126.02   |
| 11  | bB    | 829 | CLA  | C1D-CHD-C4C | -3.74 | 118.06      | 126.02   |
| 11  | bB    | 803 | CLA  | C3B-C4B-NB  | 3.74  | 113.87      | 110.53   |
| 11  | cL    | 205 | CLA  | C1D-CHD-C4C | -3.74 | 118.07      | 126.02   |
| 15  | bI    | 101 | BCR  | C2-C1-C6    | 3.74  | 115.87      | 110.44   |
| 11  | bA    | 804 | CLA  | C1C-C2C-C3C | -3.74 | 103.05      | 106.98   |
| 11  | bA    | 842 | CLA  | C1D-CHD-C4C | -3.74 | 118.07      | 126.02   |
| 11  | bB    | 803 | CLA  | C4C-C3C-C2C | -3.74 | 101.45      | 106.89   |
| 11  | aA    | 829 | CLA  | C1C-C2C-C3C | -3.74 | 103.05      | 106.98   |
| 12  | cA    | 830 | F6C  | C4C-CHD-C1D | -3.74 | 117.45      | 126.25   |
| 11  | aB    | 830 | CLA  | CHD-C1D-ND  | -3.74 | 119.54      | 124.80   |
| 11  | cA    | 837 | CLA  | C1C-C2C-C3C | -3.74 | 103.05      | 106.98   |
| 11  | aB    | 821 | CLA  | C3C-C4C-NC  | 3.74  | 115.22      | 110.43   |
| 11  | aA    | 842 | CLA  | C1D-CHD-C4C | -3.74 | 118.08      | 126.02   |
| 11  | bA    | 808 | CLA  | C1C-C2C-C3C | -3.74 | 103.05      | 106.98   |
| 11  | bA    | 810 | CLA  | C1C-C2C-C3C | -3.74 | 103.05      | 106.98   |
| 11  | bA    | 803 | CLA  | C3C-C4C-NC  | 3.74  | 115.22      | 110.43   |
| 11  | bB    | 814 | CLA  | CHD-C1D-ND  | -3.73 | 119.55      | 124.80   |
| 12  | aA    | 830 | F6C  | C4C-CHD-C1D | -3.73 | 117.47      | 126.25   |
| 11  | aL    | 205 | CLA  | C1D-CHD-C4C | -3.73 | 118.08      | 126.02   |
| 11  | bK    | 101 | CLA  | C1D-CHD-C4C | -3.73 | 118.08      | 126.02   |
| 11  | bA    | 820 | CLA  | C3B-C4B-NB  | 3.73  | 113.86      | 110.53   |
| 11  | aB    | 829 | CLA  | C1D-CHD-C4C | -3.73 | 118.09      | 126.02   |
| 12  | bB    | 824 | F6C  | CHD-C4C-C3C | -3.73 | 117.13      | 125.30   |
| 11  | bB    | 830 | CLA  | CHD-C1D-ND  | -3.73 | 119.55      | 124.80   |
| 11  | bB    | 822 | CLA  | CAC-C3C-C4C | 3.73  | 129.65      | 124.79   |
| 11  | bA    | 819 | CLA  | CHD-C1D-ND  | -3.73 | 119.55      | 124.80   |
| 11  | aA    | 820 | CLA  | C3B-C4B-NB  | 3.73  | 113.86      | 110.53   |
| 11  | bA    | 824 | CLA  | C4A-NA-C1A  | -3.73 | 104.98      | 106.68   |
| 11  | bL    | 205 | CLA  | C1D-CHD-C4C | -3.73 | 118.09      | 126.02   |
| 11  | aB    | 827 | CLA  | C1C-C2C-C3C | -3.73 | 103.06      | 106.98   |
| 11  | cA    | 808 | CLA  | C1C-C2C-C3C | -3.73 | 103.06      | 106.98   |
| 11  | aA    | 803 | CLA  | C3C-C4C-NC  | 3.73  | 115.21      | 110.43   |
| 11  | aA    | 813 | CLA  | C3C-C4C-NC  | 3.73  | 115.21      | 110.43   |
| 11  | bA    | 805 | CLA  | C3C-C4C-NC  | 3.73  | 115.21      | 110.43   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cA    | 837 | CLA  | C3C-C4C-NC  | 3.73  | 115.21      | 110.43   |
| 11  | cB    | 815 | CLA  | C4A-NA-C1A  | -3.73 | 104.98      | 106.68   |
| 11  | aB    | 822 | CLA  | CAC-C3C-C4C | 3.73  | 129.64      | 124.79   |
| 11  | cB    | 814 | CLA  | CHD-C1D-ND  | -3.73 | 119.56      | 124.80   |
| 11  | cB    | 830 | CLA  | CHD-C1D-ND  | -3.73 | 119.56      | 124.80   |
| 11  | bB    | 817 | CLA  | C1D-CHD-C4C | -3.73 | 118.10      | 126.02   |
| 11  | aB    | 815 | CLA  | C4A-NA-C1A  | -3.73 | 104.98      | 106.68   |
| 11  | aB    | 835 | CLA  | C4A-NA-C1A  | -3.73 | 104.98      | 106.68   |
| 12  | aB    | 824 | F6C  | CHD-C4C-C3C | -3.73 | 117.14      | 125.30   |
| 11  | aA    | 805 | CLA  | C3C-C4C-NC  | 3.73  | 115.20      | 110.43   |
| 11  | bB    | 830 | CLA  | C1D-CHD-C4C | -3.72 | 118.10      | 126.02   |
| 11  | bA    | 836 | CLA  | C2B-C1B-NB  | 3.72  | 114.19      | 110.33   |
| 11  | aB    | 817 | CLA  | C1D-CHD-C4C | -3.72 | 118.11      | 126.02   |
| 11  | cB    | 822 | CLA  | CAC-C3C-C4C | 3.72  | 129.63      | 124.79   |
| 12  | aL    | 202 | F6C  | C1-C2-C3    | -3.72 | 120.10      | 126.20   |
| 11  | bB    | 834 | CLA  | CHD-C1D-ND  | -3.72 | 119.56      | 124.80   |
| 12  | bA    | 830 | F6C  | C4C-CHD-C1D | -3.72 | 117.50      | 126.25   |
| 11  | aB    | 814 | CLA  | CHD-C1D-ND  | -3.72 | 119.57      | 124.80   |
| 11  | cA    | 805 | CLA  | C3C-C4C-NC  | 3.72  | 115.20      | 110.43   |
| 11  | cA    | 835 | CLA  | C1C-C2C-C3C | -3.72 | 103.07      | 106.98   |
| 11  | cB    | 827 | CLA  | C1C-C2C-C3C | -3.72 | 103.07      | 106.98   |
| 11  | bB    | 802 | CLA  | C3B-C4B-NB  | 3.72  | 113.85      | 110.53   |
| 11  | aA    | 837 | CLA  | C3C-C4C-NC  | 3.72  | 115.19      | 110.43   |
| 11  | aK    | 101 | CLA  | C1D-CHD-C4C | -3.72 | 118.12      | 126.02   |
| 11  | cB    | 817 | CLA  | C1D-CHD-C4C | -3.72 | 118.12      | 126.02   |
| 12  | bL    | 202 | F6C  | C1-C2-C3    | -3.72 | 120.11      | 126.20   |
| 12  | cB    | 824 | F6C  | CHD-C4C-C3C | -3.72 | 117.16      | 125.30   |
| 11  | aB    | 835 | CLA  | C1D-CHD-C4C | -3.72 | 118.12      | 126.02   |
| 11  | bA    | 842 | CLA  | O2D-CGD-CBD | 3.72  | 117.73      | 111.23   |
| 11  | aA    | 804 | CLA  | C1D-CHD-C4C | -3.72 | 118.12      | 126.02   |
| 11  | aL    | 204 | CLA  | C3C-C4C-NC  | 3.72  | 115.19      | 110.43   |
| 11  | aK    | 101 | CLA  | C1C-C2C-C3C | -3.72 | 103.07      | 106.98   |
| 11  | cB    | 835 | CLA  | C1D-CHD-C4C | -3.72 | 118.12      | 126.02   |
| 11  | aA    | 804 | CLA  | C1C-C2C-C3C | -3.71 | 103.07      | 106.98   |
| 11  | bA    | 828 | CLA  | C4C-C3C-C2C | -3.71 | 101.48      | 106.89   |
| 11  | aA    | 828 | CLA  | C4C-C3C-C2C | -3.71 | 101.49      | 106.89   |
| 11  | aA    | 837 | CLA  | C1C-C2C-C3C | -3.71 | 103.08      | 106.98   |
| 12  | cL    | 202 | F6C  | C1-C2-C3    | -3.71 | 120.11      | 126.20   |
| 11  | bB    | 827 | CLA  | C1C-C2C-C3C | -3.71 | 103.08      | 106.98   |
| 11  | aB    | 830 | CLA  | C1D-CHD-C4C | -3.71 | 118.13      | 126.02   |
| 11  | aA    | 836 | CLA  | C2B-C1B-NB  | 3.71  | 114.17      | 110.33   |
| 11  | cL    | 204 | CLA  | C3C-C4C-NC  | 3.71  | 115.18      | 110.43   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cB    | 834 | CLA  | CHD-C1D-ND  | -3.71 | 119.58      | 124.80   |
| 11  | bA    | 814 | CLA  | C1D-CHD-C4C | -3.71 | 118.14      | 126.02   |
| 11  | cA    | 834 | CLA  | C4A-NA-C1A  | -3.71 | 104.99      | 106.68   |
| 11  | cA    | 836 | CLA  | C4A-NA-C1A  | -3.71 | 104.99      | 106.68   |
| 11  | cB    | 809 | CLA  | C4A-NA-C1A  | -3.71 | 104.99      | 106.68   |
| 11  | bB    | 834 | CLA  | C3B-C4B-NB  | 3.71  | 113.84      | 110.53   |
| 11  | cA    | 842 | CLA  | O2D-CGD-CBD | 3.71  | 117.71      | 111.23   |
| 11  | cB    | 830 | CLA  | C1D-CHD-C4C | -3.71 | 118.14      | 126.02   |
| 11  | bB    | 835 | CLA  | C1D-CHD-C4C | -3.70 | 118.15      | 126.02   |
| 11  | aB    | 813 | CLA  | C3C-C4C-NC  | 3.70  | 115.17      | 110.43   |
| 11  | cA    | 831 | CLA  | C3C-C4C-NC  | 3.70  | 115.17      | 110.43   |
| 11  | aA    | 841 | CLA  | C1C-C2C-C3C | -3.70 | 103.09      | 106.98   |
| 11  | aA    | 829 | CLA  | C1D-CHD-C4C | -3.70 | 118.15      | 126.02   |
| 11  | aA    | 842 | CLA  | O2D-CGD-CBD | 3.70  | 117.70      | 111.23   |
| 11  | aA    | 829 | CLA  | C3C-C4C-NC  | 3.70  | 115.17      | 110.43   |
| 11  | bK    | 103 | CLA  | CHD-C1D-ND  | -3.70 | 119.59      | 124.80   |
| 11  | bK    | 101 | CLA  | C1C-C2C-C3C | -3.70 | 103.09      | 106.98   |
| 11  | aB    | 812 | CLA  | C1D-CHD-C4C | -3.70 | 118.16      | 126.02   |
| 11  | bB    | 812 | CLA  | C1D-CHD-C4C | -3.70 | 118.16      | 126.02   |
| 11  | cB    | 837 | CLA  | C1D-CHD-C4C | -3.70 | 118.16      | 126.02   |
| 11  | bB    | 809 | CLA  | C3C-C4C-NC  | 3.70  | 115.17      | 110.43   |
| 11  | cA    | 814 | CLA  | C1D-CHD-C4C | -3.70 | 118.16      | 126.02   |
| 11  | aA    | 811 | CLA  | C1D-CHD-C4C | -3.70 | 118.16      | 126.02   |
| 11  | aA    | 833 | CLA  | C1D-CHD-C4C | -3.70 | 118.16      | 126.02   |
| 11  | aB    | 810 | CLA  | C3B-C4B-NB  | 3.70  | 113.83      | 110.53   |
| 11  | cA    | 829 | CLA  | C1D-CHD-C4C | -3.70 | 118.16      | 126.02   |
| 11  | cA    | 838 | CLA  | C3C-C4C-NC  | 3.70  | 115.17      | 110.43   |
| 12  | cA    | 830 | F6C  | C3D-C2D-C1D | -3.70 | 100.47      | 105.83   |
| 11  | cB    | 838 | CLA  | C1D-CHD-C4C | -3.70 | 118.16      | 126.02   |
| 11  | bB    | 823 | CLA  | C3B-C4B-NB  | 3.70  | 113.83      | 110.53   |
| 11  | aB    | 834 | CLA  | CHD-C1D-ND  | -3.70 | 119.60      | 124.80   |
| 11  | bA    | 835 | CLA  | C1C-C2C-C3C | -3.70 | 103.09      | 106.98   |
| 11  | bA    | 838 | CLA  | CHD-C1D-ND  | -3.70 | 119.60      | 124.80   |
| 11  | aA    | 835 | CLA  | C1C-C2C-C3C | -3.70 | 103.09      | 106.98   |
| 11  | bA    | 817 | CLA  | C4A-NA-C1A  | -3.70 | 104.99      | 106.68   |
| 11  | bA    | 829 | CLA  | C1D-CHD-C4C | -3.70 | 118.17      | 126.02   |
| 11  | aA    | 834 | CLA  | CHD-C1D-ND  | -3.69 | 119.60      | 124.80   |
| 11  | bK    | 103 | CLA  | C3C-C4C-NC  | 3.69  | 115.16      | 110.43   |
| 11  | bA    | 837 | CLA  | C1C-C2C-C3C | -3.69 | 103.09      | 106.98   |
| 11  | bB    | 837 | CLA  | C1D-CHD-C4C | -3.69 | 118.17      | 126.02   |
| 11  | bB    | 814 | CLA  | C1C-C2C-C3C | -3.69 | 103.10      | 106.98   |
| 11  | aB    | 809 | CLA  | C3C-C4C-NC  | 3.69  | 115.16      | 110.43   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bL    | 204 | CLA  | C3C-C4C-NC  | 3.69  | 115.16      | 110.43   |
| 11  | aB    | 838 | CLA  | C1D-CHD-C4C | -3.69 | 118.17      | 126.02   |
| 11  | bB    | 808 | CLA  | CAA-C2A-C3A | -3.69 | 103.02      | 113.00   |
| 11  | cB    | 802 | CLA  | C3B-C4B-NB  | 3.69  | 113.83      | 110.53   |
| 11  | bB    | 805 | CLA  | C1C-C2C-C3C | -3.69 | 103.10      | 106.98   |
| 11  | cB    | 809 | CLA  | C3C-C4C-NC  | 3.69  | 115.16      | 110.43   |
| 11  | bA    | 834 | CLA  | CHD-C1D-ND  | -3.69 | 119.61      | 124.80   |
| 11  | bA    | 833 | CLA  | C1D-CHD-C4C | -3.69 | 118.18      | 126.02   |
| 11  | cB    | 813 | CLA  | C3C-C4C-NC  | 3.69  | 115.16      | 110.43   |
| 11  | cA    | 838 | CLA  | C3B-C4B-NB  | 3.69  | 113.82      | 110.53   |
| 11  | bA    | 809 | CLA  | C1D-CHD-C4C | -3.69 | 118.18      | 126.02   |
| 11  | cB    | 812 | CLA  | C1D-CHD-C4C | -3.69 | 118.18      | 126.02   |
| 11  | cA    | 829 | CLA  | C3C-C4C-NC  | 3.69  | 115.16      | 110.43   |
| 11  | bA    | 828 | CLA  | C3B-C4B-NB  | 3.69  | 113.82      | 110.53   |
| 11  | bB    | 810 | CLA  | C3B-C4B-NB  | 3.69  | 113.82      | 110.53   |
| 11  | cA    | 820 | CLA  | C3B-C4B-NB  | 3.69  | 113.82      | 110.53   |
| 11  | aA    | 809 | CLA  | C1D-CHD-C4C | -3.69 | 118.18      | 126.02   |
| 11  | cK    | 101 | CLA  | C1C-C2C-C3C | -3.69 | 103.10      | 106.98   |
| 11  | aK    | 103 | CLA  | CHD-C1D-ND  | -3.69 | 119.61      | 124.80   |
| 11  | cA    | 834 | CLA  | CHD-C1D-ND  | -3.69 | 119.62      | 124.80   |
| 11  | cA    | 813 | CLA  | C1C-C2C-C3C | -3.69 | 103.10      | 106.98   |
| 12  | aA    | 830 | F6C  | C3D-C2D-C1D | -3.68 | 100.50      | 105.83   |
| 11  | aB    | 802 | CLA  | C3B-C4B-NB  | 3.68  | 113.82      | 110.53   |
| 11  | bA    | 813 | CLA  | C3C-C4C-NC  | 3.68  | 115.15      | 110.43   |
| 11  | aB    | 805 | CLA  | C1C-C2C-C3C | -3.68 | 103.11      | 106.98   |
| 11  | aB    | 807 | CLA  | CHD-C1D-ND  | -3.68 | 119.62      | 124.80   |
| 11  | cA    | 836 | CLA  | C2B-C1B-NB  | 3.68  | 114.14      | 110.33   |
| 11  | cA    | 809 | CLA  | C1D-CHD-C4C | -3.68 | 118.20      | 126.02   |
| 11  | aB    | 808 | CLA  | CAA-C2A-C3A | -3.68 | 103.05      | 113.00   |
| 11  | cB    | 837 | CLA  | C3C-C4C-NC  | 3.68  | 115.14      | 110.43   |
| 11  | aB    | 837 | CLA  | C1D-CHD-C4C | -3.68 | 118.20      | 126.02   |
| 11  | bB    | 838 | CLA  | C1D-CHD-C4C | -3.68 | 118.20      | 126.02   |
| 11  | cA    | 805 | CLA  | C4A-NA-C1A  | -3.68 | 105.00      | 106.68   |
| 11  | cB    | 808 | CLA  | CAA-C2A-C3A | -3.68 | 103.06      | 113.00   |
| 11  | aA    | 816 | CLA  | C3C-C4C-NC  | 3.68  | 115.14      | 110.43   |
| 11  | cA    | 816 | CLA  | C3C-C4C-NC  | 3.68  | 115.14      | 110.43   |
| 11  | aA    | 823 | CLA  | C3C-C4C-NC  | 3.68  | 115.14      | 110.43   |
| 11  | aA    | 831 | CLA  | C3C-C4C-NC  | 3.68  | 115.14      | 110.43   |
| 11  | bB    | 820 | CLA  | C1D-CHD-C4C | -3.68 | 118.20      | 126.02   |
| 11  | aA    | 828 | CLA  | C3B-C4B-NB  | 3.68  | 113.81      | 110.53   |
| 11  | aB    | 838 | CLA  | C3C-C4C-NC  | 3.68  | 115.14      | 110.43   |
| 11  | bB    | 830 | CLA  | C1C-C2C-C3C | -3.67 | 103.11      | 106.98   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bB    | 828 | CLA  | C3B-C2B-C1B | -3.67 | 102.84      | 107.17   |
| 11  | bA    | 829 | CLA  | C3C-C4C-NC  | 3.67  | 115.14      | 110.43   |
| 11  | aA    | 825 | CLA  | C1C-C2C-C3C | -3.67 | 103.12      | 106.98   |
| 11  | bA    | 836 | CLA  | C4A-NA-C1A  | -3.67 | 105.00      | 106.68   |
| 11  | cB    | 820 | CLA  | C1D-CHD-C4C | -3.67 | 118.21      | 126.02   |
| 11  | bB    | 813 | CLA  | C3C-C4C-NC  | 3.67  | 115.14      | 110.43   |
| 11  | aA    | 814 | CLA  | C1D-CHD-C4C | -3.67 | 118.22      | 126.02   |
| 11  | bA    | 811 | CLA  | C1D-CHD-C4C | -3.67 | 118.22      | 126.02   |
| 11  | cB    | 834 | CLA  | C3B-C4B-NB  | 3.67  | 113.81      | 110.53   |
| 11  | cB    | 830 | CLA  | C1C-C2C-C3C | -3.67 | 103.12      | 106.98   |
| 11  | cA    | 838 | CLA  | CHD-C1D-ND  | -3.67 | 119.64      | 124.80   |
| 11  | bL    | 206 | CLA  | C1-C2-C3    | -3.67 | 120.18      | 126.20   |
| 11  | cB    | 828 | CLA  | C3B-C2B-C1B | -3.67 | 102.84      | 107.17   |
| 11  | bA    | 813 | CLA  | C1C-C2C-C3C | -3.67 | 103.12      | 106.98   |
| 11  | cA    | 833 | CLA  | C1D-CHD-C4C | -3.67 | 118.22      | 126.02   |
| 11  | cB    | 807 | CLA  | C1D-CHD-C4C | -3.67 | 118.22      | 126.02   |
| 11  | aA    | 805 | CLA  | C1D-CHD-C4C | -3.67 | 118.22      | 126.02   |
| 11  | cA    | 811 | CLA  | C1D-CHD-C4C | -3.67 | 118.22      | 126.02   |
| 11  | aB    | 807 | CLA  | C1D-CHD-C4C | -3.67 | 118.22      | 126.02   |
| 11  | cA    | 813 | CLA  | C3C-C4C-NC  | 3.67  | 115.13      | 110.43   |
| 11  | bA    | 813 | CLA  | C4A-NA-C1A  | -3.67 | 105.01      | 106.68   |
| 12  | bA    | 844 | F6C  | C1-C2-C3    | -3.67 | 120.19      | 126.20   |
| 11  | cB    | 809 | CLA  | C3B-C4B-NB  | 3.67  | 113.80      | 110.53   |
| 11  | cB    | 810 | CLA  | C3B-C4B-NB  | 3.67  | 113.80      | 110.53   |
| 11  | bB    | 832 | CLA  | C1D-CHD-C4C | -3.67 | 118.23      | 126.02   |
| 11  | cB    | 833 | CLA  | C1C-C2C-C3C | -3.67 | 103.12      | 106.98   |
| 11  | bA    | 834 | CLA  | C3C-C4C-NC  | 3.66  | 115.12      | 110.43   |
| 11  | cB    | 801 | CLA  | C3B-C4B-NB  | 3.66  | 113.80      | 110.53   |
| 11  | bA    | 823 | CLA  | C3C-C4C-NC  | 3.66  | 115.12      | 110.43   |
| 11  | aA    | 838 | CLA  | CHD-C1D-ND  | -3.66 | 119.65      | 124.80   |
| 11  | bB    | 830 | CLA  | C4A-NA-C1A  | -3.66 | 105.01      | 106.68   |
| 11  | bA    | 831 | CLA  | C3C-C4C-NC  | 3.66  | 115.12      | 110.43   |
| 11  | aB    | 832 | CLA  | C1D-CHD-C4C | -3.66 | 118.24      | 126.02   |
| 12  | bA    | 832 | F6C  | OMB-CMB-C2B | -3.66 | 117.36      | 125.62   |
| 11  | aA    | 813 | CLA  | C1C-C2C-C3C | -3.66 | 103.13      | 106.98   |
| 11  | aB    | 830 | CLA  | C1C-C2C-C3C | -3.66 | 103.13      | 106.98   |
| 11  | aA    | 838 | CLA  | C3C-C4C-NC  | 3.66  | 115.12      | 110.43   |
| 11  | cA    | 823 | CLA  | C3C-C4C-NC  | 3.66  | 115.12      | 110.43   |
| 11  | aB    | 817 | CLA  | C4-C3-C5    | 3.66  | 121.58      | 115.23   |
| 12  | aA    | 826 | F6C  | CHA-C1A-C2A | -3.66 | 120.57      | 130.41   |
| 11  | bB    | 807 | CLA  | CHD-C1D-ND  | -3.66 | 119.66      | 124.80   |
| 11  | cB    | 805 | CLA  | C1C-C2C-C3C | -3.66 | 103.13      | 106.98   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12  | bA    | 830 | F6C  | C3D-C2D-C1D | -3.66 | 100.54      | 105.83   |
| 11  | bB    | 807 | CLA  | C1D-CHD-C4C | -3.66 | 118.25      | 126.02   |
| 12  | bA    | 826 | F6C  | CHA-C1A-C2A | -3.66 | 120.58      | 130.41   |
| 11  | aB    | 820 | CLA  | C1D-CHD-C4C | -3.66 | 118.25      | 126.02   |
| 11  | aB    | 833 | CLA  | C1C-C2C-C3C | -3.65 | 103.14      | 106.98   |
| 11  | bL    | 205 | CLA  | C1C-C2C-C3C | -3.65 | 103.14      | 106.98   |
| 11  | cB    | 814 | CLA  | C1C-C2C-C3C | -3.65 | 103.14      | 106.98   |
| 11  | bA    | 834 | CLA  | C4A-NA-C1A  | -3.65 | 105.01      | 106.68   |
| 11  | aB    | 814 | CLA  | C1C-C2C-C3C | -3.65 | 103.14      | 106.98   |
| 12  | cA    | 826 | F6C  | CHA-C1A-C2A | -3.65 | 120.58      | 130.41   |
| 11  | aK    | 103 | CLA  | C3C-C4C-NC  | 3.65  | 115.11      | 110.43   |
| 11  | cB    | 817 | CLA  | C4-C3-C5    | 3.65  | 121.57      | 115.23   |
| 11  | cB    | 823 | CLA  | C3B-C4B-NB  | 3.65  | 113.79      | 110.53   |
| 11  | aL    | 206 | CLA  | C1-C2-C3    | -3.65 | 120.21      | 126.20   |
| 11  | cB    | 832 | CLA  | C1D-CHD-C4C | -3.65 | 118.26      | 126.02   |
| 11  | aA    | 816 | CLA  | C4A-NA-C1A  | -3.65 | 105.01      | 106.68   |
| 11  | bA    | 838 | CLA  | C3C-C4C-NC  | 3.65  | 115.11      | 110.43   |
| 11  | cL    | 205 | CLA  | C3C-C4C-NC  | 3.65  | 115.11      | 110.43   |
| 11  | bB    | 809 | CLA  | C3B-C4B-NB  | 3.65  | 113.79      | 110.53   |
| 11  | bA    | 804 | CLA  | C4A-NA-C1A  | -3.65 | 105.01      | 106.68   |
| 11  | aB    | 834 | CLA  | C3B-C4B-NB  | 3.65  | 113.79      | 110.53   |
| 11  | bB    | 817 | CLA  | C4-C3-C5    | 3.65  | 121.56      | 115.23   |
| 11  | aA    | 838 | CLA  | C3B-C4B-NB  | 3.65  | 113.79      | 110.53   |
| 11  | bA    | 838 | CLA  | C3B-C4B-NB  | 3.65  | 113.79      | 110.53   |
| 11  | cA    | 828 | CLA  | C3B-C4B-NB  | 3.65  | 113.78      | 110.53   |
| 11  | bB    | 812 | CLA  | C3C-C4C-NC  | 3.65  | 115.10      | 110.43   |
| 11  | cL    | 205 | CLA  | C1C-C2C-C3C | -3.65 | 103.15      | 106.98   |
| 11  | aA    | 815 | CLA  | CHD-C1D-ND  | -3.64 | 119.67      | 124.80   |
| 11  | bA    | 816 | CLA  | C3C-C4C-NC  | 3.64  | 115.10      | 110.43   |
| 11  | bA    | 805 | CLA  | C1D-CHD-C4C | -3.64 | 118.28      | 126.02   |
| 11  | bB    | 834 | CLA  | C1D-CHD-C4C | -3.64 | 118.28      | 126.02   |
| 12  | cA    | 832 | F6C  | OMB-CMB-C2B | -3.64 | 117.40      | 125.62   |
| 15  | bL    | 207 | BCR  | C2-C1-C6    | 3.64  | 115.73      | 110.44   |
| 12  | aA    | 832 | F6C  | OMB-CMB-C2B | -3.64 | 117.40      | 125.62   |
| 11  | aB    | 827 | CLA  | C3D-C2D-C1D | -3.64 | 100.86      | 105.83   |
| 11  | bB    | 827 | CLA  | C3D-C2D-C1D | -3.64 | 100.86      | 105.83   |
| 11  | cK    | 103 | CLA  | C3C-C4C-NC  | 3.64  | 115.09      | 110.43   |
| 11  | bB    | 833 | CLA  | C1C-C2C-C3C | -3.64 | 103.15      | 106.98   |
| 11  | bA    | 811 | CLA  | CAA-C2A-C3A | -3.64 | 103.17      | 113.00   |
| 11  | cA    | 825 | CLA  | CAC-C3C-C4C | 3.64  | 129.53      | 124.79   |
| 12  | cA    | 844 | F6C  | C1-C2-C3    | -3.64 | 120.24      | 126.20   |
| 11  | aB    | 818 | CLA  | CHD-C1D-ND  | -3.64 | 119.68      | 124.80   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cB    | 825 | CLA  | CHD-C1D-ND  | -3.64 | 119.68      | 124.80   |
| 11  | cA    | 815 | CLA  | CHD-C1D-ND  | -3.64 | 119.68      | 124.80   |
| 11  | cB    | 808 | CLA  | C3B-C4B-NB  | 3.64  | 113.78      | 110.53   |
| 11  | cB    | 827 | CLA  | C3D-C2D-C1D | -3.64 | 100.87      | 105.83   |
| 11  | aB    | 837 | CLA  | C3C-C4C-NC  | 3.64  | 115.09      | 110.43   |
| 11  | bA    | 841 | CLA  | C3C-C4C-NC  | 3.64  | 115.09      | 110.43   |
| 11  | aB    | 812 | CLA  | CHD-C1D-ND  | -3.63 | 119.69      | 124.80   |
| 11  | cB    | 807 | CLA  | CHD-C1D-ND  | -3.63 | 119.69      | 124.80   |
| 11  | bB    | 830 | CLA  | C3C-C4C-NC  | 3.63  | 115.09      | 110.43   |
| 11  | cA    | 834 | CLA  | C3C-C4C-NC  | 3.63  | 115.09      | 110.43   |
| 11  | bB    | 808 | CLA  | C3B-C4B-NB  | 3.63  | 113.77      | 110.53   |
| 11  | cB    | 818 | CLA  | CHD-C1D-ND  | -3.63 | 119.69      | 124.80   |
| 11  | cB    | 830 | CLA  | C3C-C4C-NC  | 3.63  | 115.08      | 110.43   |
| 11  | aA    | 834 | CLA  | C3C-C4C-NC  | 3.63  | 115.08      | 110.43   |
| 11  | aA    | 834 | CLA  | C4A-NA-C1A  | -3.63 | 105.02      | 106.68   |
| 11  | aB    | 809 | CLA  | C3B-C4B-NB  | 3.63  | 113.77      | 110.53   |
| 11  | cB    | 834 | CLA  | C1D-CHD-C4C | -3.63 | 118.30      | 126.02   |
| 15  | aB    | 848 | BCR  | C2-C1-C6    | 3.63  | 115.71      | 110.44   |
| 11  | cA    | 811 | CLA  | CAA-C2A-C3A | -3.63 | 103.19      | 113.00   |
| 11  | aB    | 815 | CLA  | CHD-C1D-ND  | -3.63 | 119.69      | 124.80   |
| 11  | bB    | 815 | CLA  | CHD-C1D-ND  | -3.63 | 119.69      | 124.80   |
| 11  | aL    | 205 | CLA  | C1C-C2C-C3C | -3.63 | 103.16      | 106.98   |
| 11  | aB    | 812 | CLA  | C3C-C4C-NC  | 3.63  | 115.08      | 110.43   |
| 11  | cB    | 838 | CLA  | C3C-C4C-NC  | 3.63  | 115.08      | 110.43   |
| 11  | cA    | 805 | CLA  | C1D-CHD-C4C | -3.63 | 118.31      | 126.02   |
| 12  | aA    | 844 | F6C  | C1-C2-C3    | -3.63 | 120.25      | 126.20   |
| 11  | aB    | 828 | CLA  | C3B-C2B-C1B | -3.63 | 102.89      | 107.17   |
| 11  | aA    | 811 | CLA  | CAA-C2A-C3A | -3.63 | 103.20      | 113.00   |
| 11  | cA    | 817 | CLA  | C4A-NA-C1A  | -3.63 | 105.02      | 106.68   |
| 11  | bL    | 205 | CLA  | C3C-C4C-NC  | 3.63  | 115.08      | 110.43   |
| 11  | aA    | 825 | CLA  | CAC-C3C-C4C | 3.63  | 129.51      | 124.79   |
| 11  | bB    | 812 | CLA  | CHD-C1D-ND  | -3.63 | 119.70      | 124.80   |
| 11  | aB    | 811 | CLA  | C1C-C2C-C3C | -3.63 | 103.17      | 106.98   |
| 11  | cB    | 806 | CLA  | C3C-C4C-NC  | 3.63  | 115.07      | 110.43   |
| 11  | bL    | 204 | CLA  | CHD-C1D-ND  | -3.62 | 119.70      | 124.80   |
| 11  | aB    | 834 | CLA  | C3C-C4C-NC  | 3.62  | 115.07      | 110.43   |
| 15  | cB    | 848 | BCR  | C2-C1-C6    | 3.62  | 115.70      | 110.44   |
| 11  | bA    | 815 | CLA  | CHD-C1D-ND  | -3.62 | 119.70      | 124.80   |
| 11  | aA    | 813 | CLA  | C4A-NA-C1A  | -3.62 | 105.03      | 106.68   |
| 11  | aA    | 836 | CLA  | C4A-NA-C1A  | -3.62 | 105.03      | 106.68   |
| 11  | cA    | 813 | CLA  | C4A-NA-C1A  | -3.62 | 105.03      | 106.68   |
| 11  | cB    | 815 | CLA  | CHD-C1D-ND  | -3.62 | 119.70      | 124.80   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cB    | 811 | CLA  | C1C-C2C-C3C | -3.62 | 103.17      | 106.98   |
| 11  | aB    | 834 | CLA  | C1D-CHD-C4C | -3.62 | 118.32      | 126.02   |
| 15  | aL    | 207 | BCR  | C2-C1-C6    | 3.62  | 115.70      | 110.44   |
| 11  | bB    | 818 | CLA  | CHD-C1D-ND  | -3.62 | 119.71      | 124.80   |
| 11  | bA    | 825 | CLA  | CAC-C3C-C4C | 3.62  | 129.50      | 124.79   |
| 11  | aA    | 841 | CLA  | C3C-C4C-NC  | 3.62  | 115.07      | 110.43   |
| 11  | aB    | 801 | CLA  | C3B-C4B-NB  | 3.62  | 113.76      | 110.53   |
| 11  | aB    | 828 | CLA  | C3D-C2D-C1D | -3.62 | 100.89      | 105.83   |
| 11  | cA    | 837 | CLA  | CAA-C2A-C3A | -3.62 | 103.22      | 113.00   |
| 11  | aB    | 830 | CLA  | C3C-C4C-NC  | 3.62  | 115.06      | 110.43   |
| 15  | aB    | 848 | BCR  | C3-C4-C5    | -3.62 | 107.60      | 114.06   |
| 15  | cL    | 207 | BCR  | C2-C1-C6    | 3.62  | 115.69      | 110.44   |
| 11  | bB    | 814 | CLA  | C3B-C4B-NB  | 3.62  | 113.76      | 110.53   |
| 11  | cB    | 812 | CLA  | C3C-C4C-NC  | 3.62  | 115.06      | 110.43   |
| 11  | cL    | 206 | CLA  | C1-C2-C3    | -3.62 | 120.27      | 126.20   |
| 11  | cA    | 813 | CLA  | CHD-C1D-ND  | -3.62 | 119.71      | 124.80   |
| 11  | aA    | 825 | CLA  | CHD-C1D-ND  | -3.61 | 119.72      | 124.80   |
| 11  | cA    | 825 | CLA  | CHD-C1D-ND  | -3.61 | 119.72      | 124.80   |
| 11  | cB    | 833 | CLA  | C1D-CHD-C4C | -3.61 | 118.34      | 126.02   |
| 11  | cB    | 811 | CLA  | CHD-C1D-ND  | -3.61 | 119.72      | 124.80   |
| 11  | cA    | 841 | CLA  | C3C-C4C-NC  | 3.61  | 115.06      | 110.43   |
| 11  | bB    | 801 | CLA  | C3B-C4B-NB  | 3.61  | 113.75      | 110.53   |
| 11  | cA    | 824 | CLA  | C4A-NA-C1A  | -3.61 | 105.03      | 106.68   |
| 11  | cB    | 812 | CLA  | CHD-C1D-ND  | -3.61 | 119.72      | 124.80   |
| 11  | aB    | 833 | CLA  | C1D-CHD-C4C | -3.61 | 118.35      | 126.02   |
| 11  | bA    | 833 | CLA  | C4A-NA-C1A  | -3.61 | 105.03      | 106.68   |
| 12  | cA    | 826 | F6C  | C4C-CHD-C1D | -3.61 | 117.76      | 126.25   |
| 11  | cB    | 834 | CLA  | C4B-C3B-C2B | -3.61 | 102.81      | 107.30   |
| 11  | bB    | 825 | CLA  | CHD-C1D-ND  | -3.61 | 119.72      | 124.80   |
| 11  | aB    | 809 | CLA  | C4A-NA-C1A  | -3.61 | 105.03      | 106.68   |
| 11  | cA    | 804 | CLA  | C4A-NA-C1A  | -3.61 | 105.03      | 106.68   |
| 11  | bB    | 837 | CLA  | C3C-C4C-NC  | 3.61  | 115.05      | 110.43   |
| 11  | aB    | 823 | CLA  | C3B-C4B-NB  | 3.60  | 113.75      | 110.53   |
| 11  | aA    | 841 | CLA  | C1D-CHD-C4C | -3.60 | 118.36      | 126.02   |
| 11  | aB    | 811 | CLA  | CHD-C1D-ND  | -3.60 | 119.73      | 124.80   |
| 11  | bA    | 825 | CLA  | CHD-C1D-ND  | -3.60 | 119.73      | 124.80   |
| 15  | cB    | 848 | BCR  | C3-C4-C5    | -3.60 | 107.63      | 114.06   |
| 12  | bB    | 824 | F6C  | C1C-C2C-C3C | -3.60 | 102.69      | 106.82   |
| 11  | aB    | 806 | CLA  | C3C-C4C-NC  | 3.60  | 115.05      | 110.43   |
| 11  | bA    | 841 | CLA  | C1D-CHD-C4C | -3.60 | 118.36      | 126.02   |
| 11  | cB    | 814 | CLA  | C3B-C4B-NB  | 3.60  | 113.75      | 110.53   |
| 15  | bB    | 848 | BCR  | C2-C1-C6    | 3.60  | 115.67      | 110.44   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aA    | 837 | CLA  | CAA-C2A-C3A | -3.60 | 103.27      | 113.00   |
| 11  | bB    | 838 | CLA  | C3C-C4C-NC  | 3.60  | 115.04      | 110.43   |
| 11  | aB    | 832 | CLA  | C1C-C2C-C3C | -3.60 | 103.20      | 106.98   |
| 11  | aL    | 206 | CLA  | C1C-C2C-C3C | -3.60 | 103.20      | 106.98   |
| 11  | cB    | 828 | CLA  | C3D-C2D-C1D | -3.60 | 100.92      | 105.83   |
| 15  | bB    | 848 | BCR  | C3-C4-C5    | -3.60 | 107.64      | 114.06   |
| 11  | bB    | 833 | CLA  | C1D-CHD-C4C | -3.60 | 118.38      | 126.02   |
| 11  | aB    | 802 | CLA  | O2D-CGD-O1D | -3.60 | 116.85      | 123.85   |
| 11  | bB    | 822 | CLA  | C2C-C1C-NC  | 3.60  | 113.76      | 109.98   |
| 11  | cB    | 812 | CLA  | C3B-C4B-NB  | 3.60  | 113.74      | 110.53   |
| 11  | bB    | 811 | CLA  | CHD-C1D-ND  | -3.60 | 119.74      | 124.80   |
| 11  | aA    | 808 | CLA  | C3C-C4C-NC  | 3.60  | 115.04      | 110.43   |
| 11  | bA    | 837 | CLA  | CAA-C2A-C3A | -3.60 | 103.28      | 113.00   |
| 11  | bB    | 802 | CLA  | O2D-CGD-O1D | -3.59 | 116.85      | 123.85   |
| 11  | aB    | 822 | CLA  | C2C-C1C-NC  | 3.59  | 113.76      | 109.98   |
| 11  | cB    | 802 | CLA  | O2D-CGD-O1D | -3.59 | 116.85      | 123.85   |
| 11  | bB    | 806 | CLA  | C3C-C4C-NC  | 3.59  | 115.03      | 110.43   |
| 11  | bB    | 828 | CLA  | C3D-C2D-C1D | -3.59 | 100.93      | 105.83   |
| 11  | aL    | 205 | CLA  | C3C-C4C-NC  | 3.59  | 115.03      | 110.43   |
| 12  | aA    | 826 | F6C  | C4C-CHD-C1D | -3.59 | 117.80      | 126.25   |
| 11  | bA    | 813 | CLA  | CHD-C1D-ND  | -3.59 | 119.75      | 124.80   |
| 11  | aA    | 824 | CLA  | C4A-NA-C1A  | -3.59 | 105.04      | 106.68   |
| 11  | bB    | 811 | CLA  | C1C-C2C-C3C | -3.59 | 103.20      | 106.98   |
| 11  | aA    | 835 | CLA  | C3C-C4C-NC  | 3.59  | 115.03      | 110.43   |
| 12  | bA    | 826 | F6C  | C4C-CHD-C1D | -3.59 | 117.82      | 126.25   |
| 11  | cA    | 841 | CLA  | C1D-CHD-C4C | -3.58 | 118.40      | 126.02   |
| 11  | bB    | 834 | CLA  | C4B-C3B-C2B | -3.58 | 102.84      | 107.30   |
| 11  | cB    | 822 | CLA  | C2C-C1C-NC  | 3.58  | 113.75      | 109.98   |
| 11  | bA    | 816 | CLA  | CHD-C1D-ND  | -3.58 | 119.76      | 124.80   |
| 11  | bB    | 817 | CLA  | C3B-C4B-NB  | 3.58  | 113.73      | 110.53   |
| 11  | aB    | 811 | CLA  | C4A-NA-C1A  | -3.58 | 105.05      | 106.68   |
| 11  | aL    | 204 | CLA  | CHD-C1D-ND  | -3.58 | 119.76      | 124.80   |
| 11  | aB    | 803 | CLA  | CHC-C1C-C2C | -3.58 | 116.77      | 126.95   |
| 11  | cL    | 206 | CLA  | C1C-C2C-C3C | -3.58 | 103.21      | 106.98   |
| 11  | cB    | 834 | CLA  | C3C-C4C-NC  | 3.58  | 115.02      | 110.43   |
| 11  | aB    | 821 | CLA  | CHD-C1D-ND  | -3.58 | 119.77      | 124.80   |
| 11  | aB    | 825 | CLA  | CHD-C1D-ND  | -3.58 | 119.77      | 124.80   |
| 11  | bA    | 816 | CLA  | C4A-NA-C1A  | -3.58 | 105.05      | 106.68   |
| 11  | aB    | 834 | CLA  | C4B-C3B-C2B | -3.58 | 102.86      | 107.30   |
| 11  | bL    | 206 | CLA  | C1C-C2C-C3C | -3.58 | 103.22      | 106.98   |
| 11  | bB    | 826 | CLA  | C3B-C4B-NB  | 3.57  | 113.72      | 110.53   |
| 11  | aB    | 808 | CLA  | O2A-CGA-CBA | 3.57  | 122.73      | 111.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aA    | 813 | CLA  | CHD-C1D-ND  | -3.57 | 119.77      | 124.80   |
| 11  | aA    | 809 | CLA  | C4A-NA-C1A  | -3.57 | 105.05      | 106.68   |
| 11  | aB    | 809 | CLA  | CMA-C3A-C2A | -3.57 | 100.17      | 113.98   |
| 11  | cA    | 837 | CLA  | C3B-C4B-NB  | 3.57  | 113.72      | 110.53   |
| 11  | aA    | 806 | CLA  | C1C-C2C-C3C | -3.57 | 103.22      | 106.98   |
| 11  | bB    | 809 | CLA  | CMA-C3A-C2A | -3.57 | 100.17      | 113.98   |
| 11  | bB    | 808 | CLA  | O2A-CGA-CBA | 3.57  | 122.72      | 111.83   |
| 11  | aA    | 804 | CLA  | C3C-C4C-NC  | 3.57  | 115.00      | 110.43   |
| 12  | aB    | 824 | F6C  | C1C-C2C-C3C | -3.57 | 102.73      | 106.82   |
| 11  | cL    | 204 | CLA  | CHD-C1D-ND  | -3.57 | 119.78      | 124.80   |
| 11  | cA    | 835 | CLA  | C3C-C4C-NC  | 3.57  | 115.00      | 110.43   |
| 11  | bB    | 836 | CLA  | C4C-C3C-C2C | -3.57 | 101.70      | 106.89   |
| 11  | cB    | 809 | CLA  | CMA-C3A-C2A | -3.57 | 100.19      | 113.98   |
| 11  | aB    | 808 | CLA  | C3B-C4B-NB  | 3.57  | 113.71      | 110.53   |
| 11  | cA    | 816 | CLA  | CHD-C1D-ND  | -3.57 | 119.78      | 124.80   |
| 11  | bA    | 817 | CLA  | C3C-C4C-NC  | 3.57  | 115.00      | 110.43   |
| 11  | cB    | 803 | CLA  | CHC-C1C-C2C | -3.56 | 116.82      | 126.95   |
| 11  | bA    | 808 | CLA  | C3C-C4C-NC  | 3.56  | 115.00      | 110.43   |
| 11  | cB    | 808 | CLA  | O2A-CGA-CBA | 3.56  | 122.70      | 111.83   |
| 11  | aA    | 816 | CLA  | CHD-C1D-ND  | -3.56 | 119.79      | 124.80   |
| 11  | aB    | 814 | CLA  | C3B-C4B-NB  | 3.56  | 113.71      | 110.53   |
| 11  | cA    | 804 | CLA  | C3C-C4C-NC  | 3.56  | 114.99      | 110.43   |
| 11  | bB    | 812 | CLA  | C3B-C4B-NB  | 3.56  | 113.71      | 110.53   |
| 11  | bA    | 835 | CLA  | C3C-C4C-NC  | 3.56  | 114.99      | 110.43   |
| 11  | cK    | 103 | CLA  | C1C-C2C-C3C | -3.56 | 103.23      | 106.98   |
| 11  | bB    | 803 | CLA  | CHC-C1C-C2C | -3.56 | 116.83      | 126.95   |
| 11  | cL    | 205 | CLA  | CHD-C1D-ND  | -3.56 | 119.79      | 124.80   |
| 15  | aB    | 848 | BCR  | C15-C16-C17 | -3.56 | 116.23      | 123.52   |
| 11  | bA    | 836 | CLA  | C3B-C4B-NB  | 3.56  | 113.71      | 110.53   |
| 11  | cA    | 817 | CLA  | C3C-C4C-NC  | 3.56  | 114.99      | 110.43   |
| 11  | aL    | 205 | CLA  | CHD-C1D-ND  | -3.56 | 119.79      | 124.80   |
| 11  | cA    | 823 | CLA  | CHD-C1D-ND  | -3.56 | 119.80      | 124.80   |
| 15  | cB    | 848 | BCR  | C15-C16-C17 | -3.56 | 116.24      | 123.52   |
| 11  | aB    | 825 | CLA  | C1C-C2C-C3C | -3.56 | 103.24      | 106.98   |
| 12  | cA    | 827 | F6C  | C4C-CHD-C1D | -3.56 | 117.88      | 126.25   |
| 11  | aA    | 842 | CLA  | C3C-C4C-NC  | 3.56  | 114.99      | 110.43   |
| 11  | bB    | 835 | CLA  | C3C-C4C-NC  | 3.56  | 114.99      | 110.43   |
| 11  | aA    | 806 | CLA  | C1D-CHD-C4C | -3.56 | 118.46      | 126.02   |
| 11  | bB    | 827 | CLA  | C4-C3-C5    | 3.56  | 121.40      | 115.23   |
| 11  | cA    | 808 | CLA  | C3C-C4C-NC  | 3.56  | 114.98      | 110.43   |
| 11  | aB    | 835 | CLA  | C3B-C4B-NB  | 3.56  | 113.70      | 110.53   |
| 11  | cB    | 835 | CLA  | C3C-C4C-NC  | 3.55  | 114.98      | 110.43   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cA    | 806 | CLA  | C1D-CHD-C4C | -3.55 | 118.47      | 126.02   |
| 11  | cB    | 826 | CLA  | C3B-C4B-NB  | 3.55  | 113.70      | 110.53   |
| 11  | aB    | 817 | CLA  | C3B-C4B-NB  | 3.55  | 113.70      | 110.53   |
| 12  | cB    | 824 | F6C  | C1C-C2C-C3C | -3.55 | 102.75      | 106.82   |
| 11  | cB    | 827 | CLA  | C4-C3-C5    | 3.55  | 121.39      | 115.23   |
| 12  | bA    | 826 | F6C  | C1C-C2C-C3C | -3.55 | 102.75      | 106.82   |
| 11  | cB    | 821 | CLA  | CHD-C1D-ND  | -3.55 | 119.81      | 124.80   |
| 11  | bB    | 834 | CLA  | C3C-C4C-NC  | 3.55  | 114.98      | 110.43   |
| 11  | aA    | 804 | CLA  | C4A-NA-C1A  | -3.55 | 105.06      | 106.68   |
| 12  | aA    | 826 | F6C  | C1C-C2C-C3C | -3.55 | 102.75      | 106.82   |
| 11  | aB    | 835 | CLA  | C3C-C4C-NC  | 3.55  | 114.97      | 110.43   |
| 11  | aA    | 817 | CLA  | C3C-C4C-NC  | 3.55  | 114.97      | 110.43   |
| 11  | cA    | 840 | CLA  | C3C-C4C-NC  | 3.55  | 114.97      | 110.43   |
| 11  | bA    | 806 | CLA  | C1D-CHD-C4C | -3.55 | 118.48      | 126.02   |
| 11  | bA    | 808 | CLA  | C3B-C4B-NB  | 3.55  | 113.69      | 110.53   |
| 11  | bA    | 837 | CLA  | C3B-C4B-NB  | 3.55  | 113.69      | 110.53   |
| 11  | aB    | 836 | CLA  | C4C-C3C-C2C | -3.55 | 101.73      | 106.89   |
| 11  | cB    | 832 | CLA  | C1C-C2C-C3C | -3.54 | 103.25      | 106.98   |
| 11  | bA    | 804 | CLA  | C3C-C4C-NC  | 3.54  | 114.97      | 110.43   |
| 11  | bL    | 205 | CLA  | CHD-C1D-ND  | -3.54 | 119.82      | 124.80   |
| 11  | bB    | 821 | CLA  | CHD-C1D-ND  | -3.54 | 119.82      | 124.80   |
| 11  | bB    | 828 | CLA  | CHC-C1C-C2C | -3.54 | 116.88      | 126.95   |
| 11  | cA    | 816 | CLA  | C4A-NA-C1A  | -3.54 | 105.06      | 106.68   |
| 11  | bB    | 835 | CLA  | C3B-C4B-NB  | 3.54  | 113.69      | 110.53   |
| 11  | aA    | 822 | CLA  | CHD-C1D-ND  | -3.54 | 119.82      | 124.80   |
| 11  | bB    | 827 | CLA  | CMD-C2D-C1D | 3.54  | 130.97      | 124.73   |
| 11  | cA    | 806 | CLA  | C1C-C2C-C3C | -3.54 | 103.25      | 106.98   |
| 11  | cA    | 842 | CLA  | C3C-C4C-NC  | 3.54  | 114.97      | 110.43   |
| 11  | aA    | 808 | CLA  | C1D-CHD-C4C | -3.54 | 118.49      | 126.02   |
| 12  | bA    | 827 | F6C  | C4C-CHD-C1D | -3.54 | 117.92      | 126.25   |
| 11  | bA    | 806 | CLA  | C1C-C2C-C3C | -3.54 | 103.26      | 106.98   |
| 11  | cA    | 817 | CLA  | C4B-C3B-C2B | -3.54 | 102.90      | 107.30   |
| 11  | aA    | 802 | CLA  | C4B-C3B-C2B | -3.54 | 102.90      | 107.30   |
| 11  | bK    | 103 | CLA  | C1C-C2C-C3C | -3.54 | 103.26      | 106.98   |
| 11  | cA    | 803 | CLA  | C3B-C4B-NB  | 3.54  | 113.69      | 110.53   |
| 12  | aA    | 827 | F6C  | C4C-CHD-C1D | -3.54 | 117.93      | 126.25   |
| 11  | cA    | 802 | CLA  | C4B-C3B-C2B | -3.54 | 102.90      | 107.30   |
| 11  | bB    | 818 | CLA  | C4A-NA-C1A  | -3.54 | 105.06      | 106.68   |
| 11  | aB    | 828 | CLA  | CHC-C1C-C2C | -3.54 | 116.89      | 126.95   |
| 11  | aB    | 840 | CLA  | C4B-C3B-C2B | -3.54 | 102.90      | 107.30   |
| 11  | cB    | 835 | CLA  | C3B-C4B-NB  | 3.54  | 113.69      | 110.53   |
| 15  | bB    | 848 | BCR  | C15-C16-C17 | -3.54 | 116.28      | 123.52   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aB    | 827 | CLA  | C4-C3-C5    | 3.54  | 121.37      | 115.23   |
| 11  | cA    | 808 | CLA  | C1D-CHD-C4C | -3.54 | 118.50      | 126.02   |
| 11  | cB    | 828 | CLA  | CAC-C3C-C4C | 3.54  | 129.39      | 124.79   |
| 11  | aB    | 816 | CLA  | C1D-CHD-C4C | -3.53 | 118.51      | 126.02   |
| 11  | bL    | 206 | CLA  | CHD-C1D-ND  | -3.53 | 119.83      | 124.80   |
| 12  | bL    | 202 | F6C  | C1C-C2C-C3C | -3.53 | 102.77      | 106.82   |
| 11  | bA    | 817 | CLA  | C4B-C3B-C2B | -3.53 | 102.91      | 107.30   |
| 11  | cA    | 809 | CLA  | C3C-C4C-NC  | 3.53  | 114.96      | 110.43   |
| 11  | cB    | 828 | CLA  | CHC-C1C-C2C | -3.53 | 116.91      | 126.95   |
| 11  | cA    | 822 | CLA  | CHD-C1D-ND  | -3.53 | 119.83      | 124.80   |
| 11  | aA    | 837 | CLA  | C3B-C4B-NB  | 3.53  | 113.68      | 110.53   |
| 11  | bB    | 840 | CLA  | C3C-C4C-NC  | 3.53  | 114.95      | 110.43   |
| 11  | cA    | 803 | CLA  | C1D-CHD-C4C | -3.53 | 118.52      | 126.02   |
| 11  | aB    | 840 | CLA  | C3B-C4B-NB  | 3.53  | 113.68      | 110.53   |
| 11  | cA    | 836 | CLA  | C3B-C4B-NB  | 3.53  | 113.68      | 110.53   |
| 11  | bA    | 835 | CLA  | C4A-NA-C1A  | -3.53 | 105.07      | 106.68   |
| 11  | cB    | 836 | CLA  | C4C-C3C-C2C | -3.53 | 101.76      | 106.89   |
| 11  | aB    | 816 | CLA  | C1C-C2C-C3C | -3.53 | 103.27      | 106.98   |
| 11  | bB    | 832 | CLA  | C1C-C2C-C3C | -3.53 | 103.27      | 106.98   |
| 11  | bB    | 831 | CLA  | C3C-C4C-NC  | 3.53  | 114.95      | 110.43   |
| 11  | aA    | 836 | CLA  | C3B-C4B-NB  | 3.53  | 113.68      | 110.53   |
| 11  | aB    | 830 | CLA  | C4A-NA-C1A  | -3.52 | 105.07      | 106.68   |
| 11  | aK    | 103 | CLA  | C1C-C2C-C3C | -3.52 | 103.27      | 106.98   |
| 11  | bB    | 816 | CLA  | C1C-C2C-C3C | -3.52 | 103.27      | 106.98   |
| 11  | bA    | 842 | CLA  | C3C-C4C-NC  | 3.52  | 114.94      | 110.43   |
| 11  | bA    | 808 | CLA  | C1D-CHD-C4C | -3.52 | 118.53      | 126.02   |
| 11  | bA    | 822 | CLA  | CHD-C1D-ND  | -3.52 | 119.85      | 124.80   |
| 12  | aL    | 202 | F6C  | C1C-C2C-C3C | -3.52 | 102.78      | 106.82   |
| 11  | aA    | 823 | CLA  | CHD-C1D-ND  | -3.52 | 119.85      | 124.80   |
| 11  | bA    | 828 | CLA  | CHD-C1D-ND  | -3.52 | 119.85      | 124.80   |
| 11  | bA    | 803 | CLA  | C1D-CHD-C4C | -3.52 | 118.54      | 126.02   |
| 11  | cA    | 835 | CLA  | C4A-NA-C1A  | -3.52 | 105.07      | 106.68   |
| 11  | aB    | 812 | CLA  | C3B-C4B-NB  | 3.52  | 113.67      | 110.53   |
| 11  | aB    | 826 | CLA  | C3B-C4B-NB  | 3.52  | 113.67      | 110.53   |
| 11  | cA    | 808 | CLA  | C3B-C4B-NB  | 3.52  | 113.67      | 110.53   |
| 12  | cL    | 202 | F6C  | C1C-C2C-C3C | -3.52 | 102.79      | 106.82   |
| 11  | cA    | 833 | CLA  | C3B-C4B-NB  | 3.52  | 113.67      | 110.53   |
| 11  | bA    | 802 | CLA  | C4B-C3B-C2B | -3.52 | 102.93      | 107.30   |
| 11  | cB    | 840 | CLA  | C3C-C4C-NC  | 3.52  | 114.94      | 110.43   |
| 11  | bB    | 825 | CLA  | C1C-C2C-C3C | -3.52 | 103.28      | 106.98   |
| 11  | bA    | 823 | CLA  | CHD-C1D-ND  | -3.52 | 119.85      | 124.80   |
| 11  | aB    | 837 | CLA  | C1C-C2C-C3C | -3.52 | 103.28      | 106.98   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cB    | 816 | CLA  | C1C-C2C-C3C | -3.52 | 103.28      | 106.98   |
| 11  | cL    | 206 | CLA  | CHD-C1D-ND  | -3.52 | 119.85      | 124.80   |
| 11  | aA    | 840 | CLA  | C3C-C4C-NC  | 3.52  | 114.93      | 110.43   |
| 11  | aA    | 815 | CLA  | C4B-C3B-C2B | -3.52 | 102.93      | 107.30   |
| 11  | cB    | 809 | CLA  | C1C-C2C-C3C | -3.52 | 103.28      | 106.98   |
| 12  | aA    | 844 | F6C  | CHD-C1D-ND  | -3.51 | 119.02      | 124.31   |
| 11  | cB    | 825 | CLA  | C1C-C2C-C3C | -3.51 | 103.28      | 106.98   |
| 11  | aA    | 828 | CLA  | CHD-C1D-ND  | -3.51 | 119.86      | 124.80   |
| 11  | aL    | 206 | CLA  | CHD-C1D-ND  | -3.51 | 119.86      | 124.80   |
| 11  | cB    | 810 | CLA  | C3C-C4C-NC  | 3.51  | 114.93      | 110.43   |
| 12  | cA    | 844 | F6C  | CHD-C1D-ND  | -3.51 | 119.02      | 124.31   |
| 11  | aB    | 828 | CLA  | CAC-C3C-C4C | 3.51  | 129.36      | 124.79   |
| 11  | cA    | 828 | CLA  | CHD-C1D-ND  | -3.51 | 119.86      | 124.80   |
| 11  | bA    | 803 | CLA  | C3B-C4B-NB  | 3.51  | 113.66      | 110.53   |
| 11  | cA    | 815 | CLA  | C4B-C3B-C2B | -3.51 | 102.94      | 107.30   |
| 12  | cA    | 826 | F6C  | C1C-C2C-C3C | -3.51 | 102.80      | 106.82   |
| 11  | bB    | 803 | CLA  | C3C-C4C-NC  | 3.51  | 114.92      | 110.43   |
| 11  | bA    | 842 | CLA  | CAA-C2A-C3A | -3.51 | 103.52      | 113.00   |
| 11  | aA    | 833 | CLA  | C3B-C4B-NB  | 3.51  | 113.66      | 110.53   |
| 11  | cB    | 817 | CLA  | C3B-C4B-NB  | 3.51  | 113.66      | 110.53   |
| 11  | bB    | 810 | CLA  | C3C-C4C-NC  | 3.51  | 114.92      | 110.43   |
| 11  | bB    | 816 | CLA  | C1D-CHD-C4C | -3.51 | 118.57      | 126.02   |
| 11  | cB    | 803 | CLA  | C3C-C4C-NC  | 3.51  | 114.92      | 110.43   |
| 11  | cB    | 804 | CLA  | C1C-C2C-C3C | -3.51 | 103.29      | 106.98   |
| 11  | bB    | 840 | CLA  | C4B-C3B-C2B | -3.50 | 102.95      | 107.30   |
| 12  | bA    | 832 | F6C  | C1C-C2C-C3C | -3.50 | 102.81      | 106.82   |
| 11  | aB    | 803 | CLA  | C3C-C4C-NC  | 3.50  | 114.92      | 110.43   |
| 11  | aB    | 840 | CLA  | C3C-C4C-NC  | 3.50  | 114.92      | 110.43   |
| 11  | aB    | 809 | CLA  | C1C-C2C-C3C | -3.50 | 103.30      | 106.98   |
| 11  | cA    | 843 | CLA  | CHD-C1D-ND  | -3.50 | 119.88      | 124.80   |
| 11  | cB    | 837 | CLA  | C1C-C2C-C3C | -3.50 | 103.30      | 106.98   |
| 11  | cA    | 809 | CLA  | C4A-NA-C1A  | -3.50 | 105.08      | 106.68   |
| 11  | cL    | 206 | CLA  | C4A-NA-C1A  | -3.50 | 105.08      | 106.68   |
| 11  | aA    | 806 | CLA  | C3B-C4B-NB  | 3.50  | 113.65      | 110.53   |
| 11  | aB    | 810 | CLA  | C3C-C4C-NC  | 3.50  | 114.91      | 110.43   |
| 11  | cB    | 811 | CLA  | C4A-NA-C1A  | -3.50 | 105.08      | 106.68   |
| 11  | aA    | 803 | CLA  | C1D-CHD-C4C | -3.50 | 118.59      | 126.02   |
| 11  | cB    | 809 | CLA  | C4B-C3B-C2B | -3.50 | 102.95      | 107.30   |
| 11  | bA    | 840 | CLA  | C3C-C4C-NC  | 3.50  | 114.91      | 110.43   |
| 11  | bB    | 811 | CLA  | C4A-NA-C1A  | -3.50 | 105.08      | 106.68   |
| 12  | cA    | 844 | F6C  | C4C-CHD-C1D | -3.50 | 118.03      | 126.25   |
| 12  | bA    | 844 | F6C  | C4C-CHD-C1D | -3.50 | 118.03      | 126.25   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bB    | 837 | CLA  | C1C-C2C-C3C | -3.50 | 103.30      | 106.98   |
| 11  | cA    | 806 | CLA  | C3B-C4B-NB  | 3.50  | 113.65      | 110.53   |
| 11  | cL    | 206 | CLA  | C3B-C4B-NB  | 3.50  | 113.65      | 110.53   |
| 11  | cA    | 811 | CLA  | C3C-C4C-NC  | 3.49  | 114.90      | 110.43   |
| 11  | aB    | 827 | CLA  | CMD-C2D-C1D | 3.49  | 130.88      | 124.73   |
| 11  | aB    | 804 | CLA  | C1C-C2C-C3C | -3.49 | 103.31      | 106.98   |
| 11  | bA    | 806 | CLA  | C3B-C4B-NB  | 3.49  | 113.65      | 110.53   |
| 11  | aA    | 842 | CLA  | CAA-C2A-C3A | -3.49 | 103.56      | 113.00   |
| 11  | bB    | 813 | CLA  | CHD-C1D-ND  | -3.49 | 119.89      | 124.80   |
| 11  | bB    | 809 | CLA  | C1C-C2C-C3C | -3.49 | 103.31      | 106.98   |
| 11  | aA    | 843 | CLA  | CHD-C1D-ND  | -3.49 | 119.89      | 124.80   |
| 11  | cB    | 827 | CLA  | CMD-C2D-C1D | 3.49  | 130.87      | 124.73   |
| 11  | cB    | 840 | CLA  | C4B-C3B-C2B | -3.49 | 102.96      | 107.30   |
| 11  | cA    | 842 | CLA  | CAA-C2A-C3A | -3.49 | 103.57      | 113.00   |
| 11  | aA    | 808 | CLA  | C3B-C4B-NB  | 3.49  | 113.64      | 110.53   |
| 11  | aA    | 809 | CLA  | C3C-C4C-NC  | 3.49  | 114.90      | 110.43   |
| 12  | cB    | 824 | F6C  | CHD-C1D-ND  | -3.49 | 119.06      | 124.31   |
| 11  | aA    | 817 | CLA  | C4B-C3B-C2B | -3.49 | 102.97      | 107.30   |
| 11  | bA    | 824 | CLA  | C4-C3-C5    | 3.48  | 120.23      | 116.13   |
| 11  | bB    | 828 | CLA  | CAC-C3C-C4C | 3.48  | 129.32      | 124.79   |
| 11  | bA    | 833 | CLA  | C3B-C4B-NB  | 3.48  | 113.64      | 110.53   |
| 12  | bA    | 844 | F6C  | CHD-C1D-ND  | -3.48 | 119.06      | 124.31   |
| 11  | bA    | 811 | CLA  | O2D-CGD-CBD | 3.48  | 117.32      | 111.23   |
| 11  | aA    | 824 | CLA  | C4-C3-C5    | 3.48  | 120.23      | 116.13   |
| 11  | bA    | 815 | CLA  | C4B-C3B-C2B | -3.48 | 102.97      | 107.30   |
| 11  | aA    | 803 | CLA  | CHD-C1D-ND  | -3.48 | 119.91      | 124.80   |
| 11  | cB    | 831 | CLA  | C3C-C4C-NC  | 3.48  | 114.89      | 110.43   |
| 11  | cB    | 816 | CLA  | C1D-CHD-C4C | -3.48 | 118.62      | 126.02   |
| 11  | bA    | 843 | CLA  | CHD-C1D-ND  | -3.48 | 119.91      | 124.80   |
| 11  | aA    | 820 | CLA  | CAC-C3C-C4C | 3.48  | 129.31      | 124.79   |
| 11  | cB    | 803 | CLA  | C1D-CHD-C4C | -3.48 | 118.63      | 126.02   |
| 11  | aA    | 803 | CLA  | C3B-C4B-NB  | 3.48  | 113.63      | 110.53   |
| 12  | cA    | 832 | F6C  | C1C-C2C-C3C | -3.48 | 102.83      | 106.82   |
| 11  | aA    | 811 | CLA  | C3C-C4C-NC  | 3.48  | 114.88      | 110.43   |
| 11  | cB    | 840 | CLA  | C3B-C4B-NB  | 3.48  | 113.63      | 110.53   |
| 11  | cB    | 835 | CLA  | CAA-C2A-C3A | -3.48 | 103.61      | 113.00   |
| 11  | aB    | 831 | CLA  | C3C-C4C-NC  | 3.48  | 114.88      | 110.43   |
| 11  | bB    | 801 | CLA  | CHD-C1D-ND  | -3.47 | 119.91      | 124.80   |
| 11  | aA    | 813 | CLA  | C4B-C3B-C2B | -3.47 | 102.98      | 107.30   |
| 11  | bA    | 809 | CLA  | C3C-C4C-NC  | 3.47  | 114.88      | 110.43   |
| 11  | aB    | 818 | CLA  | C4A-NA-C1A  | -3.47 | 105.09      | 106.68   |
| 11  | cA    | 811 | CLA  | O2D-CGD-CBD | 3.47  | 117.30      | 111.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12  | aA    | 844 | F6C  | C4C-CHD-C1D | -3.47 | 118.08      | 126.25   |
| 11  | aA    | 835 | CLA  | C4A-NA-C1A  | -3.47 | 105.09      | 106.68   |
| 11  | bA    | 811 | CLA  | C3C-C4C-NC  | 3.47  | 114.88      | 110.43   |
| 11  | aA    | 811 | CLA  | O2D-CGD-CBD | 3.47  | 117.30      | 111.23   |
| 11  | cA    | 812 | CLA  | C3B-C4B-NB  | 3.47  | 113.63      | 110.53   |
| 11  | bL    | 206 | CLA  | C4A-NA-C1A  | -3.47 | 105.10      | 106.68   |
| 11  | aB    | 813 | CLA  | CHD-C1D-ND  | -3.47 | 119.92      | 124.80   |
| 11  | aA    | 820 | CLA  | CBA-CAA-C2A | 3.47  | 124.11      | 113.79   |
| 11  | bB    | 835 | CLA  | CAA-C2A-C3A | -3.47 | 103.63      | 113.00   |
| 11  | bB    | 809 | CLA  | C4B-C3B-C2B | -3.47 | 102.99      | 107.30   |
| 11  | bA    | 809 | CLA  | C4A-NA-C1A  | -3.47 | 105.10      | 106.68   |
| 12  | aA    | 832 | F6C  | C1C-C2C-C3C | -3.46 | 102.85      | 106.82   |
| 11  | bL    | 206 | CLA  | C3B-C4B-NB  | 3.46  | 113.62      | 110.53   |
| 11  | aB    | 801 | CLA  | CHD-C1D-ND  | -3.46 | 119.93      | 124.80   |
| 11  | bL    | 205 | CLA  | C4A-NA-C1A  | -3.46 | 105.10      | 106.68   |
| 11  | aB    | 803 | CLA  | C1D-CHD-C4C | -3.46 | 118.66      | 126.02   |
| 11  | aA    | 839 | CLA  | C3C-C4C-NC  | 3.46  | 114.87      | 110.43   |
| 12  | aB    | 824 | F6C  | CHD-C1D-ND  | -3.46 | 119.10      | 124.31   |
| 12  | cA    | 832 | F6C  | C4C-CHD-C1D | -3.46 | 118.11      | 126.25   |
| 11  | bA    | 820 | CLA  | CAC-C3C-C4C | 3.46  | 129.29      | 124.79   |
| 11  | aB    | 835 | CLA  | CAA-C2A-C3A | -3.46 | 103.64      | 113.00   |
| 11  | aB    | 809 | CLA  | C4B-C3B-C2B | -3.46 | 103.00      | 107.30   |
| 11  | cA    | 824 | CLA  | C4-C3-C5    | 3.46  | 120.20      | 116.13   |
| 11  | cB    | 818 | CLA  | C4A-NA-C1A  | -3.46 | 105.10      | 106.68   |
| 11  | aB    | 808 | CLA  | C1C-C2C-C3C | -3.46 | 103.34      | 106.98   |
| 11  | cB    | 801 | CLA  | CHD-C1D-ND  | -3.46 | 119.93      | 124.80   |
| 11  | bB    | 803 | CLA  | C1D-CHD-C4C | -3.46 | 118.67      | 126.02   |
| 11  | aB    | 832 | CLA  | C3B-C4B-NB  | 3.46  | 113.62      | 110.53   |
| 11  | aK    | 101 | CLA  | C3C-C4C-NC  | 3.46  | 114.86      | 110.43   |
| 11  | bB    | 821 | CLA  | C4A-NA-C1A  | -3.46 | 105.10      | 106.68   |
| 11  | bA    | 814 | CLA  | C3B-C4B-NB  | 3.46  | 113.62      | 110.53   |
| 11  | bA    | 820 | CLA  | CBA-CAA-C2A | 3.46  | 124.08      | 113.79   |
| 12  | aA    | 827 | F6C  | CHD-C1D-ND  | -3.46 | 119.10      | 124.31   |
| 12  | aA    | 832 | F6C  | CHD-C1D-ND  | -3.46 | 119.10      | 124.31   |
| 11  | bK    | 101 | CLA  | C3C-C4C-NC  | 3.46  | 114.86      | 110.43   |
| 11  | cA    | 813 | CLA  | C4B-C3B-C2B | -3.45 | 103.01      | 107.30   |
| 11  | cA    | 820 | CLA  | CBA-CAA-C2A | 3.45  | 124.07      | 113.79   |
| 12  | bA    | 832 | F6C  | C4C-CHD-C1D | -3.45 | 118.13      | 126.25   |
| 11  | bA    | 803 | CLA  | CHD-C1D-ND  | -3.45 | 119.94      | 124.80   |
| 11  | cB    | 832 | CLA  | C3B-C4B-NB  | 3.45  | 113.61      | 110.53   |
| 11  | cK    | 101 | CLA  | C3C-C4C-NC  | 3.45  | 114.85      | 110.43   |
| 11  | bB    | 804 | CLA  | C1C-C2C-C3C | -3.45 | 103.35      | 106.98   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aA    | 824 | CLA  | C3B-C4B-NB  | 3.45  | 113.61      | 110.53   |
| 11  | bB    | 834 | CLA  | C4A-NA-C1A  | -3.45 | 105.11      | 106.68   |
| 11  | bA    | 839 | CLA  | C3C-C4C-NC  | 3.45  | 114.85      | 110.43   |
| 11  | cA    | 839 | CLA  | C3C-C4C-NC  | 3.45  | 114.85      | 110.43   |
| 11  | cA    | 834 | CLA  | CMB-C2B-C1B | 3.45  | 130.67      | 125.42   |
| 12  | aA    | 832 | F6C  | C4C-CHD-C1D | -3.44 | 118.15      | 126.25   |
| 11  | cA    | 820 | CLA  | CAC-C3C-C4C | 3.44  | 129.27      | 124.79   |
| 11  | aA    | 834 | CLA  | CMB-C2B-C1B | 3.44  | 130.66      | 125.42   |
| 11  | cA    | 843 | CLA  | C1C-C2C-C3C | -3.44 | 103.36      | 106.98   |
| 11  | bA    | 834 | CLA  | C3B-C4B-NB  | 3.44  | 113.60      | 110.53   |
| 15  | aB    | 846 | BCR  | C2-C1-C6    | 3.44  | 115.44      | 110.44   |
| 15  | cB    | 846 | BCR  | C2-C1-C6    | 3.44  | 115.44      | 110.44   |
| 11  | bB    | 825 | CLA  | C3B-C4B-NB  | 3.44  | 113.60      | 110.53   |
| 11  | aA    | 815 | CLA  | C3C-C4C-NC  | 3.44  | 114.83      | 110.43   |
| 12  | bA    | 827 | F6C  | CHD-C1D-ND  | -3.44 | 119.14      | 124.31   |
| 11  | aA    | 811 | CLA  | C3B-C4B-NB  | 3.44  | 113.60      | 110.53   |
| 11  | bA    | 813 | CLA  | C4B-C3B-C2B | -3.44 | 103.03      | 107.30   |
| 11  | aA    | 837 | CLA  | C4A-NA-C1A  | -3.43 | 105.11      | 106.68   |
| 11  | cA    | 803 | CLA  | CHD-C1D-ND  | -3.43 | 119.97      | 124.80   |
| 11  | aA    | 803 | CLA  | CHB-C4A-NA  | 3.43  | 129.36      | 124.40   |
| 11  | aB    | 815 | CLA  | CAC-C3C-C4C | 3.43  | 129.26      | 124.79   |
| 11  | bB    | 832 | CLA  | C3B-C4B-NB  | 3.43  | 113.59      | 110.53   |
| 11  | cA    | 834 | CLA  | C3B-C4B-NB  | 3.43  | 113.59      | 110.53   |
| 12  | bB    | 824 | F6C  | CHD-C1D-ND  | -3.43 | 119.14      | 124.31   |
| 11  | bA    | 812 | CLA  | C3B-C4B-NB  | 3.43  | 113.59      | 110.53   |
| 11  | aB    | 818 | CLA  | C4C-C3C-C2C | -3.43 | 101.90      | 106.89   |
| 11  | bB    | 803 | CLA  | O2D-CGD-CBD | 3.43  | 117.23      | 111.23   |
| 11  | aA    | 814 | CLA  | C3B-C4B-NB  | 3.43  | 113.59      | 110.53   |
| 15  | bB    | 846 | BCR  | C2-C1-C6    | 3.43  | 115.42      | 110.44   |
| 11  | cA    | 815 | CLA  | CHC-C1C-C2C | -3.43 | 117.21      | 126.95   |
| 11  | bA    | 811 | CLA  | C3B-C4B-NB  | 3.43  | 113.59      | 110.53   |
| 11  | bB    | 840 | CLA  | C3B-C4B-NB  | 3.43  | 113.59      | 110.53   |
| 11  | cA    | 814 | CLA  | C3B-C4B-NB  | 3.43  | 113.59      | 110.53   |
| 11  | bA    | 814 | CLA  | C3C-C4C-NC  | 3.43  | 114.82      | 110.43   |
| 11  | cB    | 815 | CLA  | CAC-C3C-C4C | 3.43  | 129.25      | 124.79   |
| 11  | aB    | 808 | CLA  | O2A-CGA-O1A | -3.43 | 115.06      | 123.63   |
| 11  | cB    | 813 | CLA  | CHD-C1D-ND  | -3.43 | 119.98      | 124.80   |
| 11  | bA    | 843 | CLA  | C1C-C2C-C3C | -3.42 | 103.38      | 106.98   |
| 11  | aB    | 803 | CLA  | O2D-CGD-CBD | 3.42  | 117.22      | 111.23   |
| 11  | bA    | 815 | CLA  | C3C-C4C-NC  | 3.42  | 114.81      | 110.43   |
| 11  | cB    | 803 | CLA  | O2D-CGD-CBD | 3.42  | 117.21      | 111.23   |
| 11  | aA    | 843 | CLA  | C1C-C2C-C3C | -3.42 | 103.38      | 106.98   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bB    | 815 | CLA  | CAC-C3C-C4C | 3.42  | 129.24      | 124.79   |
| 12  | cA    | 827 | F6C  | CHD-C1D-ND  | -3.42 | 119.16      | 124.31   |
| 11  | cB    | 818 | CLA  | C4C-C3C-C2C | -3.42 | 101.91      | 106.89   |
| 11  | cB    | 808 | CLA  | O2A-CGA-O1A | -3.42 | 115.07      | 123.63   |
| 12  | bA    | 832 | F6C  | CHD-C1D-ND  | -3.42 | 119.16      | 124.31   |
| 11  | aB    | 831 | CLA  | O2D-CGD-O1D | -3.42 | 117.19      | 123.85   |
| 11  | cB    | 805 | CLA  | C3C-C4C-NC  | 3.42  | 114.81      | 110.43   |
| 11  | bA    | 831 | CLA  | CHD-C1D-ND  | -3.42 | 119.99      | 124.80   |
| 11  | cA    | 818 | CLA  | C3B-C4B-NB  | 3.42  | 113.58      | 110.53   |
| 11  | bB    | 808 | CLA  | C1C-C2C-C3C | -3.42 | 103.39      | 106.98   |
| 11  | aA    | 818 | CLA  | C3B-C4B-NB  | 3.42  | 113.58      | 110.53   |
| 11  | aA    | 834 | CLA  | C3B-C4B-NB  | 3.42  | 113.58      | 110.53   |
| 11  | bB    | 818 | CLA  | C4C-C3C-C2C | -3.42 | 101.92      | 106.89   |
| 11  | cB    | 831 | CLA  | O2D-CGD-O1D | -3.42 | 117.20      | 123.85   |
| 11  | bA    | 834 | CLA  | CMB-C2B-C1B | 3.42  | 130.62      | 125.42   |
| 11  | aL    | 206 | CLA  | C3B-C4B-NB  | 3.42  | 113.58      | 110.53   |
| 11  | bB    | 807 | CLA  | C3B-C4B-NB  | 3.41  | 113.58      | 110.53   |
| 11  | cA    | 814 | CLA  | C3C-C4C-NC  | 3.41  | 114.80      | 110.43   |
| 12  | bA    | 830 | F6C  | C1C-C2C-C3C | -3.41 | 102.91      | 106.82   |
| 11  | aA    | 809 | CLA  | C3B-C4B-NB  | 3.41  | 113.57      | 110.53   |
| 11  | bA    | 823 | CLA  | C3B-C4B-NB  | 3.41  | 113.57      | 110.53   |
| 11  | cA    | 811 | CLA  | C3B-C4B-NB  | 3.41  | 113.57      | 110.53   |
| 11  | aA    | 815 | CLA  | CHC-C1C-C2C | -3.41 | 117.27      | 126.95   |
| 11  | aL    | 205 | CLA  | C4A-NA-C1A  | -3.41 | 105.12      | 106.68   |
| 13  | cB    | 841 | PQN  | C11-C12-C13 | -3.41 | 120.96      | 126.83   |
| 11  | bB    | 834 | CLA  | CHC-C1C-C2C | -3.41 | 117.27      | 126.95   |
| 11  | bA    | 818 | CLA  | CMC-C2C-C1C | 3.41  | 130.36      | 125.03   |
| 11  | bB    | 808 | CLA  | O2A-CGA-O1A | -3.41 | 115.11      | 123.63   |
| 11  | cA    | 815 | CLA  | C3C-C4C-NC  | 3.41  | 114.79      | 110.43   |
| 11  | cA    | 803 | CLA  | CHB-C4A-NA  | 3.40  | 129.31      | 124.40   |
| 11  | cA    | 820 | CLA  | CHC-C1C-C2C | -3.40 | 117.27      | 126.95   |
| 11  | cB    | 834 | CLA  | CHC-C1C-C2C | -3.40 | 117.27      | 126.95   |
| 11  | bA    | 820 | CLA  | C4B-C3B-C2B | -3.40 | 103.07      | 107.30   |
| 11  | bA    | 837 | CLA  | C4A-NA-C1A  | -3.40 | 105.13      | 106.68   |
| 11  | aB    | 834 | CLA  | CHC-C1C-C2C | -3.40 | 117.27      | 126.95   |
| 11  | bA    | 815 | CLA  | CHC-C1C-C2C | -3.40 | 117.27      | 126.95   |
| 11  | bA    | 820 | CLA  | CHC-C1C-C2C | -3.40 | 117.28      | 126.95   |
| 11  | cB    | 826 | CLA  | C1-C2-C3    | -3.40 | 120.62      | 126.20   |
| 11  | bB    | 805 | CLA  | C3C-C4C-NC  | 3.40  | 114.79      | 110.43   |
| 11  | aA    | 814 | CLA  | C3C-C4C-NC  | 3.40  | 114.79      | 110.43   |
| 11  | aA    | 820 | CLA  | C4B-C3B-C2B | -3.40 | 103.07      | 107.30   |
| 11  | aA    | 820 | CLA  | CHC-C1C-C2C | -3.40 | 117.29      | 126.95   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aB    | 807 | CLA  | C3B-C4B-NB  | 3.40  | 113.56      | 110.53   |
| 12  | bB    | 824 | F6C  | CHC-C1C-C2C | -3.40 | 117.56      | 127.43   |
| 11  | bA    | 824 | CLA  | C3B-C4B-NB  | 3.40  | 113.56      | 110.53   |
| 11  | aB    | 833 | CLA  | C4A-NA-C1A  | -3.40 | 105.13      | 106.68   |
| 12  | cA    | 830 | F6C  | C1C-C2C-C3C | -3.40 | 102.93      | 106.82   |
| 11  | cB    | 839 | CLA  | C1C-C2C-C3C | -3.40 | 103.41      | 106.98   |
| 11  | bA    | 803 | CLA  | CHB-C4A-NA  | 3.40  | 129.30      | 124.40   |
| 11  | bA    | 818 | CLA  | C3B-C4B-NB  | 3.40  | 113.56      | 110.53   |
| 11  | aB    | 817 | CLA  | C4A-NA-C1A  | -3.40 | 105.13      | 106.68   |
| 11  | aL    | 204 | CLA  | C4A-NA-C1A  | -3.40 | 105.13      | 106.68   |
| 12  | aA    | 830 | F6C  | C1C-C2C-C3C | -3.39 | 102.93      | 106.82   |
| 11  | aB    | 826 | CLA  | C1-C2-C3    | -3.39 | 120.64      | 126.20   |
| 12  | cA    | 832 | F6C  | CHD-C1D-ND  | -3.39 | 119.20      | 124.31   |
| 11  | aB    | 814 | CLA  | C3C-C4C-NC  | 3.39  | 114.78      | 110.43   |
| 11  | aB    | 818 | CLA  | C4B-C3B-C2B | -3.39 | 103.08      | 107.30   |
| 11  | bB    | 831 | CLA  | O2D-CGD-O1D | -3.39 | 117.25      | 123.85   |
| 12  | aB    | 824 | F6C  | CHC-C1C-C2C | -3.39 | 117.58      | 127.43   |
| 11  | bA    | 819 | CLA  | C1-C2-C3    | -3.39 | 120.64      | 126.20   |
| 11  | bB    | 826 | CLA  | C1-C2-C3    | -3.39 | 120.64      | 126.20   |
| 11  | aA    | 807 | CLA  | C3C-C4C-NC  | 3.39  | 114.77      | 110.43   |
| 11  | cA    | 837 | CLA  | C4A-NA-C1A  | -3.39 | 105.13      | 106.68   |
| 11  | bB    | 826 | CLA  | CAC-C3C-C4C | 3.39  | 129.20      | 124.79   |
| 11  | aB    | 810 | CLA  | C4B-C3B-C2B | -3.39 | 103.09      | 107.30   |
| 11  | aA    | 816 | CLA  | C1C-C2C-C3C | -3.39 | 103.42      | 106.98   |
| 11  | bB    | 814 | CLA  | C4A-NA-C1A  | -3.39 | 105.13      | 106.68   |
| 11  | cA    | 807 | CLA  | C3C-C4C-NC  | 3.39  | 114.77      | 110.43   |
| 11  | cB    | 804 | CLA  | C1-C2-C3    | -3.39 | 121.28      | 126.76   |
| 11  | bB    | 826 | CLA  | C4C-C3C-C2C | -3.38 | 101.97      | 106.89   |
| 11  | aB    | 814 | CLA  | C4A-NA-C1A  | -3.38 | 105.14      | 106.68   |
| 11  | bA    | 808 | CLA  | C4A-NA-C1A  | -3.38 | 105.14      | 106.68   |
| 11  | aB    | 836 | CLA  | CHD-C1D-ND  | -3.38 | 120.04      | 124.80   |
| 11  | cB    | 808 | CLA  | C1C-C2C-C3C | -3.38 | 103.42      | 106.98   |
| 11  | cA    | 824 | CLA  | C3B-C4B-NB  | 3.38  | 113.55      | 110.53   |
| 11  | cB    | 807 | CLA  | C3B-C4B-NB  | 3.38  | 113.55      | 110.53   |
| 11  | cL    | 205 | CLA  | C4A-NA-C1A  | -3.38 | 105.14      | 106.68   |
| 11  | aA    | 825 | CLA  | C3B-C4B-NB  | 3.38  | 113.55      | 110.53   |
| 11  | aB    | 826 | CLA  | CAC-C3C-C4C | 3.38  | 129.19      | 124.79   |
| 11  | bB    | 810 | CLA  | C4B-C3B-C2B | -3.38 | 103.10      | 107.30   |
| 11  | bA    | 814 | CLA  | CAC-C3C-C4C | 3.38  | 129.19      | 124.79   |
| 11  | cA    | 834 | CLA  | CAA-C2A-C3A | -3.38 | 103.87      | 113.00   |
| 11  | cA    | 812 | CLA  | C3C-C4C-NC  | 3.38  | 114.76      | 110.43   |
| 11  | cA    | 820 | CLA  | C4B-C3B-C2B | -3.38 | 103.10      | 107.30   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cA    | 818 | CLA  | CMC-C2C-C1C | 3.38  | 130.31      | 125.03   |
| 11  | bA    | 831 | CLA  | CHC-C1C-C2C | -3.38 | 117.35      | 126.95   |
| 11  | aA    | 812 | CLA  | C3B-C4B-NB  | 3.38  | 113.55      | 110.53   |
| 11  | bA    | 807 | CLA  | C3B-C4B-NB  | 3.38  | 113.54      | 110.53   |
| 11  | bA    | 816 | CLA  | C1C-C2C-C3C | -3.38 | 103.43      | 106.98   |
| 11  | aA    | 812 | CLA  | C3C-C4C-NC  | 3.38  | 114.75      | 110.43   |
| 11  | bA    | 833 | CLA  | C3C-C4C-NC  | 3.38  | 114.75      | 110.43   |
| 11  | bB    | 833 | CLA  | C4A-NA-C1A  | -3.38 | 105.14      | 106.68   |
| 11  | cA    | 816 | CLA  | C1C-C2C-C3C | -3.37 | 103.43      | 106.98   |
| 11  | cB    | 826 | CLA  | C4C-C3C-C2C | -3.37 | 101.98      | 106.89   |
| 11  | aA    | 823 | CLA  | C3B-C4B-NB  | 3.37  | 113.54      | 110.53   |
| 11  | bA    | 812 | CLA  | C3C-C4C-NC  | 3.37  | 114.75      | 110.43   |
| 11  | cB    | 814 | CLA  | C3C-C4C-NC  | 3.37  | 114.75      | 110.43   |
| 11  | bB    | 804 | CLA  | C1-C2-C3    | -3.37 | 121.31      | 126.76   |
| 11  | aB    | 815 | CLA  | CMC-C2C-C1C | 3.37  | 130.30      | 125.03   |
| 11  | aA    | 814 | CLA  | CAC-C3C-C4C | 3.37  | 129.18      | 124.79   |
| 11  | bA    | 807 | CLA  | C3C-C4C-NC  | 3.37  | 114.75      | 110.43   |
| 13  | aB    | 841 | PQN  | C11-C12-C13 | -3.37 | 121.02      | 126.83   |
| 13  | bB    | 841 | PQN  | C11-C12-C13 | -3.37 | 121.02      | 126.83   |
| 11  | aB    | 832 | CLA  | C3C-C4C-NC  | 3.37  | 114.75      | 110.43   |
| 11  | aA    | 831 | CLA  | CHD-C1D-ND  | -3.37 | 120.06      | 124.80   |
| 11  | bA    | 812 | CLA  | C1C-C2C-C3C | -3.37 | 103.44      | 106.98   |
| 11  | cB    | 818 | CLA  | C4B-C3B-C2B | -3.37 | 103.11      | 107.30   |
| 11  | aB    | 826 | CLA  | C4C-C3C-C2C | -3.37 | 101.99      | 106.89   |
| 11  | bB    | 814 | CLA  | C3C-C4C-NC  | 3.37  | 114.75      | 110.43   |
| 11  | aL    | 206 | CLA  | C4A-NA-C1A  | -3.37 | 105.14      | 106.68   |
| 11  | cB    | 825 | CLA  | C3B-C4B-NB  | 3.37  | 113.54      | 110.53   |
| 11  | aA    | 825 | CLA  | C3C-C4C-NC  | 3.37  | 114.74      | 110.43   |
| 11  | aA    | 833 | CLA  | C3C-C4C-NC  | 3.37  | 114.74      | 110.43   |
| 11  | bB    | 818 | CLA  | C4B-C3B-C2B | -3.37 | 103.12      | 107.30   |
| 11  | aB    | 825 | CLA  | C3B-C4B-NB  | 3.37  | 113.53      | 110.53   |
| 11  | cA    | 807 | CLA  | C3B-C4B-NB  | 3.37  | 113.53      | 110.53   |
| 11  | cA    | 823 | CLA  | C3B-C4B-NB  | 3.37  | 113.53      | 110.53   |
| 11  | cB    | 815 | CLA  | CMC-C2C-C1C | 3.36  | 130.29      | 125.03   |
| 11  | aB    | 825 | CLA  | CAA-C2A-C3A | -3.36 | 103.91      | 113.00   |
| 11  | bB    | 826 | CLA  | CHD-C1D-ND  | -3.36 | 120.07      | 124.80   |
| 11  | cA    | 833 | CLA  | C3C-C4C-NC  | 3.36  | 114.74      | 110.43   |
| 11  | aB    | 834 | CLA  | C4A-NA-C1A  | -3.36 | 105.14      | 106.68   |
| 11  | cA    | 825 | CLA  | C4A-NA-C1A  | -3.36 | 105.14      | 106.68   |
| 12  | cB    | 824 | F6C  | CHC-C1C-C2C | -3.36 | 117.67      | 127.43   |
| 11  | cA    | 831 | CLA  | CHC-C1C-C2C | -3.36 | 117.39      | 126.95   |
| 11  | bB    | 832 | CLA  | C3C-C4C-NC  | 3.36  | 114.73      | 110.43   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aA    | 831 | CLA  | CHC-C1C-C2C | -3.36 | 117.40      | 126.95   |
| 11  | bB    | 802 | CLA  | C1C-C2C-C3C | -3.36 | 103.45      | 106.98   |
| 11  | aA    | 834 | CLA  | CAA-C2A-C3A | -3.36 | 103.92      | 113.00   |
| 11  | cA    | 817 | CLA  | CHC-C1C-C2C | -3.36 | 117.40      | 126.95   |
| 11  | bB    | 825 | CLA  | C4A-NA-C1A  | -3.36 | 105.15      | 106.68   |
| 12  | bB    | 824 | F6C  | C4C-CHD-C1D | -3.36 | 118.35      | 126.25   |
| 11  | aA    | 819 | CLA  | C1-C2-C3    | -3.36 | 120.70      | 126.20   |
| 11  | aB    | 821 | CLA  | C4A-NA-C1A  | -3.36 | 105.15      | 106.68   |
| 11  | bA    | 809 | CLA  | C3B-C4B-NB  | 3.36  | 113.53      | 110.53   |
| 11  | bA    | 834 | CLA  | CAA-C2A-C3A | -3.35 | 103.93      | 113.00   |
| 11  | cA    | 812 | CLA  | C1C-C2C-C3C | -3.35 | 103.45      | 106.98   |
| 11  | cA    | 831 | CLA  | CHD-C1D-ND  | -3.35 | 120.08      | 124.80   |
| 11  | aB    | 805 | CLA  | C3C-C4C-NC  | 3.35  | 114.73      | 110.43   |
| 11  | cB    | 826 | CLA  | CHD-C1D-ND  | -3.35 | 120.08      | 124.80   |
| 11  | bA    | 805 | CLA  | C1C-C2C-C3C | -3.35 | 103.45      | 106.98   |
| 11  | cA    | 819 | CLA  | C1-C2-C3    | -3.35 | 120.70      | 126.20   |
| 11  | aA    | 818 | CLA  | CMC-C2C-C1C | 3.35  | 130.27      | 125.03   |
| 11  | cB    | 836 | CLA  | CHD-C1D-ND  | -3.35 | 120.09      | 124.80   |
| 11  | bB    | 825 | CLA  | CAA-C2A-C3A | -3.35 | 103.94      | 113.00   |
| 11  | cA    | 814 | CLA  | CAC-C3C-C4C | 3.35  | 129.15      | 124.79   |
| 11  | bA    | 817 | CLA  | CHC-C1C-C2C | -3.35 | 117.43      | 126.95   |
| 11  | aB    | 826 | CLA  | CHD-C1D-ND  | -3.35 | 120.09      | 124.80   |
| 11  | aA    | 812 | CLA  | C1C-C2C-C3C | -3.35 | 103.46      | 106.98   |
| 11  | bB    | 836 | CLA  | CHD-C1D-ND  | -3.35 | 120.09      | 124.80   |
| 11  | bB    | 815 | CLA  | CMC-C2C-C1C | 3.35  | 130.26      | 125.03   |
| 11  | bB    | 817 | CLA  | C4A-NA-C1A  | -3.34 | 105.15      | 106.68   |
| 11  | bA    | 814 | CLA  | C1C-C2C-C3C | -3.34 | 103.46      | 106.98   |
| 11  | bA    | 825 | CLA  | C3B-C4B-NB  | 3.34  | 113.52      | 110.53   |
| 11  | cB    | 816 | CLA  | C3C-C4C-NC  | 3.34  | 114.71      | 110.43   |
| 11  | cB    | 826 | CLA  | CAC-C3C-C4C | 3.34  | 129.14      | 124.79   |
| 11  | cB    | 810 | CLA  | C4B-C3B-C2B | -3.34 | 103.15      | 107.30   |
| 11  | cL    | 206 | CLA  | CAA-C2A-C3A | -3.34 | 103.97      | 113.00   |
| 11  | bB    | 803 | CLA  | CHB-C4A-NA  | 3.34  | 129.22      | 124.40   |
| 11  | bB    | 826 | CLA  | C1C-C2C-C3C | -3.34 | 103.47      | 106.98   |
| 11  | cB    | 834 | CLA  | C4A-NA-C1A  | -3.34 | 105.16      | 106.68   |
| 11  | cB    | 840 | CLA  | C4A-NA-C1A  | -3.34 | 105.16      | 106.68   |
| 12  | aB    | 824 | F6C  | C4C-CHD-C1D | -3.34 | 118.39      | 126.25   |
| 11  | aA    | 817 | CLA  | CHC-C1C-C2C | -3.34 | 117.46      | 126.95   |
| 11  | cA    | 825 | CLA  | C3C-C4C-NC  | 3.34  | 114.71      | 110.43   |
| 11  | cB    | 825 | CLA  | CAA-C2A-C3A | -3.34 | 103.98      | 113.00   |
| 11  | aB    | 802 | CLA  | C1C-C2C-C3C | -3.34 | 103.47      | 106.98   |
| 11  | aB    | 804 | CLA  | C1-C2-C3    | -3.34 | 121.36      | 126.76   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cB    | 821 | CLA  | C4A-NA-C1A  | -3.34 | 105.16      | 106.68   |
| 11  | cA    | 809 | CLA  | C3B-C4B-NB  | 3.34  | 113.51      | 110.53   |
| 11  | cB    | 832 | CLA  | C3C-C4C-NC  | 3.34  | 114.70      | 110.43   |
| 11  | aA    | 807 | CLA  | C3B-C4B-NB  | 3.33  | 113.51      | 110.53   |
| 11  | bA    | 808 | CLA  | C1-C2-C3    | -3.33 | 120.73      | 126.20   |
| 11  | bA    | 825 | CLA  | C4A-NA-C1A  | -3.33 | 105.16      | 106.68   |
| 11  | cB    | 814 | CLA  | C4A-NA-C1A  | -3.33 | 105.16      | 106.68   |
| 12  | cB    | 824 | F6C  | C4C-CHD-C1D | -3.33 | 118.41      | 126.25   |
| 11  | cB    | 817 | CLA  | C3C-C4C-NC  | 3.33  | 114.70      | 110.43   |
| 11  | cA    | 821 | CLA  | CAC-C3C-C4C | 3.33  | 129.13      | 124.79   |
| 11  | aB    | 839 | CLA  | C1C-C2C-C3C | -3.33 | 103.47      | 106.98   |
| 11  | aB    | 803 | CLA  | CHB-C4A-NA  | 3.33  | 129.21      | 124.40   |
| 11  | aL    | 206 | CLA  | CAA-C2A-C3A | -3.33 | 104.00      | 113.00   |
| 11  | bA    | 825 | CLA  | C3C-C4C-NC  | 3.33  | 114.70      | 110.43   |
| 11  | cA    | 808 | CLA  | C1-C2-C3    | -3.33 | 120.74      | 126.20   |
| 11  | bA    | 803 | CLA  | C4B-C3B-C2B | -3.33 | 103.16      | 107.30   |
| 11  | cA    | 803 | CLA  | CAA-C2A-C3A | -3.33 | 104.01      | 113.00   |
| 11  | aA    | 803 | CLA  | CAA-C2A-C3A | -3.33 | 104.01      | 113.00   |
| 11  | aA    | 814 | CLA  | C1C-C2C-C3C | -3.33 | 103.48      | 106.98   |
| 11  | cA    | 823 | CLA  | O2D-CGD-O1D | -3.33 | 117.37      | 123.85   |
| 11  | bL    | 206 | CLA  | CAA-C2A-C3A | -3.33 | 104.01      | 113.00   |
| 11  | bA    | 829 | CLA  | C4A-NA-C1A  | -3.33 | 105.16      | 106.68   |
| 11  | bA    | 803 | CLA  | C4C-C3C-C2C | -3.32 | 102.05      | 106.89   |
| 11  | aB    | 815 | CLA  | C1C-C2C-C3C | -3.32 | 103.49      | 106.98   |
| 11  | bA    | 821 | CLA  | CAC-C3C-C4C | 3.32  | 129.11      | 124.79   |
| 11  | cA    | 814 | CLA  | C1C-C2C-C3C | -3.32 | 103.49      | 106.98   |
| 11  | aA    | 808 | CLA  | C1-C2-C3    | -3.32 | 120.76      | 126.20   |
| 11  | bB    | 817 | CLA  | C3C-C4C-NC  | 3.32  | 114.68      | 110.43   |
| 11  | aB    | 817 | CLA  | C3C-C4C-NC  | 3.32  | 114.68      | 110.43   |
| 11  | aB    | 826 | CLA  | C1C-C2C-C3C | -3.32 | 103.49      | 106.98   |
| 11  | bB    | 816 | CLA  | C3C-C4C-NC  | 3.32  | 114.68      | 110.43   |
| 11  | aA    | 821 | CLA  | CAC-C3C-C4C | 3.32  | 129.10      | 124.79   |
| 11  | bB    | 814 | CLA  | CHC-C1C-C2C | -3.31 | 117.53      | 126.95   |
| 12  | aA    | 844 | F6C  | C1C-C2C-C3C | -3.31 | 103.02      | 106.82   |
| 11  | aA    | 805 | CLA  | C1C-C2C-C3C | -3.31 | 103.50      | 106.98   |
| 11  | aA    | 803 | CLA  | C4B-C3B-C2B | -3.31 | 103.19      | 107.30   |
| 11  | cA    | 805 | CLA  | C1C-C2C-C3C | -3.31 | 103.50      | 106.98   |
| 11  | bB    | 828 | CLA  | CHD-C1D-ND  | -3.31 | 120.15      | 124.80   |
| 11  | bA    | 823 | CLA  | O2D-CGD-O1D | -3.31 | 117.41      | 123.85   |
| 11  | cB    | 815 | CLA  | C1C-C2C-C3C | -3.31 | 103.50      | 106.98   |
| 11  | bB    | 815 | CLA  | C1C-C2C-C3C | -3.31 | 103.50      | 106.98   |
| 11  | aB    | 814 | CLA  | CHC-C1C-C2C | -3.31 | 117.56      | 126.95   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aB    | 816 | CLA  | C3C-C4C-NC  | 3.31  | 114.66      | 110.43   |
| 11  | bB    | 839 | CLA  | C1C-C2C-C3C | -3.30 | 103.50      | 106.98   |
| 12  | cA    | 844 | F6C  | C1C-C2C-C3C | -3.30 | 103.03      | 106.82   |
| 11  | aB    | 828 | CLA  | CHD-C1D-ND  | -3.30 | 120.16      | 124.80   |
| 11  | cB    | 820 | CLA  | C3C-C4C-NC  | 3.30  | 114.66      | 110.43   |
| 11  | aB    | 832 | CLA  | C4A-NA-C1A  | -3.30 | 105.17      | 106.68   |
| 11  | cB    | 814 | CLA  | CHC-C1C-C2C | -3.30 | 117.57      | 126.95   |
| 11  | cA    | 825 | CLA  | C3B-C4B-NB  | 3.30  | 113.48      | 110.53   |
| 11  | bA    | 803 | CLA  | CAA-C2A-C3A | -3.30 | 104.08      | 113.00   |
| 11  | cA    | 803 | CLA  | C4B-C3B-C2B | -3.30 | 103.20      | 107.30   |
| 17  | aA    | 853 | LMT  | O3'-C3'-C2' | -3.30 | 102.60      | 110.38   |
| 17  | cA    | 853 | LMT  | O3'-C3'-C2' | -3.30 | 102.60      | 110.38   |
| 11  | cB    | 802 | CLA  | C1C-C2C-C3C | -3.30 | 103.51      | 106.98   |
| 11  | aB    | 820 | CLA  | C3C-C4C-NC  | 3.30  | 114.65      | 110.43   |
| 11  | cB    | 828 | CLA  | C3C-C4C-NC  | 3.30  | 114.65      | 110.43   |
| 11  | cB    | 817 | CLA  | CAA-C2A-C3A | -3.30 | 104.09      | 113.00   |
| 11  | bB    | 825 | CLA  | C4C-C3C-C2C | -3.29 | 102.10      | 106.89   |
| 11  | bB    | 832 | CLA  | C4A-NA-C1A  | -3.29 | 105.18      | 106.68   |
| 11  | bA    | 807 | CLA  | C1-C2-C3    | -3.29 | 120.80      | 126.20   |
| 12  | bA    | 844 | F6C  | C1C-C2C-C3C | -3.29 | 103.05      | 106.82   |
| 11  | cB    | 828 | CLA  | CHD-C1D-ND  | -3.29 | 120.17      | 124.80   |
| 11  | aA    | 828 | CLA  | CHD-C4C-NC  | 3.29  | 129.34      | 124.23   |
| 11  | cB    | 833 | CLA  | C4A-NA-C1A  | -3.29 | 105.18      | 106.68   |
| 11  | cB    | 802 | CLA  | C4C-C3C-C2C | -3.29 | 102.10      | 106.89   |
| 11  | bB    | 808 | CLA  | C4B-C3B-C2B | -3.29 | 103.21      | 107.30   |
| 11  | cB    | 826 | CLA  | C1C-C2C-C3C | -3.29 | 103.52      | 106.98   |
| 11  | aA    | 829 | CLA  | C4A-NA-C1A  | -3.29 | 105.18      | 106.68   |
| 11  | aL    | 204 | CLA  | C4B-C3B-C2B | -3.29 | 103.21      | 107.30   |
| 11  | cB    | 829 | CLA  | C4B-C3B-C2B | -3.29 | 103.21      | 107.30   |
| 17  | bA    | 853 | LMT  | O3'-C3'-C2' | -3.29 | 102.62      | 110.38   |
| 11  | cB    | 803 | CLA  | CHB-C4A-NA  | 3.29  | 129.15      | 124.40   |
| 11  | bA    | 836 | CLA  | C4B-C3B-C2B | -3.29 | 103.21      | 107.30   |
| 11  | bA    | 828 | CLA  | CHD-C4C-NC  | 3.29  | 129.33      | 124.23   |
| 12  | bA    | 832 | F6C  | CHC-C1C-C2C | -3.29 | 117.89      | 127.43   |
| 17  | cA    | 853 | LMT  | C1'-C2'-C3' | 3.29  | 116.92      | 110.01   |
| 17  | bA    | 853 | LMT  | C1'-C2'-C3' | 3.29  | 116.92      | 110.01   |
| 11  | bB    | 807 | CLA  | CAC-C3C-C4C | 3.28  | 129.06      | 124.79   |
| 11  | bB    | 817 | CLA  | CAA-C2A-C3A | -3.28 | 104.13      | 113.00   |
| 12  | cA    | 832 | F6C  | CHC-C1C-C2C | -3.28 | 117.90      | 127.43   |
| 11  | cA    | 803 | CLA  | C4C-C3C-C2C | -3.28 | 102.11      | 106.89   |
| 11  | aA    | 807 | CLA  | C1-C2-C3    | -3.28 | 120.82      | 126.20   |
| 11  | bA    | 839 | CLA  | C3B-C4B-NB  | 3.28  | 113.46      | 110.53   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cB    | 833 | CLA  | C3C-C4C-NC  | 3.28  | 114.63      | 110.43   |
| 11  | bB    | 828 | CLA  | C3C-C4C-NC  | 3.28  | 114.63      | 110.43   |
| 11  | cA    | 807 | CLA  | C4A-NA-C1A  | -3.28 | 105.18      | 106.68   |
| 11  | aB    | 807 | CLA  | CAC-C3C-C4C | 3.28  | 129.06      | 124.79   |
| 11  | aB    | 817 | CLA  | CAA-C2A-C3A | -3.28 | 104.14      | 113.00   |
| 11  | bL    | 204 | CLA  | C4B-C3B-C2B | -3.28 | 103.23      | 107.30   |
| 11  | cL    | 204 | CLA  | C4B-C3B-C2B | -3.28 | 103.23      | 107.30   |
| 11  | cL    | 204 | CLA  | C4A-NA-C1A  | -3.27 | 105.19      | 106.68   |
| 11  | aB    | 833 | CLA  | C3C-C4C-NC  | 3.27  | 114.62      | 110.43   |
| 11  | cB    | 825 | CLA  | C4C-C3C-C2C | -3.27 | 102.13      | 106.89   |
| 11  | aB    | 828 | CLA  | C3C-C4C-NC  | 3.27  | 114.62      | 110.43   |
| 11  | aA    | 841 | CLA  | C4A-NA-C1A  | -3.27 | 105.19      | 106.68   |
| 17  | aA    | 853 | LMT  | C1'-C2'-C3' | 3.27  | 116.89      | 110.01   |
| 12  | aA    | 827 | F6C  | C1C-C2C-C3C | -3.27 | 103.07      | 106.82   |
| 11  | cA    | 831 | CLA  | C4A-NA-C1A  | -3.27 | 105.19      | 106.68   |
| 11  | bA    | 824 | CLA  | C3C-C4C-NC  | 3.27  | 114.62      | 110.43   |
| 11  | cA    | 818 | CLA  | CHD-C1D-ND  | -3.27 | 120.20      | 124.80   |
| 11  | cB    | 817 | CLA  | CHC-C1C-C2C | -3.27 | 117.66      | 126.95   |
| 11  | aA    | 823 | CLA  | O2D-CGD-O1D | -3.27 | 117.48      | 123.85   |
| 12  | cA    | 827 | F6C  | C1C-C2C-C3C | -3.27 | 103.08      | 106.82   |
| 11  | cA    | 836 | CLA  | C4B-C3B-C2B | -3.27 | 103.24      | 107.30   |
| 11  | aA    | 836 | CLA  | C4B-C3B-C2B | -3.27 | 103.24      | 107.30   |
| 11  | aB    | 808 | CLA  | C4B-C3B-C2B | -3.27 | 103.24      | 107.30   |
| 11  | aB    | 829 | CLA  | C4B-C3B-C2B | -3.27 | 103.24      | 107.30   |
| 11  | bB    | 805 | CLA  | CAC-C3C-C4C | 3.26  | 129.04      | 124.79   |
| 11  | aB    | 812 | CLA  | C4C-C3C-C2C | -3.26 | 102.14      | 106.89   |
| 11  | cA    | 807 | CLA  | C1-C2-C3    | -3.26 | 120.85      | 126.20   |
| 11  | bB    | 808 | CLA  | C4A-NA-C1A  | -3.26 | 105.19      | 106.68   |
| 11  | bL    | 204 | CLA  | C4A-NA-C1A  | -3.26 | 105.19      | 106.68   |
| 11  | cB    | 822 | CLA  | C3B-C4B-NB  | 3.26  | 113.44      | 110.53   |
| 11  | bB    | 812 | CLA  | C4C-C3C-C2C | -3.26 | 102.14      | 106.89   |
| 11  | aB    | 820 | CLA  | C3B-C4B-NB  | 3.26  | 113.44      | 110.53   |
| 11  | cA    | 828 | CLA  | CHD-C4C-NC  | 3.26  | 129.29      | 124.23   |
| 11  | aB    | 817 | CLA  | CHC-C1C-C2C | -3.26 | 117.68      | 126.95   |
| 11  | cA    | 808 | CLA  | C4A-NA-C1A  | -3.26 | 105.19      | 106.68   |
| 11  | aB    | 825 | CLA  | C4C-C3C-C2C | -3.26 | 102.14      | 106.89   |
| 11  | aA    | 825 | CLA  | C4A-NA-C1A  | -3.26 | 105.19      | 106.68   |
| 11  | bB    | 829 | CLA  | C4B-C3B-C2B | -3.26 | 103.25      | 107.30   |
| 11  | aB    | 806 | CLA  | O2D-CGD-CBD | 3.26  | 116.93      | 111.23   |
| 11  | bA    | 824 | CLA  | CHC-C1C-C2C | -3.26 | 117.69      | 126.95   |
| 11  | bB    | 817 | CLA  | CHC-C1C-C2C | -3.26 | 117.69      | 126.95   |
| 11  | aA    | 812 | CLA  | CHC-C1C-C2C | -3.26 | 117.69      | 126.95   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bA    | 807 | CLA  | C4A-NA-C1A  | -3.26 | 105.19      | 106.68   |
| 11  | bB    | 833 | CLA  | C3C-C4C-NC  | 3.26  | 114.60      | 110.43   |
| 11  | aA    | 803 | CLA  | C4C-C3C-C2C | -3.26 | 102.15      | 106.89   |
| 11  | bB    | 839 | CLA  | C4C-C3C-C2C | -3.26 | 102.15      | 106.89   |
| 11  | cB    | 808 | CLA  | C4B-C3B-C2B | -3.26 | 103.25      | 107.30   |
| 11  | cB    | 840 | CLA  | CHC-C1C-C2C | -3.26 | 117.69      | 126.95   |
| 11  | cA    | 812 | CLA  | CAC-C3C-C4C | 3.26  | 129.03      | 124.79   |
| 12  | cA    | 826 | F6C  | C1-C2-C3    | -3.26 | 120.86      | 126.20   |
| 12  | aA    | 832 | F6C  | CHC-C1C-C2C | -3.26 | 117.98      | 127.43   |
| 11  | bB    | 840 | CLA  | CHC-C1C-C2C | -3.26 | 117.70      | 126.95   |
| 11  | bB    | 820 | CLA  | C3C-C4C-NC  | 3.26  | 114.60      | 110.43   |
| 11  | aA    | 812 | CLA  | CAC-C3C-C4C | 3.25  | 129.02      | 124.79   |
| 11  | aB    | 840 | CLA  | CHC-C1C-C2C | -3.25 | 117.70      | 126.95   |
| 11  | cA    | 824 | CLA  | C3C-C4C-NC  | 3.25  | 114.60      | 110.43   |
| 11  | bB    | 840 | CLA  | C4A-NA-C1A  | -3.25 | 105.19      | 106.68   |
| 12  | bA    | 826 | F6C  | C1-C2-C3    | -3.25 | 120.87      | 126.20   |
| 11  | cB    | 806 | CLA  | O2D-CGD-CBD | 3.25  | 116.91      | 111.23   |
| 11  | cA    | 812 | CLA  | CHC-C1C-C2C | -3.25 | 117.71      | 126.95   |
| 11  | cA    | 824 | CLA  | CHC-C1C-C2C | -3.25 | 117.71      | 126.95   |
| 11  | cB    | 805 | CLA  | CAC-C3C-C4C | 3.25  | 129.02      | 124.79   |
| 11  | bA    | 812 | CLA  | CHC-C1C-C2C | -3.25 | 117.71      | 126.95   |
| 11  | cB    | 801 | CLA  | C1C-C2C-C3C | -3.25 | 103.56      | 106.98   |
| 15  | cB    | 845 | BCR  | C15-C16-C17 | -3.25 | 116.87      | 123.52   |
| 11  | cB    | 808 | CLA  | C4C-C3C-C2C | -3.25 | 102.16      | 106.89   |
| 11  | cA    | 841 | CLA  | C4A-NA-C1A  | -3.25 | 105.20      | 106.68   |
| 11  | cA    | 825 | CLA  | CHC-C1C-C2C | -3.25 | 117.72      | 126.95   |
| 11  | cB    | 807 | CLA  | CAC-C3C-C4C | 3.25  | 129.01      | 124.79   |
| 11  | cA    | 823 | CLA  | CHD-C4C-NC  | 3.25  | 129.26      | 124.23   |
| 11  | cB    | 832 | CLA  | C4A-NA-C1A  | -3.25 | 105.20      | 106.68   |
| 12  | aA    | 826 | F6C  | C1-C2-C3    | -3.25 | 120.88      | 126.20   |
| 11  | cB    | 831 | CLA  | C3B-C4B-NB  | 3.25  | 113.43      | 110.53   |
| 11  | aB    | 802 | CLA  | C4C-C3C-C2C | -3.24 | 102.17      | 106.89   |
| 11  | aA    | 824 | CLA  | CHC-C1C-C2C | -3.24 | 117.73      | 126.95   |
| 12  | bA    | 827 | F6C  | C1C-C2C-C3C | -3.24 | 103.10      | 106.82   |
| 11  | bB    | 802 | CLA  | C4C-C3C-C2C | -3.24 | 102.17      | 106.89   |
| 11  | cB    | 820 | CLA  | C3B-C4B-NB  | 3.24  | 113.43      | 110.53   |
| 15  | aB    | 845 | BCR  | C15-C16-C17 | -3.24 | 116.88      | 123.52   |
| 11  | cB    | 816 | CLA  | C1-C2-C3    | -3.24 | 120.88      | 126.20   |
| 11  | aA    | 806 | CLA  | CHC-C1C-C2C | -3.24 | 117.73      | 126.95   |
| 12  | bL    | 202 | F6C  | CHD-C1D-ND  | -3.24 | 119.43      | 124.31   |
| 11  | cB    | 812 | CLA  | C1C-C2C-C3C | -3.24 | 103.57      | 106.98   |
| 11  | cB    | 817 | CLA  | C4A-NA-C1A  | -3.24 | 105.20      | 106.68   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bA    | 825 | CLA  | CHC-C1C-C2C | -3.24 | 117.74      | 126.95   |
| 15  | bB    | 845 | BCR  | C15-C16-C17 | -3.24 | 116.89      | 123.52   |
| 11  | aA    | 825 | CLA  | CHC-C1C-C2C | -3.24 | 117.74      | 126.95   |
| 11  | aB    | 840 | CLA  | C4A-NA-C1A  | -3.24 | 105.20      | 106.68   |
| 11  | bB    | 801 | CLA  | C1C-C2C-C3C | -3.24 | 103.57      | 106.98   |
| 11  | bB    | 805 | CLA  | C4B-C3B-C2B | -3.24 | 103.28      | 107.30   |
| 11  | bB    | 806 | CLA  | CHD-C4C-NC  | 3.24  | 129.25      | 124.23   |
| 11  | aB    | 808 | CLA  | C4A-NA-C1A  | -3.24 | 105.20      | 106.68   |
| 12  | aL    | 202 | F6C  | CHD-C1D-ND  | -3.24 | 119.44      | 124.31   |
| 11  | bA    | 818 | CLA  | CHD-C1D-ND  | -3.24 | 120.25      | 124.80   |
| 11  | bB    | 826 | CLA  | C4B-C3B-C2B | -3.24 | 103.28      | 107.30   |
| 11  | aA    | 818 | CLA  | CHD-C1D-ND  | -3.24 | 120.25      | 124.80   |
| 11  | aA    | 811 | CLA  | C4B-C3B-C2B | -3.24 | 103.28      | 107.30   |
| 11  | bB    | 806 | CLA  | O2D-CGD-CBD | 3.24  | 116.89      | 111.23   |
| 11  | aA    | 824 | CLA  | C3C-C4C-NC  | 3.24  | 114.58      | 110.43   |
| 12  | cL    | 202 | F6C  | CHD-C1D-ND  | -3.24 | 119.44      | 124.31   |
| 11  | cB    | 804 | CLA  | C3B-C4B-NB  | 3.24  | 113.42      | 110.53   |
| 11  | aB    | 801 | CLA  | C1C-C2C-C3C | -3.23 | 103.58      | 106.98   |
| 11  | bB    | 816 | CLA  | C1-C2-C3    | -3.23 | 120.90      | 126.20   |
| 11  | bB    | 820 | CLA  | C3B-C4B-NB  | 3.23  | 113.42      | 110.53   |
| 11  | bK    | 103 | CLA  | C3B-C4B-NB  | 3.23  | 113.42      | 110.53   |
| 11  | bA    | 806 | CLA  | CHC-C1C-C2C | -3.23 | 117.76      | 126.95   |
| 11  | cA    | 806 | CLA  | CHC-C1C-C2C | -3.23 | 117.76      | 126.95   |
| 11  | aB    | 812 | CLA  | C1C-C2C-C3C | -3.23 | 103.58      | 106.98   |
| 11  | bB    | 812 | CLA  | C1C-C2C-C3C | -3.23 | 103.58      | 106.98   |
| 11  | bA    | 812 | CLA  | CAC-C3C-C4C | 3.23  | 129.00      | 124.79   |
| 11  | bB    | 808 | CLA  | C4C-C3C-C2C | -3.23 | 102.19      | 106.89   |
| 11  | cK    | 103 | CLA  | C4A-NA-C1A  | -3.23 | 105.20      | 106.68   |
| 11  | bB    | 802 | CLA  | CAC-C3C-C4C | 3.23  | 128.99      | 124.79   |
| 11  | cB    | 822 | CLA  | CAA-C2A-C3A | -3.23 | 104.27      | 113.00   |
| 11  | bA    | 823 | CLA  | CHD-C4C-NC  | 3.23  | 129.24      | 124.23   |
| 11  | bA    | 811 | CLA  | C4B-C3B-C2B | -3.23 | 103.29      | 107.30   |
| 11  | cA    | 843 | CLA  | C4B-C3B-C2B | -3.23 | 103.29      | 107.30   |
| 11  | aB    | 808 | CLA  | C4C-C3C-C2C | -3.23 | 102.19      | 106.89   |
| 11  | cA    | 819 | CLA  | C4C-C3C-C2C | -3.23 | 102.19      | 106.89   |
| 11  | aA    | 810 | CLA  | CHD-C1D-ND  | -3.23 | 120.26      | 124.80   |
| 11  | aB    | 839 | CLA  | C4C-C3C-C2C | -3.23 | 102.20      | 106.89   |
| 11  | bB    | 822 | CLA  | CAA-C2A-C3A | -3.23 | 104.28      | 113.00   |
| 11  | bA    | 819 | CLA  | C4C-C3C-C2C | -3.22 | 102.20      | 106.89   |
| 11  | cB    | 801 | CLA  | C4C-C3C-C2C | -3.22 | 102.20      | 106.89   |
| 12  | bB    | 824 | F6C  | C1-C2-C3    | -3.22 | 120.92      | 126.20   |
| 11  | cB    | 826 | CLA  | C4B-C3B-C2B | -3.22 | 103.30      | 107.30   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aB    | 802 | CLA  | CAC-C3C-C4C | 3.22  | 128.98      | 124.79   |
| 11  | aA    | 819 | CLA  | C4C-C3C-C2C | -3.22 | 102.20      | 106.89   |
| 11  | cB    | 812 | CLA  | C4C-C3C-C2C | -3.22 | 102.20      | 106.89   |
| 12  | cB    | 824 | F6C  | C1-C2-C3    | -3.22 | 120.92      | 126.20   |
| 11  | aA    | 823 | CLA  | CHD-C4C-NC  | 3.22  | 129.22      | 124.23   |
| 11  | aA    | 838 | CLA  | C4B-C3B-C2B | -3.22 | 103.30      | 107.30   |
| 11  | cA    | 829 | CLA  | C4A-NA-C1A  | -3.22 | 105.21      | 106.68   |
| 11  | bB    | 821 | CLA  | C3B-C4B-NB  | 3.22  | 113.40      | 110.53   |
| 11  | aB    | 822 | CLA  | CAA-C2A-C3A | -3.22 | 104.30      | 113.00   |
| 11  | aB    | 816 | CLA  | C1-C2-C3    | -3.22 | 120.92      | 126.20   |
| 11  | cA    | 833 | CLA  | CAA-C2A-C3A | -3.22 | 104.30      | 113.00   |
| 11  | cB    | 817 | CLA  | O2A-CGA-CBA | 3.22  | 121.64      | 111.83   |
| 11  | aB    | 826 | CLA  | C4B-C3B-C2B | -3.22 | 103.30      | 107.30   |
| 11  | aB    | 822 | CLA  | C3B-C4B-NB  | 3.22  | 113.40      | 110.53   |
| 11  | bB    | 831 | CLA  | C3B-C4B-NB  | 3.22  | 113.40      | 110.53   |
| 11  | cB    | 810 | CLA  | CAA-C2A-C3A | -3.22 | 104.31      | 113.00   |
| 11  | cB    | 802 | CLA  | CAC-C3C-C4C | 3.22  | 128.97      | 124.79   |
| 11  | cB    | 825 | CLA  | C4A-NA-C1A  | -3.22 | 105.21      | 106.68   |
| 11  | aB    | 831 | CLA  | C3B-C4B-NB  | 3.21  | 113.40      | 110.53   |
| 11  | aA    | 818 | CLA  | C4C-C3C-C2C | -3.21 | 102.21      | 106.89   |
| 11  | bB    | 801 | CLA  | C4C-C3C-C2C | -3.21 | 102.21      | 106.89   |
| 11  | aA    | 843 | CLA  | C4B-C3B-C2B | -3.21 | 103.31      | 107.30   |
| 11  | cA    | 838 | CLA  | C4B-C3B-C2B | -3.21 | 103.31      | 107.30   |
| 11  | bB    | 822 | CLA  | C3B-C4B-NB  | 3.21  | 113.40      | 110.53   |
| 11  | aB    | 813 | CLA  | C4B-C3B-C2B | -3.21 | 103.31      | 107.30   |
| 11  | aB    | 805 | CLA  | C4B-C3B-C2B | -3.21 | 103.31      | 107.30   |
| 11  | aA    | 818 | CLA  | CAC-C3C-C4C | 3.21  | 128.97      | 124.79   |
| 11  | bA    | 843 | CLA  | C4B-C3B-C2B | -3.21 | 103.31      | 107.30   |
| 11  | bB    | 817 | CLA  | O2A-CGA-CBA | 3.21  | 121.62      | 111.83   |
| 11  | cA    | 840 | CLA  | CBA-CAA-C2A | 3.21  | 123.34      | 113.79   |
| 11  | aA    | 807 | CLA  | C4A-NA-C1A  | -3.21 | 105.22      | 106.68   |
| 11  | bA    | 831 | CLA  | C1-C2-C3    | -3.21 | 120.94      | 126.20   |
| 11  | aB    | 801 | CLA  | C4C-C3C-C2C | -3.21 | 102.22      | 106.89   |
| 11  | aB    | 806 | CLA  | CHD-C4C-NC  | 3.21  | 129.21      | 124.23   |
| 11  | aB    | 817 | CLA  | O2A-CGA-CBA | 3.21  | 121.61      | 111.83   |
| 11  | aA    | 808 | CLA  | C4A-NA-C1A  | -3.21 | 105.22      | 106.68   |
| 11  | cB    | 808 | CLA  | C4A-NA-C1A  | -3.21 | 105.22      | 106.68   |
| 15  | cA    | 851 | BCR  | C15-C16-C17 | -3.21 | 116.96      | 123.52   |
| 11  | aA    | 833 | CLA  | CAA-C2A-C3A | -3.21 | 104.34      | 113.00   |
| 11  | cB    | 821 | CLA  | C3B-C4B-NB  | 3.20  | 113.39      | 110.53   |
| 11  | aB    | 835 | CLA  | CHC-C1C-C2C | -3.20 | 117.84      | 126.95   |
| 15  | bA    | 851 | BCR  | C15-C16-C17 | -3.20 | 116.96      | 123.52   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aA    | 831 | CLA  | C1-C2-C3    | -3.20 | 120.95      | 126.20   |
| 12  | aB    | 824 | F6C  | C1-C2-C3    | -3.20 | 120.95      | 126.20   |
| 11  | aA    | 840 | CLA  | CBA-CAA-C2A | 3.20  | 123.32      | 113.79   |
| 11  | aB    | 821 | CLA  | C3B-C4B-NB  | 3.20  | 113.39      | 110.53   |
| 11  | aA    | 824 | CLA  | C4B-C3B-C2B | -3.20 | 103.32      | 107.30   |
| 11  | bB    | 811 | CLA  | C4C-C3C-C2C | -3.20 | 102.23      | 106.89   |
| 11  | cA    | 831 | CLA  | C1-C2-C3    | -3.20 | 120.95      | 126.20   |
| 11  | cB    | 839 | CLA  | C4C-C3C-C2C | -3.20 | 102.23      | 106.89   |
| 11  | aB    | 809 | CLA  | CHC-C1C-C2C | -3.20 | 117.85      | 126.95   |
| 11  | bB    | 810 | CLA  | CAA-C2A-C3A | -3.20 | 104.35      | 113.00   |
| 12  | cA    | 826 | F6C  | CHD-C4C-NC  | 3.20  | 128.85      | 124.05   |
| 11  | cB    | 806 | CLA  | CHD-C4C-NC  | 3.20  | 129.19      | 124.23   |
| 11  | bB    | 835 | CLA  | CHC-C1C-C2C | -3.20 | 117.86      | 126.95   |
| 11  | bB    | 809 | CLA  | CHC-C1C-C2C | -3.20 | 117.86      | 126.95   |
| 11  | bA    | 833 | CLA  | CAA-C2A-C3A | -3.20 | 104.36      | 113.00   |
| 11  | cB    | 838 | CLA  | CAA-C2A-C3A | -3.20 | 104.36      | 113.00   |
| 11  | aA    | 821 | CLA  | CHC-C1C-C2C | -3.20 | 117.86      | 126.95   |
| 11  | cB    | 835 | CLA  | CHC-C1C-C2C | -3.20 | 117.86      | 126.95   |
| 11  | bA    | 840 | CLA  | CBA-CAA-C2A | 3.19  | 123.30      | 113.79   |
| 11  | aB    | 811 | CLA  | C4C-C3C-C2C | -3.19 | 102.24      | 106.89   |
| 11  | aB    | 838 | CLA  | C3B-C4B-NB  | 3.19  | 113.38      | 110.53   |
| 11  | aA    | 836 | CLA  | CHC-C1C-C2C | -3.19 | 117.87      | 126.95   |
| 11  | cB    | 818 | CLA  | CAC-C3C-C4C | 3.19  | 128.95      | 124.79   |
| 11  | aB    | 810 | CLA  | CAA-C2A-C3A | -3.19 | 104.37      | 113.00   |
| 11  | cB    | 814 | CLA  | CAC-C3C-C4C | 3.19  | 128.94      | 124.79   |
| 11  | bA    | 810 | CLA  | CHD-C1D-ND  | -3.19 | 120.31      | 124.80   |
| 11  | bA    | 821 | CLA  | CHC-C1C-C2C | -3.19 | 117.88      | 126.95   |
| 11  | cB    | 809 | CLA  | CHC-C1C-C2C | -3.19 | 117.88      | 126.95   |
| 11  | bB    | 838 | CLA  | C3B-C4B-NB  | 3.19  | 113.38      | 110.53   |
| 11  | bA    | 818 | CLA  | C4C-C3C-C2C | -3.19 | 102.25      | 106.89   |
| 15  | aA    | 851 | BCR  | C15-C16-C17 | -3.19 | 116.99      | 123.52   |
| 11  | aK    | 103 | CLA  | C3B-C4B-NB  | 3.19  | 113.38      | 110.53   |
| 11  | cK    | 103 | CLA  | C3B-C4B-NB  | 3.19  | 113.38      | 110.53   |
| 11  | cA    | 821 | CLA  | CHC-C1C-C2C | -3.19 | 117.88      | 126.95   |
| 11  | cA    | 807 | CLA  | CHD-C4C-NC  | 3.19  | 129.18      | 124.23   |
| 11  | bB    | 804 | CLA  | C3B-C4B-NB  | 3.19  | 113.38      | 110.53   |
| 11  | cB    | 827 | CLA  | C4C-C3C-C2C | -3.19 | 102.25      | 106.89   |
| 11  | bA    | 810 | CLA  | CAC-C3C-C4C | 3.19  | 128.94      | 124.79   |
| 11  | cA    | 811 | CLA  | C4B-C3B-C2B | -3.19 | 103.34      | 107.30   |
| 11  | cA    | 839 | CLA  | C3B-C4B-NB  | 3.19  | 113.38      | 110.53   |
| 11  | bA    | 824 | CLA  | C4B-C3B-C2B | -3.19 | 103.34      | 107.30   |
| 11  | cA    | 818 | CLA  | C4C-C3C-C2C | -3.19 | 102.25      | 106.89   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cA    | 836 | CLA  | CHC-C1C-C2C | -3.19 | 117.90      | 126.95   |
| 11  | bK    | 103 | CLA  | C4A-NA-C1A  | -3.18 | 105.23      | 106.68   |
| 11  | aB    | 818 | CLA  | CAC-C3C-C4C | 3.18  | 128.93      | 124.79   |
| 11  | cA    | 820 | CLA  | C3C-C4C-NC  | 3.18  | 114.51      | 110.43   |
| 11  | bB    | 814 | CLA  | CAC-C3C-C4C | 3.18  | 128.93      | 124.79   |
| 11  | bB    | 832 | CLA  | CAC-C3C-C4C | 3.18  | 128.93      | 124.79   |
| 11  | aB    | 810 | CLA  | CHC-C1C-C2C | -3.18 | 117.90      | 126.95   |
| 11  | aA    | 831 | CLA  | C4A-NA-C1A  | -3.18 | 105.23      | 106.68   |
| 11  | cA    | 816 | CLA  | C4C-C3C-C2C | -3.18 | 102.26      | 106.89   |
| 11  | bB    | 833 | CLA  | CMA-C3A-C2A | -3.18 | 101.68      | 113.98   |
| 11  | cB    | 810 | CLA  | CHC-C1C-C2C | -3.18 | 117.91      | 126.95   |
| 12  | bA    | 832 | F6C  | C1-C2-C3    | -3.18 | 121.61      | 126.76   |
| 11  | aB    | 833 | CLA  | CMA-C3A-C2A | -3.18 | 101.69      | 113.98   |
| 11  | aB    | 825 | CLA  | C4A-NA-C1A  | -3.18 | 105.23      | 106.68   |
| 11  | aB    | 814 | CLA  | CAC-C3C-C4C | 3.18  | 128.93      | 124.79   |
| 11  | bA    | 838 | CLA  | C4B-C3B-C2B | -3.18 | 103.35      | 107.30   |
| 11  | cB    | 805 | CLA  | C4B-C3B-C2B | -3.18 | 103.35      | 107.30   |
| 11  | cA    | 810 | CLA  | CAC-C3C-C4C | 3.18  | 128.93      | 124.79   |
| 11  | bB    | 813 | CLA  | C4B-C3B-C2B | -3.18 | 103.35      | 107.30   |
| 11  | bA    | 841 | CLA  | C4A-NA-C1A  | -3.18 | 105.23      | 106.68   |
| 11  | aB    | 838 | CLA  | CAA-C2A-C3A | -3.18 | 104.41      | 113.00   |
| 11  | bA    | 836 | CLA  | CHC-C1C-C2C | -3.18 | 117.92      | 126.95   |
| 11  | aB    | 805 | CLA  | CAC-C3C-C4C | 3.18  | 128.92      | 124.79   |
| 11  | aB    | 816 | CLA  | CAA-C2A-C3A | -3.18 | 104.42      | 113.00   |
| 11  | bA    | 839 | CLA  | C4B-C3B-C2B | -3.18 | 103.35      | 107.30   |
| 11  | bB    | 809 | CLA  | C4C-C3C-C2C | -3.18 | 102.27      | 106.89   |
| 11  | bB    | 838 | CLA  | CAA-C2A-C3A | -3.17 | 104.42      | 113.00   |
| 11  | bB    | 827 | CLA  | C4C-C3C-C2C | -3.17 | 102.27      | 106.89   |
| 11  | cB    | 804 | CLA  | CAA-C2A-C3A | -3.17 | 104.42      | 113.00   |
| 11  | aA    | 810 | CLA  | CAC-C3C-C4C | 3.17  | 128.92      | 124.79   |
| 11  | aA    | 824 | CLA  | CBC-CAC-C3C | -3.17 | 103.82      | 112.42   |
| 11  | bB    | 816 | CLA  | CAA-C2A-C3A | -3.17 | 104.42      | 113.00   |
| 11  | cB    | 833 | CLA  | CMA-C3A-C2A | -3.17 | 101.72      | 113.98   |
| 11  | aB    | 804 | CLA  | C3B-C4B-NB  | 3.17  | 113.36      | 110.53   |
| 11  | bB    | 810 | CLA  | CHC-C1C-C2C | -3.17 | 117.93      | 126.95   |
| 11  | bA    | 831 | CLA  | C4A-NA-C1A  | -3.17 | 105.23      | 106.68   |
| 11  | bB    | 830 | CLA  | C3B-C4B-NB  | 3.17  | 113.36      | 110.53   |
| 11  | cB    | 809 | CLA  | C4C-C3C-C2C | -3.17 | 102.28      | 106.89   |
| 11  | cA    | 824 | CLA  | C4B-C3B-C2B | -3.17 | 103.36      | 107.30   |
| 11  | aB    | 804 | CLA  | CAA-C2A-C3A | -3.17 | 104.44      | 113.00   |
| 11  | cA    | 843 | CLA  | C3B-C4B-NB  | 3.17  | 113.36      | 110.53   |
| 11  | cB    | 838 | CLA  | C3B-C4B-NB  | 3.17  | 113.36      | 110.53   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bA    | 807 | CLA  | CHD-C4C-NC  | 3.17  | 129.14      | 124.23   |
| 11  | aB    | 810 | CLA  | CMA-C3A-C2A | -3.17 | 101.73      | 113.98   |
| 11  | cA    | 818 | CLA  | CAC-C3C-C4C | 3.17  | 128.91      | 124.79   |
| 11  | cA    | 810 | CLA  | CHD-C1D-ND  | -3.17 | 120.34      | 124.80   |
| 12  | cA    | 832 | F6C  | C1-C2-C3    | -3.17 | 121.64      | 126.76   |
| 11  | aB    | 827 | CLA  | C4C-C3C-C2C | -3.17 | 102.28      | 106.89   |
| 11  | bB    | 804 | CLA  | CAA-C2A-C3A | -3.17 | 104.44      | 113.00   |
| 11  | bA    | 821 | CLA  | C4B-C3B-C2B | -3.17 | 103.36      | 107.30   |
| 11  | cB    | 811 | CLA  | C4C-C3C-C2C | -3.17 | 102.28      | 106.89   |
| 11  | bA    | 824 | CLA  | CBC-CAC-C3C | -3.17 | 103.84      | 112.42   |
| 11  | aL    | 206 | CLA  | CMB-C2B-C1B | 3.17  | 130.24      | 125.42   |
| 11  | bB    | 817 | CLA  | C4B-C3B-C2B | -3.17 | 103.36      | 107.30   |
| 11  | cB    | 813 | CLA  | C4B-C3B-C2B | -3.17 | 103.36      | 107.30   |
| 12  | aA    | 826 | F6C  | CHD-C4C-NC  | 3.17  | 128.80      | 124.05   |
| 11  | cA    | 835 | CLA  | CAA-C2A-C3A | -3.16 | 104.45      | 113.00   |
| 11  | bA    | 816 | CLA  | C4C-C3C-C2C | -3.16 | 102.29      | 106.89   |
| 11  | cA    | 839 | CLA  | C4B-C3B-C2B | -3.16 | 103.37      | 107.30   |
| 11  | aA    | 829 | CLA  | CAC-C3C-C4C | 3.16  | 128.91      | 124.79   |
| 11  | cB    | 810 | CLA  | CMA-C3A-C2A | -3.16 | 101.75      | 113.98   |
| 11  | aK    | 103 | CLA  | C4A-NA-C1A  | -3.16 | 105.24      | 106.68   |
| 11  | bB    | 821 | CLA  | O2D-CGD-O1D | -3.16 | 117.69      | 123.85   |
| 11  | cA    | 843 | CLA  | C4C-C3C-C2C | -3.16 | 102.29      | 106.89   |
| 11  | aA    | 835 | CLA  | CAA-C2A-C3A | -3.16 | 104.45      | 113.00   |
| 11  | aB    | 809 | CLA  | C4C-C3C-C2C | -3.16 | 102.29      | 106.89   |
| 12  | aA    | 826 | F6C  | CHD-C1D-ND  | -3.16 | 119.55      | 124.31   |
| 11  | bA    | 829 | CLA  | CAC-C3C-C4C | 3.16  | 128.90      | 124.79   |
| 11  | cA    | 819 | CLA  | CAC-C3C-C4C | 3.16  | 128.90      | 124.79   |
| 11  | aA    | 816 | CLA  | C4C-C3C-C2C | -3.16 | 102.29      | 106.89   |
| 11  | bA    | 835 | CLA  | CAA-C2A-C3A | -3.16 | 104.46      | 113.00   |
| 11  | bB    | 835 | CLA  | CMB-C2B-C1B | 3.16  | 130.23      | 125.42   |
| 11  | bB    | 830 | CLA  | CHC-C1C-C2C | -3.16 | 117.98      | 126.95   |
| 11  | aA    | 843 | CLA  | C4C-C3C-C2C | -3.16 | 102.30      | 106.89   |
| 11  | bA    | 819 | CLA  | CHD-C4C-NC  | 3.15  | 129.12      | 124.23   |
| 12  | bA    | 826 | F6C  | CHD-C1D-ND  | -3.15 | 119.56      | 124.31   |
| 11  | bB    | 818 | CLA  | CAC-C3C-C4C | 3.15  | 128.89      | 124.79   |
| 11  | cA    | 824 | CLA  | CBC-CAC-C3C | -3.15 | 103.87      | 112.42   |
| 11  | bA    | 822 | CLA  | C4B-C3B-C2B | -3.15 | 103.38      | 107.30   |
| 11  | cB    | 816 | CLA  | CAA-C2A-C3A | -3.15 | 104.48      | 113.00   |
| 11  | aB    | 817 | CLA  | C4B-C3B-C2B | -3.15 | 103.38      | 107.30   |
| 11  | bA    | 820 | CLA  | C3C-C4C-NC  | 3.15  | 114.47      | 110.43   |
| 11  | aA    | 802 | CLA  | CHC-C1C-C2C | -3.15 | 117.99      | 126.95   |
| 11  | bA    | 843 | CLA  | C4C-C3C-C2C | -3.15 | 102.30      | 106.89   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bB    | 810 | CLA  | CMA-C3A-C2A | -3.15 | 101.80      | 113.98   |
| 11  | aA    | 839 | CLA  | C3B-C4B-NB  | 3.15  | 113.34      | 110.53   |
| 11  | bA    | 802 | CLA  | CHC-C1C-C2C | -3.15 | 117.99      | 126.95   |
| 12  | aA    | 832 | F6C  | C1-C2-C3    | -3.15 | 121.66      | 126.76   |
| 13  | cA    | 845 | PQN  | C14-C13-C15 | 3.15  | 120.70      | 115.23   |
| 11  | aB    | 835 | CLA  | CMB-C2B-C1B | 3.15  | 130.22      | 125.42   |
| 11  | aB    | 832 | CLA  | CAC-C3C-C4C | 3.15  | 128.89      | 124.79   |
| 13  | aA    | 845 | PQN  | C14-C13-C15 | 3.15  | 120.69      | 115.23   |
| 12  | cL    | 202 | F6C  | CHA-C1A-C2A | -3.15 | 121.94      | 130.41   |
| 11  | cA    | 802 | CLA  | CHC-C1C-C2C | -3.15 | 118.00      | 126.95   |
| 12  | aA    | 827 | F6C  | CHD-C4C-NC  | 3.15  | 128.77      | 124.05   |
| 11  | bB    | 804 | CLA  | C4C-C3C-C2C | -3.15 | 102.31      | 106.89   |
| 11  | cB    | 821 | CLA  | O2D-CGD-O1D | -3.15 | 117.72      | 123.85   |
| 11  | bA    | 835 | CLA  | CMB-C2B-C1B | 3.15  | 130.21      | 125.42   |
| 11  | bA    | 843 | CLA  | C3B-C4B-NB  | 3.15  | 113.34      | 110.53   |
| 11  | cA    | 822 | CLA  | C4B-C3B-C2B | -3.15 | 103.39      | 107.30   |
| 11  | bB    | 821 | CLA  | CHC-C1C-C2C | -3.15 | 118.01      | 126.95   |
| 12  | bL    | 202 | F6C  | CHA-C1A-C2A | -3.14 | 121.95      | 130.41   |
| 12  | aL    | 202 | F6C  | CHA-C1A-C2A | -3.14 | 121.95      | 130.41   |
| 11  | aA    | 821 | CLA  | C4B-C3B-C2B | -3.14 | 103.39      | 107.30   |
| 11  | aA    | 839 | CLA  | C4B-C3B-C2B | -3.14 | 103.39      | 107.30   |
| 10  | bA    | 801 | CL0  | C1-C2-C3    | -3.14 | 121.05      | 126.20   |
| 11  | aA    | 820 | CLA  | C3C-C4C-NC  | 3.14  | 114.46      | 110.43   |
| 11  | cA    | 829 | CLA  | CAC-C3C-C4C | 3.14  | 128.88      | 124.79   |
| 11  | aA    | 807 | CLA  | CHD-C4C-NC  | 3.14  | 129.10      | 124.23   |
| 11  | aB    | 821 | CLA  | O2D-CGD-O1D | -3.14 | 117.73      | 123.85   |
| 11  | bB    | 820 | CLA  | CHD-C4C-NC  | 3.14  | 129.10      | 124.23   |
| 11  | cA    | 819 | CLA  | CHD-C4C-NC  | 3.14  | 129.10      | 124.23   |
| 11  | cA    | 835 | CLA  | CMB-C2B-C1B | 3.14  | 130.20      | 125.42   |
| 11  | cL    | 206 | CLA  | CMB-C2B-C1B | 3.14  | 130.20      | 125.42   |
| 12  | cA    | 826 | F6C  | CHD-C1D-ND  | -3.14 | 119.58      | 124.31   |
| 11  | aA    | 836 | CLA  | CHD-C1D-ND  | -3.14 | 120.38      | 124.80   |
| 11  | aA    | 835 | CLA  | CMB-C2B-C1B | 3.14  | 130.20      | 125.42   |
| 11  | aA    | 819 | CLA  | CHD-C4C-NC  | 3.14  | 129.10      | 124.23   |
| 11  | aB    | 821 | CLA  | CHC-C1C-C2C | -3.14 | 118.02      | 126.95   |
| 15  | cB    | 842 | BCR  | C15-C16-C17 | -3.14 | 117.09      | 123.52   |
| 11  | aK    | 103 | CLA  | C4C-C3C-C2C | -3.14 | 102.32      | 106.89   |
| 11  | aL    | 206 | CLA  | C4C-C3C-C2C | -3.14 | 102.32      | 106.89   |
| 11  | bK    | 103 | CLA  | C4C-C3C-C2C | -3.14 | 102.32      | 106.89   |
| 11  | cK    | 103 | CLA  | CHC-C1C-C2C | -3.14 | 118.03      | 126.95   |
| 11  | cA    | 839 | CLA  | CHC-C1C-C2C | -3.14 | 118.03      | 126.95   |
| 11  | cB    | 820 | CLA  | CHD-C4C-NC  | 3.14  | 129.09      | 124.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cA    | 843 | CLA  | CAC-C3C-C4C | 3.14  | 128.87      | 124.79   |
| 11  | aA    | 825 | CLA  | C4B-C3B-C2B | -3.14 | 103.40      | 107.30   |
| 11  | bA    | 829 | CLA  | C4B-C3B-C2B | -3.14 | 103.40      | 107.30   |
| 11  | bA    | 833 | CLA  | C4B-C3B-C2B | -3.14 | 103.40      | 107.30   |
| 11  | cA    | 818 | CLA  | C4B-C3B-C2B | -3.14 | 103.40      | 107.30   |
| 11  | aA    | 839 | CLA  | CHC-C1C-C2C | -3.14 | 118.04      | 126.95   |
| 11  | aB    | 830 | CLA  | CHC-C1C-C2C | -3.14 | 118.04      | 126.95   |
| 11  | bB    | 805 | CLA  | CHC-C1C-C2C | -3.14 | 118.04      | 126.95   |
| 11  | bA    | 818 | CLA  | CAC-C3C-C4C | 3.14  | 128.87      | 124.79   |
| 18  | aB    | 847 | LMG  | O6-C1-O1    | -3.13 | 102.64      | 110.04   |
| 11  | cB    | 817 | CLA  | C4B-C3B-C2B | -3.13 | 103.40      | 107.30   |
| 10  | aA    | 801 | CL0  | C1-C2-C3    | -3.13 | 121.06      | 126.20   |
| 13  | bA    | 845 | PQN  | C14-C13-C15 | 3.13  | 120.67      | 115.23   |
| 11  | cA    | 821 | CLA  | C4B-C3B-C2B | -3.13 | 103.41      | 107.30   |
| 12  | bA    | 826 | F6C  | CHD-C4C-NC  | 3.13  | 128.75      | 124.05   |
| 11  | cB    | 821 | CLA  | CHC-C1C-C2C | -3.13 | 118.05      | 126.95   |
| 12  | cA    | 826 | F6C  | C4C-C3C-C2C | -3.13 | 102.02      | 106.87   |
| 11  | cB    | 830 | CLA  | CHC-C1C-C2C | -3.13 | 118.05      | 126.95   |
| 11  | cB    | 804 | CLA  | C4C-C3C-C2C | -3.13 | 102.33      | 106.89   |
| 11  | cB    | 820 | CLA  | CHC-C1C-C2C | -3.13 | 118.05      | 126.95   |
| 12  | cA    | 827 | F6C  | CHD-C4C-NC  | 3.13  | 128.74      | 124.05   |
| 11  | aA    | 825 | CLA  | O2A-CGA-CBA | 3.13  | 121.37      | 111.83   |
| 11  | bB    | 839 | CLA  | CHD-C1D-ND  | -3.13 | 120.40      | 124.80   |
| 15  | bA    | 848 | BCR  | C24-C23-C22 | -3.13 | 121.61      | 126.23   |
| 11  | aA    | 843 | CLA  | C3B-C4B-NB  | 3.13  | 113.32      | 110.53   |
| 12  | bA    | 826 | F6C  | C4C-C3C-C2C | -3.13 | 102.03      | 106.87   |
| 10  | cA    | 801 | CL0  | C1-C2-C3    | -3.13 | 121.08      | 126.20   |
| 11  | bA    | 839 | CLA  | CHC-C1C-C2C | -3.12 | 118.07      | 126.95   |
| 11  | bK    | 103 | CLA  | CHC-C1C-C2C | -3.12 | 118.07      | 126.95   |
| 11  | aA    | 818 | CLA  | C4B-C3B-C2B | -3.12 | 103.42      | 107.30   |
| 11  | aA    | 819 | CLA  | CAC-C3C-C4C | 3.12  | 128.85      | 124.79   |
| 11  | aA    | 839 | CLA  | CAC-C3C-C4C | 3.12  | 128.85      | 124.79   |
| 15  | bB    | 842 | BCR  | C15-C16-C17 | -3.12 | 117.13      | 123.52   |
| 11  | aB    | 805 | CLA  | CHC-C1C-C2C | -3.12 | 118.07      | 126.95   |
| 11  | bA    | 825 | CLA  | C4B-C3B-C2B | -3.12 | 103.42      | 107.30   |
| 11  | aA    | 819 | CLA  | CMC-C2C-C1C | 3.12  | 129.91      | 125.03   |
| 11  | bL    | 206 | CLA  | CMB-C2B-C1B | 3.12  | 130.17      | 125.42   |
| 18  | bB    | 847 | LMG  | O6-C1-O1    | -3.12 | 102.67      | 110.04   |
| 18  | cB    | 847 | LMG  | O6-C1-O1    | -3.12 | 102.67      | 110.04   |
| 11  | aA    | 843 | CLA  | CAC-C3C-C4C | 3.12  | 128.85      | 124.79   |
| 11  | cB    | 832 | CLA  | CAC-C3C-C4C | 3.12  | 128.85      | 124.79   |
| 12  | aA    | 826 | F6C  | CHC-C1C-C2C | -3.12 | 118.37      | 127.43   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aB    | 808 | CLA  | CHC-C1C-C2C | -3.12 | 118.08      | 126.95   |
| 11  | aK    | 103 | CLA  | CHC-C1C-C2C | -3.12 | 118.08      | 126.95   |
| 11  | bA    | 819 | CLA  | CAC-C3C-C4C | 3.12  | 128.85      | 124.79   |
| 11  | bA    | 825 | CLA  | O2A-CGA-CBA | 3.12  | 121.34      | 111.83   |
| 11  | bA    | 818 | CLA  | CHD-C4C-NC  | 3.12  | 129.06      | 124.23   |
| 11  | cK    | 103 | CLA  | C4C-C3C-C2C | -3.12 | 102.35      | 106.89   |
| 11  | cL    | 206 | CLA  | C4C-C3C-C2C | -3.12 | 102.35      | 106.89   |
| 11  | cB    | 839 | CLA  | CHD-C1D-ND  | -3.12 | 120.42      | 124.80   |
| 11  | aB    | 830 | CLA  | O2D-CGD-O1D | -3.12 | 117.78      | 123.85   |
| 11  | cB    | 831 | CLA  | CHC-C1C-C2C | -3.12 | 118.09      | 126.95   |
| 15  | aL    | 208 | BCR  | C2-C1-C6    | 3.12  | 114.96      | 110.44   |
| 11  | aA    | 818 | CLA  | CHD-C4C-NC  | 3.11  | 129.06      | 124.23   |
| 11  | cA    | 836 | CLA  | CHD-C1D-ND  | -3.11 | 120.42      | 124.80   |
| 11  | bA    | 818 | CLA  | C4B-C3B-C2B | -3.11 | 103.43      | 107.30   |
| 11  | bL    | 206 | CLA  | C4C-C3C-C2C | -3.11 | 102.36      | 106.89   |
| 11  | cB    | 813 | CLA  | CHC-C1C-C2C | -3.11 | 118.10      | 126.95   |
| 12  | bA    | 826 | F6C  | CHC-C1C-C2C | -3.11 | 118.39      | 127.43   |
| 12  | bA    | 827 | F6C  | CHD-C4C-NC  | 3.11  | 128.72      | 124.05   |
| 11  | aB    | 813 | CLA  | CHC-C1C-C2C | -3.11 | 118.10      | 126.95   |
| 11  | bA    | 812 | CLA  | C4C-C3C-C2C | -3.11 | 102.36      | 106.89   |
| 11  | aA    | 841 | CLA  | C3B-C4B-NB  | 3.11  | 113.31      | 110.53   |
| 11  | aB    | 830 | CLA  | C3B-C4B-NB  | 3.11  | 113.31      | 110.53   |
| 11  | aA    | 833 | CLA  | C4B-C3B-C2B | -3.11 | 103.43      | 107.30   |
| 11  | cA    | 825 | CLA  | O2A-CGA-CBA | 3.11  | 121.33      | 111.83   |
| 15  | aB    | 842 | BCR  | C15-C16-C17 | -3.11 | 117.15      | 123.52   |
| 11  | bB    | 820 | CLA  | CHC-C1C-C2C | -3.11 | 118.10      | 126.95   |
| 11  | cB    | 805 | CLA  | CHC-C1C-C2C | -3.11 | 118.10      | 126.95   |
| 11  | aA    | 840 | CLA  | C4B-C3B-C2B | -3.11 | 103.43      | 107.30   |
| 12  | aA    | 826 | F6C  | C4C-C3C-C2C | -3.11 | 102.05      | 106.87   |
| 11  | aB    | 820 | CLA  | CHD-C4C-NC  | 3.11  | 129.06      | 124.23   |
| 11  | aB    | 818 | CLA  | CAA-C2A-C3A | -3.11 | 104.59      | 113.00   |
| 11  | aA    | 822 | CLA  | C4B-C3B-C2B | -3.11 | 103.43      | 107.30   |
| 11  | aA    | 812 | CLA  | C4C-C3C-C2C | -3.11 | 102.36      | 106.89   |
| 11  | cA    | 819 | CLA  | CMC-C2C-C1C | 3.11  | 129.89      | 125.03   |
| 11  | cA    | 840 | CLA  | C4B-C3B-C2B | -3.11 | 103.44      | 107.30   |
| 11  | aB    | 801 | CLA  | CHD-C4C-NC  | 3.11  | 129.05      | 124.23   |
| 11  | cB    | 835 | CLA  | CMB-C2B-C1B | 3.11  | 130.15      | 125.42   |
| 11  | aA    | 808 | CLA  | CAC-C3C-C4C | 3.11  | 128.84      | 124.79   |
| 11  | bA    | 819 | CLA  | CMC-C2C-C1C | 3.11  | 129.89      | 125.03   |
| 11  | bB    | 830 | CLA  | O2D-CGD-O1D | -3.11 | 117.80      | 123.85   |
| 11  | bA    | 841 | CLA  | C3B-C4B-NB  | 3.11  | 113.31      | 110.53   |
| 11  | cB    | 830 | CLA  | O2D-CGD-O1D | -3.11 | 117.80      | 123.85   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bA    | 836 | CLA  | C4C-C3C-C2C | -3.11 | 102.37      | 106.89   |
| 15  | aA    | 848 | BCR  | C24-C23-C22 | -3.11 | 121.64      | 126.23   |
| 15  | cL    | 208 | BCR  | C2-C1-C6    | 3.11  | 114.95      | 110.44   |
| 11  | cA    | 812 | CLA  | C4C-C3C-C2C | -3.11 | 102.37      | 106.89   |
| 11  | cA    | 839 | CLA  | CAC-C3C-C4C | 3.11  | 128.83      | 124.79   |
| 11  | cA    | 829 | CLA  | C4B-C3B-C2B | -3.11 | 103.44      | 107.30   |
| 11  | aB    | 807 | CLA  | CHC-C1C-C2C | -3.11 | 118.12      | 126.95   |
| 11  | bB    | 814 | CLA  | C4B-C3B-C2B | -3.10 | 103.44      | 107.30   |
| 11  | cB    | 815 | CLA  | CHD-C4C-NC  | 3.10  | 129.04      | 124.23   |
| 11  | aA    | 813 | CLA  | CAC-C3C-C4C | 3.10  | 128.83      | 124.79   |
| 11  | cB    | 801 | CLA  | C1-C2-C3    | -3.10 | 121.11      | 126.20   |
| 11  | aB    | 820 | CLA  | CHC-C1C-C2C | -3.10 | 118.13      | 126.95   |
| 11  | aB    | 827 | CLA  | C3B-C4B-NB  | 3.10  | 113.30      | 110.53   |
| 11  | bB    | 818 | CLA  | CAA-C2A-C3A | -3.10 | 104.61      | 113.00   |
| 11  | aB    | 804 | CLA  | C4C-C3C-C2C | -3.10 | 102.38      | 106.89   |
| 11  | cA    | 836 | CLA  | C4C-C3C-C2C | -3.10 | 102.38      | 106.89   |
| 11  | bB    | 801 | CLA  | C1-C2-C3    | -3.10 | 121.12      | 126.20   |
| 11  | aA    | 829 | CLA  | C4B-C3B-C2B | -3.10 | 103.45      | 107.30   |
| 11  | aB    | 823 | CLA  | CHD-C1D-ND  | -3.10 | 120.44      | 124.80   |
| 13  | cB    | 841 | PQN  | C11-C3-C2   | -3.10 | 119.58      | 124.89   |
| 11  | cB    | 818 | CLA  | CAA-C2A-C3A | -3.10 | 104.62      | 113.00   |
| 11  | cA    | 808 | CLA  | CAC-C3C-C4C | 3.10  | 128.82      | 124.79   |
| 12  | cL    | 202 | F6C  | O2D-CGD-O1D | -3.10 | 117.82      | 123.85   |
| 11  | bB    | 807 | CLA  | CHC-C1C-C2C | -3.10 | 118.14      | 126.95   |
| 11  | bA    | 840 | CLA  | C4B-C3B-C2B | -3.10 | 103.45      | 107.30   |
| 11  | bB    | 819 | CLA  | CHD-C1D-ND  | -3.10 | 120.44      | 124.80   |
| 11  | cA    | 831 | CLA  | C4C-C3C-C2C | -3.10 | 102.38      | 106.89   |
| 11  | aA    | 808 | CLA  | CAA-C2A-C3A | -3.10 | 104.63      | 113.00   |
| 11  | cA    | 833 | CLA  | C4B-C3B-C2B | -3.10 | 103.45      | 107.30   |
| 11  | bA    | 839 | CLA  | CAC-C3C-C4C | 3.10  | 128.82      | 124.79   |
| 11  | cA    | 808 | CLA  | CAA-C2A-C3A | -3.10 | 104.63      | 113.00   |
| 11  | cB    | 819 | CLA  | CHD-C1D-ND  | -3.10 | 120.44      | 124.80   |
| 11  | aB    | 801 | CLA  | C1-C2-C3    | -3.10 | 121.12      | 126.20   |
| 15  | bL    | 208 | BCR  | C2-C1-C6    | 3.10  | 114.94      | 110.44   |
| 11  | bB    | 831 | CLA  | CHC-C1C-C2C | -3.10 | 118.15      | 126.95   |
| 11  | cA    | 821 | CLA  | C3B-C4B-NB  | 3.10  | 113.29      | 110.53   |
| 11  | cA    | 818 | CLA  | CHD-C4C-NC  | 3.10  | 129.03      | 124.23   |
| 11  | bB    | 827 | CLA  | C3B-C4B-NB  | 3.10  | 113.29      | 110.53   |
| 12  | cA    | 826 | F6C  | CHC-C1C-C2C | -3.09 | 118.44      | 127.43   |
| 11  | cA    | 840 | CLA  | CAC-C3C-C4C | 3.09  | 128.82      | 124.79   |
| 11  | bA    | 822 | CLA  | C3B-C4B-NB  | 3.09  | 113.29      | 110.53   |
| 11  | bA    | 843 | CLA  | CAC-C3C-C4C | 3.09  | 128.81      | 124.79   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aB    | 839 | CLA  | CHD-C1D-ND  | -3.09 | 120.45      | 124.80   |
| 11  | cB    | 807 | CLA  | CHC-C1C-C2C | -3.09 | 118.16      | 126.95   |
| 11  | cB    | 833 | CLA  | CHB-C4A-NA  | 3.09  | 128.86      | 124.40   |
| 11  | bB    | 808 | CLA  | CHC-C1C-C2C | -3.09 | 118.16      | 126.95   |
| 11  | aB    | 838 | CLA  | C4B-C3B-C2B | -3.09 | 103.46      | 107.30   |
| 11  | aB    | 831 | CLA  | CHC-C1C-C2C | -3.09 | 118.16      | 126.95   |
| 11  | aA    | 821 | CLA  | C3B-C4B-NB  | 3.09  | 113.29      | 110.53   |
| 11  | cB    | 830 | CLA  | C3B-C4B-NB  | 3.09  | 113.29      | 110.53   |
| 11  | aA    | 807 | CLA  | CHC-C1C-C2C | -3.09 | 118.17      | 126.95   |
| 11  | bB    | 813 | CLA  | CHC-C1C-C2C | -3.09 | 118.17      | 126.95   |
| 12  | bL    | 202 | F6C  | O2D-CGD-O1D | -3.09 | 117.83      | 123.85   |
| 11  | cA    | 807 | CLA  | CHC-C1C-C2C | -3.09 | 118.17      | 126.95   |
| 11  | bA    | 804 | CLA  | C3B-C4B-NB  | 3.09  | 113.29      | 110.53   |
| 11  | cA    | 825 | CLA  | C4B-C3B-C2B | -3.09 | 103.46      | 107.30   |
| 12  | aL    | 202 | F6C  | O2D-CGD-O1D | -3.09 | 117.84      | 123.85   |
| 11  | cB    | 808 | CLA  | CHC-C1C-C2C | -3.09 | 118.18      | 126.95   |
| 11  | bA    | 818 | CLA  | C1C-C2C-C3C | -3.09 | 103.73      | 106.98   |
| 11  | bA    | 808 | CLA  | CAC-C3C-C4C | 3.09  | 128.81      | 124.79   |
| 11  | bK    | 103 | CLA  | CAC-C3C-C4C | 3.09  | 128.81      | 124.79   |
| 12  | bL    | 202 | F6C  | CHC-C1C-C2C | -3.09 | 118.47      | 127.43   |
| 11  | aB    | 814 | CLA  | C4B-C3B-C2B | -3.09 | 103.47      | 107.30   |
| 11  | cB    | 814 | CLA  | C4B-C3B-C2B | -3.09 | 103.47      | 107.30   |
| 11  | bB    | 823 | CLA  | CHD-C1D-ND  | -3.09 | 120.46      | 124.80   |
| 13  | aB    | 841 | PQN  | C11-C3-C2   | -3.09 | 119.60      | 124.89   |
| 12  | aA    | 844 | F6C  | CHC-C1C-C2C | -3.09 | 118.47      | 127.43   |
| 11  | bA    | 836 | CLA  | CHD-C1D-ND  | -3.08 | 120.46      | 124.80   |
| 11  | bB    | 838 | CLA  | C4B-C3B-C2B | -3.08 | 103.47      | 107.30   |
| 11  | cK    | 101 | CLA  | C3B-C4B-NB  | 3.08  | 113.28      | 110.53   |
| 11  | bB    | 814 | CLA  | CAA-C2A-C3A | -3.08 | 104.67      | 113.00   |
| 11  | cB    | 801 | CLA  | CHD-C4C-NC  | 3.08  | 129.01      | 124.23   |
| 11  | cB    | 838 | CLA  | C4B-C3B-C2B | -3.08 | 103.47      | 107.30   |
| 11  | bA    | 814 | CLA  | C4C-C3C-C2C | -3.08 | 102.41      | 106.89   |
| 11  | bA    | 808 | CLA  | CAA-C2A-C3A | -3.08 | 104.67      | 113.00   |
| 12  | bA    | 844 | F6C  | CHC-C1C-C2C | -3.08 | 118.48      | 127.43   |
| 11  | aA    | 811 | CLA  | CHC-C1C-C2C | -3.08 | 118.19      | 126.95   |
| 11  | aB    | 819 | CLA  | CHD-C1D-ND  | -3.08 | 120.47      | 124.80   |
| 11  | aB    | 811 | CLA  | C3B-C4B-NB  | 3.08  | 113.28      | 110.53   |
| 11  | bA    | 821 | CLA  | C3B-C4B-NB  | 3.08  | 113.28      | 110.53   |
| 13  | bB    | 841 | PQN  | C11-C3-C2   | -3.08 | 119.61      | 124.89   |
| 11  | bB    | 833 | CLA  | CHB-C4A-NA  | 3.08  | 128.84      | 124.40   |
| 12  | cA    | 844 | F6C  | CHC-C1C-C2C | -3.08 | 118.49      | 127.43   |
| 11  | aA    | 831 | CLA  | C4C-C3C-C2C | -3.08 | 102.41      | 106.89   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cA    | 822 | CLA  | C3B-C4B-NB  | 3.08  | 113.28      | 110.53   |
| 11  | cB    | 814 | CLA  | CAA-C2A-C3A | -3.08 | 104.69      | 113.00   |
| 11  | aB    | 814 | CLA  | CAA-C2A-C3A | -3.08 | 104.69      | 113.00   |
| 11  | aA    | 836 | CLA  | C4C-C3C-C2C | -3.08 | 102.41      | 106.89   |
| 11  | bA    | 831 | CLA  | C4C-C3C-C2C | -3.08 | 102.41      | 106.89   |
| 11  | cA    | 814 | CLA  | C4C-C3C-C2C | -3.08 | 102.41      | 106.89   |
| 11  | aB    | 840 | CLA  | CHD-C4C-NC  | 3.08  | 129.00      | 124.23   |
| 11  | cB    | 840 | CLA  | CHD-C4C-NC  | 3.07  | 129.00      | 124.23   |
| 11  | bB    | 815 | CLA  | CHD-C4C-NC  | 3.07  | 129.00      | 124.23   |
| 11  | bB    | 801 | CLA  | CHD-C4C-NC  | 3.07  | 128.99      | 124.23   |
| 11  | bA    | 807 | CLA  | CHC-C1C-C2C | -3.07 | 118.22      | 126.95   |
| 12  | cL    | 202 | F6C  | CHC-C1C-C2C | -3.07 | 118.52      | 127.43   |
| 11  | cA    | 811 | CLA  | CHC-C1C-C2C | -3.07 | 118.23      | 126.95   |
| 11  | aB    | 833 | CLA  | CHB-C4A-NA  | 3.07  | 128.83      | 124.40   |
| 11  | cB    | 805 | CLA  | CHB-C4A-NA  | 3.07  | 128.83      | 124.40   |
| 11  | aB    | 815 | CLA  | CHD-C4C-NC  | 3.07  | 128.99      | 124.23   |
| 11  | bB    | 807 | CLA  | C4B-C3B-C2B | -3.07 | 103.49      | 107.30   |
| 12  | aL    | 202 | F6C  | CHC-C1C-C2C | -3.07 | 118.53      | 127.43   |
| 11  | aK    | 101 | CLA  | CHC-C1C-C2C | -3.07 | 118.24      | 126.95   |
| 11  | bA    | 811 | CLA  | CHC-C1C-C2C | -3.06 | 118.24      | 126.95   |
| 11  | bL    | 205 | CLA  | C3B-C4B-NB  | 3.06  | 113.27      | 110.53   |
| 11  | aA    | 813 | CLA  | CHC-C1C-C2C | -3.06 | 118.24      | 126.95   |
| 11  | aB    | 832 | CLA  | CHC-C1C-C2C | -3.06 | 118.24      | 126.95   |
| 11  | aB    | 807 | CLA  | C4B-C3B-C2B | -3.06 | 103.49      | 107.30   |
| 11  | bA    | 813 | CLA  | CAC-C3C-C4C | 3.06  | 128.77      | 124.79   |
| 11  | aA    | 813 | CLA  | C4C-C3C-C2C | -3.06 | 102.44      | 106.89   |
| 11  | bB    | 840 | CLA  | CHD-C4C-NC  | 3.06  | 128.98      | 124.23   |
| 11  | aA    | 840 | CLA  | CAC-C3C-C4C | 3.06  | 128.77      | 124.79   |
| 11  | cK    | 101 | CLA  | CHC-C1C-C2C | -3.06 | 118.25      | 126.95   |
| 15  | cA    | 848 | BCR  | C24-C23-C22 | -3.06 | 121.71      | 126.23   |
| 15  | aB    | 848 | BCR  | C27-C26-C25 | 3.06  | 126.84      | 122.70   |
| 11  | cA    | 816 | CLA  | CHC-C1C-C2C | -3.06 | 118.26      | 126.95   |
| 11  | cA    | 843 | CLA  | CHC-C1C-C2C | -3.06 | 118.26      | 126.95   |
| 11  | aA    | 814 | CLA  | C4C-C3C-C2C | -3.06 | 102.44      | 106.89   |
| 11  | bA    | 805 | CLA  | CMC-C2C-C1C | 3.06  | 129.81      | 125.03   |
| 11  | aA    | 834 | CLA  | CHC-C1C-C2C | -3.06 | 118.27      | 126.95   |
| 15  | aA    | 849 | BCR  | C15-C16-C17 | -3.05 | 117.27      | 123.52   |
| 11  | cB    | 811 | CLA  | C3B-C4B-NB  | 3.05  | 113.26      | 110.53   |
| 11  | cA    | 821 | CLA  | C4C-C3C-C2C | -3.05 | 102.45      | 106.89   |
| 11  | bA    | 816 | CLA  | CHC-C1C-C2C | -3.05 | 118.27      | 126.95   |
| 11  | bA    | 843 | CLA  | CHC-C1C-C2C | -3.05 | 118.27      | 126.95   |
| 11  | cA    | 841 | CLA  | C3B-C4B-NB  | 3.05  | 113.25      | 110.53   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cB    | 827 | CLA  | C3B-C4B-NB  | 3.05  | 113.25      | 110.53   |
| 11  | bA    | 833 | CLA  | CHC-C1C-C2C | -3.05 | 118.27      | 126.95   |
| 11  | aA    | 823 | CLA  | CHC-C1C-C2C | -3.05 | 118.28      | 126.95   |
| 11  | aA    | 816 | CLA  | CHC-C1C-C2C | -3.05 | 118.28      | 126.95   |
| 11  | cA    | 818 | CLA  | C1C-C2C-C3C | -3.05 | 103.77      | 106.98   |
| 11  | bK    | 101 | CLA  | CHC-C1C-C2C | -3.05 | 118.28      | 126.95   |
| 11  | bA    | 810 | CLA  | C4C-C3C-C2C | -3.05 | 102.45      | 106.89   |
| 11  | cA    | 813 | CLA  | CAC-C3C-C4C | 3.05  | 128.76      | 124.79   |
| 11  | bB    | 838 | CLA  | O2A-CGA-CBA | 3.05  | 121.14      | 111.83   |
| 11  | aA    | 810 | CLA  | CHC-C1C-C2C | -3.05 | 118.28      | 126.95   |
| 11  | cB    | 838 | CLA  | O2A-CGA-CBA | 3.05  | 121.14      | 111.83   |
| 11  | aA    | 818 | CLA  | C1C-C2C-C3C | -3.05 | 103.77      | 106.98   |
| 11  | aB    | 817 | CLA  | CBA-CAA-C2A | 3.05  | 122.87      | 113.79   |
| 11  | aB    | 812 | CLA  | CHC-C1C-C2C | -3.05 | 118.28      | 126.95   |
| 11  | bB    | 838 | CLA  | CHC-C1C-C2C | -3.05 | 118.28      | 126.95   |
| 11  | bB    | 819 | CLA  | CHC-C1C-C2C | -3.05 | 118.28      | 126.95   |
| 11  | cA    | 813 | CLA  | CHC-C1C-C2C | -3.05 | 118.28      | 126.95   |
| 11  | cB    | 832 | CLA  | CHC-C1C-C2C | -3.05 | 118.28      | 126.95   |
| 11  | aK    | 103 | CLA  | CAC-C3C-C4C | 3.05  | 128.76      | 124.79   |
| 11  | cB    | 817 | CLA  | CBA-CAA-C2A | 3.05  | 122.86      | 113.79   |
| 11  | aA    | 810 | CLA  | C4C-C3C-C2C | -3.05 | 102.46      | 106.89   |
| 11  | bA    | 821 | CLA  | C4C-C3C-C2C | -3.05 | 102.46      | 106.89   |
| 11  | aA    | 843 | CLA  | CHC-C1C-C2C | -3.05 | 118.29      | 126.95   |
| 11  | aB    | 836 | CLA  | C1C-C2C-C3C | -3.05 | 103.78      | 106.98   |
| 11  | bB    | 811 | CLA  | C3B-C4B-NB  | 3.05  | 113.25      | 110.53   |
| 11  | bA    | 821 | CLA  | CHD-C1D-ND  | -3.05 | 120.52      | 124.80   |
| 11  | cB    | 823 | CLA  | CHD-C1D-ND  | -3.05 | 120.52      | 124.80   |
| 11  | bA    | 834 | CLA  | CHC-C1C-C2C | -3.05 | 118.29      | 126.95   |
| 11  | bA    | 813 | CLA  | CHC-C1C-C2C | -3.05 | 118.29      | 126.95   |
| 11  | aB    | 838 | CLA  | O2A-CGA-CBA | 3.04  | 121.12      | 111.83   |
| 11  | bA    | 840 | CLA  | C3B-C4B-NB  | 3.04  | 113.25      | 110.53   |
| 11  | cB    | 807 | CLA  | C4B-C3B-C2B | -3.04 | 103.52      | 107.30   |
| 11  | bB    | 804 | CLA  | C4A-NA-C1A  | -3.04 | 105.29      | 106.68   |
| 11  | cA    | 815 | CLA  | C4A-NA-C1A  | -3.04 | 105.29      | 106.68   |
| 11  | cB    | 811 | CLA  | CHC-C1C-C2C | -3.04 | 118.30      | 126.95   |
| 11  | bA    | 823 | CLA  | CHC-C1C-C2C | -3.04 | 118.30      | 126.95   |
| 11  | cA    | 834 | CLA  | CHC-C1C-C2C | -3.04 | 118.30      | 126.95   |
| 11  | aA    | 822 | CLA  | C3B-C4B-NB  | 3.04  | 113.25      | 110.53   |
| 11  | bB    | 811 | CLA  | CHC-C1C-C2C | -3.04 | 118.30      | 126.95   |
| 11  | cB    | 812 | CLA  | CHC-C1C-C2C | -3.04 | 118.30      | 126.95   |
| 11  | bB    | 828 | CLA  | O2D-CGD-O1D | -3.04 | 117.93      | 123.85   |
| 12  | cA    | 830 | F6C  | CHC-C1C-C2C | -3.04 | 118.60      | 127.43   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aB    | 811 | CLA  | CHC-C1C-C2C | -3.04 | 118.30      | 126.95   |
| 11  | cB    | 819 | CLA  | CHC-C1C-C2C | -3.04 | 118.30      | 126.95   |
| 11  | cL    | 204 | CLA  | CHC-C1C-C2C | -3.04 | 118.30      | 126.95   |
| 11  | aA    | 803 | CLA  | C1C-C2C-C3C | -3.04 | 103.78      | 106.98   |
| 11  | bA    | 843 | CLA  | C4-C3-C5    | 3.04  | 119.71      | 116.13   |
| 11  | aL    | 205 | CLA  | C3B-C4B-NB  | 3.04  | 113.25      | 110.53   |
| 15  | cA    | 849 | BCR  | C15-C16-C17 | -3.04 | 117.30      | 123.52   |
| 11  | bA    | 829 | CLA  | CAA-C2A-C3A | -3.04 | 104.78      | 113.00   |
| 11  | aA    | 804 | CLA  | C3B-C4B-NB  | 3.04  | 113.24      | 110.53   |
| 11  | cB    | 836 | CLA  | C1C-C2C-C3C | -3.04 | 103.78      | 106.98   |
| 11  | bA    | 806 | CLA  | C4A-NA-C1A  | -3.04 | 105.29      | 106.68   |
| 11  | bB    | 817 | CLA  | CBA-CAA-C2A | 3.04  | 122.83      | 113.79   |
| 12  | aA    | 830 | F6C  | CHC-C1C-C2C | -3.04 | 118.61      | 127.43   |
| 15  | cB    | 848 | BCR  | C27-C26-C25 | 3.04  | 126.81      | 122.70   |
| 11  | cB    | 804 | CLA  | CHD-C4C-NC  | 3.04  | 128.94      | 124.23   |
| 11  | cB    | 828 | CLA  | O2D-CGD-O1D | -3.04 | 117.94      | 123.85   |
| 11  | cK    | 103 | CLA  | CAC-C3C-C4C | 3.04  | 128.74      | 124.79   |
| 11  | cA    | 823 | CLA  | CHC-C1C-C2C | -3.04 | 118.32      | 126.95   |
| 11  | aA    | 833 | CLA  | CHC-C1C-C2C | -3.04 | 118.32      | 126.95   |
| 11  | cA    | 837 | CLA  | C4B-C3B-C2B | -3.04 | 103.53      | 107.30   |
| 11  | aA    | 821 | CLA  | C4C-C3C-C2C | -3.04 | 102.47      | 106.89   |
| 11  | aA    | 829 | CLA  | CAA-C2A-C3A | -3.04 | 104.80      | 113.00   |
| 11  | cA    | 804 | CLA  | C3B-C4B-NB  | 3.03  | 113.24      | 110.53   |
| 11  | aA    | 816 | CLA  | C4B-C3B-C2B | -3.03 | 103.53      | 107.30   |
| 11  | bB    | 836 | CLA  | C1C-C2C-C3C | -3.03 | 103.79      | 106.98   |
| 11  | cA    | 829 | CLA  | CHC-C1C-C2C | -3.03 | 118.33      | 126.95   |
| 11  | bB    | 812 | CLA  | CHC-C1C-C2C | -3.03 | 118.33      | 126.95   |
| 12  | bA    | 830 | F6C  | CHC-C1C-C2C | -3.03 | 118.62      | 127.43   |
| 11  | cA    | 829 | CLA  | CAA-C2A-C3A | -3.03 | 104.80      | 113.00   |
| 11  | cA    | 810 | CLA  | CHC-C1C-C2C | -3.03 | 118.33      | 126.95   |
| 11  | cA    | 833 | CLA  | CHC-C1C-C2C | -3.03 | 118.33      | 126.95   |
| 11  | bL    | 204 | CLA  | CHC-C1C-C2C | -3.03 | 118.33      | 126.95   |
| 11  | aA    | 837 | CLA  | C4B-C3B-C2B | -3.03 | 103.53      | 107.30   |
| 11  | aB    | 819 | CLA  | CHC-C1C-C2C | -3.03 | 118.33      | 126.95   |
| 11  | bB    | 832 | CLA  | CHC-C1C-C2C | -3.03 | 118.33      | 126.95   |
| 11  | cA    | 831 | CLA  | CAC-C3C-C4C | 3.03  | 128.73      | 124.79   |
| 11  | aL    | 204 | CLA  | CHC-C1C-C2C | -3.03 | 118.34      | 126.95   |
| 11  | bB    | 835 | CLA  | C4B-C3B-C2B | -3.03 | 103.53      | 107.30   |
| 11  | cB    | 815 | CLA  | C4C-C3C-C2C | -3.03 | 102.48      | 106.89   |
| 11  | aA    | 805 | CLA  | CMC-C2C-C1C | 3.03  | 129.77      | 125.03   |
| 11  | cA    | 806 | CLA  | C4A-NA-C1A  | -3.03 | 105.30      | 106.68   |
| 11  | cA    | 840 | CLA  | C3B-C4B-NB  | 3.03  | 113.23      | 110.53   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cA    | 841 | CLA  | O2A-CGA-CBA | 3.03  | 121.07      | 111.83   |
| 11  | cA    | 805 | CLA  | CMC-C2C-C1C | 3.03  | 129.77      | 125.03   |
| 11  | cA    | 802 | CLA  | CAC-C3C-C4C | 3.03  | 128.73      | 124.79   |
| 12  | aA    | 827 | F6C  | CHC-C1C-C2C | -3.03 | 118.64      | 127.43   |
| 11  | aB    | 838 | CLA  | CHC-C1C-C2C | -3.03 | 118.34      | 126.95   |
| 11  | aB    | 828 | CLA  | O2D-CGD-O1D | -3.03 | 117.95      | 123.85   |
| 11  | aB    | 814 | CLA  | C4C-C3C-C2C | -3.03 | 102.49      | 106.89   |
| 11  | bA    | 816 | CLA  | C4B-C3B-C2B | -3.03 | 103.54      | 107.30   |
| 11  | bB    | 830 | CLA  | C4B-C3B-C2B | -3.03 | 103.54      | 107.30   |
| 11  | aK    | 101 | CLA  | C3B-C4B-NB  | 3.03  | 113.23      | 110.53   |
| 11  | bB    | 815 | CLA  | C4C-C3C-C2C | -3.03 | 102.49      | 106.89   |
| 11  | aB    | 804 | CLA  | C4A-NA-C1A  | -3.02 | 105.30      | 106.68   |
| 11  | bK    | 101 | CLA  | C3B-C4B-NB  | 3.02  | 113.23      | 110.53   |
| 11  | cB    | 838 | CLA  | CHC-C1C-C2C | -3.02 | 118.35      | 126.95   |
| 12  | cA    | 827 | F6C  | CHC-C1C-C2C | -3.02 | 118.65      | 127.43   |
| 11  | aB    | 818 | CLA  | C3B-C4B-NB  | 3.02  | 113.23      | 110.53   |
| 11  | cA    | 841 | CLA  | CHC-C1C-C2C | -3.02 | 118.36      | 126.95   |
| 11  | aB    | 801 | CLA  | CAC-C3C-C4C | 3.02  | 128.72      | 124.79   |
| 11  | aB    | 815 | CLA  | C4C-C3C-C2C | -3.02 | 102.49      | 106.89   |
| 11  | cL    | 205 | CLA  | C3B-C4B-NB  | 3.02  | 113.23      | 110.53   |
| 11  | cL    | 205 | CLA  | CAC-C3C-C4C | 3.02  | 128.72      | 124.79   |
| 15  | bA    | 849 | BCR  | C15-C16-C17 | -3.02 | 117.34      | 123.52   |
| 11  | bA    | 837 | CLA  | C4B-C3B-C2B | -3.02 | 103.55      | 107.30   |
| 11  | bL    | 206 | CLA  | C4B-C3B-C2B | -3.02 | 103.55      | 107.30   |
| 11  | aA    | 814 | CLA  | CAA-C2A-C3A | -3.02 | 104.83      | 113.00   |
| 11  | bA    | 829 | CLA  | CHC-C1C-C2C | -3.02 | 118.36      | 126.95   |
| 11  | cA    | 835 | CLA  | C1-C2-C3    | -3.02 | 121.25      | 126.20   |
| 11  | bB    | 801 | CLA  | CAC-C3C-C4C | 3.02  | 128.72      | 124.79   |
| 11  | aA    | 810 | CLA  | C3B-C4B-NB  | 3.02  | 113.23      | 110.53   |
| 11  | aA    | 831 | CLA  | CAC-C3C-C4C | 3.02  | 128.72      | 124.79   |
| 11  | aB    | 825 | CLA  | CHC-C1C-C2C | -3.02 | 118.37      | 126.95   |
| 11  | bA    | 810 | CLA  | CHC-C1C-C2C | -3.02 | 118.37      | 126.95   |
| 11  | bA    | 814 | CLA  | CAA-C2A-C3A | -3.02 | 104.84      | 113.00   |
| 11  | cB    | 814 | CLA  | C4C-C3C-C2C | -3.02 | 102.50      | 106.89   |
| 11  | aA    | 815 | CLA  | C4A-NA-C1A  | -3.02 | 105.30      | 106.68   |
| 11  | bA    | 840 | CLA  | CAC-C3C-C4C | 3.02  | 128.72      | 124.79   |
| 11  | cB    | 802 | CLA  | C4B-C3B-C2B | -3.02 | 103.55      | 107.30   |
| 11  | bB    | 814 | CLA  | C4C-C3C-C2C | -3.02 | 102.50      | 106.89   |
| 11  | aB    | 805 | CLA  | CHB-C4A-NA  | 3.02  | 128.75      | 124.40   |
| 12  | bA    | 827 | F6C  | CHC-C1C-C2C | -3.02 | 118.67      | 127.43   |
| 11  | cA    | 821 | CLA  | CHD-C1D-ND  | -3.02 | 120.56      | 124.80   |
| 11  | aB    | 804 | CLA  | CHD-C4C-NC  | 3.02  | 128.91      | 124.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cL    | 206 | CLA  | C4B-C3B-C2B | -3.02 | 103.55      | 107.30   |
| 11  | cA    | 810 | CLA  | C4C-C3C-C2C | -3.02 | 102.50      | 106.89   |
| 11  | cA    | 836 | CLA  | CAC-C3C-C4C | 3.02  | 128.71      | 124.79   |
| 11  | cA    | 803 | CLA  | C1C-C2C-C3C | -3.01 | 103.81      | 106.98   |
| 11  | aB    | 821 | CLA  | C4C-C3C-C2C | -3.01 | 102.50      | 106.89   |
| 11  | bB    | 805 | CLA  | CHB-C4A-NA  | 3.01  | 128.75      | 124.40   |
| 11  | bA    | 841 | CLA  | O2A-CGA-CBA | 3.01  | 121.02      | 111.83   |
| 11  | bA    | 835 | CLA  | C1-C2-C3    | -3.01 | 121.26      | 126.20   |
| 11  | aA    | 829 | CLA  | CHC-C1C-C2C | -3.01 | 118.39      | 126.95   |
| 11  | bB    | 822 | CLA  | CHD-C4C-NC  | 3.01  | 128.90      | 124.23   |
| 11  | bL    | 205 | CLA  | CHC-C1C-C2C | -3.01 | 118.39      | 126.95   |
| 11  | aB    | 802 | CLA  | C4B-C3B-C2B | -3.01 | 103.56      | 107.30   |
| 11  | bA    | 841 | CLA  | CHC-C1C-C2C | -3.01 | 118.39      | 126.95   |
| 11  | aA    | 802 | CLA  | CAC-C3C-C4C | 3.01  | 128.71      | 124.79   |
| 11  | bA    | 822 | CLA  | CHC-C1C-C2C | -3.01 | 118.39      | 126.95   |
| 11  | bA    | 813 | CLA  | C4C-C3C-C2C | -3.01 | 102.51      | 106.89   |
| 11  | cB    | 801 | CLA  | CAC-C3C-C4C | 3.01  | 128.71      | 124.79   |
| 11  | bA    | 809 | CLA  | CHC-C1C-C2C | -3.01 | 118.40      | 126.95   |
| 11  | bB    | 825 | CLA  | CHC-C1C-C2C | -3.01 | 118.40      | 126.95   |
| 11  | aA    | 840 | CLA  | C3B-C4B-NB  | 3.01  | 113.22      | 110.53   |
| 11  | cB    | 808 | CLA  | C4-C3-C5    | 3.01  | 120.45      | 115.23   |
| 11  | bB    | 804 | CLA  | CHD-C4C-NC  | 3.01  | 128.89      | 124.23   |
| 11  | bA    | 831 | CLA  | CAC-C3C-C4C | 3.01  | 128.70      | 124.79   |
| 11  | cL    | 205 | CLA  | CHC-C1C-C2C | -3.01 | 118.40      | 126.95   |
| 11  | cA    | 816 | CLA  | C4B-C3B-C2B | -3.01 | 103.56      | 107.30   |
| 11  | cB    | 825 | CLA  | CHC-C1C-C2C | -3.01 | 118.41      | 126.95   |
| 11  | bA    | 835 | CLA  | CHD-C4C-NC  | 3.01  | 128.89      | 124.23   |
| 11  | aA    | 841 | CLA  | O2A-CGA-CBA | 3.01  | 121.00      | 111.83   |
| 11  | bB    | 830 | CLA  | C4C-C3C-C2C | -3.01 | 102.52      | 106.89   |
| 11  | aA    | 806 | CLA  | C4A-NA-C1A  | -3.01 | 105.31      | 106.68   |
| 11  | cB    | 827 | CLA  | CHC-C1C-C2C | -3.00 | 118.41      | 126.95   |
| 11  | bB    | 821 | CLA  | C4C-C3C-C2C | -3.00 | 102.52      | 106.89   |
| 11  | aB    | 808 | CLA  | C4-C3-C5    | 3.00  | 120.44      | 115.23   |
| 11  | aA    | 821 | CLA  | CHD-C1D-ND  | -3.00 | 120.58      | 124.80   |
| 11  | aB    | 816 | CLA  | CHC-C1C-C2C | -3.00 | 118.41      | 126.95   |
| 11  | aB    | 821 | CLA  | C4B-C3B-C2B | -3.00 | 103.57      | 107.30   |
| 11  | bB    | 808 | CLA  | C4-C3-C5    | 3.00  | 120.44      | 115.23   |
| 11  | aL    | 205 | CLA  | CHC-C1C-C2C | -3.00 | 118.42      | 126.95   |
| 11  | bB    | 827 | CLA  | CHC-C1C-C2C | -3.00 | 118.42      | 126.95   |
| 11  | cB    | 809 | CLA  | CAC-C3C-C4C | 3.00  | 128.70      | 124.79   |
| 11  | aB    | 830 | CLA  | C4B-C3B-C2B | -3.00 | 103.57      | 107.30   |
| 11  | aA    | 841 | CLA  | CHC-C1C-C2C | -3.00 | 118.42      | 126.95   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aB    | 827 | CLA  | CHC-C1C-C2C | -3.00 | 118.42      | 126.95   |
| 11  | aA    | 843 | CLA  | C4-C3-C5    | 3.00  | 119.66      | 116.13   |
| 11  | bB    | 809 | CLA  | CAC-C3C-C4C | 3.00  | 128.69      | 124.79   |
| 11  | aB    | 835 | CLA  | C4B-C3B-C2B | -3.00 | 103.57      | 107.30   |
| 11  | cB    | 835 | CLA  | C4B-C3B-C2B | -3.00 | 103.57      | 107.30   |
| 11  | bB    | 818 | CLA  | CHC-C1C-C2C | -3.00 | 118.42      | 126.95   |
| 11  | cB    | 816 | CLA  | CHC-C1C-C2C | -3.00 | 118.42      | 126.95   |
| 11  | cA    | 837 | CLA  | CHD-C4C-NC  | 3.00  | 128.88      | 124.23   |
| 11  | bA    | 837 | CLA  | C4C-C3C-C2C | -3.00 | 102.53      | 106.89   |
| 11  | bB    | 817 | CLA  | CHD-C4C-NC  | 3.00  | 128.88      | 124.23   |
| 11  | cA    | 835 | CLA  | CHD-C4C-NC  | 3.00  | 128.88      | 124.23   |
| 11  | bA    | 810 | CLA  | C3B-C4B-NB  | 3.00  | 113.21      | 110.53   |
| 12  | bA    | 827 | F6C  | C4-C3-C5    | 3.00  | 120.43      | 115.23   |
| 11  | aA    | 836 | CLA  | CAC-C3C-C4C | 3.00  | 128.69      | 124.79   |
| 12  | cA    | 827 | F6C  | C4-C3-C5    | 3.00  | 120.43      | 115.23   |
| 11  | cL    | 205 | CLA  | C4C-C3C-C2C | -3.00 | 102.53      | 106.89   |
| 11  | bB    | 818 | CLA  | C3B-C4B-NB  | 3.00  | 113.21      | 110.53   |
| 11  | cA    | 822 | CLA  | CHC-C1C-C2C | -3.00 | 118.43      | 126.95   |
| 11  | cA    | 805 | CLA  | C4C-C3C-C2C | -3.00 | 102.53      | 106.89   |
| 11  | cA    | 814 | CLA  | CAA-C2A-C3A | -3.00 | 104.90      | 113.00   |
| 11  | cA    | 835 | CLA  | CHC-C1C-C2C | -3.00 | 118.43      | 126.95   |
| 11  | bA    | 836 | CLA  | CAC-C3C-C4C | 3.00  | 128.69      | 124.79   |
| 15  | bB    | 848 | BCR  | C27-C26-C25 | 3.00  | 126.75      | 122.70   |
| 11  | aA    | 835 | CLA  | C1-C2-C3    | -3.00 | 121.29      | 126.20   |
| 11  | bB    | 802 | CLA  | C4B-C3B-C2B | -3.00 | 103.58      | 107.30   |
| 11  | bB    | 816 | CLA  | CHC-C1C-C2C | -2.99 | 118.44      | 126.95   |
| 11  | cA    | 843 | CLA  | C4-C3-C5    | 2.99  | 119.65      | 116.13   |
| 11  | aB    | 822 | CLA  | CHD-C4C-NC  | 2.99  | 128.87      | 124.23   |
| 11  | aA    | 810 | CLA  | C4A-NA-C1A  | -2.99 | 105.31      | 106.68   |
| 12  | aA    | 832 | F6C  | CHD-C4C-NC  | 2.99  | 128.54      | 124.05   |
| 11  | aA    | 824 | CLA  | CHD-C4C-NC  | 2.99  | 128.87      | 124.23   |
| 11  | cA    | 813 | CLA  | C4C-C3C-C2C | -2.99 | 102.53      | 106.89   |
| 11  | aB    | 817 | CLA  | CHD-C4C-NC  | 2.99  | 128.87      | 124.23   |
| 11  | aA    | 809 | CLA  | CHC-C1C-C2C | -2.99 | 118.44      | 126.95   |
| 11  | aA    | 805 | CLA  | C4C-C3C-C2C | -2.99 | 102.54      | 106.89   |
| 11  | cB    | 821 | CLA  | C4C-C3C-C2C | -2.99 | 102.54      | 106.89   |
| 11  | bA    | 802 | CLA  | CAC-C3C-C4C | 2.99  | 128.68      | 124.79   |
| 11  | aL    | 206 | CLA  | C4B-C3B-C2B | -2.99 | 103.58      | 107.30   |
| 11  | aA    | 805 | CLA  | CAC-C3C-C4C | 2.99  | 128.68      | 124.79   |
| 11  | aB    | 809 | CLA  | CAC-C3C-C4C | 2.99  | 128.68      | 124.79   |
| 11  | aA    | 822 | CLA  | CHC-C1C-C2C | -2.99 | 118.45      | 126.95   |
| 11  | cB    | 804 | CLA  | CMC-C2C-C1C | 2.99  | 129.71      | 125.03   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aB    | 818 | CLA  | CHC-C1C-C2C | -2.99 | 118.45      | 126.95   |
| 11  | cA    | 810 | CLA  | C3B-C4B-NB  | 2.99  | 113.20      | 110.53   |
| 11  | aB    | 838 | CLA  | C4C-C3C-C2C | -2.99 | 102.54      | 106.89   |
| 11  | bA    | 835 | CLA  | CHC-C1C-C2C | -2.99 | 118.46      | 126.95   |
| 11  | cA    | 809 | CLA  | CHC-C1C-C2C | -2.99 | 118.46      | 126.95   |
| 11  | aA    | 835 | CLA  | CHD-C4C-NC  | 2.99  | 128.86      | 124.23   |
| 11  | cB    | 822 | CLA  | CHD-C4C-NC  | 2.99  | 128.86      | 124.23   |
| 11  | aB    | 830 | CLA  | C4C-C3C-C2C | -2.99 | 102.54      | 106.89   |
| 11  | bB    | 821 | CLA  | C4B-C3B-C2B | -2.99 | 103.59      | 107.30   |
| 11  | bA    | 824 | CLA  | CHD-C4C-NC  | 2.99  | 128.86      | 124.23   |
| 11  | cA    | 819 | CLA  | C1C-C2C-C3C | -2.99 | 103.84      | 106.98   |
| 11  | bA    | 829 | CLA  | C4C-C3C-C2C | -2.99 | 102.55      | 106.89   |
| 11  | cB    | 837 | CLA  | C4C-C3C-C2C | -2.99 | 102.55      | 106.89   |
| 11  | cA    | 802 | CLA  | C1-C2-C3    | -2.98 | 121.31      | 126.20   |
| 11  | aA    | 819 | CLA  | C1C-C2C-C3C | -2.98 | 103.84      | 106.98   |
| 11  | cA    | 809 | CLA  | CAC-C3C-C4C | 2.98  | 128.67      | 124.79   |
| 11  | aB    | 806 | CLA  | CAA-C2A-C3A | -2.98 | 104.94      | 113.00   |
| 11  | bA    | 815 | CLA  | C4A-NA-C1A  | -2.98 | 105.32      | 106.68   |
| 12  | cA    | 832 | F6C  | CHD-C4C-NC  | 2.98  | 128.52      | 124.05   |
| 11  | bA    | 819 | CLA  | C1C-C2C-C3C | -2.98 | 103.84      | 106.98   |
| 11  | cB    | 838 | CLA  | C4C-C3C-C2C | -2.98 | 102.55      | 106.89   |
| 11  | aA    | 835 | CLA  | CHC-C1C-C2C | -2.98 | 118.47      | 126.95   |
| 11  | cB    | 818 | CLA  | CHC-C1C-C2C | -2.98 | 118.47      | 126.95   |
| 11  | bK    | 103 | CLA  | O2A-CGA-CBA | 2.98  | 120.92      | 111.83   |
| 11  | cB    | 836 | CLA  | CMB-C2B-C1B | 2.98  | 129.96      | 125.42   |
| 11  | bA    | 841 | CLA  | CAC-C3C-C4C | 2.98  | 128.67      | 124.79   |
| 11  | cA    | 817 | CLA  | CAA-C2A-C3A | -2.98 | 104.95      | 113.00   |
| 15  | cM    | 101 | BCR  | C15-C16-C17 | -2.98 | 117.42      | 123.52   |
| 12  | cA    | 826 | F6C  | O2D-CGD-O1D | -2.98 | 118.05      | 123.85   |
| 11  | bA    | 805 | CLA  | C4C-C3C-C2C | -2.98 | 102.56      | 106.89   |
| 15  | aM    | 101 | BCR  | C15-C16-C17 | -2.98 | 117.43      | 123.52   |
| 11  | aK    | 101 | CLA  | CAC-C3C-C4C | 2.98  | 128.66      | 124.79   |
| 11  | cA    | 805 | CLA  | CAC-C3C-C4C | 2.98  | 128.66      | 124.79   |
| 11  | cB    | 821 | CLA  | C4B-C3B-C2B | -2.98 | 103.60      | 107.30   |
| 11  | bA    | 837 | CLA  | CHD-C4C-NC  | 2.98  | 128.85      | 124.23   |
| 11  | bA    | 840 | CLA  | CHC-C1C-C2C | -2.98 | 118.49      | 126.95   |
| 11  | cK    | 103 | CLA  | O2A-CGA-CBA | 2.98  | 120.91      | 111.83   |
| 11  | aL    | 205 | CLA  | C4C-C3C-C2C | -2.98 | 102.56      | 106.89   |
| 11  | cA    | 829 | CLA  | C4C-C3C-C2C | -2.98 | 102.56      | 106.89   |
| 11  | bB    | 839 | CLA  | CHD-C4C-NC  | 2.97  | 128.84      | 124.23   |
| 11  | aL    | 205 | CLA  | CAC-C3C-C4C | 2.97  | 128.66      | 124.79   |
| 11  | cB    | 830 | CLA  | C4C-C3C-C2C | -2.97 | 102.56      | 106.89   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aB    | 833 | CLA  | CHC-C1C-C2C | -2.97 | 118.50      | 126.95   |
| 11  | cA    | 824 | CLA  | CHD-C4C-NC  | 2.97  | 128.84      | 124.23   |
| 11  | aB    | 838 | CLA  | CAC-C3C-C4C | 2.97  | 128.66      | 124.79   |
| 11  | bB    | 806 | CLA  | CAA-C2A-C3A | -2.97 | 104.97      | 113.00   |
| 11  | cB    | 833 | CLA  | CHC-C1C-C2C | -2.97 | 118.50      | 126.95   |
| 11  | bB    | 836 | CLA  | CMB-C2B-C1B | 2.97  | 129.94      | 125.42   |
| 11  | aA    | 829 | CLA  | C4C-C3C-C2C | -2.97 | 102.57      | 106.89   |
| 11  | cK    | 101 | CLA  | CAC-C3C-C4C | 2.97  | 128.66      | 124.79   |
| 11  | bB    | 832 | CLA  | CMB-C2B-C1B | 2.97  | 129.94      | 125.42   |
| 12  | aA    | 844 | F6C  | CHD-C4C-NC  | 2.97  | 128.51      | 124.05   |
| 11  | bA    | 803 | CLA  | C1C-C2C-C3C | -2.97 | 103.86      | 106.98   |
| 11  | aB    | 836 | CLA  | CMB-C2B-C1B | 2.97  | 129.94      | 125.42   |
| 11  | cB    | 813 | CLA  | C4C-C3C-C2C | -2.97 | 102.57      | 106.89   |
| 11  | cB    | 806 | CLA  | CAA-C2A-C3A | -2.97 | 104.98      | 113.00   |
| 11  | aB    | 832 | CLA  | CMB-C2B-C1B | 2.97  | 129.94      | 125.42   |
| 11  | bB    | 838 | CLA  | C4C-C3C-C2C | -2.97 | 102.57      | 106.89   |
| 12  | cA    | 844 | F6C  | CHD-C4C-NC  | 2.97  | 128.50      | 124.05   |
| 11  | bA    | 805 | CLA  | CAC-C3C-C4C | 2.97  | 128.65      | 124.79   |
| 11  | bA    | 804 | CLA  | CHC-C1C-C2C | -2.97 | 118.52      | 126.95   |
| 11  | cB    | 830 | CLA  | C4B-C3B-C2B | -2.97 | 103.61      | 107.30   |
| 11  | bA    | 817 | CLA  | CAA-C2A-C3A | -2.97 | 104.99      | 113.00   |
| 11  | cA    | 840 | CLA  | CHC-C1C-C2C | -2.97 | 118.52      | 126.95   |
| 11  | aK    | 103 | CLA  | O2A-CGA-CBA | 2.97  | 120.88      | 111.83   |
| 11  | aA    | 806 | CLA  | C4B-C3B-C2B | -2.97 | 103.61      | 107.30   |
| 11  | aA    | 837 | CLA  | C4C-C3C-C2C | -2.96 | 102.58      | 106.89   |
| 11  | aB    | 813 | CLA  | C4C-C3C-C2C | -2.96 | 102.58      | 106.89   |
| 11  | cB    | 817 | CLA  | CHD-C4C-NC  | 2.96  | 128.83      | 124.23   |
| 11  | aA    | 828 | CLA  | C4B-C3B-C2B | -2.96 | 103.62      | 107.30   |
| 11  | cA    | 806 | CLA  | C4-C3-C5    | 2.96  | 120.37      | 115.23   |
| 11  | aA    | 837 | CLA  | CHD-C4C-NC  | 2.96  | 128.82      | 124.23   |
| 11  | cB    | 839 | CLA  | CHD-C4C-NC  | 2.96  | 128.82      | 124.23   |
| 11  | bL    | 205 | CLA  | C4C-C3C-C2C | -2.96 | 102.58      | 106.89   |
| 11  | cA    | 837 | CLA  | C4C-C3C-C2C | -2.96 | 102.58      | 106.89   |
| 11  | bK    | 101 | CLA  | CAC-C3C-C4C | 2.96  | 128.64      | 124.79   |
| 11  | bB    | 813 | CLA  | C4C-C3C-C2C | -2.96 | 102.58      | 106.89   |
| 11  | bA    | 806 | CLA  | C4B-C3B-C2B | -2.96 | 103.62      | 107.30   |
| 11  | bA    | 828 | CLA  | C4B-C3B-C2B | -2.96 | 103.62      | 107.30   |
| 11  | aA    | 804 | CLA  | CHC-C1C-C2C | -2.96 | 118.53      | 126.95   |
| 11  | aA    | 817 | CLA  | CAA-C2A-C3A | -2.96 | 105.00      | 113.00   |
| 11  | aB    | 837 | CLA  | C4C-C3C-C2C | -2.96 | 102.58      | 106.89   |
| 11  | bA    | 841 | CLA  | C4C-C3C-C2C | -2.96 | 102.58      | 106.89   |
| 11  | cA    | 804 | CLA  | CHC-C1C-C2C | -2.96 | 118.53      | 126.95   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cA    | 820 | CLA  | C1-C2-C3    | -2.96 | 121.35      | 126.20   |
| 11  | cA    | 814 | CLA  | C4B-C3B-C2B | -2.96 | 103.62      | 107.30   |
| 11  | cA    | 828 | CLA  | C4B-C3B-C2B | -2.96 | 103.62      | 107.30   |
| 11  | bB    | 833 | CLA  | CHC-C1C-C2C | -2.96 | 118.54      | 126.95   |
| 12  | aA    | 826 | F6C  | O2D-CGD-O1D | -2.96 | 118.09      | 123.85   |
| 12  | bA    | 826 | F6C  | O2D-CGD-O1D | -2.96 | 118.09      | 123.85   |
| 12  | bA    | 832 | F6C  | CHD-C4C-NC  | 2.96  | 128.49      | 124.05   |
| 12  | bA    | 844 | F6C  | CHD-C4C-NC  | 2.96  | 128.49      | 124.05   |
| 11  | aA    | 841 | CLA  | CAC-C3C-C4C | 2.96  | 128.64      | 124.79   |
| 11  | bL    | 205 | CLA  | CAC-C3C-C4C | 2.96  | 128.64      | 124.79   |
| 11  | cA    | 806 | CLA  | C4B-C3B-C2B | -2.96 | 103.62      | 107.30   |
| 11  | bA    | 835 | CLA  | C3B-C4B-NB  | 2.96  | 113.17      | 110.53   |
| 12  | aA    | 827 | F6C  | C4-C3-C5    | 2.96  | 120.36      | 115.23   |
| 11  | aA    | 840 | CLA  | CHC-C1C-C2C | -2.96 | 118.55      | 126.95   |
| 11  | cA    | 835 | CLA  | C3B-C4B-NB  | 2.96  | 113.17      | 110.53   |
| 11  | cB    | 826 | CLA  | CAA-C2A-C3A | -2.95 | 105.01      | 113.00   |
| 11  | bA    | 808 | CLA  | CHC-C1C-C2C | -2.95 | 118.55      | 126.95   |
| 13  | bA    | 845 | PQN  | C11-C3-C2   | -2.95 | 119.83      | 124.89   |
| 12  | cA    | 830 | F6C  | CHD-C4C-NC  | 2.95  | 128.48      | 124.05   |
| 11  | bA    | 804 | CLA  | CHD-C4C-NC  | 2.95  | 128.81      | 124.23   |
| 15  | aL    | 207 | BCR  | C27-C26-C25 | 2.95  | 126.69      | 122.70   |
| 11  | bB    | 837 | CLA  | C4C-C3C-C2C | -2.95 | 102.60      | 106.89   |
| 11  | cB    | 832 | CLA  | CMB-C2B-C1B | 2.95  | 129.91      | 125.42   |
| 11  | cB    | 838 | CLA  | CAC-C3C-C4C | 2.95  | 128.63      | 124.79   |
| 11  | aA    | 808 | CLA  | CHC-C1C-C2C | -2.95 | 118.57      | 126.95   |
| 11  | cB    | 804 | CLA  | C4A-NA-C1A  | -2.95 | 105.33      | 106.68   |
| 11  | cA    | 804 | CLA  | CHD-C4C-NC  | 2.95  | 128.80      | 124.23   |
| 11  | aB    | 812 | CLA  | C1-C2-C3    | -2.95 | 121.37      | 126.20   |
| 11  | bA    | 802 | CLA  | C1-C2-C3    | -2.95 | 121.37      | 126.20   |
| 11  | aA    | 814 | CLA  | C4B-C3B-C2B | -2.95 | 103.64      | 107.30   |
| 11  | aB    | 834 | CLA  | CAC-C3C-C4C | 2.95  | 128.62      | 124.79   |
| 15  | bM    | 101 | BCR  | C15-C16-C17 | -2.95 | 117.49      | 123.52   |
| 11  | cA    | 841 | CLA  | CAC-C3C-C4C | 2.95  | 128.62      | 124.79   |
| 11  | cA    | 837 | CLA  | CHC-C1C-C2C | -2.95 | 118.58      | 126.95   |
| 11  | bA    | 814 | CLA  | C4B-C3B-C2B | -2.94 | 103.64      | 107.30   |
| 11  | aA    | 841 | CLA  | C4C-C3C-C2C | -2.94 | 102.61      | 106.89   |
| 11  | cA    | 841 | CLA  | C4C-C3C-C2C | -2.94 | 102.61      | 106.89   |
| 11  | aA    | 805 | CLA  | CHD-C4C-NC  | 2.94  | 128.80      | 124.23   |
| 11  | cA    | 808 | CLA  | CHC-C1C-C2C | -2.94 | 118.58      | 126.95   |
| 11  | bA    | 822 | CLA  | C4C-C3C-C2C | -2.94 | 102.61      | 106.89   |
| 11  | cB    | 807 | CLA  | O2D-CGD-O1D | -2.94 | 118.12      | 123.85   |
| 11  | aA    | 802 | CLA  | C1-C2-C3    | -2.94 | 121.38      | 126.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aB    | 826 | CLA  | CAA-C2A-C3A | -2.94 | 105.05      | 113.00   |
| 11  | bB    | 807 | CLA  | O2D-CGD-O1D | -2.94 | 118.12      | 123.85   |
| 11  | cB    | 823 | CLA  | CHC-C1C-C2C | -2.94 | 118.58      | 126.95   |
| 11  | bB    | 812 | CLA  | C1-C2-C3    | -2.94 | 121.38      | 126.20   |
| 11  | bB    | 804 | CLA  | CMC-C2C-C1C | 2.94  | 129.63      | 125.03   |
| 11  | bB    | 823 | CLA  | CHC-C1C-C2C | -2.94 | 118.59      | 126.95   |
| 11  | bA    | 806 | CLA  | C4-C3-C5    | 2.94  | 120.33      | 115.23   |
| 11  | cA    | 816 | CLA  | CAC-C3C-C4C | 2.94  | 128.62      | 124.79   |
| 11  | cA    | 842 | CLA  | CHD-C4C-NC  | 2.94  | 128.79      | 124.23   |
| 12  | aA    | 827 | F6C  | O2D-CGD-O1D | -2.94 | 118.12      | 123.85   |
| 11  | bB    | 826 | CLA  | CAA-C2A-C3A | -2.94 | 105.05      | 113.00   |
| 11  | bB    | 818 | CLA  | C1C-C2C-C3C | -2.94 | 103.89      | 106.98   |
| 11  | aA    | 828 | CLA  | CHC-C1C-C2C | -2.94 | 118.60      | 126.95   |
| 11  | aA    | 837 | CLA  | CHC-C1C-C2C | -2.94 | 118.60      | 126.95   |
| 11  | aA    | 822 | CLA  | C4C-C3C-C2C | -2.94 | 102.61      | 106.89   |
| 11  | bB    | 807 | CLA  | C4C-C3C-C2C | -2.94 | 102.61      | 106.89   |
| 15  | bL    | 207 | BCR  | C27-C26-C25 | 2.94  | 126.67      | 122.70   |
| 11  | aB    | 804 | CLA  | CMC-C2C-C1C | 2.94  | 129.62      | 125.03   |
| 11  | bA    | 837 | CLA  | CHC-C1C-C2C | -2.94 | 118.60      | 126.95   |
| 12  | bA    | 827 | F6C  | O2D-CGD-O1D | -2.94 | 118.13      | 123.85   |
| 12  | aA    | 830 | F6C  | CHD-C4C-NC  | 2.94  | 128.45      | 124.05   |
| 11  | aA    | 835 | CLA  | C3B-C4B-NB  | 2.94  | 113.15      | 110.53   |
| 11  | cB    | 818 | CLA  | C3B-C4B-NB  | 2.94  | 113.15      | 110.53   |
| 13  | cA    | 845 | PQN  | C11-C3-C2   | -2.94 | 119.86      | 124.89   |
| 11  | cA    | 810 | CLA  | C4A-NA-C1A  | -2.93 | 105.34      | 106.68   |
| 11  | cB    | 833 | CLA  | C3B-C4B-NB  | 2.93  | 113.15      | 110.53   |
| 11  | bA    | 809 | CLA  | CAC-C3C-C4C | 2.93  | 128.61      | 124.79   |
| 12  | bA    | 830 | F6C  | CHD-C4C-NC  | 2.93  | 128.45      | 124.05   |
| 11  | cA    | 822 | CLA  | C4C-C3C-C2C | -2.93 | 102.62      | 106.89   |
| 11  | cB    | 807 | CLA  | C4C-C3C-C2C | -2.93 | 102.62      | 106.89   |
| 11  | aB    | 823 | CLA  | CHC-C1C-C2C | -2.93 | 118.62      | 126.95   |
| 11  | cB    | 818 | CLA  | C1C-C2C-C3C | -2.93 | 103.90      | 106.98   |
| 11  | cB    | 812 | CLA  | C1-C2-C3    | -2.93 | 121.39      | 126.20   |
| 11  | aB    | 839 | CLA  | CHD-C4C-NC  | 2.93  | 128.77      | 124.23   |
| 11  | cB    | 834 | CLA  | CAC-C3C-C4C | 2.93  | 128.60      | 124.79   |
| 11  | aA    | 820 | CLA  | C1-C2-C3    | -2.93 | 121.40      | 126.20   |
| 11  | cB    | 806 | CLA  | C1-C2-C3    | -2.93 | 121.40      | 126.20   |
| 10  | cA    | 801 | CL0  | O2A-CGA-CBA | 2.93  | 120.77      | 111.83   |
| 11  | aB    | 806 | CLA  | C1-C2-C3    | -2.93 | 121.40      | 126.20   |
| 11  | aA    | 809 | CLA  | CAC-C3C-C4C | 2.93  | 128.60      | 124.79   |
| 11  | aA    | 815 | CLA  | C4C-C3C-C2C | -2.93 | 102.63      | 106.89   |
| 11  | bA    | 815 | CLA  | C4C-C3C-C2C | -2.93 | 102.63      | 106.89   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bB    | 823 | CLA  | CAC-C3C-C4C | 2.93  | 128.60      | 124.79   |
| 11  | aA    | 808 | CLA  | C4C-C3C-C2C | -2.93 | 102.63      | 106.89   |
| 11  | aA    | 838 | CLA  | CHC-C1C-C2C | -2.93 | 118.63      | 126.95   |
| 11  | bA    | 828 | CLA  | CHC-C1C-C2C | -2.93 | 118.63      | 126.95   |
| 11  | cA    | 828 | CLA  | CHC-C1C-C2C | -2.93 | 118.63      | 126.95   |
| 11  | aA    | 816 | CLA  | CAC-C3C-C4C | 2.92  | 128.59      | 124.79   |
| 11  | bA    | 842 | CLA  | CHC-C1C-C2C | -2.92 | 118.64      | 126.95   |
| 11  | bA    | 810 | CLA  | C4A-NA-C1A  | -2.92 | 105.34      | 106.68   |
| 10  | bA    | 801 | CL0  | O2A-CGA-CBA | 2.92  | 120.75      | 111.83   |
| 10  | aA    | 801 | CL0  | O2A-CGA-CBA | 2.92  | 120.75      | 111.83   |
| 11  | bA    | 808 | CLA  | C4C-C3C-C2C | -2.92 | 102.64      | 106.89   |
| 11  | bB    | 832 | CLA  | C4C-C3C-C2C | -2.92 | 102.64      | 106.89   |
| 11  | cA    | 808 | CLA  | C4C-C3C-C2C | -2.92 | 102.64      | 106.89   |
| 11  | aA    | 806 | CLA  | C4-C3-C5    | 2.92  | 120.30      | 115.23   |
| 11  | aB    | 831 | CLA  | CBA-CAA-C2A | 2.92  | 122.48      | 113.79   |
| 12  | bL    | 202 | F6C  | O2A-CGA-O1A | -2.92 | 116.32      | 123.63   |
| 11  | bA    | 814 | CLA  | CHC-C1C-C2C | -2.92 | 118.65      | 126.95   |
| 11  | bB    | 806 | CLA  | C1-C2-C3    | -2.92 | 121.41      | 126.20   |
| 11  | cB    | 832 | CLA  | C4C-C3C-C2C | -2.92 | 102.64      | 106.89   |
| 11  | aB    | 825 | CLA  | O2A-CGA-CBA | 2.92  | 120.74      | 111.83   |
| 11  | bA    | 838 | CLA  | CHC-C1C-C2C | -2.92 | 118.65      | 126.95   |
| 15  | cB    | 845 | BCR  | C27-C26-C25 | 2.92  | 126.65      | 122.70   |
| 11  | bA    | 803 | CLA  | CAC-C3C-C4C | 2.92  | 128.59      | 124.79   |
| 11  | bA    | 820 | CLA  | C1-C2-C3    | -2.92 | 121.42      | 126.20   |
| 11  | cB    | 806 | CLA  | CHC-C1C-C2C | -2.92 | 118.66      | 126.95   |
| 11  | cB    | 805 | CLA  | C4C-C3C-C2C | -2.92 | 102.65      | 106.89   |
| 11  | cA    | 814 | CLA  | CHC-C1C-C2C | -2.92 | 118.66      | 126.95   |
| 11  | cA    | 805 | CLA  | CHD-C4C-NC  | 2.92  | 128.75      | 124.23   |
| 11  | aB    | 818 | CLA  | C1C-C2C-C3C | -2.92 | 103.91      | 106.98   |
| 11  | cA    | 807 | CLA  | C4B-C3B-C2B | -2.92 | 103.68      | 107.30   |
| 11  | aA    | 814 | CLA  | CHC-C1C-C2C | -2.92 | 118.66      | 126.95   |
| 11  | bA    | 842 | CLA  | CHD-C4C-NC  | 2.92  | 128.75      | 124.23   |
| 11  | aA    | 842 | CLA  | CHC-C1C-C2C | -2.92 | 118.66      | 126.95   |
| 11  | aL    | 206 | CLA  | CHC-C1C-C2C | -2.92 | 118.66      | 126.95   |
| 11  | bB    | 808 | CLA  | CAC-C3C-C4C | 2.92  | 128.58      | 124.79   |
| 11  | bB    | 819 | CLA  | C4C-C3C-C2C | -2.92 | 102.65      | 106.89   |
| 11  | bB    | 823 | CLA  | C4C-C3C-C2C | -2.91 | 102.65      | 106.89   |
| 15  | bB    | 845 | BCR  | C27-C26-C25 | 2.91  | 126.64      | 122.70   |
| 13  | aA    | 845 | PQN  | C11-C3-C2   | -2.91 | 119.90      | 124.89   |
| 11  | aA    | 842 | CLA  | CHD-C4C-NC  | 2.91  | 128.75      | 124.23   |
| 11  | bA    | 805 | CLA  | CHD-C4C-NC  | 2.91  | 128.75      | 124.23   |
| 11  | aB    | 808 | CLA  | CAC-C3C-C4C | 2.91  | 128.58      | 124.79   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bB    | 828 | CLA  | C1-C2-C3    | -2.91 | 121.43      | 126.20   |
| 11  | bB    | 831 | CLA  | CBA-CAA-C2A | 2.91  | 122.46      | 113.79   |
| 11  | bA    | 840 | CLA  | O2D-CGD-O1D | -2.91 | 118.18      | 123.85   |
| 11  | cA    | 842 | CLA  | CHC-C1C-C2C | -2.91 | 118.67      | 126.95   |
| 11  | bB    | 825 | CLA  | C4B-C3B-C2B | -2.91 | 103.68      | 107.30   |
| 11  | aB    | 832 | CLA  | C4C-C3C-C2C | -2.91 | 102.65      | 106.89   |
| 11  | cA    | 838 | CLA  | CHC-C1C-C2C | -2.91 | 118.67      | 126.95   |
| 11  | bB    | 834 | CLA  | CAC-C3C-C4C | 2.91  | 128.58      | 124.79   |
| 11  | bB    | 838 | CLA  | CAC-C3C-C4C | 2.91  | 128.58      | 124.79   |
| 11  | aB    | 807 | CLA  | C4C-C3C-C2C | -2.91 | 102.66      | 106.89   |
| 12  | aL    | 202 | F6C  | O2A-CGA-O1A | -2.91 | 116.35      | 123.63   |
| 11  | cB    | 831 | CLA  | CBA-CAA-C2A | 2.91  | 122.45      | 113.79   |
| 11  | aB    | 807 | CLA  | O2D-CGD-O1D | -2.91 | 118.18      | 123.85   |
| 11  | bB    | 817 | CLA  | C1-O2A-CGA  | 2.91  | 123.69      | 116.65   |
| 11  | bB    | 806 | CLA  | CHC-C1C-C2C | -2.91 | 118.68      | 126.95   |
| 12  | cL    | 202 | F6C  | O2A-CGA-O1A | -2.91 | 116.35      | 123.63   |
| 11  | bB    | 830 | CLA  | CAC-C3C-C4C | 2.91  | 128.57      | 124.79   |
| 11  | bB    | 833 | CLA  | C3B-C4B-NB  | 2.91  | 113.13      | 110.53   |
| 11  | bB    | 837 | CLA  | CHD-C4C-NC  | 2.91  | 128.74      | 124.23   |
| 11  | cB    | 830 | CLA  | CAC-C3C-C4C | 2.91  | 128.57      | 124.79   |
| 11  | cK    | 103 | CLA  | C4-C3-C5    | 2.91  | 119.55      | 116.13   |
| 11  | aB    | 821 | CLA  | C4-C3-C5    | 2.91  | 120.27      | 115.23   |
| 11  | cB    | 827 | CLA  | CAC-C3C-C4C | 2.91  | 128.57      | 124.79   |
| 11  | aL    | 205 | CLA  | O2D-CGD-O1D | -2.91 | 118.19      | 123.85   |
| 11  | cL    | 206 | CLA  | CHC-C1C-C2C | -2.91 | 118.69      | 126.95   |
| 11  | bK    | 103 | CLA  | C4-C3-C5    | 2.90  | 119.55      | 116.13   |
| 11  | aB    | 828 | CLA  | C1-C2-C3    | -2.90 | 121.44      | 126.20   |
| 15  | cL    | 207 | BCR  | C27-C26-C25 | 2.90  | 126.63      | 122.70   |
| 11  | bA    | 816 | CLA  | CAC-C3C-C4C | 2.90  | 128.57      | 124.79   |
| 11  | bB    | 825 | CLA  | O2A-CGA-CBA | 2.90  | 120.69      | 111.83   |
| 11  | bL    | 205 | CLA  | O2D-CGD-O1D | -2.90 | 118.20      | 123.85   |
| 12  | cA    | 827 | F6C  | O2D-CGD-O1D | -2.90 | 118.20      | 123.85   |
| 11  | bA    | 807 | CLA  | C4B-C3B-C2B | -2.90 | 103.69      | 107.30   |
| 11  | cB    | 823 | CLA  | CAC-C3C-C4C | 2.90  | 128.57      | 124.79   |
| 11  | cA    | 815 | CLA  | C4C-C3C-C2C | -2.90 | 102.67      | 106.89   |
| 15  | aA    | 849 | BCR  | C11-C10-C9  | -2.90 | 123.21      | 127.28   |
| 11  | aA    | 804 | CLA  | CHD-C4C-NC  | 2.90  | 128.73      | 124.23   |
| 11  | cB    | 823 | CLA  | C4C-C3C-C2C | -2.90 | 102.67      | 106.89   |
| 15  | aB    | 845 | BCR  | C27-C26-C25 | 2.90  | 126.62      | 122.70   |
| 11  | cB    | 819 | CLA  | C4C-C3C-C2C | -2.90 | 102.67      | 106.89   |
| 11  | aB    | 806 | CLA  | CHC-C1C-C2C | -2.90 | 118.71      | 126.95   |
| 11  | bL    | 206 | CLA  | CHC-C1C-C2C | -2.90 | 118.71      | 126.95   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aB    | 802 | CLA  | CMC-C2C-C1C | 2.90  | 129.56      | 125.03   |
| 11  | aB    | 823 | CLA  | CAC-C3C-C4C | 2.90  | 128.56      | 124.79   |
| 11  | bB    | 812 | CLA  | C4B-C3B-C2B | -2.90 | 103.70      | 107.30   |
| 11  | bB    | 805 | CLA  | C4C-C3C-C2C | -2.90 | 102.67      | 106.89   |
| 11  | aB    | 823 | CLA  | C1-O2A-CGA  | 2.90  | 123.67      | 116.65   |
| 11  | cB    | 825 | CLA  | O2A-CGA-CBA | 2.90  | 120.66      | 111.83   |
| 11  | bB    | 826 | CLA  | CHC-C1C-C2C | -2.89 | 118.72      | 126.95   |
| 11  | cB    | 828 | CLA  | C1-C2-C3    | -2.89 | 121.45      | 126.20   |
| 11  | cB    | 825 | CLA  | C4B-C3B-C2B | -2.89 | 103.70      | 107.30   |
| 11  | cL    | 205 | CLA  | O2D-CGD-O1D | -2.89 | 118.22      | 123.85   |
| 11  | bA    | 834 | CLA  | C4C-C3C-C2C | -2.89 | 102.68      | 106.89   |
| 11  | bB    | 827 | CLA  | CAC-C3C-C4C | 2.89  | 128.55      | 124.79   |
| 15  | bA    | 849 | BCR  | C11-C10-C9  | -2.89 | 123.22      | 127.28   |
| 11  | cB    | 836 | CLA  | O2A-CGA-CBA | 2.89  | 120.65      | 111.83   |
| 11  | aA    | 840 | CLA  | O2D-CGD-O1D | -2.89 | 118.22      | 123.85   |
| 11  | bB    | 839 | CLA  | C4B-C3B-C2B | -2.89 | 103.71      | 107.30   |
| 12  | bA    | 832 | F6C  | O2A-CGA-CBA | 2.89  | 120.65      | 111.83   |
| 11  | aB    | 834 | CLA  | C4C-C3C-C2C | -2.89 | 102.69      | 106.89   |
| 11  | cB    | 802 | CLA  | CMC-C2C-C1C | 2.89  | 129.55      | 125.03   |
| 12  | aA    | 832 | F6C  | O2A-CGA-CBA | 2.89  | 120.64      | 111.83   |
| 11  | bB    | 802 | CLA  | CMC-C2C-C1C | 2.89  | 129.55      | 125.03   |
| 11  | aB    | 826 | CLA  | CHC-C1C-C2C | -2.89 | 118.75      | 126.95   |
| 11  | cA    | 808 | CLA  | C4B-C3B-C2B | -2.89 | 103.71      | 107.30   |
| 11  | aB    | 823 | CLA  | C4C-C3C-C2C | -2.89 | 102.69      | 106.89   |
| 11  | aA    | 833 | CLA  | CHD-C4C-NC  | 2.89  | 128.71      | 124.23   |
| 11  | cB    | 833 | CLA  | CHD-C4C-NC  | 2.89  | 128.71      | 124.23   |
| 11  | cB    | 816 | CLA  | C4C-C3C-C2C | -2.89 | 102.69      | 106.89   |
| 11  | aA    | 834 | CLA  | CHD-C4C-NC  | 2.88  | 128.70      | 124.23   |
| 11  | cA    | 833 | CLA  | CHD-C4C-NC  | 2.88  | 128.70      | 124.23   |
| 11  | aB    | 833 | CLA  | C3B-C4B-NB  | 2.88  | 113.11      | 110.53   |
| 11  | bB    | 836 | CLA  | O2A-CGA-CBA | 2.88  | 120.63      | 111.83   |
| 11  | cL    | 204 | CLA  | C4C-C3C-C2C | -2.88 | 102.69      | 106.89   |
| 11  | cA    | 803 | CLA  | CAC-C3C-C4C | 2.88  | 128.54      | 124.79   |
| 11  | aB    | 817 | CLA  | C1-O2A-CGA  | 2.88  | 123.63      | 116.65   |
| 11  | cB    | 817 | CLA  | C1-O2A-CGA  | 2.88  | 123.63      | 116.65   |
| 11  | cB    | 826 | CLA  | CHC-C1C-C2C | -2.88 | 118.75      | 126.95   |
| 11  | aB    | 823 | CLA  | C4B-C3B-C2B | -2.88 | 103.72      | 107.30   |
| 11  | aB    | 825 | CLA  | C4B-C3B-C2B | -2.88 | 103.72      | 107.30   |
| 11  | bB    | 837 | CLA  | CHC-C1C-C2C | -2.88 | 118.75      | 126.95   |
| 11  | aK    | 103 | CLA  | C4-C3-C5    | 2.88  | 119.52      | 116.13   |
| 11  | cB    | 834 | CLA  | C4C-C3C-C2C | -2.88 | 102.70      | 106.89   |
| 11  | bB    | 821 | CLA  | C4-C3-C5    | 2.88  | 120.23      | 115.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aB    | 837 | CLA  | CHC-C1C-C2C | -2.88 | 118.76      | 126.95   |
| 11  | cB    | 823 | CLA  | C1-O2A-CGA  | 2.88  | 123.63      | 116.65   |
| 12  | cA    | 832 | F6C  | O2A-CGA-CBA | 2.88  | 120.62      | 111.83   |
| 11  | cA    | 839 | CLA  | C4C-C3C-C2C | -2.88 | 102.70      | 106.89   |
| 11  | bA    | 823 | CLA  | C4B-C3B-C2B | -2.88 | 103.72      | 107.30   |
| 11  | cA    | 803 | CLA  | CMB-C2B-C3B | 2.88  | 133.33      | 126.55   |
| 11  | cB    | 808 | CLA  | CHD-C1D-ND  | -2.88 | 120.75      | 124.80   |
| 11  | aB    | 837 | CLA  | CHD-C4C-NC  | 2.88  | 128.70      | 124.23   |
| 11  | bA    | 808 | CLA  | C4B-C3B-C2B | -2.88 | 103.72      | 107.30   |
| 11  | cA    | 840 | CLA  | O2D-CGD-O1D | -2.88 | 118.24      | 123.85   |
| 11  | cB    | 815 | CLA  | C3B-C4B-NB  | 2.88  | 113.10      | 110.53   |
| 11  | bA    | 822 | CLA  | CMB-C2B-C1B | 2.88  | 129.80      | 125.42   |
| 15  | aB    | 844 | BCR  | C27-C26-C25 | 2.88  | 126.59      | 122.70   |
| 11  | bB    | 810 | CLA  | CAC-C3C-C4C | 2.88  | 128.54      | 124.79   |
| 11  | cB    | 801 | CLA  | CHC-C1C-C2C | -2.88 | 118.77      | 126.95   |
| 11  | aA    | 807 | CLA  | C4B-C3B-C2B | -2.88 | 103.72      | 107.30   |
| 11  | aB    | 808 | CLA  | CHD-C1D-ND  | -2.88 | 120.75      | 124.80   |
| 11  | bB    | 808 | CLA  | CHD-C1D-ND  | -2.88 | 120.75      | 124.80   |
| 11  | aA    | 803 | CLA  | CMB-C2B-C3B | 2.88  | 133.32      | 126.55   |
| 11  | bB    | 804 | CLA  | CBA-CAA-C2A | 2.88  | 122.36      | 113.79   |
| 15  | cB    | 844 | BCR  | C27-C26-C25 | 2.88  | 126.59      | 122.70   |
| 11  | cB    | 837 | CLA  | CHC-C1C-C2C | -2.88 | 118.77      | 126.95   |
| 11  | bB    | 823 | CLA  | C4B-C3B-C2B | -2.88 | 103.72      | 107.30   |
| 15  | cA    | 849 | BCR  | C11-C10-C9  | -2.88 | 123.24      | 127.28   |
| 11  | aL    | 204 | CLA  | C4C-C3C-C2C | -2.88 | 102.70      | 106.89   |
| 11  | bA    | 835 | CLA  | C4C-C3C-C2C | -2.88 | 102.70      | 106.89   |
| 11  | cA    | 839 | CLA  | CMB-C2B-C1B | 2.88  | 129.80      | 125.42   |
| 11  | cB    | 823 | CLA  | CMC-C2C-C1C | 2.88  | 129.53      | 125.03   |
| 11  | cA    | 834 | CLA  | CHD-C4C-NC  | 2.88  | 128.69      | 124.23   |
| 11  | cB    | 837 | CLA  | CHD-C4C-NC  | 2.88  | 128.69      | 124.23   |
| 11  | cB    | 821 | CLA  | C4-C3-C5    | 2.88  | 120.22      | 115.23   |
| 11  | cB    | 808 | CLA  | CAC-C3C-C4C | 2.88  | 128.53      | 124.79   |
| 11  | aB    | 804 | CLA  | CBA-CAA-C2A | 2.87  | 122.35      | 113.79   |
| 11  | aA    | 835 | CLA  | C4C-C3C-C2C | -2.87 | 102.71      | 106.89   |
| 11  | aB    | 830 | CLA  | CAC-C3C-C4C | 2.87  | 128.53      | 124.79   |
| 11  | aB    | 833 | CLA  | CHD-C4C-NC  | 2.87  | 128.69      | 124.23   |
| 11  | aA    | 839 | CLA  | C4C-C3C-C2C | -2.87 | 102.71      | 106.89   |
| 11  | cA    | 834 | CLA  | C4C-C3C-C2C | -2.87 | 102.71      | 106.89   |
| 11  | cA    | 835 | CLA  | C4C-C3C-C2C | -2.87 | 102.71      | 106.89   |
| 11  | aB    | 801 | CLA  | CHC-C1C-C2C | -2.87 | 118.78      | 126.95   |
| 11  | aB    | 831 | CLA  | C4C-C3C-C2C | -2.87 | 102.71      | 106.89   |
| 11  | bA    | 833 | CLA  | CHD-C4C-NC  | 2.87  | 128.69      | 124.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aB    | 836 | CLA  | CHC-C1C-C2C | -2.87 | 118.78      | 126.95   |
| 11  | cB    | 804 | CLA  | CBA-CAA-C2A | 2.87  | 122.34      | 113.79   |
| 11  | bA    | 840 | CLA  | O2A-CGA-CBA | 2.87  | 120.59      | 111.83   |
| 11  | bB    | 801 | CLA  | CHC-C1C-C2C | -2.87 | 118.79      | 126.95   |
| 11  | aA    | 821 | CLA  | CMB-C2B-C1B | 2.87  | 129.79      | 125.42   |
| 11  | bB    | 823 | CLA  | C1-O2A-CGA  | 2.87  | 123.60      | 116.65   |
| 12  | aL    | 202 | F6C  | CAC-C3C-C4C | 2.87  | 128.86      | 124.91   |
| 11  | bB    | 806 | CLA  | C3B-C4B-NB  | 2.87  | 113.09      | 110.53   |
| 11  | aK    | 101 | CLA  | C4C-C3C-C2C | -2.87 | 102.71      | 106.89   |
| 11  | bA    | 822 | CLA  | CHD-C4C-NC  | 2.87  | 128.68      | 124.23   |
| 11  | bB    | 833 | CLA  | CHD-C4C-NC  | 2.87  | 128.68      | 124.23   |
| 11  | bB    | 831 | CLA  | C4C-C3C-C2C | -2.87 | 102.71      | 106.89   |
| 11  | cK    | 101 | CLA  | C4C-C3C-C2C | -2.87 | 102.71      | 106.89   |
| 11  | cA    | 823 | CLA  | C4B-C3B-C2B | -2.87 | 103.73      | 107.30   |
| 11  | cB    | 803 | CLA  | C4B-C3B-C2B | -2.87 | 103.73      | 107.30   |
| 11  | aB    | 819 | CLA  | C4C-C3C-C2C | -2.87 | 102.72      | 106.89   |
| 11  | bL    | 204 | CLA  | C4C-C3C-C2C | -2.87 | 102.72      | 106.89   |
| 11  | aA    | 803 | CLA  | CAC-C3C-C4C | 2.87  | 128.52      | 124.79   |
| 11  | aB    | 836 | CLA  | O2A-CGA-CBA | 2.87  | 120.58      | 111.83   |
| 11  | bA    | 803 | CLA  | CMB-C2B-C3B | 2.87  | 133.30      | 126.55   |
| 11  | cB    | 836 | CLA  | CHC-C1C-C2C | -2.87 | 118.80      | 126.95   |
| 11  | cA    | 822 | CLA  | CMB-C2B-C1B | 2.87  | 129.79      | 125.42   |
| 11  | bB    | 836 | CLA  | CHC-C1C-C2C | -2.87 | 118.80      | 126.95   |
| 11  | bA    | 834 | CLA  | CHD-C4C-NC  | 2.87  | 128.68      | 124.23   |
| 11  | aA    | 802 | CLA  | C4C-C3C-C2C | -2.87 | 102.72      | 106.89   |
| 11  | aB    | 803 | CLA  | C4B-C3B-C2B | -2.87 | 103.74      | 107.30   |
| 11  | cB    | 812 | CLA  | C4B-C3B-C2B | -2.87 | 103.74      | 107.30   |
| 11  | aB    | 816 | CLA  | C4C-C3C-C2C | -2.87 | 102.72      | 106.89   |
| 11  | bA    | 838 | CLA  | CHD-C4C-NC  | 2.86  | 128.67      | 124.23   |
| 11  | bB    | 834 | CLA  | C4C-C3C-C2C | -2.86 | 102.72      | 106.89   |
| 11  | cA    | 835 | CLA  | O2D-CGD-O1D | -2.86 | 118.27      | 123.85   |
| 11  | bL    | 206 | CLA  | C4-C3-C5    | 2.86  | 120.20      | 115.23   |
| 11  | aB    | 812 | CLA  | C4B-C3B-C2B | -2.86 | 103.74      | 107.30   |
| 11  | bB    | 803 | CLA  | C4B-C3B-C2B | -2.86 | 103.74      | 107.30   |
| 11  | aA    | 834 | CLA  | C4C-C3C-C2C | -2.86 | 102.72      | 106.89   |
| 11  | cA    | 840 | CLA  | C4C-C3C-C2C | -2.86 | 102.72      | 106.89   |
| 11  | aA    | 838 | CLA  | CHD-C4C-NC  | 2.86  | 128.67      | 124.23   |
| 11  | aA    | 840 | CLA  | O2A-CGA-CBA | 2.86  | 120.56      | 111.83   |
| 11  | bA    | 802 | CLA  | C4C-C3C-C2C | -2.86 | 102.73      | 106.89   |
| 11  | bK    | 101 | CLA  | C4C-C3C-C2C | -2.86 | 102.73      | 106.89   |
| 11  | bA    | 839 | CLA  | CMB-C2B-C1B | 2.86  | 129.77      | 125.42   |
| 11  | bB    | 815 | CLA  | C3B-C4B-NB  | 2.86  | 113.08      | 110.53   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bA    | 835 | CLA  | O2D-CGD-O1D | -2.86 | 118.28      | 123.85   |
| 11  | aA    | 825 | CLA  | C4C-C3C-C2C | -2.86 | 102.73      | 106.89   |
| 11  | bA    | 839 | CLA  | C4C-C3C-C2C | -2.86 | 102.73      | 106.89   |
| 11  | aB    | 822 | CLA  | C4A-NA-C1A  | -2.86 | 105.38      | 106.68   |
| 11  | cB    | 839 | CLA  | C4B-C3B-C2B | -2.86 | 103.75      | 107.30   |
| 11  | aA    | 839 | CLA  | CMB-C2B-C1B | 2.86  | 129.77      | 125.42   |
| 11  | aB    | 805 | CLA  | C4C-C3C-C2C | -2.86 | 102.73      | 106.89   |
| 12  | bL    | 202 | F6C  | CAC-C3C-C4C | 2.86  | 128.84      | 124.91   |
| 11  | aB    | 839 | CLA  | C4B-C3B-C2B | -2.85 | 103.75      | 107.30   |
| 11  | bB    | 816 | CLA  | C4C-C3C-C2C | -2.85 | 102.74      | 106.89   |
| 11  | aA    | 823 | CLA  | C4B-C3B-C2B | -2.85 | 103.75      | 107.30   |
| 11  | aA    | 803 | CLA  | CHC-C1C-C2C | -2.85 | 118.84      | 126.95   |
| 11  | aA    | 807 | CLA  | CAA-C2A-C3A | -2.85 | 105.29      | 113.00   |
| 11  | bL    | 205 | CLA  | C4B-C3B-C2B | -2.85 | 103.75      | 107.30   |
| 11  | bB    | 816 | CLA  | CAC-C3C-C4C | 2.85  | 128.50      | 124.79   |
| 15  | bB    | 844 | BCR  | C27-C26-C25 | 2.85  | 126.56      | 122.70   |
| 11  | aL    | 205 | CLA  | C4B-C3B-C2B | -2.85 | 103.75      | 107.30   |
| 11  | bB    | 823 | CLA  | O2D-CGD-O1D | -2.85 | 118.30      | 123.85   |
| 12  | bB    | 824 | F6C  | C4-C3-C5    | 2.85  | 120.18      | 115.23   |
| 12  | cL    | 202 | F6C  | CAC-C3C-C4C | 2.85  | 128.84      | 124.91   |
| 11  | bA    | 821 | CLA  | CMB-C2B-C1B | 2.85  | 129.76      | 125.42   |
| 11  | cA    | 803 | CLA  | CHC-C1C-C2C | -2.85 | 118.84      | 126.95   |
| 11  | cA    | 840 | CLA  | O2A-CGA-CBA | 2.85  | 120.53      | 111.83   |
| 11  | aB    | 827 | CLA  | CAC-C3C-C4C | 2.85  | 128.50      | 124.79   |
| 11  | cA    | 811 | CLA  | C4C-C3C-C2C | -2.85 | 102.74      | 106.89   |
| 11  | aA    | 840 | CLA  | CHD-C4C-NC  | 2.85  | 128.65      | 124.23   |
| 11  | bB    | 823 | CLA  | CMC-C2C-C1C | 2.85  | 129.49      | 125.03   |
| 11  | aB    | 831 | CLA  | CHD-C4C-NC  | 2.85  | 128.65      | 124.23   |
| 11  | aA    | 840 | CLA  | C4C-C3C-C2C | -2.85 | 102.74      | 106.89   |
| 11  | bB    | 819 | CLA  | CAC-C3C-C4C | 2.85  | 128.50      | 124.79   |
| 15  | cL    | 203 | BCR  | C7-C8-C9    | -2.85 | 122.02      | 126.23   |
| 11  | aB    | 823 | CLA  | CMC-C2C-C1C | 2.85  | 129.49      | 125.03   |
| 11  | aB    | 810 | CLA  | CAC-C3C-C4C | 2.85  | 128.50      | 124.79   |
| 11  | cB    | 810 | CLA  | CAC-C3C-C4C | 2.85  | 128.50      | 124.79   |
| 12  | bL    | 202 | F6C  | C4C-C3C-C2C | -2.85 | 102.46      | 106.87   |
| 11  | bA    | 803 | CLA  | CHC-C1C-C2C | -2.85 | 118.86      | 126.95   |
| 11  | bA    | 840 | CLA  | CHD-C4C-NC  | 2.85  | 128.65      | 124.23   |
| 11  | cB    | 831 | CLA  | CHD-C4C-NC  | 2.85  | 128.65      | 124.23   |
| 11  | aB    | 815 | CLA  | C3B-C4B-NB  | 2.85  | 113.07      | 110.53   |
| 11  | aA    | 822 | CLA  | CMB-C2B-C1B | 2.85  | 129.75      | 125.42   |
| 11  | bB    | 831 | CLA  | CAC-C3C-C4C | 2.85  | 128.49      | 124.79   |
| 11  | aA    | 816 | CLA  | C3B-C4B-NB  | 2.85  | 113.07      | 110.53   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bB    | 835 | CLA  | C4C-C3C-C2C | -2.85 | 102.75      | 106.89   |
| 11  | cB    | 816 | CLA  | CAC-C3C-C4C | 2.84  | 128.49      | 124.79   |
| 11  | aA    | 808 | CLA  | C4B-C3B-C2B | -2.84 | 103.77      | 107.30   |
| 11  | cA    | 807 | CLA  | CAA-C2A-C3A | -2.84 | 105.31      | 113.00   |
| 11  | bA    | 834 | CLA  | C4B-C3B-C2B | -2.84 | 103.77      | 107.30   |
| 11  | cK    | 101 | CLA  | C4B-C3B-C2B | -2.84 | 103.77      | 107.30   |
| 11  | bA    | 833 | CLA  | C1-C2-C3    | -2.84 | 121.54      | 126.20   |
| 11  | bB    | 822 | CLA  | C4A-NA-C1A  | -2.84 | 105.38      | 106.68   |
| 11  | cA    | 842 | CLA  | C4C-C3C-C2C | -2.84 | 102.75      | 106.89   |
| 11  | cB    | 835 | CLA  | C4C-C3C-C2C | -2.84 | 102.75      | 106.89   |
| 12  | bB    | 824 | F6C  | CHD-C4C-NC  | 2.84  | 128.31      | 124.05   |
| 11  | aL    | 206 | CLA  | C4-C3-C5    | 2.84  | 120.16      | 115.23   |
| 12  | aB    | 824 | F6C  | C4-C3-C5    | 2.84  | 120.16      | 115.23   |
| 11  | cB    | 837 | CLA  | CAC-C3C-C4C | 2.84  | 128.49      | 124.79   |
| 12  | aA    | 826 | F6C  | O2A-CGA-CBA | 2.84  | 120.50      | 111.83   |
| 11  | bK    | 103 | CLA  | C4B-C3B-C2B | -2.84 | 103.77      | 107.30   |
| 11  | aA    | 822 | CLA  | CHD-C4C-NC  | 2.84  | 128.63      | 124.23   |
| 11  | aB    | 808 | CLA  | CBA-CAA-C2A | 2.84  | 122.24      | 113.79   |
| 12  | cB    | 824 | F6C  | CHD-C4C-NC  | 2.84  | 128.31      | 124.05   |
| 11  | cA    | 802 | CLA  | C4C-C3C-C2C | -2.84 | 102.76      | 106.89   |
| 11  | cB    | 831 | CLA  | C4C-C3C-C2C | -2.84 | 102.76      | 106.89   |
| 12  | bA    | 844 | F6C  | CAC-C3C-C4C | 2.84  | 128.82      | 124.91   |
| 12  | cA    | 844 | F6C  | CAC-C3C-C4C | 2.84  | 128.82      | 124.91   |
| 11  | aB    | 835 | CLA  | C4C-C3C-C2C | -2.84 | 102.76      | 106.89   |
| 11  | cA    | 816 | CLA  | C3B-C4B-NB  | 2.84  | 113.06      | 110.53   |
| 11  | cL    | 206 | CLA  | C4-C3-C5    | 2.84  | 120.15      | 115.23   |
| 11  | bB    | 826 | CLA  | O2A-CGA-CBA | 2.84  | 120.49      | 111.83   |
| 11  | cB    | 819 | CLA  | CAC-C3C-C4C | 2.84  | 128.48      | 124.79   |
| 11  | cA    | 834 | CLA  | C4B-C3B-C2B | -2.84 | 103.78      | 107.30   |
| 11  | aB    | 816 | CLA  | C3B-C4B-NB  | 2.84  | 113.06      | 110.53   |
| 12  | aB    | 824 | F6C  | CHD-C4C-NC  | 2.84  | 128.30      | 124.05   |
| 11  | aA    | 835 | CLA  | O2D-CGD-O1D | -2.83 | 118.33      | 123.85   |
| 11  | bB    | 811 | CLA  | C4B-C3B-C2B | -2.83 | 103.78      | 107.30   |
| 11  | aA    | 811 | CLA  | CHD-C4C-NC  | 2.83  | 128.63      | 124.23   |
| 11  | aB    | 826 | CLA  | O2A-CGA-CBA | 2.83  | 120.47      | 111.83   |
| 11  | aA    | 811 | CLA  | C4C-C3C-C2C | -2.83 | 102.77      | 106.89   |
| 11  | bA    | 811 | CLA  | C4C-C3C-C2C | -2.83 | 102.77      | 106.89   |
| 11  | bA    | 840 | CLA  | C4C-C3C-C2C | -2.83 | 102.77      | 106.89   |
| 11  | cA    | 812 | CLA  | C4B-C3B-C2B | -2.83 | 103.78      | 107.30   |
| 12  | aA    | 844 | F6C  | CAC-C3C-C4C | 2.83  | 128.81      | 124.91   |
| 11  | bA    | 807 | CLA  | CAA-C2A-C3A | -2.83 | 105.34      | 113.00   |
| 11  | cA    | 821 | CLA  | CMB-C2B-C1B | 2.83  | 129.73      | 125.42   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aB    | 823 | CLA  | O2D-CGD-O1D | -2.83 | 118.33      | 123.85   |
| 11  | cA    | 814 | CLA  | CAA-CBA-CGA | -2.83 | 105.17      | 113.21   |
| 11  | aB    | 820 | CLA  | C4B-C3B-C2B | -2.83 | 103.78      | 107.30   |
| 11  | cB    | 808 | CLA  | CBA-CAA-C2A | 2.83  | 122.22      | 113.79   |
| 11  | bB    | 831 | CLA  | CHD-C4C-NC  | 2.83  | 128.62      | 124.23   |
| 12  | cB    | 824 | F6C  | C4-C3-C5    | 2.83  | 120.14      | 115.23   |
| 11  | cB    | 823 | CLA  | C4B-C3B-C2B | -2.83 | 103.78      | 107.30   |
| 11  | cB    | 823 | CLA  | O2D-CGD-O1D | -2.83 | 118.34      | 123.85   |
| 11  | aB    | 806 | CLA  | C3B-C4B-NB  | 2.83  | 113.06      | 110.53   |
| 11  | bB    | 808 | CLA  | CBA-CAA-C2A | 2.83  | 122.21      | 113.79   |
| 12  | cL    | 202 | F6C  | C4C-C3C-C2C | -2.83 | 102.49      | 106.87   |
| 11  | aA    | 838 | CLA  | CAC-C3C-C4C | 2.83  | 128.47      | 124.79   |
| 12  | bA    | 826 | F6C  | O2A-CGA-CBA | 2.83  | 120.46      | 111.83   |
| 11  | aA    | 804 | CLA  | C4C-C3C-C2C | -2.83 | 102.77      | 106.89   |
| 11  | aB    | 810 | CLA  | CHD-C4C-NC  | 2.83  | 128.62      | 124.23   |
| 15  | aL    | 203 | BCR  | C7-C8-C9    | -2.83 | 122.05      | 126.23   |
| 12  | cA    | 826 | F6C  | O2A-CGA-CBA | 2.83  | 120.46      | 111.83   |
| 11  | bA    | 814 | CLA  | CAA-CBA-CGA | -2.83 | 105.18      | 113.21   |
| 11  | cA    | 804 | CLA  | C4C-C3C-C2C | -2.83 | 102.78      | 106.89   |
| 11  | cA    | 833 | CLA  | C1-C2-C3    | -2.83 | 121.57      | 126.20   |
| 11  | bB    | 831 | CLA  | C4B-C3B-C2B | -2.83 | 103.79      | 107.30   |
| 11  | cB    | 839 | CLA  | C1-C2-C3    | -2.82 | 121.57      | 126.20   |
| 11  | bK    | 101 | CLA  | C4B-C3B-C2B | -2.82 | 103.79      | 107.30   |
| 15  | cA    | 850 | BCR  | C15-C16-C17 | -2.82 | 117.74      | 123.52   |
| 12  | aL    | 202 | F6C  | C4C-C3C-C2C | -2.82 | 102.50      | 106.87   |
| 11  | cB    | 826 | CLA  | O2A-CGA-CBA | 2.82  | 120.44      | 111.83   |
| 11  | aL    | 204 | CLA  | O2D-CGD-O1D | -2.82 | 118.36      | 123.85   |
| 11  | aA    | 834 | CLA  | C4B-C3B-C2B | -2.82 | 103.79      | 107.30   |
| 11  | aA    | 814 | CLA  | CAA-CBA-CGA | -2.82 | 105.20      | 113.21   |
| 11  | cA    | 840 | CLA  | CHD-C4C-NC  | 2.82  | 128.60      | 124.23   |
| 11  | bA    | 824 | CLA  | C4C-C3C-C2C | -2.82 | 102.79      | 106.89   |
| 11  | aK    | 103 | CLA  | C4B-C3B-C2B | -2.82 | 103.80      | 107.30   |
| 11  | cA    | 825 | CLA  | C4C-C3C-C2C | -2.82 | 102.79      | 106.89   |
| 11  | aA    | 812 | CLA  | C4B-C3B-C2B | -2.82 | 103.80      | 107.30   |
| 11  | aB    | 831 | CLA  | C4B-C3B-C2B | -2.82 | 103.80      | 107.30   |
| 11  | aA    | 842 | CLA  | C4C-C3C-C2C | -2.82 | 102.79      | 106.89   |
| 11  | bB    | 810 | CLA  | CHD-C4C-NC  | 2.82  | 128.60      | 124.23   |
| 11  | cB    | 833 | CLA  | C4B-C3B-C2B | -2.82 | 103.80      | 107.30   |
| 11  | aB    | 839 | CLA  | C1-C2-C3    | -2.82 | 121.58      | 126.20   |
| 11  | cA    | 838 | CLA  | CHD-C4C-NC  | 2.82  | 128.60      | 124.23   |
| 11  | cA    | 811 | CLA  | CHD-C4C-NC  | 2.82  | 128.60      | 124.23   |
| 11  | cB    | 810 | CLA  | CHD-C4C-NC  | 2.82  | 128.60      | 124.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bA    | 805 | CLA  | O2D-CGD-O1D | -2.81 | 118.37      | 123.85   |
| 11  | cA    | 805 | CLA  | O2D-CGD-O1D | -2.81 | 118.37      | 123.85   |
| 11  | aB    | 828 | CLA  | C4C-C3C-C2C | -2.81 | 102.80      | 106.89   |
| 11  | bA    | 825 | CLA  | C4C-C3C-C2C | -2.81 | 102.80      | 106.89   |
| 11  | cB    | 806 | CLA  | C3B-C4B-NB  | 2.81  | 113.04      | 110.53   |
| 11  | bA    | 804 | CLA  | C4C-C3C-C2C | -2.81 | 102.80      | 106.89   |
| 11  | cB    | 827 | CLA  | C4B-C3B-C2B | -2.81 | 103.80      | 107.30   |
| 11  | bA    | 816 | CLA  | C3B-C4B-NB  | 2.81  | 113.04      | 110.53   |
| 11  | aA    | 805 | CLA  | O2D-CGD-O1D | -2.81 | 118.37      | 123.85   |
| 12  | cA    | 830 | F6C  | C4C-C3C-C2C | -2.81 | 102.52      | 106.87   |
| 15  | bL    | 203 | BCR  | C7-C8-C9    | -2.81 | 122.07      | 126.23   |
| 11  | bA    | 841 | CLA  | C4B-C3B-C2B | -2.81 | 103.81      | 107.30   |
| 11  | bB    | 833 | CLA  | C4C-C3C-C2C | -2.81 | 102.80      | 106.89   |
| 11  | cA    | 838 | CLA  | CAC-C3C-C4C | 2.81  | 128.45      | 124.79   |
| 15  | bA    | 850 | BCR  | C15-C16-C17 | -2.81 | 117.77      | 123.52   |
| 11  | aB    | 816 | CLA  | CAC-C3C-C4C | 2.81  | 128.45      | 124.79   |
| 11  | aA    | 842 | CLA  | C4B-C3B-C2B | -2.81 | 103.81      | 107.30   |
| 15  | aA    | 849 | BCR  | C15-C14-C13 | -2.81 | 123.34      | 127.28   |
| 11  | aB    | 827 | CLA  | C4B-C3B-C2B | -2.81 | 103.81      | 107.30   |
| 12  | aA    | 830 | F6C  | C4C-C3C-C2C | -2.81 | 102.52      | 106.87   |
| 11  | cB    | 835 | CLA  | CAC-C3C-C4C | 2.81  | 128.44      | 124.79   |
| 11  | cB    | 813 | CLA  | CHD-C4C-NC  | 2.81  | 128.59      | 124.23   |
| 11  | cK    | 101 | CLA  | CHD-C4C-NC  | 2.81  | 128.59      | 124.23   |
| 11  | cL    | 204 | CLA  | O2D-CGD-O1D | -2.81 | 118.38      | 123.85   |
| 11  | cB    | 819 | CLA  | C3B-C4B-NB  | 2.81  | 113.04      | 110.53   |
| 11  | cK    | 103 | CLA  | C4B-C3B-C2B | -2.81 | 103.81      | 107.30   |
| 11  | aB    | 833 | CLA  | C4C-C3C-C2C | -2.81 | 102.80      | 106.89   |
| 15  | bA    | 849 | BCR  | C15-C14-C13 | -2.81 | 123.34      | 127.28   |
| 11  | bB    | 807 | CLA  | CMB-C2B-C1B | 2.81  | 129.69      | 125.42   |
| 11  | cB    | 816 | CLA  | C3B-C4B-NB  | 2.81  | 113.04      | 110.53   |
| 11  | cA    | 822 | CLA  | CHD-C4C-NC  | 2.81  | 128.58      | 124.23   |
| 11  | bL    | 204 | CLA  | O2D-CGD-O1D | -2.81 | 118.39      | 123.85   |
| 11  | bB    | 810 | CLA  | C4C-C3C-C2C | -2.81 | 102.81      | 106.89   |
| 11  | cB    | 833 | CLA  | C4C-C3C-C2C | -2.81 | 102.81      | 106.89   |
| 11  | aB    | 813 | CLA  | CHD-C4C-NC  | 2.81  | 128.58      | 124.23   |
| 11  | bB    | 827 | CLA  | C4B-C3B-C2B | -2.81 | 103.81      | 107.30   |
| 11  | cL    | 205 | CLA  | C4B-C3B-C2B | -2.80 | 103.81      | 107.30   |
| 11  | bA    | 842 | CLA  | C4C-C3C-C2C | -2.80 | 102.81      | 106.89   |
| 11  | bB    | 828 | CLA  | C4C-C3C-C2C | -2.80 | 102.81      | 106.89   |
| 11  | bB    | 833 | CLA  | C4B-C3B-C2B | -2.80 | 103.81      | 107.30   |
| 11  | cB    | 801 | CLA  | CMC-C2C-C1C | 2.80  | 129.42      | 125.03   |
| 11  | aB    | 816 | CLA  | CHD-C4C-NC  | 2.80  | 128.58      | 124.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cB    | 831 | CLA  | C4B-C3B-C2B | -2.80 | 103.82      | 107.30   |
| 11  | aK    | 101 | CLA  | C4B-C3B-C2B | -2.80 | 103.82      | 107.30   |
| 11  | cB    | 807 | CLA  | CMB-C2B-C1B | 2.80  | 129.69      | 125.42   |
| 11  | aK    | 101 | CLA  | CHD-C4C-NC  | 2.80  | 128.58      | 124.23   |
| 11  | bA    | 811 | CLA  | CHD-C4C-NC  | 2.80  | 128.58      | 124.23   |
| 11  | cA    | 817 | CLA  | CHD-C4C-NC  | 2.80  | 128.57      | 124.23   |
| 11  | aB    | 807 | CLA  | CMB-C2B-C1B | 2.80  | 129.68      | 125.42   |
| 15  | aA    | 850 | BCR  | C15-C16-C17 | -2.80 | 117.79      | 123.52   |
| 11  | aB    | 837 | CLA  | CAC-C3C-C4C | 2.80  | 128.43      | 124.79   |
| 11  | cB    | 831 | CLA  | CAC-C3C-C4C | 2.80  | 128.43      | 124.79   |
| 11  | cB    | 835 | CLA  | CHD-C4C-NC  | 2.80  | 128.57      | 124.23   |
| 11  | cB    | 811 | CLA  | C4B-C3B-C2B | -2.80 | 103.82      | 107.30   |
| 11  | aB    | 835 | CLA  | CHD-C4C-NC  | 2.80  | 128.57      | 124.23   |
| 15  | cA    | 849 | BCR  | C15-C14-C13 | -2.80 | 123.35      | 127.28   |
| 11  | aB    | 811 | CLA  | C4B-C3B-C2B | -2.80 | 103.82      | 107.30   |
| 11  | bA    | 809 | CLA  | CHD-C4C-NC  | 2.80  | 128.57      | 124.23   |
| 11  | cA    | 809 | CLA  | C4C-C3C-C2C | -2.80 | 102.82      | 106.89   |
| 11  | aB    | 833 | CLA  | CAC-C3C-C4C | 2.80  | 128.43      | 124.79   |
| 11  | bA    | 818 | CLA  | C4A-NA-C1A  | -2.80 | 105.40      | 106.68   |
| 11  | aB    | 831 | CLA  | CAC-C3C-C4C | 2.80  | 128.43      | 124.79   |
| 11  | bB    | 820 | CLA  | C4B-C3B-C2B | -2.80 | 103.83      | 107.30   |
| 11  | aA    | 802 | CLA  | O2D-CGD-O1D | -2.80 | 118.41      | 123.85   |
| 11  | bB    | 839 | CLA  | C1-C2-C3    | -2.80 | 121.62      | 126.20   |
| 11  | bA    | 842 | CLA  | C4B-C3B-C2B | -2.80 | 103.83      | 107.30   |
| 11  | bB    | 835 | CLA  | CHD-C4C-NC  | 2.79  | 128.56      | 124.23   |
| 11  | bB    | 812 | CLA  | O2A-CGA-CBA | 2.79  | 120.36      | 111.83   |
| 11  | aA    | 818 | CLA  | C4A-NA-C1A  | -2.79 | 105.40      | 106.68   |
| 11  | aL    | 206 | CLA  | CAC-C3C-C4C | 2.79  | 128.43      | 124.79   |
| 11  | bB    | 835 | CLA  | CAC-C3C-C4C | 2.79  | 128.43      | 124.79   |
| 12  | bA    | 830 | F6C  | C4C-C3C-C2C | -2.79 | 102.55      | 106.87   |
| 11  | cB    | 816 | CLA  | C4B-C3B-C2B | -2.79 | 103.83      | 107.30   |
| 11  | cB    | 820 | CLA  | C4B-C3B-C2B | -2.79 | 103.83      | 107.30   |
| 11  | aB    | 833 | CLA  | C4B-C3B-C2B | -2.79 | 103.83      | 107.30   |
| 11  | cB    | 818 | CLA  | CHD-C4C-NC  | 2.79  | 128.56      | 124.23   |
| 11  | bB    | 806 | CLA  | C4C-C3C-C2C | -2.79 | 102.83      | 106.89   |
| 11  | cB    | 806 | CLA  | C4C-C3C-C2C | -2.79 | 102.83      | 106.89   |
| 11  | cA    | 805 | CLA  | C3B-C4B-NB  | 2.79  | 113.02      | 110.53   |
| 11  | cB    | 815 | CLA  | CHC-C1C-C2C | -2.79 | 119.02      | 126.95   |
| 11  | bA    | 822 | CLA  | C4-C3-C5    | 2.79  | 120.07      | 115.23   |
| 11  | cB    | 828 | CLA  | C4C-C3C-C2C | -2.79 | 102.83      | 106.89   |
| 11  | aA    | 833 | CLA  | C1-C2-C3    | -2.79 | 121.62      | 126.20   |
| 11  | cA    | 842 | CLA  | C4B-C3B-C2B | -2.79 | 103.83      | 107.30   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aA    | 817 | CLA  | CHD-C4C-NC  | 2.79  | 128.56      | 124.23   |
| 11  | bB    | 818 | CLA  | CHD-C4C-NC  | 2.79  | 128.56      | 124.23   |
| 11  | bB    | 819 | CLA  | C3B-C4B-NB  | 2.79  | 113.02      | 110.53   |
| 11  | cB    | 825 | CLA  | CHD-C4C-NC  | 2.79  | 128.55      | 124.23   |
| 11  | cA    | 824 | CLA  | C4C-C3C-C2C | -2.79 | 102.83      | 106.89   |
| 11  | cA    | 838 | CLA  | C4C-C3C-C2C | -2.79 | 102.83      | 106.89   |
| 11  | aB    | 812 | CLA  | O2A-CGA-CBA | 2.79  | 120.33      | 111.83   |
| 11  | bA    | 810 | CLA  | C4B-C3B-C2B | -2.79 | 103.84      | 107.30   |
| 11  | cB    | 833 | CLA  | CAC-C3C-C4C | 2.79  | 128.41      | 124.79   |
| 11  | bA    | 812 | CLA  | C4B-C3B-C2B | -2.79 | 103.84      | 107.30   |
| 11  | cB    | 836 | CLA  | C4-C3-C5    | 2.78  | 119.41      | 116.13   |
| 11  | cB    | 812 | CLA  | O2A-CGA-CBA | 2.78  | 120.33      | 111.83   |
| 11  | aB    | 815 | CLA  | CHC-C1C-C2C | -2.78 | 119.03      | 126.95   |
| 11  | aL    | 206 | CLA  | CHD-C4C-NC  | 2.78  | 128.55      | 124.23   |
| 11  | aA    | 841 | CLA  | C1-C2-C3    | -2.78 | 122.26      | 126.76   |
| 11  | bA    | 805 | CLA  | C3B-C4B-NB  | 2.78  | 113.02      | 110.53   |
| 11  | cA    | 802 | CLA  | O2D-CGD-O1D | -2.78 | 118.43      | 123.85   |
| 11  | bK    | 101 | CLA  | CHD-C4C-NC  | 2.78  | 128.55      | 124.23   |
| 11  | aB    | 808 | CLA  | CHD-C4C-NC  | 2.78  | 128.54      | 124.23   |
| 11  | bA    | 838 | CLA  | C4C-C3C-C2C | -2.78 | 102.84      | 106.89   |
| 11  | bA    | 802 | CLA  | O2D-CGD-O1D | -2.78 | 118.44      | 123.85   |
| 11  | bB    | 822 | CLA  | C4B-C3B-C2B | -2.78 | 103.84      | 107.30   |
| 11  | aA    | 809 | CLA  | CHD-C4C-NC  | 2.78  | 128.54      | 124.23   |
| 11  | cL    | 206 | CLA  | CHD-C4C-NC  | 2.78  | 128.54      | 124.23   |
| 11  | cB    | 810 | CLA  | C4C-C3C-C2C | -2.78 | 102.84      | 106.89   |
| 11  | bB    | 816 | CLA  | CHD-C4C-NC  | 2.78  | 128.54      | 124.23   |
| 15  | cK    | 102 | BCR  | C20-C21-C22 | -2.78 | 123.38      | 127.28   |
| 11  | aB    | 835 | CLA  | CAC-C3C-C4C | 2.78  | 128.41      | 124.79   |
| 11  | bA    | 838 | CLA  | CAC-C3C-C4C | 2.78  | 128.41      | 124.79   |
| 11  | bA    | 817 | CLA  | CHD-C4C-NC  | 2.78  | 128.54      | 124.23   |
| 11  | bB    | 813 | CLA  | CHD-C4C-NC  | 2.78  | 128.54      | 124.23   |
| 11  | cB    | 808 | CLA  | CHD-C4C-NC  | 2.78  | 128.54      | 124.23   |
| 11  | aB    | 810 | CLA  | C4C-C3C-C2C | -2.78 | 102.85      | 106.89   |
| 11  | aA    | 824 | CLA  | C4C-C3C-C2C | -2.78 | 102.85      | 106.89   |
| 11  | cB    | 813 | CLA  | C1-C2-C3    | -2.78 | 121.65      | 126.20   |
| 11  | aB    | 819 | CLA  | CAC-C3C-C4C | 2.78  | 128.40      | 124.79   |
| 11  | bB    | 837 | CLA  | CAC-C3C-C4C | 2.78  | 128.40      | 124.79   |
| 11  | bA    | 839 | CLA  | O2D-CGD-O1D | -2.78 | 118.45      | 123.85   |
| 11  | aB    | 801 | CLA  | CMC-C2C-C1C | 2.77  | 129.37      | 125.03   |
| 11  | bB    | 815 | CLA  | CHC-C1C-C2C | -2.77 | 119.06      | 126.95   |
| 11  | cA    | 821 | CLA  | C1-C2-C3    | -2.77 | 121.65      | 126.20   |
| 11  | aA    | 838 | CLA  | C4C-C3C-C2C | -2.77 | 102.85      | 106.89   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bL    | 204 | CLA  | CHD-C4C-NC  | 2.77  | 128.53      | 124.23   |
| 11  | cA    | 802 | CLA  | O2A-CGA-CBA | 2.77  | 120.29      | 111.83   |
| 11  | bB    | 833 | CLA  | CAC-C3C-C4C | 2.77  | 128.40      | 124.79   |
| 11  | aB    | 806 | CLA  | C4C-C3C-C2C | -2.77 | 102.86      | 106.89   |
| 11  | bB    | 808 | CLA  | CHD-C4C-NC  | 2.77  | 128.53      | 124.23   |
| 11  | aB    | 831 | CLA  | C1-C2-C3    | -2.77 | 121.66      | 126.20   |
| 11  | bB    | 801 | CLA  | CMC-C2C-C1C | 2.77  | 129.36      | 125.03   |
| 11  | cL    | 206 | CLA  | CAC-C3C-C4C | 2.77  | 128.40      | 124.79   |
| 11  | cA    | 809 | CLA  | CHD-C4C-NC  | 2.77  | 128.53      | 124.23   |
| 11  | aA    | 806 | CLA  | CMC-C2C-C1C | 2.77  | 129.36      | 125.03   |
| 11  | bB    | 840 | CLA  | CBC-CAC-C3C | -2.77 | 104.91      | 112.42   |
| 11  | aA    | 802 | CLA  | O2A-CGA-CBA | 2.77  | 120.28      | 111.83   |
| 11  | aA    | 811 | CLA  | CAC-C3C-C4C | 2.77  | 128.39      | 124.79   |
| 11  | bA    | 822 | CLA  | CAC-C3C-C4C | 2.77  | 128.39      | 124.79   |
| 11  | cA    | 806 | CLA  | CMC-C2C-C1C | 2.77  | 129.36      | 125.03   |
| 11  | cB    | 832 | CLA  | C4B-C3B-C2B | -2.77 | 103.86      | 107.30   |
| 12  | aA    | 827 | F6C  | O2A-CGA-CBA | 2.77  | 120.28      | 111.83   |
| 11  | aB    | 823 | CLA  | CHD-C4C-NC  | 2.77  | 128.52      | 124.23   |
| 11  | bA    | 841 | CLA  | C1-C2-C3    | -2.77 | 122.28      | 126.76   |
| 12  | aB    | 824 | F6C  | CAC-C3C-C4C | 2.77  | 128.72      | 124.91   |
| 11  | cA    | 824 | CLA  | O2A-CGA-CBA | 2.77  | 120.27      | 111.83   |
| 15  | bK    | 102 | BCR  | C20-C21-C22 | -2.77 | 123.40      | 127.28   |
| 11  | cA    | 822 | CLA  | C4-C3-C5    | 2.77  | 120.03      | 115.23   |
| 11  | cB    | 823 | CLA  | CHD-C4C-NC  | 2.77  | 128.52      | 124.23   |
| 11  | aA    | 840 | CLA  | CMB-C2B-C1B | 2.76  | 129.63      | 125.42   |
| 11  | bB    | 832 | CLA  | C4B-C3B-C2B | -2.76 | 103.86      | 107.30   |
| 11  | bB    | 813 | CLA  | C1-C2-C3    | -2.76 | 121.67      | 126.20   |
| 11  | cA    | 817 | CLA  | C4C-C3C-C2C | -2.76 | 102.87      | 106.89   |
| 11  | cB    | 802 | CLA  | CHB-C1B-C2B | -2.76 | 119.40      | 127.43   |
| 11  | bA    | 817 | CLA  | C4C-C3C-C2C | -2.76 | 102.87      | 106.89   |
| 15  | cL    | 207 | BCR  | C15-C16-C17 | -2.76 | 117.87      | 123.52   |
| 11  | aA    | 809 | CLA  | C4C-C3C-C2C | -2.76 | 102.87      | 106.89   |
| 11  | cA    | 841 | CLA  | C4B-C3B-C2B | -2.76 | 103.87      | 107.30   |
| 11  | aB    | 840 | CLA  | CBC-CAC-C3C | -2.76 | 104.93      | 112.42   |
| 11  | cB    | 822 | CLA  | C4A-NA-C1A  | -2.76 | 105.42      | 106.68   |
| 11  | cA    | 810 | CLA  | C4B-C3B-C2B | -2.76 | 103.87      | 107.30   |
| 11  | aA    | 842 | CLA  | C3B-C4B-NB  | 2.76  | 113.00      | 110.53   |
| 11  | cB    | 840 | CLA  | CBC-CAC-C3C | -2.76 | 104.94      | 112.42   |
| 12  | bA    | 827 | F6C  | O2A-CGA-CBA | 2.76  | 120.25      | 111.83   |
| 11  | bB    | 816 | CLA  | C3B-C4B-NB  | 2.76  | 112.99      | 110.53   |
| 11  | bL    | 206 | CLA  | CHD-C4C-NC  | 2.76  | 128.51      | 124.23   |
| 11  | bA    | 821 | CLA  | C1-C2-C3    | -2.76 | 121.68      | 126.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bA    | 807 | CLA  | O2A-CGA-CBA | 2.76  | 120.25      | 111.83   |
| 10  | aA    | 801 | CL0  | C4C-C3C-C2C | -2.76 | 102.48      | 113.37   |
| 11  | aA    | 822 | CLA  | CAC-C3C-C4C | 2.76  | 128.38      | 124.79   |
| 11  | bB    | 816 | CLA  | C4B-C3B-C2B | -2.76 | 103.87      | 107.30   |
| 11  | aB    | 813 | CLA  | C1-C2-C3    | -2.76 | 121.68      | 126.20   |
| 10  | cA    | 801 | CL0  | C4C-C3C-C2C | -2.76 | 102.48      | 113.37   |
| 11  | bB    | 811 | CLA  | CAA-C2A-C3A | -2.76 | 105.55      | 113.00   |
| 11  | bA    | 809 | CLA  | C4C-C3C-C2C | -2.76 | 102.88      | 106.89   |
| 11  | bL    | 206 | CLA  | CAC-C3C-C4C | 2.76  | 128.38      | 124.79   |
| 11  | cB    | 819 | CLA  | CHD-C4C-NC  | 2.76  | 128.51      | 124.23   |
| 11  | aA    | 822 | CLA  | C4-C3-C5    | 2.76  | 120.01      | 115.23   |
| 12  | bB    | 824 | F6C  | CAC-C3C-C4C | 2.76  | 128.70      | 124.91   |
| 11  | bA    | 824 | CLA  | O2A-CGA-CBA | 2.76  | 120.24      | 111.83   |
| 11  | bA    | 802 | CLA  | CHA-C1A-NA  | -2.76 | 120.15      | 126.39   |
| 11  | aA    | 841 | CLA  | C4B-C3B-C2B | -2.76 | 103.88      | 107.30   |
| 11  | aB    | 832 | CLA  | C4B-C3B-C2B | -2.76 | 103.88      | 107.30   |
| 11  | bB    | 802 | CLA  | CHB-C1B-C2B | -2.76 | 119.43      | 127.43   |
| 15  | aL    | 207 | BCR  | C15-C16-C17 | -2.76 | 117.88      | 123.52   |
| 11  | bB    | 819 | CLA  | CHD-C4C-NC  | 2.75  | 128.50      | 124.23   |
| 11  | aA    | 824 | CLA  | O2A-CGA-CBA | 2.75  | 120.23      | 111.83   |
| 11  | bA    | 806 | CLA  | CMC-C2C-C1C | 2.75  | 129.34      | 125.03   |
| 11  | aA    | 835 | CLA  | CAC-C3C-C4C | 2.75  | 128.37      | 124.79   |
| 15  | aK    | 102 | BCR  | C20-C21-C22 | -2.75 | 123.42      | 127.28   |
| 11  | cA    | 840 | CLA  | CMB-C2B-C1B | 2.75  | 129.61      | 125.42   |
| 11  | cA    | 841 | CLA  | C1-C2-C3    | -2.75 | 122.31      | 126.76   |
| 11  | cL    | 204 | CLA  | CHD-C4C-NC  | 2.75  | 128.50      | 124.23   |
| 11  | bA    | 808 | CLA  | CHD-C4C-NC  | 2.75  | 128.50      | 124.23   |
| 12  | cA    | 827 | F6C  | O2A-CGA-CBA | 2.75  | 120.23      | 111.83   |
| 11  | aA    | 807 | CLA  | O2A-CGA-CBA | 2.75  | 120.23      | 111.83   |
| 11  | aL    | 205 | CLA  | CHD-C4C-NC  | 2.75  | 128.50      | 124.23   |
| 15  | bL    | 207 | BCR  | C15-C16-C17 | -2.75 | 117.89      | 123.52   |
| 11  | aB    | 802 | CLA  | CHB-C1B-C2B | -2.75 | 119.44      | 127.43   |
| 11  | bB    | 836 | CLA  | C4-C3-C5    | 2.75  | 119.36      | 116.13   |
| 11  | aA    | 808 | CLA  | CHD-C4C-NC  | 2.75  | 128.49      | 124.23   |
| 11  | cA    | 833 | CLA  | C4C-C3C-C2C | -2.75 | 102.89      | 106.89   |
| 11  | aB    | 805 | CLA  | CHD-C4C-NC  | 2.75  | 128.49      | 124.23   |
| 11  | bB    | 831 | CLA  | C1-C2-C3    | -2.75 | 121.69      | 126.20   |
| 11  | aB    | 811 | CLA  | CAA-C2A-C3A | -2.75 | 105.57      | 113.00   |
| 11  | cB    | 822 | CLA  | C4B-C3B-C2B | -2.75 | 103.89      | 107.30   |
| 11  | cA    | 808 | CLA  | CHD-C4C-NC  | 2.75  | 128.49      | 124.23   |
| 11  | cB    | 816 | CLA  | CHD-C4C-NC  | 2.75  | 128.49      | 124.23   |
| 12  | bA    | 827 | F6C  | C4C-C3C-C2C | -2.75 | 102.62      | 106.87   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bA    | 840 | CLA  | CMB-C2B-C1B | 2.75  | 129.60      | 125.42   |
| 11  | aA    | 810 | CLA  | C4B-C3B-C2B | -2.75 | 103.89      | 107.30   |
| 11  | bA    | 802 | CLA  | O2A-CGA-CBA | 2.75  | 120.21      | 111.83   |
| 11  | aB    | 822 | CLA  | C4B-C3B-C2B | -2.75 | 103.89      | 107.30   |
| 10  | bA    | 801 | CL0  | C4C-C3C-C2C | -2.75 | 102.53      | 113.37   |
| 11  | bA    | 823 | CLA  | CMB-C2B-C1B | 2.75  | 129.60      | 125.42   |
| 11  | aA    | 805 | CLA  | C3B-C4B-NB  | 2.75  | 112.98      | 110.53   |
| 11  | aB    | 819 | CLA  | C3B-C4B-NB  | 2.75  | 112.98      | 110.53   |
| 11  | aA    | 813 | CLA  | C3B-C4B-NB  | 2.74  | 112.98      | 110.53   |
| 11  | cA    | 818 | CLA  | C4A-NA-C1A  | -2.74 | 105.43      | 106.68   |
| 11  | cA    | 807 | CLA  | O2A-CGA-CBA | 2.74  | 120.20      | 111.83   |
| 11  | aB    | 818 | CLA  | CHD-C4C-NC  | 2.74  | 128.49      | 124.23   |
| 11  | cB    | 811 | CLA  | CAA-C2A-C3A | -2.74 | 105.58      | 113.00   |
| 11  | bA    | 818 | CLA  | C1-O2A-CGA  | 2.74  | 123.29      | 116.65   |
| 11  | bB    | 825 | CLA  | CHD-C4C-NC  | 2.74  | 128.49      | 124.23   |
| 11  | aL    | 204 | CLA  | CHD-C4C-NC  | 2.74  | 128.48      | 124.23   |
| 11  | cA    | 811 | CLA  | CAC-C3C-C4C | 2.74  | 128.36      | 124.79   |
| 15  | bI    | 101 | BCR  | C11-C10-C9  | -2.74 | 123.43      | 127.28   |
| 11  | aB    | 819 | CLA  | CHD-C4C-NC  | 2.74  | 128.48      | 124.23   |
| 11  | cA    | 843 | CLA  | CHD-C4C-NC  | 2.74  | 128.48      | 124.23   |
| 11  | cA    | 822 | CLA  | CAC-C3C-C4C | 2.74  | 128.35      | 124.79   |
| 11  | cA    | 835 | CLA  | CAC-C3C-C4C | 2.74  | 128.35      | 124.79   |
| 11  | cA    | 839 | CLA  | O2D-CGD-O1D | -2.74 | 118.52      | 123.85   |
| 11  | aB    | 816 | CLA  | C4B-C3B-C2B | -2.74 | 103.90      | 107.30   |
| 11  | bK    | 103 | CLA  | CMB-C2B-C1B | 2.74  | 129.59      | 125.42   |
| 11  | aA    | 821 | CLA  | C1-C2-C3    | -2.74 | 121.71      | 126.20   |
| 11  | aA    | 839 | CLA  | O2D-CGD-O1D | -2.74 | 118.52      | 123.85   |
| 11  | aB    | 836 | CLA  | C4-C3-C5    | 2.74  | 119.35      | 116.13   |
| 11  | bA    | 838 | CLA  | CMC-C2C-C1C | 2.74  | 129.31      | 125.03   |
| 11  | aB    | 825 | CLA  | CHD-C4C-NC  | 2.73  | 128.47      | 124.23   |
| 11  | bB    | 823 | CLA  | CHD-C4C-NC  | 2.73  | 128.47      | 124.23   |
| 11  | bB    | 802 | CLA  | C4-C3-C5    | 2.73  | 119.97      | 115.23   |
| 11  | cL    | 205 | CLA  | CHD-C4C-NC  | 2.73  | 128.47      | 124.23   |
| 11  | aA    | 819 | CLA  | C4B-C3B-C2B | -2.73 | 103.90      | 107.30   |
| 11  | cA    | 818 | CLA  | C1-O2A-CGA  | 2.73  | 123.27      | 116.65   |
| 12  | cA    | 827 | F6C  | C4C-C3C-C2C | -2.73 | 102.64      | 106.87   |
| 11  | cB    | 802 | CLA  | C4-C3-C5    | 2.73  | 119.97      | 115.23   |
| 15  | bI    | 101 | BCR  | C3-C4-C5    | -2.73 | 109.18      | 114.06   |
| 11  | bA    | 836 | CLA  | CMB-C2B-C1B | 2.73  | 129.58      | 125.42   |
| 11  | bA    | 835 | CLA  | CAC-C3C-C4C | 2.73  | 128.34      | 124.79   |
| 11  | bA    | 836 | CLA  | O2D-CGD-CBD | 2.73  | 116.00      | 111.23   |
| 11  | aA    | 838 | CLA  | CMC-C2C-C1C | 2.73  | 129.30      | 125.03   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aB    | 807 | CLA  | CAA-C2A-C3A | -2.73 | 105.62      | 113.00   |
| 11  | bB    | 805 | CLA  | CHD-C4C-NC  | 2.73  | 128.46      | 124.23   |
| 12  | cB    | 824 | F6C  | CAC-C3C-C4C | 2.73  | 128.67      | 124.91   |
| 11  | bA    | 805 | CLA  | C4B-C3B-C2B | -2.73 | 103.91      | 107.30   |
| 11  | cA    | 804 | CLA  | CAA-C2A-C3A | -2.73 | 105.62      | 113.00   |
| 11  | aA    | 833 | CLA  | C4C-C3C-C2C | -2.73 | 102.92      | 106.89   |
| 11  | cA    | 802 | CLA  | C6-C5-C3    | -2.73 | 106.82      | 113.47   |
| 11  | bA    | 813 | CLA  | CHD-C4C-NC  | 2.73  | 128.46      | 124.23   |
| 11  | bA    | 837 | CLA  | CAC-C3C-C4C | 2.73  | 128.34      | 124.79   |
| 11  | cB    | 813 | CLA  | CAC-C3C-C4C | 2.73  | 128.34      | 124.79   |
| 12  | aA    | 827 | F6C  | C4C-C3C-C2C | -2.73 | 102.65      | 106.87   |
| 11  | aB    | 813 | CLA  | CAC-C3C-C4C | 2.73  | 128.34      | 124.79   |
| 11  | aB    | 802 | CLA  | C4-C3-C5    | 2.73  | 119.96      | 115.23   |
| 11  | bA    | 816 | CLA  | CHD-C4C-NC  | 2.73  | 128.46      | 124.23   |
| 11  | bA    | 833 | CLA  | C4C-C3C-C2C | -2.73 | 102.92      | 106.89   |
| 11  | aA    | 802 | CLA  | C6-C5-C3    | -2.73 | 106.83      | 113.47   |
| 11  | bA    | 804 | CLA  | C4B-C3B-C2B | -2.73 | 103.91      | 107.30   |
| 11  | cB    | 831 | CLA  | C1-C2-C3    | -2.73 | 121.73      | 126.20   |
| 11  | cA    | 836 | CLA  | CMB-C2B-C1B | 2.72  | 129.57      | 125.42   |
| 11  | bA    | 805 | CLA  | CHC-C1C-C2C | -2.72 | 119.20      | 126.95   |
| 11  | aA    | 818 | CLA  | C1-O2A-CGA  | 2.72  | 123.25      | 116.65   |
| 11  | bB    | 807 | CLA  | CAA-C2A-C3A | -2.72 | 105.64      | 113.00   |
| 11  | cB    | 807 | CLA  | CAA-C2A-C3A | -2.72 | 105.64      | 113.00   |
| 15  | cI    | 103 | BCR  | C3-C4-C5    | -2.72 | 109.20      | 114.06   |
| 11  | bA    | 819 | CLA  | O2A-CGA-CBA | 2.72  | 120.14      | 111.83   |
| 11  | cA    | 819 | CLA  | O2A-CGA-CBA | 2.72  | 120.14      | 111.83   |
| 15  | cI    | 103 | BCR  | C11-C10-C9  | -2.72 | 123.46      | 127.28   |
| 11  | cB    | 804 | CLA  | C4B-C3B-C2B | -2.72 | 103.92      | 107.30   |
| 11  | cA    | 813 | CLA  | C3B-C4B-NB  | 2.72  | 112.96      | 110.53   |
| 11  | cA    | 842 | CLA  | C3B-C4B-NB  | 2.72  | 112.96      | 110.53   |
| 11  | cA    | 805 | CLA  | CHC-C1C-C2C | -2.72 | 119.21      | 126.95   |
| 11  | aB    | 826 | CLA  | CHD-C4C-NC  | 2.72  | 128.45      | 124.23   |
| 11  | bA    | 814 | CLA  | CHD-C4C-NC  | 2.72  | 128.45      | 124.23   |
| 11  | cA    | 816 | CLA  | CHD-C4C-NC  | 2.72  | 128.45      | 124.23   |
| 11  | bB    | 802 | CLA  | CHC-C1C-C2C | -2.72 | 119.22      | 126.95   |
| 11  | aA    | 819 | CLA  | O2A-CGA-CBA | 2.72  | 120.13      | 111.83   |
| 11  | aA    | 804 | CLA  | CAA-C2A-C3A | -2.72 | 105.65      | 113.00   |
| 11  | cB    | 838 | CLA  | CHD-C4C-NC  | 2.72  | 128.45      | 124.23   |
| 11  | cA    | 802 | CLA  | CHA-C1A-NA  | -2.72 | 120.23      | 126.39   |
| 11  | aA    | 804 | CLA  | C4B-C3B-C2B | -2.72 | 103.92      | 107.30   |
| 15  | aI    | 101 | BCR  | C11-C10-C9  | -2.72 | 123.47      | 127.28   |
| 11  | bB    | 805 | CLA  | O2D-CGD-O1D | -2.72 | 118.56      | 123.85   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bB    | 816 | CLA  | CHB-C4A-NA  | 2.72  | 128.32      | 124.40   |
| 11  | bA    | 843 | CLA  | CHD-C4C-NC  | 2.72  | 128.44      | 124.23   |
| 11  | cA    | 813 | CLA  | CHD-C4C-NC  | 2.72  | 128.44      | 124.23   |
| 12  | cA    | 832 | F6C  | CAC-C3C-C4C | 2.72  | 128.65      | 124.91   |
| 11  | cK    | 103 | CLA  | CMB-C2B-C1B | 2.72  | 129.56      | 125.42   |
| 11  | bB    | 826 | CLA  | CHD-C4C-NC  | 2.72  | 128.44      | 124.23   |
| 11  | bA    | 811 | CLA  | CAC-C3C-C4C | 2.72  | 128.32      | 124.79   |
| 11  | aA    | 802 | CLA  | CHA-C1A-NA  | -2.71 | 120.24      | 126.39   |
| 11  | bA    | 842 | CLA  | C3B-C4B-NB  | 2.71  | 112.95      | 110.53   |
| 11  | cB    | 805 | CLA  | O2D-CGD-O1D | -2.71 | 118.56      | 123.85   |
| 11  | bA    | 803 | CLA  | CHD-C4C-NC  | 2.71  | 128.44      | 124.23   |
| 11  | aA    | 817 | CLA  | C4C-C3C-C2C | -2.71 | 102.94      | 106.89   |
| 11  | cA    | 828 | CLA  | CAC-C3C-C4C | 2.71  | 128.32      | 124.79   |
| 11  | cB    | 818 | CLA  | C4-C3-C5    | 2.71  | 119.94      | 115.23   |
| 11  | cB    | 839 | CLA  | CHC-C1C-C2C | -2.71 | 119.24      | 126.95   |
| 15  | aI    | 101 | BCR  | C3-C4-C5    | -2.71 | 109.22      | 114.06   |
| 15  | aA    | 848 | BCR  | C27-C26-C25 | 2.71  | 126.37      | 122.70   |
| 11  | bL    | 205 | CLA  | CHD-C4C-NC  | 2.71  | 128.44      | 124.23   |
| 11  | cA    | 837 | CLA  | CAC-C3C-C4C | 2.71  | 128.32      | 124.79   |
| 11  | cB    | 805 | CLA  | CHD-C4C-NC  | 2.71  | 128.43      | 124.23   |
| 11  | bB    | 804 | CLA  | C4B-C3B-C2B | -2.71 | 103.93      | 107.30   |
| 11  | cB    | 826 | CLA  | CHD-C4C-NC  | 2.71  | 128.43      | 124.23   |
| 11  | bA    | 802 | CLA  | C6-C5-C3    | -2.71 | 106.87      | 113.47   |
| 11  | aA    | 815 | CLA  | CAC-C3C-C4C | 2.71  | 128.31      | 124.79   |
| 11  | cA    | 804 | CLA  | C4B-C3B-C2B | -2.71 | 103.93      | 107.30   |
| 11  | cB    | 802 | CLA  | CHC-C1C-C2C | -2.71 | 119.25      | 126.95   |
| 11  | aA    | 823 | CLA  | CMB-C2B-C1B | 2.71  | 129.54      | 125.42   |
| 11  | aA    | 805 | CLA  | CHC-C1C-C2C | -2.71 | 119.25      | 126.95   |
| 11  | cA    | 836 | CLA  | O2D-CGD-CBD | 2.71  | 115.96      | 111.23   |
| 11  | aA    | 816 | CLA  | CHD-C4C-NC  | 2.71  | 128.43      | 124.23   |
| 11  | bA    | 804 | CLA  | CAA-C2A-C3A | -2.71 | 105.69      | 113.00   |
| 11  | cB    | 837 | CLA  | C3B-C4B-NB  | 2.71  | 112.95      | 110.53   |
| 11  | aA    | 828 | CLA  | CAC-C3C-C4C | 2.71  | 128.31      | 124.79   |
| 11  | cB    | 803 | CLA  | CHC-C1C-NC  | 2.71  | 128.39      | 124.31   |
| 11  | cA    | 818 | CLA  | C4-C3-C5    | 2.71  | 119.92      | 115.23   |
| 11  | cA    | 819 | CLA  | C4B-C3B-C2B | -2.71 | 103.94      | 107.30   |
| 11  | bA    | 807 | CLA  | CMB-C2B-C1B | 2.71  | 129.54      | 125.42   |
| 15  | bK    | 102 | BCR  | C27-C26-C25 | 2.70  | 126.36      | 122.70   |
| 11  | bA    | 828 | CLA  | CAC-C3C-C4C | 2.70  | 128.31      | 124.79   |
| 11  | cA    | 838 | CLA  | CMC-C2C-C1C | 2.70  | 129.26      | 125.03   |
| 11  | cA    | 814 | CLA  | CHD-C4C-NC  | 2.70  | 128.42      | 124.23   |
| 11  | bA    | 828 | CLA  | O2D-CGD-O1D | -2.70 | 118.59      | 123.85   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aK    | 103 | CLA  | CMB-C2B-C1B | 2.70  | 129.53      | 125.42   |
| 11  | cA    | 806 | CLA  | C3C-C4C-NC  | 2.70  | 113.89      | 110.43   |
| 11  | cA    | 828 | CLA  | O2D-CGD-O1D | -2.70 | 118.59      | 123.85   |
| 12  | bA    | 832 | F6C  | CAC-C3C-C4C | 2.70  | 128.63      | 124.91   |
| 12  | cA    | 827 | F6C  | CAC-C3C-C4C | 2.70  | 128.63      | 124.91   |
| 11  | aA    | 839 | CLA  | CHD-C4C-NC  | 2.70  | 128.42      | 124.23   |
| 11  | aA    | 843 | CLA  | CHD-C4C-NC  | 2.70  | 128.42      | 124.23   |
| 11  | aA    | 813 | CLA  | CHD-C4C-NC  | 2.70  | 128.42      | 124.23   |
| 11  | bB    | 838 | CLA  | CHD-C4C-NC  | 2.70  | 128.42      | 124.23   |
| 11  | aA    | 836 | CLA  | CMB-C2B-C1B | 2.70  | 129.53      | 125.42   |
| 11  | aB    | 803 | CLA  | CHC-C1C-NC  | 2.70  | 128.38      | 124.31   |
| 11  | aB    | 805 | CLA  | O2D-CGD-O1D | -2.70 | 118.59      | 123.85   |
| 11  | bB    | 839 | CLA  | CAC-C3C-C4C | 2.70  | 128.30      | 124.79   |
| 11  | aB    | 802 | CLA  | CHC-C1C-C2C | -2.70 | 119.28      | 126.95   |
| 11  | aB    | 816 | CLA  | CHB-C4A-NA  | 2.70  | 128.29      | 124.40   |
| 11  | bA    | 818 | CLA  | C4-C3-C5    | 2.70  | 119.91      | 115.23   |
| 11  | cA    | 805 | CLA  | C4B-C3B-C2B | -2.70 | 103.95      | 107.30   |
| 11  | aA    | 820 | CLA  | CHD-C4C-NC  | 2.70  | 128.41      | 124.23   |
| 11  | aA    | 828 | CLA  | O2D-CGD-O1D | -2.70 | 118.60      | 123.85   |
| 11  | aB    | 827 | CLA  | CMA-C3A-C2A | -2.70 | 103.56      | 113.98   |
| 11  | cB    | 827 | CLA  | CMA-C3A-C2A | -2.70 | 103.56      | 113.98   |
| 18  | cB    | 847 | LMG  | O1-C1-C2    | -2.70 | 104.18      | 108.27   |
| 11  | bA    | 806 | CLA  | C3C-C4C-NC  | 2.70  | 113.88      | 110.43   |
| 11  | bB    | 839 | CLA  | CHC-C1C-C2C | -2.70 | 119.29      | 126.95   |
| 11  | aA    | 818 | CLA  | C4-C3-C5    | 2.69  | 119.91      | 115.23   |
| 11  | bB    | 818 | CLA  | C4-C3-C5    | 2.69  | 119.91      | 115.23   |
| 11  | bA    | 819 | CLA  | C4B-C3B-C2B | -2.69 | 103.95      | 107.30   |
| 11  | aB    | 816 | CLA  | O2A-CGA-CBA | 2.69  | 120.05      | 111.83   |
| 11  | bB    | 827 | CLA  | CMA-C3A-C2A | -2.69 | 103.57      | 113.98   |
| 11  | bA    | 815 | CLA  | CAC-C3C-C4C | 2.69  | 128.29      | 124.79   |
| 11  | bA    | 839 | CLA  | CHD-C4C-NC  | 2.69  | 128.40      | 124.23   |
| 15  | aK    | 102 | BCR  | C27-C26-C25 | 2.69  | 126.34      | 122.70   |
| 11  | aB    | 839 | CLA  | CHC-C1C-C2C | -2.69 | 119.30      | 126.95   |
| 11  | bB    | 837 | CLA  | C3B-C4B-NB  | 2.69  | 112.93      | 110.53   |
| 11  | cB    | 839 | CLA  | CMC-C2C-C1C | 2.69  | 129.24      | 125.03   |
| 11  | bB    | 813 | CLA  | CAC-C3C-C4C | 2.69  | 128.29      | 124.79   |
| 11  | aA    | 814 | CLA  | CHD-C4C-NC  | 2.69  | 128.40      | 124.23   |
| 12  | bA    | 827 | F6C  | CAC-C3C-C4C | 2.69  | 128.61      | 124.91   |
| 12  | aA    | 844 | F6C  | OMB-CMB-C2B | -2.69 | 119.55      | 125.62   |
| 12  | bA    | 830 | F6C  | OMB-CMB-C2B | -2.69 | 119.55      | 125.62   |
| 11  | cA    | 823 | CLA  | CMB-C2B-C1B | 2.69  | 129.51      | 125.42   |
| 11  | cA    | 815 | CLA  | CAC-C3C-C4C | 2.69  | 128.29      | 124.79   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12  | aA    | 832 | F6C  | CAC-C3C-C4C | 2.69  | 128.61      | 124.91   |
| 11  | aA    | 807 | CLA  | CMB-C2B-C1B | 2.69  | 129.51      | 125.42   |
| 11  | cA    | 807 | CLA  | CMB-C2B-C1B | 2.69  | 129.51      | 125.42   |
| 11  | aB    | 818 | CLA  | C4-C3-C5    | 2.69  | 119.89      | 115.23   |
| 11  | bA    | 813 | CLA  | C3B-C4B-NB  | 2.69  | 112.93      | 110.53   |
| 11  | bA    | 805 | CLA  | CAA-C2A-C3A | -2.69 | 105.74      | 113.00   |
| 11  | cA    | 805 | CLA  | CAA-C2A-C3A | -2.69 | 105.74      | 113.00   |
| 11  | aA    | 837 | CLA  | CAC-C3C-C4C | 2.68  | 128.28      | 124.79   |
| 11  | cA    | 839 | CLA  | CHD-C4C-NC  | 2.68  | 128.39      | 124.23   |
| 11  | cA    | 804 | CLA  | CAC-C3C-C4C | 2.68  | 128.28      | 124.79   |
| 12  | aA    | 830 | F6C  | CAC-C3C-C4C | 2.68  | 128.60      | 124.91   |
| 11  | bA    | 821 | CLA  | C4A-NA-C1A  | -2.68 | 105.45      | 106.68   |
| 11  | bB    | 806 | CLA  | C4B-C3B-C2B | -2.68 | 103.97      | 107.30   |
| 11  | aA    | 803 | CLA  | CHD-C4C-NC  | 2.68  | 128.39      | 124.23   |
| 11  | cB    | 804 | CLA  | CHC-C1C-C2C | -2.68 | 119.33      | 126.95   |
| 11  | aA    | 806 | CLA  | C3C-C4C-NC  | 2.68  | 113.87      | 110.43   |
| 11  | aA    | 840 | CLA  | CAA-CBA-CGA | -2.68 | 105.59      | 113.21   |
| 11  | bB    | 830 | CLA  | CHD-C4C-NC  | 2.68  | 128.39      | 124.23   |
| 11  | aA    | 828 | CLA  | C4-C3-C5    | 2.68  | 119.88      | 115.23   |
| 11  | aA    | 836 | CLA  | O2D-CGD-CBD | 2.68  | 115.92      | 111.23   |
| 11  | aB    | 839 | CLA  | CAC-C3C-C4C | 2.68  | 128.28      | 124.79   |
| 11  | cB    | 816 | CLA  | O2A-CGA-CBA | 2.68  | 120.01      | 111.83   |
| 15  | bA    | 851 | BCR  | C27-C26-C25 | 2.68  | 126.33      | 122.70   |
| 15  | cK    | 102 | BCR  | C15-C14-C13 | -2.68 | 123.52      | 127.28   |
| 11  | bB    | 813 | CLA  | CHB-C4A-NA  | 2.68  | 128.27      | 124.40   |
| 11  | bA    | 840 | CLA  | CAA-CBA-CGA | -2.68 | 105.60      | 113.21   |
| 12  | aA    | 830 | F6C  | OMB-CMB-C2B | -2.68 | 119.57      | 125.62   |
| 11  | bB    | 804 | CLA  | CHC-C1C-C2C | -2.68 | 119.33      | 126.95   |
| 11  | aA    | 821 | CLA  | C4A-NA-C1A  | -2.68 | 105.46      | 106.68   |
| 11  | aB    | 801 | CLA  | C4A-NA-C1A  | -2.68 | 105.46      | 106.68   |
| 11  | aA    | 806 | CLA  | CHD-C4C-NC  | 2.68  | 128.38      | 124.23   |
| 11  | aB    | 822 | CLA  | CMB-C2B-C1B | 2.68  | 129.50      | 125.42   |
| 11  | bB    | 822 | CLA  | CMB-C2B-C1B | 2.68  | 129.50      | 125.42   |
| 11  | aA    | 841 | CLA  | CAA-C2A-C3A | -2.68 | 105.76      | 113.00   |
| 11  | cB    | 815 | CLA  | C4B-C3B-C2B | -2.68 | 103.97      | 107.30   |
| 11  | cB    | 819 | CLA  | C4B-C3B-C2B | -2.68 | 103.97      | 107.30   |
| 12  | cA    | 830 | F6C  | CAC-C3C-C4C | 2.68  | 128.59      | 124.91   |
| 11  | bB    | 803 | CLA  | CHC-C1C-NC  | 2.68  | 128.34      | 124.31   |
| 11  | cA    | 840 | CLA  | CAA-CBA-CGA | -2.68 | 105.61      | 113.21   |
| 12  | cA    | 830 | F6C  | OMB-CMB-C2B | -2.68 | 119.58      | 125.62   |
| 15  | aK    | 102 | BCR  | C15-C14-C13 | -2.68 | 123.53      | 127.28   |
| 11  | bB    | 836 | CLA  | CAA-C2A-C3A | -2.68 | 105.77      | 113.00   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aB    | 804 | CLA  | CHC-C1C-C2C | -2.67 | 119.35      | 126.95   |
| 12  | aA    | 827 | F6C  | CAC-C3C-C4C | 2.67  | 128.59      | 124.91   |
| 11  | cB    | 839 | CLA  | CAC-C3C-C4C | 2.67  | 128.27      | 124.79   |
| 11  | aA    | 809 | CLA  | C4B-C3B-C2B | -2.67 | 103.98      | 107.30   |
| 11  | bB    | 816 | CLA  | O2A-CGA-CBA | 2.67  | 119.98      | 111.83   |
| 11  | bA    | 820 | CLA  | CHD-C4C-NC  | 2.67  | 128.38      | 124.23   |
| 11  | bA    | 841 | CLA  | CAA-C2A-C3A | -2.67 | 105.78      | 113.00   |
| 11  | cA    | 809 | CLA  | CHB-C4A-NA  | 2.67  | 128.26      | 124.40   |
| 11  | aA    | 806 | CLA  | CMB-C2B-C1B | 2.67  | 129.49      | 125.42   |
| 11  | cA    | 841 | CLA  | CAA-C2A-C3A | -2.67 | 105.78      | 113.00   |
| 12  | bA    | 830 | F6C  | CAC-C3C-C4C | 2.67  | 128.59      | 124.91   |
| 11  | aA    | 805 | CLA  | C4B-C3B-C2B | -2.67 | 103.98      | 107.30   |
| 11  | aB    | 830 | CLA  | CHD-C4C-NC  | 2.67  | 128.37      | 124.23   |
| 11  | bA    | 815 | CLA  | CHD-C4C-NC  | 2.67  | 128.37      | 124.23   |
| 11  | cA    | 821 | CLA  | C4A-NA-C1A  | -2.67 | 105.46      | 106.68   |
| 11  | cB    | 820 | CLA  | C4A-NA-C1A  | -2.67 | 105.46      | 106.68   |
| 11  | cA    | 806 | CLA  | CMB-C2B-C1B | 2.67  | 129.48      | 125.42   |
| 12  | bA    | 844 | F6C  | OMB-CMB-C2B | -2.67 | 119.60      | 125.62   |
| 11  | aK    | 103 | CLA  | CHD-C4C-NC  | 2.67  | 128.37      | 124.23   |
| 11  | cA    | 803 | CLA  | CHD-C4C-NC  | 2.67  | 128.37      | 124.23   |
| 11  | aB    | 836 | CLA  | CAA-C2A-C3A | -2.67 | 105.79      | 113.00   |
| 12  | bA    | 844 | F6C  | C4-C3-C5    | 2.67  | 119.86      | 115.23   |
| 18  | bB    | 847 | LMG  | O1-C1-C2    | -2.67 | 104.22      | 108.27   |
| 11  | aB    | 838 | CLA  | CHD-C4C-NC  | 2.67  | 128.37      | 124.23   |
| 11  | cB    | 813 | CLA  | CHB-C4A-NA  | 2.67  | 128.25      | 124.40   |
| 11  | cB    | 822 | CLA  | CMB-C2B-C1B | 2.67  | 129.48      | 125.42   |
| 11  | bA    | 831 | CLA  | O2D-CGD-O1D | -2.67 | 118.66      | 123.85   |
| 11  | cB    | 836 | CLA  | CAA-C2A-C3A | -2.67 | 105.79      | 113.00   |
| 11  | cA    | 831 | CLA  | O2D-CGD-O1D | -2.67 | 118.66      | 123.85   |
| 12  | aA    | 844 | F6C  | C4-C3-C5    | 2.67  | 119.85      | 115.23   |
| 11  | cB    | 821 | CLA  | CHD-C4C-NC  | 2.66  | 128.36      | 124.23   |
| 11  | bA    | 804 | CLA  | CMB-C2B-C1B | 2.66  | 129.48      | 125.42   |
| 11  | aB    | 804 | CLA  | C4B-C3B-C2B | -2.66 | 103.99      | 107.30   |
| 11  | cA    | 839 | CLA  | C1-C2-C3    | -2.66 | 121.83      | 126.20   |
| 15  | cA    | 851 | BCR  | C27-C26-C25 | 2.66  | 126.30      | 122.70   |
| 15  | cK    | 102 | BCR  | C27-C26-C25 | 2.66  | 126.30      | 122.70   |
| 11  | cA    | 803 | CLA  | C4A-NA-C1A  | -2.66 | 105.46      | 106.68   |
| 12  | cA    | 844 | F6C  | OMB-CMB-C2B | -2.66 | 119.61      | 125.62   |
| 11  | aB    | 829 | CLA  | CMC-C2C-C1C | 2.66  | 129.19      | 125.03   |
| 11  | aA    | 805 | CLA  | CAA-C2A-C3A | -2.66 | 105.81      | 113.00   |
| 11  | aB    | 806 | CLA  | C4B-C3B-C2B | -2.66 | 103.99      | 107.30   |
| 11  | aB    | 813 | CLA  | CHB-C4A-NA  | 2.66  | 128.24      | 124.40   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bA    | 841 | CLA  | CHD-C4C-NC  | 2.66  | 128.36      | 124.23   |
| 11  | bB    | 811 | CLA  | CHD-C4C-NC  | 2.66  | 128.36      | 124.23   |
| 15  | bA    | 848 | BCR  | C27-C26-C25 | 2.66  | 126.30      | 122.70   |
| 11  | aA    | 804 | CLA  | CAC-C3C-C4C | 2.66  | 128.25      | 124.79   |
| 11  | bA    | 806 | CLA  | CHD-C4C-NC  | 2.66  | 128.36      | 124.23   |
| 11  | cK    | 103 | CLA  | CHD-C4C-NC  | 2.66  | 128.36      | 124.23   |
| 11  | aA    | 839 | CLA  | CAA-C2A-C3A | -2.66 | 105.81      | 113.00   |
| 11  | aB    | 822 | CLA  | CHC-C1C-C2C | -2.66 | 119.39      | 126.95   |
| 12  | aA    | 830 | F6C  | C4A-NA-C1A  | -2.66 | 104.45      | 106.31   |
| 15  | cB    | 845 | BCR  | C15-C14-C13 | -2.66 | 123.55      | 127.28   |
| 11  | cA    | 820 | CLA  | CHD-C4C-NC  | 2.66  | 128.35      | 124.23   |
| 11  | bA    | 822 | CLA  | CMC-C2C-C1C | 2.66  | 129.19      | 125.03   |
| 11  | aB    | 821 | CLA  | CHD-C4C-NC  | 2.66  | 128.35      | 124.23   |
| 11  | bA    | 809 | CLA  | CHB-C4A-NA  | 2.66  | 128.24      | 124.40   |
| 11  | bB    | 839 | CLA  | CMC-C2C-C1C | 2.66  | 129.19      | 125.03   |
| 11  | bB    | 822 | CLA  | CHC-C1C-C2C | -2.66 | 119.40      | 126.95   |
| 11  | bA    | 810 | CLA  | CMB-C2B-C1B | 2.66  | 129.46      | 125.42   |
| 12  | cA    | 844 | F6C  | C4-C3-C5    | 2.66  | 119.84      | 115.23   |
| 11  | aB    | 812 | CLA  | CMC-C2C-C1C | 2.66  | 129.18      | 125.03   |
| 11  | cA    | 822 | CLA  | CMC-C2C-C1C | 2.66  | 129.18      | 125.03   |
| 11  | aA    | 841 | CLA  | CHD-C4C-NC  | 2.66  | 128.35      | 124.23   |
| 15  | bK    | 102 | BCR  | C15-C14-C13 | -2.65 | 123.56      | 127.28   |
| 11  | cB    | 816 | CLA  | CHB-C4A-NA  | 2.65  | 128.23      | 124.40   |
| 11  | aA    | 823 | CLA  | C4C-C3C-C2C | -2.65 | 103.03      | 106.89   |
| 11  | cB    | 837 | CLA  | C4B-C3B-C2B | -2.65 | 104.00      | 107.30   |
| 15  | cA    | 848 | BCR  | C27-C26-C25 | 2.65  | 126.29      | 122.70   |
| 11  | cA    | 834 | CLA  | C4-C3-C5    | 2.65  | 119.83      | 115.23   |
| 11  | aA    | 802 | CLA  | C11-C12-C13 | -2.65 | 107.15      | 115.97   |
| 11  | cB    | 830 | CLA  | CHD-C4C-NC  | 2.65  | 128.34      | 124.23   |
| 11  | cA    | 806 | CLA  | CHD-C4C-NC  | 2.65  | 128.34      | 124.23   |
| 11  | cB    | 822 | CLA  | CHC-C1C-C2C | -2.65 | 119.42      | 126.95   |
| 11  | aB    | 831 | CLA  | CMB-C2B-C1B | 2.65  | 129.46      | 125.42   |
| 11  | cA    | 841 | CLA  | CHD-C4C-NC  | 2.65  | 128.34      | 124.23   |
| 11  | bB    | 813 | CLA  | CAA-C2A-C3A | -2.65 | 105.84      | 113.00   |
| 11  | aB    | 839 | CLA  | CMC-C2C-C1C | 2.65  | 129.18      | 125.03   |
| 11  | bA    | 809 | CLA  | C4B-C3B-C2B | -2.65 | 104.01      | 107.30   |
| 11  | bA    | 802 | CLA  | C11-C12-C13 | -2.65 | 107.16      | 115.97   |
| 11  | cA    | 823 | CLA  | C4C-C3C-C2C | -2.65 | 103.04      | 106.89   |
| 11  | cA    | 839 | CLA  | CAA-C2A-C3A | -2.65 | 105.84      | 113.00   |
| 11  | cB    | 829 | CLA  | CMC-C2C-C1C | 2.65  | 129.17      | 125.03   |
| 11  | bB    | 821 | CLA  | CHD-C4C-NC  | 2.65  | 128.34      | 124.23   |
| 11  | cA    | 828 | CLA  | C4-C3-C5    | 2.65  | 119.82      | 115.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aA    | 809 | CLA  | CHB-C4A-NA  | 2.65  | 128.22      | 124.40   |
| 11  | bA    | 839 | CLA  | CAA-C2A-C3A | -2.65 | 105.85      | 113.00   |
| 11  | bA    | 836 | CLA  | CHD-C4C-NC  | 2.65  | 128.34      | 124.23   |
| 11  | cA    | 836 | CLA  | CHD-C4C-NC  | 2.65  | 128.34      | 124.23   |
| 11  | aB    | 815 | CLA  | C4B-C3B-C2B | -2.65 | 104.01      | 107.30   |
| 15  | aB    | 845 | BCR  | C15-C14-C13 | -2.65 | 123.57      | 127.28   |
| 11  | bA    | 806 | CLA  | CMB-C2B-C1B | 2.65  | 129.45      | 125.42   |
| 11  | bA    | 823 | CLA  | C4C-C3C-C2C | -2.65 | 103.04      | 106.89   |
| 11  | cB    | 825 | CLA  | C4-C3-C5    | 2.64  | 119.82      | 115.23   |
| 11  | aA    | 822 | CLA  | CMC-C2C-C1C | 2.64  | 129.17      | 125.03   |
| 11  | bB    | 825 | CLA  | C4-C3-C5    | 2.64  | 119.82      | 115.23   |
| 11  | aA    | 810 | CLA  | CMB-C2B-C1B | 2.64  | 129.44      | 125.42   |
| 11  | cA    | 809 | CLA  | C4B-C3B-C2B | -2.64 | 104.02      | 107.30   |
| 11  | bB    | 808 | CLA  | O2D-CGD-O1D | -2.64 | 118.70      | 123.85   |
| 11  | cA    | 804 | CLA  | CMB-C2B-C1B | 2.64  | 129.44      | 125.42   |
| 11  | bA    | 828 | CLA  | C4-C3-C5    | 2.64  | 119.81      | 115.23   |
| 11  | aA    | 815 | CLA  | CHD-C4C-NC  | 2.64  | 128.33      | 124.23   |
| 11  | cB    | 813 | CLA  | CAA-C2A-C3A | -2.64 | 105.86      | 113.00   |
| 11  | cA    | 802 | CLA  | C11-C12-C13 | -2.64 | 107.19      | 115.97   |
| 11  | bK    | 103 | CLA  | CHD-C4C-NC  | 2.64  | 128.33      | 124.23   |
| 11  | cA    | 815 | CLA  | CHD-C4C-NC  | 2.64  | 128.33      | 124.23   |
| 11  | bA    | 831 | CLA  | C4-C3-C5    | 2.64  | 119.81      | 115.23   |
| 13  | bB    | 841 | PQN  | C14-C13-C15 | 2.64  | 119.81      | 115.23   |
| 11  | aB    | 813 | CLA  | CAA-C2A-C3A | -2.64 | 105.86      | 113.00   |
| 11  | aB    | 837 | CLA  | C3B-C4B-NB  | 2.64  | 112.89      | 110.53   |
| 18  | aB    | 847 | LMG  | O1-C1-C2    | -2.64 | 104.27      | 108.27   |
| 11  | bB    | 819 | CLA  | C4B-C3B-C2B | -2.64 | 104.02      | 107.30   |
| 11  | cB    | 819 | CLA  | CMB-C2B-C1B | 2.64  | 129.44      | 125.42   |
| 11  | cB    | 831 | CLA  | CMB-C2B-C1B | 2.64  | 129.44      | 125.42   |
| 15  | cL    | 208 | BCR  | C27-C26-C25 | 2.64  | 126.27      | 122.70   |
| 11  | aA    | 831 | CLA  | O2D-CGD-O1D | -2.64 | 118.72      | 123.85   |
| 11  | cA    | 810 | CLA  | CMB-C2B-C1B | 2.64  | 129.43      | 125.42   |
| 11  | cA    | 805 | CLA  | CHB-C4A-NA  | 2.64  | 128.21      | 124.40   |
| 16  | aA    | 852 | LHG  | O8-C23-C24  | 2.64  | 119.87      | 111.83   |
| 11  | aB    | 821 | CLA  | O2A-CGA-CBA | 2.64  | 119.87      | 111.83   |
| 11  | bA    | 821 | CLA  | O2D-CGD-O1D | -2.64 | 118.72      | 123.85   |
| 12  | aB    | 824 | F6C  | C4A-NA-C1A  | -2.64 | 104.46      | 106.31   |
| 11  | cB    | 820 | CLA  | CMC-C2C-C1C | 2.64  | 129.15      | 125.03   |
| 11  | aB    | 825 | CLA  | C4-C3-C5    | 2.64  | 119.80      | 115.23   |
| 11  | cB    | 819 | CLA  | C4A-NA-C1A  | -2.63 | 105.48      | 106.68   |
| 11  | cB    | 806 | CLA  | C4B-C3B-C2B | -2.63 | 104.03      | 107.30   |
| 11  | bA    | 837 | CLA  | O2D-CGD-O1D | -2.63 | 118.72      | 123.85   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cL    | 204 | CLA  | CAC-C3C-C4C | 2.63  | 128.22      | 124.79   |
| 16  | bA    | 852 | LHG  | O8-C23-C24  | 2.63  | 119.86      | 111.83   |
| 11  | bB    | 819 | CLA  | C4A-NA-C1A  | -2.63 | 105.48      | 106.68   |
| 12  | bA    | 844 | F6C  | C4C-C3C-C2C | -2.63 | 102.80      | 106.87   |
| 11  | cA    | 802 | CLA  | CHB-C1B-C2B | -2.63 | 119.79      | 127.43   |
| 11  | bB    | 815 | CLA  | C4B-C3B-C2B | -2.63 | 104.03      | 107.30   |
| 11  | bL    | 204 | CLA  | CAC-C3C-C4C | 2.63  | 128.21      | 124.79   |
| 11  | bA    | 834 | CLA  | C4-C3-C5    | 2.63  | 119.79      | 115.23   |
| 11  | bA    | 825 | CLA  | CHD-C4C-NC  | 2.63  | 128.31      | 124.23   |
| 11  | aB    | 808 | CLA  | O2D-CGD-O1D | -2.63 | 118.73      | 123.85   |
| 11  | cA    | 825 | CLA  | CHD-C4C-NC  | 2.63  | 128.31      | 124.23   |
| 11  | aB    | 819 | CLA  | C4B-C3B-C2B | -2.63 | 104.03      | 107.30   |
| 11  | bB    | 821 | CLA  | O2A-CGA-CBA | 2.63  | 119.85      | 111.83   |
| 11  | aA    | 834 | CLA  | C4-C3-C5    | 2.63  | 119.79      | 115.23   |
| 11  | cB    | 808 | CLA  | O2D-CGD-O1D | -2.63 | 118.73      | 123.85   |
| 11  | bA    | 804 | CLA  | CAC-C3C-C4C | 2.63  | 128.21      | 124.79   |
| 11  | bB    | 812 | CLA  | CMC-C2C-C1C | 2.63  | 129.14      | 125.03   |
| 11  | bA    | 810 | CLA  | CHD-C4C-NC  | 2.63  | 128.31      | 124.23   |
| 11  | aA    | 802 | CLA  | CBC-CAC-C3C | -2.63 | 105.30      | 112.42   |
| 12  | aA    | 826 | F6C  | C4-C3-C5    | 2.63  | 119.79      | 115.23   |
| 11  | bA    | 829 | CLA  | CHD-C4C-NC  | 2.63  | 128.30      | 124.23   |
| 11  | cA    | 837 | CLA  | O2D-CGD-O1D | -2.62 | 118.74      | 123.85   |
| 11  | cA    | 810 | CLA  | CHD-C4C-NC  | 2.62  | 128.30      | 124.23   |
| 11  | bA    | 839 | CLA  | C1-C2-C3    | -2.62 | 121.90      | 126.20   |
| 11  | aL    | 204 | CLA  | CAC-C3C-C4C | 2.62  | 128.20      | 124.79   |
| 11  | bB    | 829 | CLA  | CMC-C2C-C1C | 2.62  | 129.13      | 125.03   |
| 11  | aA    | 810 | CLA  | CHD-C4C-NC  | 2.62  | 128.30      | 124.23   |
| 15  | bB    | 848 | BCR  | C15-C14-C13 | -2.62 | 123.60      | 127.28   |
| 11  | cB    | 819 | CLA  | O2A-CGA-CBA | 2.62  | 119.83      | 111.83   |
| 11  | cA    | 831 | CLA  | C4-C3-C5    | 2.62  | 119.78      | 115.23   |
| 15  | bB    | 845 | BCR  | C15-C14-C13 | -2.62 | 123.60      | 127.28   |
| 11  | bA    | 802 | CLA  | CHB-C1B-C2B | -2.62 | 119.82      | 127.43   |
| 11  | cA    | 819 | CLA  | CHC-C1C-C2C | -2.62 | 119.50      | 126.95   |
| 11  | aB    | 819 | CLA  | C4A-NA-C1A  | -2.62 | 105.48      | 106.68   |
| 13  | aB    | 841 | PQN  | C14-C13-C15 | 2.62  | 119.77      | 115.23   |
| 15  | bL    | 207 | BCR  | C15-C14-C13 | -2.62 | 123.61      | 127.28   |
| 15  | cB    | 848 | BCR  | C15-C14-C13 | -2.62 | 123.61      | 127.28   |
| 11  | bA    | 819 | CLA  | CHC-C1C-C2C | -2.62 | 119.51      | 126.95   |
| 12  | cB    | 824 | F6C  | C4A-NA-C1A  | -2.62 | 104.47      | 106.31   |
| 11  | aB    | 806 | CLA  | CMC-C2C-C1C | 2.62  | 129.12      | 125.03   |
| 11  | aA    | 831 | CLA  | C4-C3-C5    | 2.62  | 119.77      | 115.23   |
| 11  | cB    | 832 | CLA  | CHD-C4C-NC  | 2.62  | 128.29      | 124.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 15  | aA    | 851 | BCR  | C27-C26-C25 | 2.62  | 126.24      | 122.70   |
| 12  | bA    | 830 | F6C  | C4-C3-C5    | 2.62  | 119.77      | 115.23   |
| 11  | bB    | 819 | CLA  | O2A-CGA-CBA | 2.62  | 119.81      | 111.83   |
| 16  | cA    | 852 | LHG  | O8-C23-C24  | 2.62  | 119.81      | 111.83   |
| 12  | cA    | 844 | F6C  | C4C-C3C-C2C | -2.62 | 102.82      | 106.87   |
| 11  | aA    | 836 | CLA  | CHD-C4C-NC  | 2.62  | 128.29      | 124.23   |
| 11  | cB    | 812 | CLA  | CMC-C2C-C1C | 2.62  | 129.12      | 125.03   |
| 11  | aA    | 839 | CLA  | C1-C2-C3    | -2.62 | 121.91      | 126.20   |
| 11  | cA    | 828 | CLA  | CAA-C2A-C3A | -2.62 | 105.93      | 113.00   |
| 11  | aA    | 819 | CLA  | CHC-C1C-C2C | -2.62 | 119.52      | 126.95   |
| 11  | bA    | 818 | CLA  | CHC-C1C-C2C | -2.62 | 119.52      | 126.95   |
| 11  | cB    | 821 | CLA  | O2A-CGA-CBA | 2.61  | 119.81      | 111.83   |
| 12  | aA    | 844 | F6C  | C4C-C3C-C2C | -2.61 | 102.82      | 106.87   |
| 11  | cA    | 829 | CLA  | CHD-C4C-NC  | 2.61  | 128.28      | 124.23   |
| 11  | cB    | 811 | CLA  | CHD-C4C-NC  | 2.61  | 128.28      | 124.23   |
| 13  | cB    | 841 | PQN  | C14-C13-C15 | 2.61  | 119.77      | 115.23   |
| 11  | cB    | 806 | CLA  | C4-C3-C5    | 2.61  | 119.76      | 115.23   |
| 12  | bA    | 826 | F6C  | C4-C3-C5    | 2.61  | 119.76      | 115.23   |
| 11  | cA    | 802 | CLA  | CBC-CAC-C3C | -2.61 | 105.34      | 112.42   |
| 11  | cB    | 806 | CLA  | CMC-C2C-C1C | 2.61  | 129.12      | 125.03   |
| 11  | aB    | 819 | CLA  | O2A-CGA-CBA | 2.61  | 119.80      | 111.83   |
| 12  | bA    | 832 | F6C  | O2D-CGD-O1D | -2.61 | 118.76      | 123.85   |
| 11  | aA    | 813 | CLA  | C1-C2-C3    | -2.61 | 121.92      | 126.20   |
| 11  | aB    | 819 | CLA  | CMB-C2B-C1B | 2.61  | 129.40      | 125.42   |
| 11  | cA    | 841 | CLA  | CMB-C2B-C1B | 2.61  | 129.40      | 125.42   |
| 12  | cA    | 830 | F6C  | C4-C3-C5    | 2.61  | 119.76      | 115.23   |
| 11  | aA    | 820 | CLA  | CAA-C2A-C3A | -2.61 | 105.94      | 113.00   |
| 11  | bB    | 820 | CLA  | CMC-C2C-C1C | 2.61  | 129.11      | 125.03   |
| 11  | cA    | 821 | CLA  | O2D-CGD-O1D | -2.61 | 118.77      | 123.85   |
| 11  | bB    | 801 | CLA  | C4B-C3B-C2B | -2.61 | 104.06      | 107.30   |
| 11  | bB    | 831 | CLA  | CMB-C2B-C1B | 2.61  | 129.39      | 125.42   |
| 11  | aA    | 829 | CLA  | CHD-C4C-NC  | 2.61  | 128.28      | 124.23   |
| 11  | bA    | 802 | CLA  | CBC-CAC-C3C | -2.61 | 105.35      | 112.42   |
| 12  | cA    | 832 | F6C  | O2D-CGD-O1D | -2.61 | 118.77      | 123.85   |
| 11  | cB    | 801 | CLA  | CBC-CAC-C3C | -2.61 | 105.35      | 112.42   |
| 11  | bA    | 834 | CLA  | CAC-C3C-C4C | 2.61  | 128.18      | 124.79   |
| 11  | aA    | 812 | CLA  | C1-C2-C3    | -2.61 | 121.92      | 126.20   |
| 12  | cA    | 826 | F6C  | C4-C3-C5    | 2.61  | 119.76      | 115.23   |
| 11  | aA    | 802 | CLA  | CHB-C1B-C2B | -2.61 | 119.86      | 127.43   |
| 11  | cA    | 812 | CLA  | C1-C2-C3    | -2.61 | 121.92      | 126.20   |
| 11  | bB    | 832 | CLA  | CHD-C4C-NC  | 2.61  | 128.27      | 124.23   |
| 11  | bB    | 806 | CLA  | CMC-C2C-C1C | 2.61  | 129.11      | 125.03   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 15  | aB    | 848 | BCR  | C15-C14-C13 | -2.61 | 123.62      | 127.28   |
| 11  | bB    | 819 | CLA  | CMB-C2B-C1B | 2.61  | 129.39      | 125.42   |
| 12  | bA    | 830 | F6C  | C4A-NA-C1A  | -2.61 | 104.48      | 106.31   |
| 11  | aB    | 811 | CLA  | CHD-C4C-NC  | 2.61  | 128.27      | 124.23   |
| 11  | cB    | 803 | CLA  | CMB-C2B-C1B | 2.61  | 129.39      | 125.42   |
| 11  | bB    | 801 | CLA  | CBC-CAC-C3C | -2.61 | 105.36      | 112.42   |
| 15  | aL    | 208 | BCR  | C27-C26-C25 | 2.60  | 126.22      | 122.70   |
| 11  | aB    | 801 | CLA  | C4B-C3B-C2B | -2.60 | 104.06      | 107.30   |
| 11  | cB    | 801 | CLA  | C4B-C3B-C2B | -2.60 | 104.06      | 107.30   |
| 11  | bA    | 820 | CLA  | CAA-C2A-C3A | -2.60 | 105.96      | 113.00   |
| 11  | aB    | 838 | CLA  | O2D-CGD-O1D | -2.60 | 118.78      | 123.85   |
| 11  | bA    | 805 | CLA  | CHB-C4A-NA  | 2.60  | 128.16      | 124.40   |
| 11  | aB    | 801 | CLA  | CBC-CAC-C3C | -2.60 | 105.36      | 112.42   |
| 11  | cA    | 812 | CLA  | CMB-C2B-C1B | 2.60  | 129.38      | 125.42   |
| 11  | bA    | 831 | CLA  | CAA-C2A-C3A | -2.60 | 105.96      | 113.00   |
| 15  | aL    | 208 | BCR  | C15-C16-C17 | -2.60 | 118.19      | 123.52   |
| 12  | aA    | 830 | F6C  | C4-C3-C5    | 2.60  | 119.75      | 115.23   |
| 11  | aA    | 804 | CLA  | CMB-C2B-C1B | 2.60  | 129.38      | 125.42   |
| 11  | bA    | 812 | CLA  | C1-C2-C3    | -2.60 | 121.93      | 126.20   |
| 11  | bA    | 803 | CLA  | C4A-NA-C1A  | -2.60 | 105.49      | 106.68   |
| 11  | cA    | 818 | CLA  | CHC-C1C-C2C | -2.60 | 119.55      | 126.95   |
| 11  | cB    | 822 | CLA  | O2D-CGD-O1D | -2.60 | 118.78      | 123.85   |
| 11  | aB    | 817 | CLA  | C4C-C3C-C2C | -2.60 | 103.11      | 106.89   |
| 11  | aA    | 821 | CLA  | O2D-CGD-O1D | -2.60 | 118.79      | 123.85   |
| 11  | cB    | 838 | CLA  | O2D-CGD-O1D | -2.60 | 118.79      | 123.85   |
| 11  | aB    | 832 | CLA  | CHD-C4C-NC  | 2.60  | 128.26      | 124.23   |
| 11  | cB    | 817 | CLA  | C4C-C3C-C2C | -2.60 | 103.11      | 106.89   |
| 11  | cA    | 820 | CLA  | CAA-C2A-C3A | -2.60 | 105.98      | 113.00   |
| 11  | aB    | 837 | CLA  | C4B-C3B-C2B | -2.60 | 104.07      | 107.30   |
| 11  | bB    | 806 | CLA  | C4-C3-C5    | 2.60  | 119.73      | 115.23   |
| 11  | cA    | 802 | CLA  | C4-C3-C5    | 2.60  | 119.73      | 115.23   |
| 11  | bA    | 834 | CLA  | C1-C2-C3    | -2.60 | 121.94      | 126.20   |
| 15  | bL    | 208 | BCR  | C27-C26-C25 | 2.60  | 126.21      | 122.70   |
| 11  | cA    | 820 | CLA  | C4C-C3C-C2C | -2.60 | 103.11      | 106.89   |
| 11  | bL    | 205 | CLA  | CMB-C2B-C1B | 2.59  | 129.37      | 125.42   |
| 11  | aA    | 834 | CLA  | C1-C2-C3    | -2.59 | 121.95      | 126.20   |
| 11  | aA    | 828 | CLA  | CAA-C2A-C3A | -2.59 | 105.99      | 113.00   |
| 12  | bA    | 832 | F6C  | C4C-C3C-C2C | -2.59 | 102.86      | 106.87   |
| 12  | aA    | 832 | F6C  | O2D-CGD-O1D | -2.59 | 118.80      | 123.85   |
| 11  | bB    | 817 | CLA  | C4C-C3C-C2C | -2.59 | 103.12      | 106.89   |
| 15  | bA    | 849 | BCR  | C27-C26-C25 | 2.59  | 126.21      | 122.70   |
| 11  | aA    | 843 | CLA  | O2A-CGA-CBA | 2.59  | 119.74      | 111.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bA    | 828 | CLA  | CAA-C2A-C3A | -2.59 | 106.00      | 113.00   |
| 11  | aA    | 829 | CLA  | O2A-CGA-CBA | 2.59  | 119.74      | 111.83   |
| 11  | bA    | 838 | CLA  | CBC-CAC-C3C | -2.59 | 105.40      | 112.42   |
| 11  | bA    | 812 | CLA  | CMB-C2B-C1B | 2.59  | 129.36      | 125.42   |
| 11  | bA    | 813 | CLA  | C1-C2-C3    | -2.59 | 121.95      | 126.20   |
| 11  | aA    | 837 | CLA  | O2D-CGD-O1D | -2.59 | 118.81      | 123.85   |
| 11  | bB    | 803 | CLA  | CMB-C2B-C1B | 2.59  | 129.36      | 125.42   |
| 11  | bB    | 837 | CLA  | C4B-C3B-C2B | -2.59 | 104.08      | 107.30   |
| 11  | cB    | 828 | CLA  | O2A-CGA-CBA | 2.59  | 119.73      | 111.83   |
| 11  | aA    | 812 | CLA  | CHD-C4C-NC  | 2.59  | 128.25      | 124.23   |
| 12  | cA    | 832 | F6C  | C4C-C3C-C2C | -2.59 | 102.86      | 106.87   |
| 15  | aL    | 207 | BCR  | C15-C14-C13 | -2.59 | 123.65      | 127.28   |
| 11  | aA    | 818 | CLA  | CHC-C1C-C2C | -2.59 | 119.59      | 126.95   |
| 11  | aA    | 817 | CLA  | CAC-C3C-C4C | 2.59  | 128.16      | 124.79   |
| 11  | aA    | 834 | CLA  | CAC-C3C-C4C | 2.59  | 128.16      | 124.79   |
| 15  | cA    | 849 | BCR  | C27-C26-C25 | 2.59  | 126.20      | 122.70   |
| 11  | cB    | 821 | CLA  | CAC-C3C-C4C | 2.59  | 128.16      | 124.79   |
| 11  | cA    | 843 | CLA  | O2A-CGA-CBA | 2.59  | 119.72      | 111.83   |
| 11  | aA    | 812 | CLA  | CMB-C2B-C1B | 2.59  | 129.36      | 125.42   |
| 11  | aA    | 825 | CLA  | CHD-C4C-NC  | 2.59  | 128.24      | 124.23   |
| 11  | bL    | 206 | CLA  | O2D-CGD-O1D | -2.59 | 118.81      | 123.85   |
| 11  | aB    | 828 | CLA  | O2A-CGA-CBA | 2.59  | 119.72      | 111.83   |
| 11  | cB    | 801 | CLA  | CHB-C4A-NA  | 2.59  | 128.13      | 124.40   |
| 11  | aB    | 820 | CLA  | CMC-C2C-C1C | 2.59  | 129.07      | 125.03   |
| 11  | cA    | 817 | CLA  | CAC-C3C-C4C | 2.59  | 128.15      | 124.79   |
| 11  | aA    | 807 | CLA  | CBC-CAC-C3C | -2.59 | 105.41      | 112.42   |
| 11  | cA    | 829 | CLA  | O2A-CGA-CBA | 2.59  | 119.72      | 111.83   |
| 11  | aB    | 803 | CLA  | C1C-C2C-C3C | -2.59 | 104.26      | 106.98   |
| 11  | bA    | 807 | CLA  | CBC-CAC-C3C | -2.59 | 105.41      | 112.42   |
| 11  | cA    | 807 | CLA  | CBC-CAC-C3C | -2.59 | 105.41      | 112.42   |
| 11  | bA    | 829 | CLA  | O2A-CGA-CBA | 2.58  | 119.72      | 111.83   |
| 11  | bA    | 824 | CLA  | CAC-C3C-C4C | 2.58  | 128.15      | 124.79   |
| 12  | cB    | 824 | F6C  | O2D-CGD-O1D | -2.58 | 118.82      | 123.85   |
| 11  | aA    | 831 | CLA  | CAA-C2A-C3A | -2.58 | 106.02      | 113.00   |
| 11  | aB    | 806 | CLA  | C4-C3-C5    | 2.58  | 119.71      | 115.23   |
| 11  | bA    | 843 | CLA  | O2A-CGA-CBA | 2.58  | 119.71      | 111.83   |
| 11  | cB    | 802 | CLA  | CHD-C4C-NC  | 2.58  | 128.24      | 124.23   |
| 15  | cL    | 208 | BCR  | C15-C16-C17 | -2.58 | 118.23      | 123.52   |
| 11  | cA    | 831 | CLA  | CAA-C2A-C3A | -2.58 | 106.02      | 113.00   |
| 11  | aA    | 805 | CLA  | CHB-C4A-NA  | 2.58  | 128.13      | 124.40   |
| 11  | cA    | 813 | CLA  | C1-C2-C3    | -2.58 | 121.97      | 126.20   |
| 11  | cB    | 809 | CLA  | CHD-C4C-NC  | 2.58  | 128.23      | 124.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12  | bB    | 824 | F6C  | C4A-NA-C1A  | -2.58 | 104.50      | 106.31   |
| 11  | cA    | 833 | CLA  | CAC-C3C-C4C | 2.58  | 128.15      | 124.79   |
| 11  | bA    | 841 | CLA  | CMB-C2B-C1B | 2.58  | 129.35      | 125.42   |
| 15  | cL    | 207 | BCR  | C15-C14-C13 | -2.58 | 123.66      | 127.28   |
| 15  | bL    | 208 | BCR  | C15-C16-C17 | -2.58 | 118.24      | 123.52   |
| 11  | bA    | 833 | CLA  | CAC-C3C-C4C | 2.58  | 128.15      | 124.79   |
| 11  | aA    | 820 | CLA  | C4C-C3C-C2C | -2.58 | 103.14      | 106.89   |
| 11  | bA    | 802 | CLA  | C4-C3-C5    | 2.58  | 119.71      | 115.23   |
| 11  | bA    | 812 | CLA  | CHD-C4C-NC  | 2.58  | 128.23      | 124.23   |
| 11  | bA    | 817 | CLA  | CAC-C3C-C4C | 2.58  | 128.15      | 124.79   |
| 11  | aA    | 815 | CLA  | CHB-C4A-NA  | 2.58  | 128.12      | 124.40   |
| 11  | aA    | 833 | CLA  | CAC-C3C-C4C | 2.58  | 128.14      | 124.79   |
| 11  | cA    | 808 | CLA  | C4-C3-C5    | 2.58  | 119.16      | 116.13   |
| 11  | cA    | 806 | CLA  | C1-C2-C3    | -2.58 | 121.97      | 126.20   |
| 12  | bB    | 824 | F6C  | O2D-CGD-O1D | -2.58 | 118.83      | 123.85   |
| 15  | cL    | 203 | BCR  | C11-C10-C9  | -2.58 | 123.66      | 127.28   |
| 13  | aA    | 845 | PQN  | C2M-C2-C3   | -2.58 | 120.22      | 124.45   |
| 11  | bB    | 822 | CLA  | O2D-CGD-O1D | -2.58 | 118.83      | 123.85   |
| 11  | aL    | 205 | CLA  | C1-C2-C3    | -2.58 | 121.98      | 126.20   |
| 15  | aA    | 849 | BCR  | C27-C26-C25 | 2.57  | 126.18      | 122.70   |
| 11  | bA    | 803 | CLA  | C1-C2-C3    | -2.57 | 121.98      | 126.20   |
| 11  | aB    | 820 | CLA  | CMB-C2B-C1B | 2.57  | 129.34      | 125.42   |
| 11  | cA    | 834 | CLA  | CAC-C3C-C4C | 2.57  | 128.14      | 124.79   |
| 11  | cA    | 838 | CLA  | CBC-CAC-C3C | -2.57 | 105.44      | 112.42   |
| 11  | bB    | 801 | CLA  | C4A-NA-C1A  | -2.57 | 105.50      | 106.68   |
| 11  | aL    | 206 | CLA  | O2D-CGD-O1D | -2.57 | 118.84      | 123.85   |
| 11  | bB    | 830 | CLA  | CAA-C2A-C3A | -2.57 | 106.05      | 113.00   |
| 11  | bB    | 838 | CLA  | CMB-C2B-C1B | 2.57  | 129.34      | 125.42   |
| 11  | aA    | 838 | CLA  | CBC-CAC-C3C | -2.57 | 105.45      | 112.42   |
| 11  | bA    | 809 | CLA  | CMC-C2C-C1C | 2.57  | 129.05      | 125.03   |
| 11  | bB    | 803 | CLA  | C1C-C2C-C3C | -2.57 | 104.28      | 106.98   |
| 11  | bA    | 815 | CLA  | CHB-C4A-NA  | 2.57  | 128.11      | 124.40   |
| 11  | cA    | 817 | CLA  | CBC-CAC-C3C | -2.57 | 105.45      | 112.42   |
| 11  | aA    | 806 | CLA  | C1-C2-C3    | -2.57 | 121.99      | 126.20   |
| 11  | bA    | 825 | CLA  | CHB-C4A-NA  | 2.57  | 128.11      | 124.40   |
| 11  | cB    | 801 | CLA  | C4A-NA-C1A  | -2.57 | 105.51      | 106.68   |
| 11  | aA    | 825 | CLA  | CHB-C4A-NA  | 2.57  | 128.11      | 124.40   |
| 11  | aB    | 803 | CLA  | CMB-C2B-C1B | 2.57  | 129.33      | 125.42   |
| 11  | cA    | 834 | CLA  | C1-C2-C3    | -2.57 | 121.99      | 126.20   |
| 11  | bA    | 814 | CLA  | O2D-CGD-O1D | -2.57 | 118.85      | 123.85   |
| 11  | cL    | 206 | CLA  | O2D-CGD-O1D | -2.57 | 118.85      | 123.85   |
| 11  | bB    | 809 | CLA  | CHD-C4C-NC  | 2.57  | 128.21      | 124.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12  | aA    | 832 | F6C  | C4C-C3C-C2C | -2.57 | 102.89      | 106.87   |
| 11  | aB    | 822 | CLA  | O2D-CGD-O1D | -2.57 | 118.85      | 123.85   |
| 12  | bA    | 844 | F6C  | C4A-NA-C1A  | -2.57 | 104.51      | 106.31   |
| 11  | cB    | 830 | CLA  | CAA-C2A-C3A | -2.57 | 106.06      | 113.00   |
| 11  | bB    | 814 | CLA  | CHD-C4C-NC  | 2.57  | 128.21      | 124.23   |
| 11  | cB    | 829 | CLA  | CHD-C4C-NC  | 2.57  | 128.21      | 124.23   |
| 11  | cB    | 806 | CLA  | CMB-C2B-C1B | 2.57  | 129.32      | 125.42   |
| 11  | cB    | 819 | CLA  | CHB-C4A-NA  | 2.57  | 128.10      | 124.40   |
| 13  | cA    | 845 | PQN  | C2M-C2-C3   | -2.56 | 120.23      | 124.45   |
| 11  | bB    | 828 | CLA  | C4-C3-C5    | 2.56  | 119.68      | 115.23   |
| 11  | cA    | 835 | CLA  | CMC-C2C-C1C | 2.56  | 129.04      | 125.03   |
| 11  | aA    | 841 | CLA  | CMB-C2B-C1B | 2.56  | 129.32      | 125.42   |
| 11  | aA    | 814 | CLA  | O2D-CGD-O1D | -2.56 | 118.86      | 123.85   |
| 11  | bA    | 840 | CLA  | CMC-C2C-C1C | 2.56  | 129.04      | 125.03   |
| 17  | cA    | 853 | LMT  | O5B-C5B-C4B | 2.56  | 114.32      | 109.70   |
| 11  | aB    | 802 | CLA  | CHD-C4C-NC  | 2.56  | 128.21      | 124.23   |
| 11  | aB    | 829 | CLA  | CHD-C4C-NC  | 2.56  | 128.21      | 124.23   |
| 11  | cA    | 812 | CLA  | CHD-C4C-NC  | 2.56  | 128.21      | 124.23   |
| 11  | aA    | 817 | CLA  | CBC-CAC-C3C | -2.56 | 105.47      | 112.42   |
| 11  | bB    | 821 | CLA  | CAC-C3C-C4C | 2.56  | 128.12      | 124.79   |
| 11  | bB    | 819 | CLA  | CHB-C4A-NA  | 2.56  | 128.10      | 124.40   |
| 11  | aA    | 809 | CLA  | CMC-C2C-C1C | 2.56  | 129.04      | 125.03   |
| 15  | aL    | 203 | BCR  | C11-C10-C9  | -2.56 | 123.69      | 127.28   |
| 11  | aA    | 802 | CLA  | C4-C3-C5    | 2.56  | 119.67      | 115.23   |
| 11  | bB    | 828 | CLA  | O2A-CGA-CBA | 2.56  | 119.65      | 111.83   |
| 11  | bB    | 820 | CLA  | CMB-C2B-C1B | 2.56  | 129.32      | 125.42   |
| 12  | aA    | 844 | F6C  | C4A-NA-C1A  | -2.56 | 104.52      | 106.31   |
| 11  | aB    | 803 | CLA  | O2A-CGA-CBA | 2.56  | 119.64      | 111.83   |
| 11  | bA    | 817 | CLA  | CBC-CAC-C3C | -2.56 | 105.48      | 112.42   |
| 11  | bA    | 820 | CLA  | C4C-C3C-C2C | -2.56 | 103.17      | 106.89   |
| 11  | cB    | 814 | CLA  | CHD-C4C-NC  | 2.56  | 128.20      | 124.23   |
| 11  | aB    | 821 | CLA  | CAC-C3C-C4C | 2.56  | 128.12      | 124.79   |
| 11  | cL    | 205 | CLA  | CMB-C2B-C1B | 2.56  | 129.31      | 125.42   |
| 11  | aB    | 828 | CLA  | C4-C3-C5    | 2.56  | 119.67      | 115.23   |
| 11  | aB    | 819 | CLA  | CHB-C4A-NA  | 2.56  | 128.09      | 124.40   |
| 11  | cA    | 814 | CLA  | O2D-CGD-O1D | -2.56 | 118.87      | 123.85   |
| 11  | cA    | 816 | CLA  | CAA-C2A-C3A | -2.56 | 106.09      | 113.00   |
| 11  | cB    | 803 | CLA  | C1C-C2C-C3C | -2.56 | 104.29      | 106.98   |
| 11  | bA    | 806 | CLA  | C1-C2-C3    | -2.56 | 122.01      | 126.20   |
| 11  | cB    | 829 | CLA  | CHB-C4A-NA  | 2.56  | 128.09      | 124.40   |
| 12  | cA    | 830 | F6C  | C4A-NA-C1A  | -2.56 | 104.52      | 106.31   |
| 11  | cA    | 803 | CLA  | C1-C2-C3    | -2.56 | 122.01      | 126.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bB    | 811 | CLA  | CMB-C2B-C1B | 2.56  | 129.31      | 125.42   |
| 12  | aL    | 202 | F6C  | CHD-C4C-NC  | 2.56  | 127.88      | 124.05   |
| 11  | cB    | 838 | CLA  | CMB-C2B-C1B | 2.56  | 129.31      | 125.42   |
| 15  | aL    | 203 | BCR  | C27-C26-C25 | 2.56  | 126.16      | 122.70   |
| 15  | bI    | 101 | BCR  | C27-C26-C25 | 2.56  | 126.16      | 122.70   |
| 11  | bA    | 816 | CLA  | CAA-C2A-C3A | -2.56 | 106.09      | 113.00   |
| 11  | bB    | 802 | CLA  | CHD-C4C-NC  | 2.56  | 128.19      | 124.23   |
| 11  | cL    | 205 | CLA  | C1-C2-C3    | -2.55 | 122.01      | 126.20   |
| 11  | cB    | 837 | CLA  | CMB-C2B-C1B | 2.55  | 129.31      | 125.42   |
| 17  | bA    | 853 | LMT  | O5B-C5B-C4B | 2.55  | 114.30      | 109.70   |
| 11  | cB    | 832 | CLA  | CHB-C4A-NA  | 2.55  | 128.09      | 124.40   |
| 11  | cB    | 815 | CLA  | CMB-C2B-C1B | 2.55  | 129.31      | 125.42   |
| 15  | aM    | 101 | BCR  | C24-C23-C22 | -2.55 | 122.46      | 126.23   |
| 11  | bL    | 205 | CLA  | C1-C2-C3    | -2.55 | 122.02      | 126.20   |
| 12  | bL    | 202 | F6C  | CHD-C4C-NC  | 2.55  | 127.88      | 124.05   |
| 15  | cM    | 101 | BCR  | C24-C23-C22 | -2.55 | 122.46      | 126.23   |
| 13  | bA    | 845 | PQN  | C2M-C2-C3   | -2.55 | 120.26      | 124.45   |
| 11  | aB    | 812 | CLA  | C4-C3-C5    | 2.55  | 119.66      | 115.23   |
| 11  | aA    | 816 | CLA  | CAA-C2A-C3A | -2.55 | 106.11      | 113.00   |
| 11  | aB    | 814 | CLA  | CHD-C4C-NC  | 2.55  | 128.19      | 124.23   |
| 11  | bB    | 811 | CLA  | CAC-C3C-C4C | 2.55  | 128.11      | 124.79   |
| 11  | cA    | 808 | CLA  | CMC-C2C-C1C | 2.55  | 129.02      | 125.03   |
| 11  | bB    | 803 | CLA  | O2A-CGA-CBA | 2.55  | 119.61      | 111.83   |
| 17  | aA    | 853 | LMT  | O5B-C5B-C4B | 2.55  | 114.29      | 109.70   |
| 11  | aB    | 830 | CLA  | CAA-C2A-C3A | -2.55 | 106.11      | 113.00   |
| 11  | bA    | 834 | CLA  | O2A-CGA-CBA | 2.55  | 119.61      | 111.83   |
| 11  | cB    | 814 | CLA  | CMB-C2B-C1B | 2.55  | 129.30      | 125.42   |
| 10  | bA    | 801 | CL0  | C1C-CHC-C4B | 2.55  | 125.19      | 116.07   |
| 11  | aB    | 829 | CLA  | CHB-C4A-NA  | 2.55  | 128.08      | 124.40   |
| 10  | aA    | 801 | CL0  | C1C-CHC-C4B | 2.55  | 125.19      | 116.07   |
| 11  | bB    | 815 | CLA  | CMB-C2B-C1B | 2.55  | 129.30      | 125.42   |
| 11  | cA    | 834 | CLA  | O2A-CGA-CBA | 2.55  | 119.60      | 111.83   |
| 11  | bB    | 829 | CLA  | CHD-C4C-NC  | 2.55  | 128.18      | 124.23   |
| 11  | cA    | 809 | CLA  | CMC-C2C-C1C | 2.55  | 129.01      | 125.03   |
| 11  | bB    | 838 | CLA  | O2D-CGD-O1D | -2.55 | 118.89      | 123.85   |
| 11  | cB    | 812 | CLA  | C4-C3-C5    | 2.55  | 119.65      | 115.23   |
| 11  | aB    | 809 | CLA  | CHD-C4C-NC  | 2.55  | 128.18      | 124.23   |
| 12  | aB    | 824 | F6C  | O2D-CGD-O1D | -2.55 | 118.89      | 123.85   |
| 10  | cA    | 801 | CL0  | C1C-CHC-C4B | 2.55  | 125.18      | 116.07   |
| 11  | aB    | 806 | CLA  | CMB-C2B-C1B | 2.55  | 129.29      | 125.42   |
| 11  | cB    | 820 | CLA  | CMB-C2B-C1B | 2.54  | 129.29      | 125.42   |
| 11  | aL    | 205 | CLA  | CMB-C2B-C1B | 2.54  | 129.29      | 125.42   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 15  | bL    | 203 | BCR  | C11-C10-C9  | -2.54 | 123.71      | 127.28   |
| 11  | aA    | 808 | CLA  | CMC-C2C-C1C | 2.54  | 129.01      | 125.03   |
| 11  | aA    | 834 | CLA  | O2A-CGA-CBA | 2.54  | 119.59      | 111.83   |
| 12  | cL    | 202 | F6C  | CHD-C4C-NC  | 2.54  | 127.86      | 124.05   |
| 11  | cA    | 824 | CLA  | CAC-C3C-C4C | 2.54  | 128.10      | 124.79   |
| 11  | aB    | 811 | CLA  | CAC-C3C-C4C | 2.54  | 128.10      | 124.79   |
| 11  | aB    | 820 | CLA  | C4A-NA-C1A  | -2.54 | 105.52      | 106.68   |
| 11  | cB    | 803 | CLA  | O2A-CGA-CBA | 2.54  | 119.58      | 111.83   |
| 11  | aA    | 803 | CLA  | C1-C2-C3    | -2.54 | 122.04      | 126.20   |
| 11  | bB    | 829 | CLA  | CHB-C4A-NA  | 2.54  | 128.06      | 124.40   |
| 11  | bB    | 806 | CLA  | CMB-C2B-C1B | 2.54  | 129.28      | 125.42   |
| 18  | cB    | 847 | LMG  | O1-C7-C8    | -2.54 | 104.65      | 110.82   |
| 15  | aL    | 208 | BCR  | C11-C10-C9  | -2.54 | 123.72      | 127.28   |
| 11  | cA    | 806 | CLA  | O2D-CGD-O1D | -2.54 | 118.91      | 123.85   |
| 15  | bM    | 101 | BCR  | C24-C23-C22 | -2.54 | 122.48      | 126.23   |
| 11  | cA    | 840 | CLA  | CMC-C2C-C1C | 2.54  | 129.00      | 125.03   |
| 11  | cA    | 840 | CLA  | C4-C3-C5    | 2.54  | 119.63      | 115.23   |
| 10  | aA    | 801 | CL0  | O2D-CGD-O1D | -2.54 | 118.91      | 123.85   |
| 12  | cA    | 844 | F6C  | O2A-CGA-CBA | 2.54  | 119.57      | 111.83   |
| 11  | bA    | 808 | CLA  | C4-C3-C5    | 2.54  | 119.11      | 116.13   |
| 12  | aA    | 844 | F6C  | O2A-CGA-CBA | 2.54  | 119.57      | 111.83   |
| 11  | cA    | 825 | CLA  | CHB-C4A-NA  | 2.54  | 128.06      | 124.40   |
| 11  | aB    | 837 | CLA  | CMC-C2C-C1C | 2.54  | 129.00      | 125.03   |
| 12  | bA    | 844 | F6C  | O2A-CGA-CBA | 2.53  | 119.56      | 111.83   |
| 11  | aB    | 838 | CLA  | CMB-C2B-C1B | 2.53  | 129.28      | 125.42   |
| 11  | aA    | 840 | CLA  | CMC-C2C-C1C | 2.53  | 128.99      | 125.03   |
| 11  | bA    | 808 | CLA  | CMC-C2C-C1C | 2.53  | 128.99      | 125.03   |
| 15  | aL    | 207 | BCR  | C7-C8-C9    | -2.53 | 122.49      | 126.23   |
| 11  | bB    | 832 | CLA  | CHB-C4A-NA  | 2.53  | 128.06      | 124.40   |
| 12  | aA    | 832 | F6C  | C4A-NA-C1A  | -2.53 | 104.53      | 106.31   |
| 11  | aA    | 824 | CLA  | CAC-C3C-C4C | 2.53  | 128.09      | 124.79   |
| 11  | cB    | 811 | CLA  | CMB-C2B-C1B | 2.53  | 129.28      | 125.42   |
| 11  | bB    | 812 | CLA  | C4-C3-C5    | 2.53  | 119.62      | 115.23   |
| 11  | cA    | 815 | CLA  | CHB-C4A-NA  | 2.53  | 128.05      | 124.40   |
| 11  | cA    | 807 | CLA  | C4C-C3C-C2C | -2.53 | 103.21      | 106.89   |
| 11  | cB    | 811 | CLA  | CAC-C3C-C4C | 2.53  | 128.08      | 124.79   |
| 11  | aA    | 835 | CLA  | CMC-C2C-C1C | 2.53  | 128.99      | 125.03   |
| 12  | aB    | 824 | F6C  | C4C-C3C-C2C | -2.53 | 102.95      | 106.87   |
| 11  | cB    | 840 | CLA  | C4C-C3C-C2C | -2.53 | 103.21      | 106.89   |
| 11  | bB    | 814 | CLA  | CMB-C2B-C1B | 2.53  | 129.27      | 125.42   |
| 11  | cB    | 837 | CLA  | CMC-C2C-C1C | 2.53  | 128.99      | 125.03   |
| 11  | aA    | 808 | CLA  | C4-C3-C5    | 2.53  | 119.10      | 116.13   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aB    | 814 | CLA  | CMB-C2B-C1B | 2.53  | 129.27      | 125.42   |
| 11  | cA    | 804 | CLA  | CMC-C2C-C1C | 2.53  | 128.98      | 125.03   |
| 11  | cA    | 810 | CLA  | CMC-C2C-C1C | 2.53  | 128.98      | 125.03   |
| 11  | aB    | 815 | CLA  | CMB-C2B-C1B | 2.53  | 129.27      | 125.42   |
| 11  | bB    | 840 | CLA  | C4C-C3C-C2C | -2.53 | 103.21      | 106.89   |
| 11  | cA    | 807 | CLA  | CMC-C2C-C1C | 2.53  | 128.98      | 125.03   |
| 10  | bA    | 801 | CL0  | O2D-CGD-O1D | -2.52 | 118.93      | 123.85   |
| 11  | bA    | 840 | CLA  | C4-C3-C5    | 2.52  | 119.61      | 115.23   |
| 18  | aB    | 847 | LMG  | O1-C7-C8    | -2.52 | 104.68      | 110.82   |
| 11  | bB    | 801 | CLA  | CHB-C4A-NA  | 2.52  | 128.04      | 124.40   |
| 11  | cA    | 828 | CLA  | O2A-CGA-CBA | 2.52  | 119.53      | 111.83   |
| 11  | bB    | 813 | CLA  | C4A-NA-C1A  | -2.52 | 105.53      | 106.68   |
| 12  | cA    | 844 | F6C  | C4A-NA-C1A  | -2.52 | 104.54      | 106.31   |
| 11  | bB    | 827 | CLA  | CHD-C4C-NC  | 2.52  | 128.14      | 124.23   |
| 15  | cI    | 103 | BCR  | C27-C26-C25 | 2.52  | 126.11      | 122.70   |
| 15  | bL    | 208 | BCR  | C11-C10-C9  | -2.52 | 123.74      | 127.28   |
| 11  | cB    | 815 | CLA  | C1-C2-C3    | -2.52 | 122.07      | 126.20   |
| 15  | bB    | 842 | BCR  | C15-C14-C13 | -2.52 | 123.74      | 127.28   |
| 11  | bA    | 835 | CLA  | CMC-C2C-C1C | 2.52  | 128.97      | 125.03   |
| 11  | cB    | 827 | CLA  | CHD-C4C-NC  | 2.52  | 128.14      | 124.23   |
| 12  | bB    | 824 | F6C  | C4C-C3C-C2C | -2.52 | 102.97      | 106.87   |
| 15  | aI    | 101 | BCR  | C27-C26-C25 | 2.52  | 126.11      | 122.70   |
| 11  | aA    | 840 | CLA  | C4-C3-C5    | 2.52  | 119.60      | 115.23   |
| 11  | aA    | 807 | CLA  | CMC-C2C-C1C | 2.52  | 128.97      | 125.03   |
| 18  | bB    | 847 | LMG  | O1-C7-C8    | -2.52 | 104.69      | 110.82   |
| 11  | bB    | 831 | CLA  | C4-C3-C5    | 2.52  | 119.60      | 115.23   |
| 15  | cL    | 208 | BCR  | C11-C10-C9  | -2.52 | 123.75      | 127.28   |
| 11  | cA    | 824 | CLA  | CAA-C2A-C3A | -2.52 | 106.19      | 113.00   |
| 11  | aA    | 810 | CLA  | CMC-C2C-C1C | 2.52  | 128.97      | 125.03   |
| 11  | cB    | 828 | CLA  | C4-C3-C5    | 2.52  | 119.60      | 115.23   |
| 11  | cA    | 835 | CLA  | C4B-C3B-C2B | -2.52 | 104.17      | 107.30   |
| 11  | bB    | 820 | CLA  | C4A-NA-C1A  | -2.52 | 105.53      | 106.68   |
| 11  | aA    | 806 | CLA  | O2D-CGD-O1D | -2.52 | 118.95      | 123.85   |
| 11  | aB    | 840 | CLA  | C4C-C3C-C2C | -2.52 | 103.23      | 106.89   |
| 10  | cA    | 801 | CL0  | O2D-CGD-O1D | -2.52 | 118.95      | 123.85   |
| 15  | cL    | 203 | BCR  | C27-C26-C25 | 2.52  | 126.11      | 122.70   |
| 11  | aB    | 837 | CLA  | CMB-C2B-C1B | 2.52  | 129.25      | 125.42   |
| 11  | aA    | 804 | CLA  | CMC-C2C-C1C | 2.52  | 128.97      | 125.03   |
| 11  | aB    | 832 | CLA  | CHB-C4A-NA  | 2.52  | 128.03      | 124.40   |
| 15  | cL    | 207 | BCR  | C7-C8-C9    | -2.52 | 122.51      | 126.23   |
| 11  | aB    | 827 | CLA  | CHD-C4C-NC  | 2.52  | 128.13      | 124.23   |
| 12  | bA    | 826 | F6C  | OMB-CMB-C2B | -2.51 | 119.95      | 125.62   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12  | cB    | 824 | F6C  | C4C-C3C-C2C | -2.51 | 102.98      | 106.87   |
| 11  | cB    | 815 | CLA  | O2D-CGD-O1D | -2.51 | 118.96      | 123.85   |
| 11  | cB    | 831 | CLA  | C4-C3-C5    | 2.51  | 119.59      | 115.23   |
| 11  | bB    | 813 | CLA  | CMB-C2B-C1B | 2.51  | 129.25      | 125.42   |
| 11  | cA    | 812 | CLA  | O2A-CGA-CBA | 2.51  | 119.50      | 111.83   |
| 15  | aB    | 842 | BCR  | C15-C14-C13 | -2.51 | 123.75      | 127.28   |
| 12  | cL    | 202 | F6C  | CAA-C2A-C1A | -2.51 | 120.99      | 128.01   |
| 11  | cB    | 813 | CLA  | C4A-NA-C1A  | -2.51 | 105.53      | 106.68   |
| 11  | bB    | 837 | CLA  | CMC-C2C-C1C | 2.51  | 128.96      | 125.03   |
| 11  | aB    | 811 | CLA  | CMB-C2B-C1B | 2.51  | 129.24      | 125.42   |
| 11  | bB    | 821 | CLA  | CMB-C2B-C1B | 2.51  | 129.24      | 125.42   |
| 12  | bL    | 202 | F6C  | CAA-C2A-C1A | -2.51 | 120.99      | 128.01   |
| 12  | bA    | 830 | F6C  | CHD-C1D-ND  | -2.51 | 120.53      | 124.31   |
| 11  | bA    | 806 | CLA  | O2D-CGD-O1D | -2.51 | 118.96      | 123.85   |
| 11  | bB    | 838 | CLA  | O2A-CGA-O1A | -2.51 | 117.35      | 123.63   |
| 11  | bA    | 824 | CLA  | CAA-C2A-C3A | -2.51 | 106.22      | 113.00   |
| 11  | bA    | 828 | CLA  | O2A-CGA-CBA | 2.51  | 119.49      | 111.83   |
| 11  | bA    | 804 | CLA  | CMC-C2C-C1C | 2.51  | 128.96      | 125.03   |
| 11  | aA    | 828 | CLA  | O2A-CGA-CBA | 2.51  | 119.48      | 111.83   |
| 15  | bB    | 846 | BCR  | C3-C4-C5    | -2.51 | 109.58      | 114.06   |
| 11  | cA    | 806 | CLA  | C4C-C3C-C2C | -2.51 | 103.24      | 106.89   |
| 11  | aB    | 815 | CLA  | C1-C2-C3    | -2.51 | 122.09      | 126.20   |
| 11  | cB    | 814 | CLA  | CHB-C4A-NA  | 2.51  | 128.02      | 124.40   |
| 11  | bB    | 837 | CLA  | CMB-C2B-C1B | 2.51  | 129.24      | 125.42   |
| 11  | bB    | 815 | CLA  | O2D-CGD-O1D | -2.51 | 118.97      | 123.85   |
| 11  | bA    | 843 | CLA  | C1-C2-C3    | -2.51 | 122.09      | 126.20   |
| 11  | aB    | 801 | CLA  | CHB-C4A-NA  | 2.51  | 128.02      | 124.40   |
| 11  | aB    | 821 | CLA  | CMB-C2B-C1B | 2.51  | 129.24      | 125.42   |
| 15  | aB    | 848 | BCR  | C7-C8-C9    | -2.51 | 122.53      | 126.23   |
| 11  | bB    | 814 | CLA  | CHB-C4A-NA  | 2.51  | 128.02      | 124.40   |
| 11  | bA    | 806 | CLA  | C4C-C3C-C2C | -2.51 | 103.24      | 106.89   |
| 11  | bB    | 826 | CLA  | CMC-C2C-C1C | 2.51  | 128.95      | 125.03   |
| 12  | aL    | 202 | F6C  | CAA-C2A-C1A | -2.50 | 121.01      | 128.01   |
| 11  | cB    | 823 | CLA  | CHA-C1A-NA  | -2.50 | 120.72      | 126.39   |
| 11  | bA    | 812 | CLA  | O2A-CGA-CBA | 2.50  | 119.47      | 111.83   |
| 18  | cB    | 847 | LMG  | C40-C39-C38 | -2.50 | 101.71      | 114.37   |
| 11  | aA    | 812 | CLA  | O2A-CGA-CBA | 2.50  | 119.47      | 111.83   |
| 11  | cB    | 821 | CLA  | CMB-C2B-C1B | 2.50  | 129.23      | 125.42   |
| 11  | aB    | 817 | CLA  | CAC-C3C-C4C | 2.50  | 128.05      | 124.79   |
| 11  | bA    | 835 | CLA  | C4B-C3B-C2B | -2.50 | 104.19      | 107.30   |
| 15  | cB    | 844 | BCR  | C40-C30-C25 | 2.50  | 114.17      | 110.24   |
| 11  | aB    | 838 | CLA  | O2A-CGA-O1A | -2.50 | 117.37      | 123.63   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12  | aA    | 830 | F6C  | CHD-C1D-ND  | -2.50 | 120.54      | 124.31   |
| 11  | bB    | 811 | CLA  | CHB-C4A-NA  | 2.50  | 128.01      | 124.40   |
| 15  | cB    | 848 | BCR  | C7-C8-C9    | -2.50 | 122.53      | 126.23   |
| 11  | aA    | 814 | CLA  | CHB-C4A-NA  | 2.50  | 128.01      | 124.40   |
| 11  | bA    | 807 | CLA  | CMC-C2C-C1C | 2.50  | 128.94      | 125.03   |
| 11  | bB    | 819 | CLA  | CMC-C2C-C1C | 2.50  | 128.94      | 125.03   |
| 11  | aB    | 823 | CLA  | CHA-C1A-NA  | -2.50 | 120.73      | 126.39   |
| 16  | cA    | 852 | LHG  | C11-C10-C9  | -2.50 | 101.73      | 114.37   |
| 11  | aB    | 813 | CLA  | CMB-C2B-C1B | 2.50  | 129.23      | 125.42   |
| 11  | cB    | 813 | CLA  | CMB-C2B-C1B | 2.50  | 129.23      | 125.42   |
| 11  | aA    | 843 | CLA  | C1-C2-C3    | -2.50 | 122.10      | 126.20   |
| 18  | bB    | 847 | LMG  | C40-C39-C38 | -2.50 | 101.73      | 114.37   |
| 11  | cB    | 838 | CLA  | O2A-CGA-O1A | -2.50 | 117.37      | 123.63   |
| 11  | bA    | 810 | CLA  | CMC-C2C-C1C | 2.50  | 128.94      | 125.03   |
| 11  | cA    | 818 | CLA  | CHB-C4A-NA  | 2.50  | 128.01      | 124.40   |
| 11  | cB    | 811 | CLA  | CHB-C4A-NA  | 2.50  | 128.01      | 124.40   |
| 11  | cA    | 838 | CLA  | CAA-C2A-C3A | -2.50 | 106.24      | 113.00   |
| 11  | bB    | 823 | CLA  | CHA-C1A-NA  | -2.50 | 120.73      | 126.39   |
| 12  | bA    | 832 | F6C  | C4A-NA-C1A  | -2.50 | 104.56      | 106.31   |
| 11  | bA    | 833 | CLA  | CBC-CAC-C3C | -2.50 | 105.65      | 112.42   |
| 18  | aB    | 847 | LMG  | C40-C39-C38 | -2.50 | 101.74      | 114.37   |
| 11  | bB    | 834 | CLA  | CHD-C4C-NC  | 2.50  | 128.10      | 124.23   |
| 15  | bL    | 207 | BCR  | C7-C8-C9    | -2.50 | 122.54      | 126.23   |
| 11  | aB    | 831 | CLA  | C4-C3-C5    | 2.50  | 119.56      | 115.23   |
| 16  | bA    | 852 | LHG  | C11-C10-C9  | -2.50 | 101.75      | 114.37   |
| 11  | aB    | 826 | CLA  | CMC-C2C-C1C | 2.50  | 128.93      | 125.03   |
| 12  | aA    | 827 | F6C  | C4A-NA-C1A  | -2.50 | 104.56      | 106.31   |
| 11  | aA    | 824 | CLA  | CAA-C2A-C3A | -2.49 | 106.26      | 113.00   |
| 11  | bA    | 837 | CLA  | CMC-C2C-C1C | 2.49  | 128.93      | 125.03   |
| 11  | aA    | 833 | CLA  | CBC-CAC-C3C | -2.49 | 105.66      | 112.42   |
| 15  | aA    | 850 | BCR  | C27-C26-C25 | 2.49  | 126.07      | 122.70   |
| 11  | bB    | 815 | CLA  | C1-C2-C3    | -2.49 | 122.11      | 126.20   |
| 11  | aB    | 814 | CLA  | CHB-C4A-NA  | 2.49  | 128.00      | 124.40   |
| 11  | cA    | 833 | CLA  | CBC-CAC-C3C | -2.49 | 105.66      | 112.42   |
| 11  | cA    | 820 | CLA  | O2D-CGD-O1D | -2.49 | 119.00      | 123.85   |
| 15  | bL    | 203 | BCR  | C27-C26-C25 | 2.49  | 126.07      | 122.70   |
| 15  | cB    | 846 | BCR  | C3-C4-C5    | -2.49 | 109.61      | 114.06   |
| 12  | cA    | 826 | F6C  | OMB-CMB-C2B | -2.49 | 119.99      | 125.62   |
| 16  | aA    | 852 | LHG  | C11-C10-C9  | -2.49 | 101.77      | 114.37   |
| 12  | cA    | 830 | F6C  | CHD-C1D-ND  | -2.49 | 120.56      | 124.31   |
| 11  | aB    | 813 | CLA  | C4A-NA-C1A  | -2.49 | 105.54      | 106.68   |
| 11  | cA    | 837 | CLA  | CMC-C2C-C1C | 2.49  | 128.93      | 125.03   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cA    | 813 | CLA  | O2A-CGA-CBA | 2.49  | 119.43      | 111.83   |
| 15  | cB    | 846 | BCR  | C27-C26-C25 | 2.49  | 126.07      | 122.70   |
| 11  | aA    | 835 | CLA  | C4B-C3B-C2B | -2.49 | 104.21      | 107.30   |
| 11  | cA    | 814 | CLA  | CHB-C4A-NA  | 2.49  | 127.99      | 124.40   |
| 11  | aA    | 803 | CLA  | C4A-NA-C1A  | -2.49 | 105.54      | 106.68   |
| 11  | bA    | 820 | CLA  | C2A-C3A-C4A | -2.49 | 97.85       | 101.87   |
| 15  | bB    | 848 | BCR  | C7-C8-C9    | -2.49 | 122.56      | 126.23   |
| 11  | aA    | 828 | CLA  | C1C-C2C-C3C | -2.49 | 104.36      | 106.98   |
| 11  | aA    | 813 | CLA  | O2A-CGA-CBA | 2.49  | 119.42      | 111.83   |
| 11  | bA    | 807 | CLA  | C4C-C3C-C2C | -2.49 | 103.27      | 106.89   |
| 15  | cB    | 842 | BCR  | C15-C14-C13 | -2.49 | 123.79      | 127.28   |
| 11  | aA    | 825 | CLA  | O2A-CGA-O1A | -2.49 | 117.41      | 123.63   |
| 11  | aA    | 806 | CLA  | C4C-C3C-C2C | -2.49 | 103.27      | 106.89   |
| 11  | bA    | 838 | CLA  | CAA-C2A-C3A | -2.49 | 106.28      | 113.00   |
| 11  | bA    | 820 | CLA  | O2D-CGD-O1D | -2.48 | 119.01      | 123.85   |
| 11  | cB    | 837 | CLA  | O2D-CGD-O1D | -2.48 | 119.01      | 123.85   |
| 11  | cA    | 802 | CLA  | CMC-C2C-C1C | 2.48  | 128.91      | 125.03   |
| 12  | bA    | 827 | F6C  | C4A-NA-C1A  | -2.48 | 104.57      | 106.31   |
| 12  | aA    | 826 | F6C  | OMB-CMB-C2B | -2.48 | 120.02      | 125.62   |
| 11  | aA    | 831 | CLA  | O1D-CGD-CBD | -2.48 | 119.62      | 124.52   |
| 11  | bA    | 835 | CLA  | CHB-C4A-NA  | 2.48  | 127.98      | 124.40   |
| 11  | bA    | 831 | CLA  | CMB-C2B-C3B | 2.48  | 132.39      | 126.55   |
| 11  | bA    | 813 | CLA  | O2A-CGA-CBA | 2.48  | 119.40      | 111.83   |
| 11  | aA    | 838 | CLA  | CAA-C2A-C3A | -2.48 | 106.30      | 113.00   |
| 11  | aA    | 809 | CLA  | O2D-CGD-O1D | -2.48 | 119.02      | 123.85   |
| 11  | aA    | 807 | CLA  | C4C-C3C-C2C | -2.48 | 103.28      | 106.89   |
| 11  | bB    | 812 | CLA  | O2D-CGD-O1D | -2.48 | 119.02      | 123.85   |
| 11  | bB    | 817 | CLA  | CAC-C3C-C4C | 2.48  | 128.01      | 124.79   |
| 11  | aB    | 819 | CLA  | CMC-C2C-C1C | 2.48  | 128.91      | 125.03   |
| 11  | cA    | 843 | CLA  | C1-C2-C3    | -2.48 | 122.14      | 126.20   |
| 11  | bA    | 831 | CLA  | O1D-CGD-CBD | -2.48 | 119.63      | 124.52   |
| 11  | bB    | 806 | CLA  | O2A-CGA-CBA | 2.48  | 119.39      | 111.83   |
| 11  | aA    | 818 | CLA  | CHB-C4A-NA  | 2.48  | 127.97      | 124.40   |
| 11  | cA    | 834 | CLA  | CHB-C4A-NA  | 2.48  | 127.97      | 124.40   |
| 11  | bA    | 809 | CLA  | O2D-CGD-O1D | -2.48 | 119.03      | 123.85   |
| 11  | cB    | 826 | CLA  | CBA-CAA-C2A | 2.48  | 121.16      | 113.79   |
| 11  | aB    | 814 | CLA  | O1D-CGD-CBD | -2.47 | 119.64      | 124.52   |
| 11  | aA    | 837 | CLA  | CMC-C2C-C1C | 2.47  | 128.90      | 125.03   |
| 15  | bM    | 101 | BCR  | C28-C27-C26 | -2.47 | 109.64      | 114.06   |
| 11  | aA    | 834 | CLA  | CHB-C4A-NA  | 2.47  | 127.97      | 124.40   |
| 11  | aB    | 826 | CLA  | CBA-CAA-C2A | 2.47  | 121.16      | 113.79   |
| 11  | cB    | 834 | CLA  | CHD-C4C-NC  | 2.47  | 128.07      | 124.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cB    | 826 | CLA  | CMC-C2C-C1C | 2.47  | 128.90      | 125.03   |
| 11  | cB    | 807 | CLA  | CMC-C2C-C1C | 2.47  | 128.90      | 125.03   |
| 11  | aB    | 815 | CLA  | O2D-CGD-O1D | -2.47 | 119.04      | 123.85   |
| 11  | aA    | 821 | CLA  | CHD-C4C-NC  | 2.47  | 128.06      | 124.23   |
| 11  | bB    | 810 | CLA  | CBC-CAC-C3C | -2.47 | 105.72      | 112.42   |
| 11  | bL    | 205 | CLA  | O2A-CGA-CBA | 2.47  | 119.37      | 111.83   |
| 11  | aB    | 811 | CLA  | CHB-C4A-NA  | 2.47  | 127.96      | 124.40   |
| 11  | cB    | 817 | CLA  | CAC-C3C-C4C | 2.47  | 128.00      | 124.79   |
| 15  | aM    | 101 | BCR  | C28-C27-C26 | -2.47 | 109.65      | 114.06   |
| 15  | aB    | 846 | BCR  | C3-C4-C5    | -2.47 | 109.65      | 114.06   |
| 11  | bB    | 825 | CLA  | C1-C2-C3    | -2.47 | 122.15      | 126.20   |
| 15  | bA    | 849 | BCR  | C29-C30-C25 | 2.47  | 114.03      | 110.44   |
| 11  | cB    | 810 | CLA  | CBC-CAC-C3C | -2.47 | 105.73      | 112.42   |
| 12  | cB    | 824 | F6C  | CBC-CAC-C3C | -2.47 | 105.73      | 112.42   |
| 11  | cA    | 831 | CLA  | CMB-C2B-C3B | 2.47  | 132.35      | 126.55   |
| 11  | cA    | 820 | CLA  | C2A-C3A-C4A | -2.47 | 97.88       | 101.87   |
| 12  | cB    | 824 | F6C  | O2A-CGA-CBA | 2.47  | 119.36      | 111.83   |
| 11  | bB    | 801 | CLA  | O2D-CGD-O1D | -2.47 | 119.05      | 123.85   |
| 11  | aA    | 802 | CLA  | CMC-C2C-C1C | 2.47  | 128.89      | 125.03   |
| 11  | aL    | 205 | CLA  | O2A-CGA-CBA | 2.47  | 119.36      | 111.83   |
| 11  | cB    | 806 | CLA  | O2A-CGA-CBA | 2.47  | 119.36      | 111.83   |
| 11  | aA    | 831 | CLA  | CMB-C2B-C3B | 2.47  | 132.35      | 126.55   |
| 11  | bA    | 818 | CLA  | CHB-C4A-NA  | 2.47  | 127.96      | 124.40   |
| 11  | bB    | 826 | CLA  | CBA-CAA-C2A | 2.47  | 121.13      | 113.79   |
| 11  | aB    | 812 | CLA  | O2D-CGD-O1D | -2.47 | 119.05      | 123.85   |
| 12  | bB    | 824 | F6C  | O2A-CGA-CBA | 2.47  | 119.35      | 111.83   |
| 11  | cA    | 808 | CLA  | CHB-C4A-NA  | 2.46  | 127.96      | 124.40   |
| 12  | aB    | 824 | F6C  | CBC-CAC-C3C | -2.46 | 105.74      | 112.42   |
| 15  | cA    | 850 | BCR  | C27-C26-C25 | 2.46  | 126.03      | 122.70   |
| 11  | cA    | 821 | CLA  | CHD-C4C-NC  | 2.46  | 128.05      | 124.23   |
| 12  | cA    | 832 | F6C  | C4A-NA-C1A  | -2.46 | 104.58      | 106.31   |
| 15  | cA    | 849 | BCR  | C29-C30-C25 | 2.46  | 114.02      | 110.44   |
| 11  | cA    | 819 | CLA  | CBA-CAA-C2A | 2.46  | 121.12      | 113.79   |
| 15  | aB    | 844 | BCR  | C40-C30-C25 | 2.46  | 114.10      | 110.24   |
| 11  | bB    | 814 | CLA  | O1D-CGD-CBD | -2.46 | 119.66      | 124.52   |
| 11  | aA    | 808 | CLA  | CHB-C4A-NA  | 2.46  | 127.95      | 124.40   |
| 11  | aB    | 806 | CLA  | O2A-CGA-CBA | 2.46  | 119.34      | 111.83   |
| 13  | cB    | 841 | PQN  | C2M-C2-C3   | -2.46 | 120.41      | 124.45   |
| 11  | cA    | 809 | CLA  | O2D-CGD-O1D | -2.46 | 119.06      | 123.85   |
| 11  | aA    | 819 | CLA  | CBA-CAA-C2A | 2.46  | 121.11      | 113.79   |
| 11  | cL    | 205 | CLA  | O2A-CGA-CBA | 2.46  | 119.33      | 111.83   |
| 12  | bB    | 824 | F6C  | CBC-CAC-C3C | -2.46 | 105.75      | 112.42   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aK    | 103 | CLA  | O2D-CGD-O1D | -2.46 | 119.06      | 123.85   |
| 11  | cA    | 836 | CLA  | CAA-C2A-C3A | -2.46 | 106.36      | 113.00   |
| 11  | aA    | 835 | CLA  | CHB-C4A-NA  | 2.46  | 127.95      | 124.40   |
| 11  | bA    | 814 | CLA  | CHB-C4A-NA  | 2.46  | 127.95      | 124.40   |
| 11  | bA    | 823 | CLA  | CHB-C4A-NA  | 2.46  | 127.95      | 124.40   |
| 15  | cA    | 851 | BCR  | C15-C14-C13 | -2.46 | 123.83      | 127.28   |
| 11  | cB    | 805 | CLA  | CMA-C3A-C2A | -2.46 | 104.48      | 113.98   |
| 13  | aB    | 841 | PQN  | C2M-C2-C3   | -2.46 | 120.41      | 124.45   |
| 11  | cB    | 819 | CLA  | CMC-C2C-C1C | 2.46  | 128.87      | 125.03   |
| 11  | bA    | 819 | CLA  | CBA-CAA-C2A | 2.46  | 121.10      | 113.79   |
| 11  | bB    | 836 | CLA  | CHD-C4C-NC  | 2.46  | 128.04      | 124.23   |
| 11  | aB    | 805 | CLA  | CMA-C3A-C2A | -2.46 | 104.49      | 113.98   |
| 11  | cA    | 831 | CLA  | O1D-CGD-CBD | -2.46 | 119.67      | 124.52   |
| 13  | bB    | 841 | PQN  | C2M-C2-C3   | -2.46 | 120.41      | 124.45   |
| 13  | cA    | 845 | PQN  | C11-C12-C13 | -2.46 | 122.60      | 126.83   |
| 11  | cB    | 804 | CLA  | O2D-CGD-O1D | -2.46 | 119.07      | 123.85   |
| 11  | aA    | 823 | CLA  | CHB-C4A-NA  | 2.46  | 127.94      | 124.40   |
| 15  | bB    | 844 | BCR  | C40-C30-C25 | 2.46  | 114.09      | 110.24   |
| 11  | cB    | 833 | CLA  | CMB-C2B-C1B | 2.45  | 129.16      | 125.42   |
| 11  | aB    | 810 | CLA  | CBC-CAC-C3C | -2.45 | 105.77      | 112.42   |
| 13  | aA    | 845 | PQN  | C11-C12-C13 | -2.45 | 122.60      | 126.83   |
| 11  | bA    | 825 | CLA  | O2A-CGA-O1A | -2.45 | 117.49      | 123.63   |
| 11  | bA    | 841 | CLA  | CHB-C4A-NA  | 2.45  | 127.94      | 124.40   |
| 12  | bL    | 202 | F6C  | OMB-CMB-C2B | -2.45 | 120.08      | 125.62   |
| 11  | bA    | 838 | CLA  | CMB-C2B-C3B | 2.45  | 132.32      | 126.55   |
| 11  | bB    | 805 | CLA  | CMA-C3A-C2A | -2.45 | 104.50      | 113.98   |
| 11  | aA    | 842 | CLA  | CAC-C3C-C4C | 2.45  | 127.98      | 124.79   |
| 11  | cB    | 813 | CLA  | CBC-CAC-C3C | -2.45 | 105.77      | 112.42   |
| 11  | cB    | 814 | CLA  | O1D-CGD-CBD | -2.45 | 119.68      | 124.52   |
| 11  | bB    | 813 | CLA  | CBC-CAC-C3C | -2.45 | 105.77      | 112.42   |
| 11  | aB    | 805 | CLA  | C1-C2-C3    | -2.45 | 122.18      | 126.20   |
| 11  | bA    | 802 | CLA  | CMC-C2C-C1C | 2.45  | 128.87      | 125.03   |
| 11  | bB    | 804 | CLA  | O2D-CGD-O1D | -2.45 | 119.07      | 123.85   |
| 11  | bB    | 837 | CLA  | O2D-CGD-O1D | -2.45 | 119.07      | 123.85   |
| 15  | bB    | 846 | BCR  | C27-C26-C25 | 2.45  | 126.02      | 122.70   |
| 15  | aA    | 849 | BCR  | C29-C30-C25 | 2.45  | 114.00      | 110.44   |
| 12  | aB    | 824 | F6C  | O2A-CGA-CBA | 2.45  | 119.31      | 111.83   |
| 11  | aB    | 807 | CLA  | CMC-C2C-C1C | 2.45  | 128.86      | 125.03   |
| 11  | bB    | 802 | CLA  | O2A-CGA-CBA | 2.45  | 119.31      | 111.83   |
| 11  | aB    | 837 | CLA  | O2D-CGD-O1D | -2.45 | 119.08      | 123.85   |
| 11  | cA    | 825 | CLA  | O2A-CGA-O1A | -2.45 | 117.50      | 123.63   |
| 11  | bA    | 828 | CLA  | C1C-C2C-C3C | -2.45 | 104.40      | 106.98   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cB    | 812 | CLA  | O2D-CGD-O1D | -2.45 | 119.08      | 123.85   |
| 11  | cA    | 842 | CLA  | CAC-C3C-C4C | 2.45  | 127.98      | 124.79   |
| 11  | aA    | 820 | CLA  | O2D-CGD-O1D | -2.45 | 119.08      | 123.85   |
| 11  | cA    | 807 | CLA  | O2D-CGD-O1D | -2.45 | 119.08      | 123.85   |
| 11  | cA    | 828 | CLA  | C4A-NA-C1A  | -2.45 | 105.56      | 106.68   |
| 12  | cA    | 830 | F6C  | O2A-CGA-CBA | 2.45  | 119.30      | 111.83   |
| 15  | bA    | 850 | BCR  | C27-C26-C25 | 2.45  | 126.01      | 122.70   |
| 15  | bA    | 851 | BCR  | C15-C14-C13 | -2.45 | 123.84      | 127.28   |
| 11  | cA    | 828 | CLA  | C1C-C2C-C3C | -2.45 | 104.41      | 106.98   |
| 11  | aK    | 101 | CLA  | CMB-C2B-C1B | 2.45  | 129.15      | 125.42   |
| 11  | aA    | 820 | CLA  | C2A-C3A-C4A | -2.45 | 97.92       | 101.87   |
| 11  | cB    | 802 | CLA  | O2A-CGA-CBA | 2.45  | 119.30      | 111.83   |
| 12  | bA    | 830 | F6C  | O2A-CGA-CBA | 2.45  | 119.30      | 111.83   |
| 11  | bA    | 834 | CLA  | O2A-CGA-O1A | -2.45 | 117.51      | 123.63   |
| 15  | aB    | 846 | BCR  | C27-C26-C25 | 2.45  | 126.01      | 122.70   |
| 11  | bK    | 101 | CLA  | CMB-C2B-C1B | 2.45  | 129.14      | 125.42   |
| 11  | aB    | 836 | CLA  | C4B-C3B-C2B | -2.45 | 104.26      | 107.30   |
| 11  | aA    | 815 | CLA  | O2D-CGD-O1D | -2.45 | 119.09      | 123.85   |
| 11  | aB    | 801 | CLA  | O2D-CGD-O1D | -2.45 | 119.09      | 123.85   |
| 11  | aB    | 825 | CLA  | C1-C2-C3    | -2.45 | 122.19      | 126.20   |
| 11  | aB    | 802 | CLA  | O2A-CGA-CBA | 2.45  | 119.29      | 111.83   |
| 12  | cL    | 202 | F6C  | OMB-CMB-C2B | -2.45 | 120.10      | 125.62   |
| 15  | aB    | 844 | BCR  | C30-C25-C26 | -2.44 | 119.30      | 122.64   |
| 15  | cM    | 101 | BCR  | C28-C27-C26 | -2.44 | 109.70      | 114.06   |
| 11  | cA    | 842 | CLA  | CMC-C2C-C1C | 2.44  | 128.85      | 125.03   |
| 12  | aA    | 830 | F6C  | O2A-CGA-CBA | 2.44  | 119.29      | 111.83   |
| 11  | cB    | 825 | CLA  | C1-C2-C3    | -2.44 | 122.19      | 126.20   |
| 11  | aA    | 836 | CLA  | CAA-C2A-C3A | -2.44 | 106.40      | 113.00   |
| 11  | cA    | 808 | CLA  | CMB-C2B-C1B | 2.44  | 129.14      | 125.42   |
| 11  | cK    | 101 | CLA  | CMB-C2B-C1B | 2.44  | 129.14      | 125.42   |
| 12  | bA    | 827 | F6C  | OMB-CMB-C2B | -2.44 | 120.11      | 125.62   |
| 11  | bB    | 823 | CLA  | CMB-C2B-C1B | 2.44  | 129.14      | 125.42   |
| 12  | aL    | 202 | F6C  | OMB-CMB-C2B | -2.44 | 120.11      | 125.62   |
| 11  | bA    | 815 | CLA  | O2D-CGD-O1D | -2.44 | 119.10      | 123.85   |
| 11  | bA    | 836 | CLA  | CAA-C2A-C3A | -2.44 | 106.40      | 113.00   |
| 11  | cA    | 835 | CLA  | CHB-C4A-NA  | 2.44  | 127.92      | 124.40   |
| 11  | aB    | 836 | CLA  | CHD-C4C-NC  | 2.44  | 128.01      | 124.23   |
| 11  | cA    | 829 | CLA  | CHB-C4A-NA  | 2.44  | 127.92      | 124.40   |
| 11  | bB    | 836 | CLA  | C4B-C3B-C2B | -2.44 | 104.27      | 107.30   |
| 11  | aB    | 813 | CLA  | CBC-CAC-C3C | -2.44 | 105.81      | 112.42   |
| 11  | cA    | 838 | CLA  | CMB-C2B-C3B | 2.44  | 132.28      | 126.55   |
| 11  | bA    | 842 | CLA  | CAC-C3C-C4C | 2.44  | 127.96      | 124.79   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cB    | 836 | CLA  | CHD-C4C-NC  | 2.44  | 128.01      | 124.23   |
| 11  | cA    | 815 | CLA  | O2D-CGD-O1D | -2.44 | 119.11      | 123.85   |
| 11  | aA    | 842 | CLA  | CMC-C2C-C1C | 2.44  | 128.84      | 125.03   |
| 11  | bB    | 807 | CLA  | CMC-C2C-C1C | 2.44  | 128.84      | 125.03   |
| 11  | aA    | 808 | CLA  | CMB-C2B-C1B | 2.44  | 129.13      | 125.42   |
| 11  | aB    | 804 | CLA  | O2D-CGD-O1D | -2.44 | 119.11      | 123.85   |
| 11  | bB    | 813 | CLA  | O2D-CGD-O1D | -2.44 | 119.11      | 123.85   |
| 11  | cA    | 823 | CLA  | CHB-C4A-NA  | 2.44  | 127.91      | 124.40   |
| 11  | bA    | 808 | CLA  | CMB-C2B-C1B | 2.43  | 129.13      | 125.42   |
| 12  | cA    | 827 | F6C  | C4A-NA-C1A  | -2.43 | 104.60      | 106.31   |
| 11  | cK    | 103 | CLA  | O2D-CGD-O1D | -2.43 | 119.11      | 123.85   |
| 15  | aB    | 843 | BCR  | C15-C16-C17 | -2.43 | 118.54      | 123.52   |
| 11  | bA    | 834 | CLA  | CHB-C4A-NA  | 2.43  | 127.91      | 124.40   |
| 11  | aA    | 838 | CLA  | CMB-C2B-C3B | 2.43  | 132.27      | 126.55   |
| 11  | aB    | 823 | CLA  | CMB-C2B-C1B | 2.43  | 129.12      | 125.42   |
| 11  | bA    | 842 | CLA  | CMC-C2C-C1C | 2.43  | 128.84      | 125.03   |
| 11  | aB    | 804 | CLA  | CHB-C4A-NA  | 2.43  | 127.91      | 124.40   |
| 11  | bB    | 833 | CLA  | CMB-C2B-C1B | 2.43  | 129.12      | 125.42   |
| 11  | aB    | 834 | CLA  | CHD-C4C-NC  | 2.43  | 128.00      | 124.23   |
| 11  | cB    | 805 | CLA  | C1-C2-C3    | -2.43 | 122.21      | 126.20   |
| 11  | bA    | 802 | CLA  | C6-C7-C8    | -2.43 | 107.89      | 115.97   |
| 11  | bA    | 829 | CLA  | CHB-C4A-NA  | 2.43  | 127.91      | 124.40   |
| 11  | bB    | 815 | CLA  | C4-C3-C5    | 2.43  | 119.45      | 115.23   |
| 12  | cA    | 827 | F6C  | OMB-CMB-C2B | -2.43 | 120.14      | 125.62   |
| 12  | bA    | 826 | F6C  | O1D-CGD-CBD | -2.43 | 119.73      | 124.52   |
| 11  | cB    | 823 | CLA  | CMB-C2B-C1B | 2.43  | 129.12      | 125.42   |
| 11  | cA    | 806 | CLA  | CAA-C2A-C3A | -2.43 | 106.44      | 113.00   |
| 11  | cB    | 839 | CLA  | C4-C3-C5    | 2.43  | 119.44      | 115.23   |
| 15  | bB    | 844 | BCR  | C30-C25-C26 | -2.43 | 119.32      | 122.64   |
| 13  | bA    | 845 | PQN  | C11-C12-C13 | -2.43 | 122.65      | 126.83   |
| 11  | cB    | 801 | CLA  | O2D-CGD-O1D | -2.43 | 119.12      | 123.85   |
| 11  | cB    | 813 | CLA  | O2D-CGD-O1D | -2.43 | 119.12      | 123.85   |
| 11  | aB    | 804 | CLA  | CAC-C3C-C4C | 2.43  | 127.95      | 124.79   |
| 11  | aB    | 839 | CLA  | C4-C3-C5    | 2.43  | 119.44      | 115.23   |
| 11  | bB    | 805 | CLA  | C1-C2-C3    | -2.43 | 122.22      | 126.20   |
| 11  | cA    | 834 | CLA  | O2A-CGA-O1A | -2.43 | 117.56      | 123.63   |
| 11  | aA    | 814 | CLA  | C4-C3-C5    | 2.43  | 119.44      | 115.23   |
| 11  | aA    | 812 | CLA  | CHB-C4A-NA  | 2.43  | 127.90      | 124.40   |
| 11  | cA    | 841 | CLA  | CHB-C4A-NA  | 2.43  | 127.90      | 124.40   |
| 11  | aB    | 826 | CLA  | O2A-CGA-O1A | -2.43 | 117.56      | 123.63   |
| 11  | aB    | 813 | CLA  | O2D-CGD-O1D | -2.42 | 119.13      | 123.85   |
| 11  | bK    | 103 | CLA  | CAA-CBA-CGA | -2.42 | 106.32      | 113.21   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cA    | 812 | CLA  | CHB-C4A-NA  | 2.42  | 127.90      | 124.40   |
| 11  | aA    | 838 | CLA  | O2D-CGD-O1D | -2.42 | 119.13      | 123.85   |
| 15  | bB    | 843 | BCR  | C15-C16-C17 | -2.42 | 118.56      | 123.52   |
| 11  | aA    | 813 | CLA  | CMC-C2C-C1C | 2.42  | 128.82      | 125.03   |
| 11  | cB    | 808 | CLA  | CBC-CAC-C3C | -2.42 | 105.85      | 112.42   |
| 11  | bA    | 814 | CLA  | C4-C3-C5    | 2.42  | 119.43      | 115.23   |
| 11  | cB    | 826 | CLA  | O2A-CGA-O1A | -2.42 | 117.57      | 123.63   |
| 12  | aA    | 826 | F6C  | O1D-CGD-CBD | -2.42 | 119.74      | 124.52   |
| 11  | aB    | 833 | CLA  | CMB-C2B-C1B | 2.42  | 129.11      | 125.42   |
| 11  | bB    | 828 | CLA  | CMB-C2B-C3B | 2.42  | 132.25      | 126.55   |
| 11  | aA    | 806 | CLA  | CAA-C2A-C3A | -2.42 | 106.45      | 113.00   |
| 11  | bB    | 817 | CLA  | O2D-CGD-O1D | -2.42 | 119.13      | 123.85   |
| 11  | cK    | 103 | CLA  | CAA-CBA-CGA | -2.42 | 106.33      | 113.21   |
| 11  | bA    | 807 | CLA  | O2D-CGD-O1D | -2.42 | 119.13      | 123.85   |
| 11  | aB    | 806 | CLA  | CBC-CAC-C3C | -2.42 | 105.86      | 112.42   |
| 12  | aA    | 827 | F6C  | OMB-CMB-C2B | -2.42 | 120.16      | 125.62   |
| 11  | aK    | 103 | CLA  | CAA-CBA-CGA | -2.42 | 106.33      | 113.21   |
| 15  | cA    | 850 | BCR  | C15-C14-C13 | -2.42 | 123.88      | 127.28   |
| 11  | aA    | 834 | CLA  | O2A-CGA-O1A | -2.42 | 117.57      | 123.63   |
| 11  | cA    | 838 | CLA  | O2D-CGD-O1D | -2.42 | 119.14      | 123.85   |
| 11  | cB    | 817 | CLA  | O2D-CGD-O1D | -2.42 | 119.14      | 123.85   |
| 11  | bB    | 804 | CLA  | CAC-C3C-C4C | 2.42  | 127.94      | 124.79   |
| 11  | bB    | 808 | CLA  | CBC-CAC-C3C | -2.42 | 105.86      | 112.42   |
| 11  | aA    | 829 | CLA  | CHB-C4A-NA  | 2.42  | 127.89      | 124.40   |
| 11  | aB    | 812 | CLA  | CAA-C2A-C3A | -2.42 | 106.47      | 113.00   |
| 15  | cB    | 843 | BCR  | C15-C16-C17 | -2.42 | 118.58      | 123.52   |
| 11  | bA    | 824 | CLA  | C1-C2-C3    | -2.42 | 122.24      | 126.20   |
| 11  | cA    | 824 | CLA  | C1-C2-C3    | -2.42 | 122.24      | 126.20   |
| 11  | aA    | 841 | CLA  | CHB-C4A-NA  | 2.42  | 127.89      | 124.40   |
| 18  | aB    | 847 | LMG  | C38-C37-C36 | -2.42 | 102.16      | 114.37   |
| 15  | aA    | 847 | BCR  | C28-C27-C26 | -2.42 | 109.75      | 114.06   |
| 11  | bB    | 826 | CLA  | O2A-CGA-O1A | -2.42 | 117.59      | 123.63   |
| 11  | bA    | 821 | CLA  | CHD-C4C-NC  | 2.42  | 127.98      | 124.23   |
| 11  | cB    | 836 | CLA  | C4B-C3B-C2B | -2.41 | 104.30      | 107.30   |
| 11  | aA    | 823 | CLA  | CMC-C2C-C1C | 2.41  | 128.81      | 125.03   |
| 11  | cB    | 839 | CLA  | O2D-CGD-O1D | -2.41 | 119.15      | 123.85   |
| 12  | aA    | 844 | F6C  | CBC-CAC-C3C | -2.41 | 105.88      | 112.42   |
| 11  | aB    | 808 | CLA  | CBC-CAC-C3C | -2.41 | 105.88      | 112.42   |
| 11  | aA    | 802 | CLA  | C6-C7-C8    | -2.41 | 107.94      | 115.97   |
| 11  | aB    | 839 | CLA  | O2D-CGD-O1D | -2.41 | 119.15      | 123.85   |
| 11  | aB    | 814 | CLA  | O2D-CGD-O1D | -2.41 | 119.15      | 123.85   |
| 11  | cB    | 812 | CLA  | CAA-C2A-C3A | -2.41 | 106.48      | 113.00   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bB    | 839 | CLA  | O2D-CGD-O1D | -2.41 | 119.15      | 123.85   |
| 12  | cA    | 826 | F6C  | O1D-CGD-CBD | -2.41 | 119.76      | 124.52   |
| 11  | aB    | 828 | CLA  | CMB-C2B-C3B | 2.41  | 132.22      | 126.55   |
| 15  | cB    | 844 | BCR  | C30-C25-C26 | -2.41 | 119.34      | 122.64   |
| 11  | bK    | 103 | CLA  | O2D-CGD-O1D | -2.41 | 119.16      | 123.85   |
| 15  | aA    | 851 | BCR  | C15-C14-C13 | -2.41 | 123.90      | 127.28   |
| 11  | bB    | 831 | CLA  | CHB-C4A-NA  | 2.41  | 127.88      | 124.40   |
| 15  | bA    | 850 | BCR  | C15-C14-C13 | -2.41 | 123.90      | 127.28   |
| 11  | cB    | 807 | CLA  | CBC-CAC-C3C | -2.41 | 105.89      | 112.42   |
| 11  | bB    | 812 | CLA  | CAA-C2A-C3A | -2.41 | 106.49      | 113.00   |
| 18  | cB    | 847 | LMG  | C38-C37-C36 | -2.41 | 102.19      | 114.37   |
| 11  | cA    | 802 | CLA  | C6-C7-C8    | -2.41 | 107.96      | 115.97   |
| 11  | aB    | 831 | CLA  | CHB-C4A-NA  | 2.41  | 127.88      | 124.40   |
| 11  | cB    | 801 | CLA  | C4-C3-C5    | 2.41  | 119.41      | 115.23   |
| 11  | bB    | 806 | CLA  | CBC-CAC-C3C | -2.41 | 105.89      | 112.42   |
| 15  | aA    | 851 | BCR  | C1-C6-C5    | -2.41 | 119.35      | 122.64   |
| 11  | bB    | 836 | CLA  | C1-C2-C3    | -2.41 | 122.25      | 126.20   |
| 11  | bB    | 804 | CLA  | CHB-C4A-NA  | 2.41  | 127.87      | 124.40   |
| 15  | cL    | 208 | BCR  | C15-C14-C13 | -2.41 | 123.90      | 127.28   |
| 11  | cB    | 815 | CLA  | C4-C3-C5    | 2.41  | 119.41      | 115.23   |
| 11  | aB    | 836 | CLA  | C1-C2-C3    | -2.41 | 122.25      | 126.20   |
| 11  | aA    | 807 | CLA  | O2D-CGD-O1D | -2.40 | 119.17      | 123.85   |
| 18  | bB    | 847 | LMG  | C38-C37-C36 | -2.40 | 102.21      | 114.37   |
| 15  | aL    | 208 | BCR  | C15-C14-C13 | -2.40 | 123.91      | 127.28   |
| 11  | bA    | 839 | CLA  | O2A-CGA-O1A | -2.40 | 117.61      | 123.63   |
| 11  | aA    | 839 | CLA  | O2A-CGA-O1A | -2.40 | 117.61      | 123.63   |
| 11  | cB    | 804 | CLA  | CAC-C3C-C4C | 2.40  | 127.92      | 124.79   |
| 11  | cB    | 828 | CLA  | CMB-C2B-C3B | 2.40  | 132.20      | 126.55   |
| 11  | cB    | 804 | CLA  | CHB-C4A-NA  | 2.40  | 127.87      | 124.40   |
| 11  | aB    | 813 | CLA  | O2A-CGA-CBA | 2.40  | 119.16      | 111.83   |
| 11  | bB    | 839 | CLA  | C4-C3-C5    | 2.40  | 119.40      | 115.23   |
| 11  | cB    | 828 | CLA  | CMD-C2D-C3D | -2.40 | 122.18      | 127.69   |
| 11  | cA    | 802 | CLA  | CHD-C4C-NC  | 2.40  | 127.95      | 124.23   |
| 11  | aB    | 805 | CLA  | C4-C3-C5    | 2.40  | 119.39      | 115.23   |
| 11  | cA    | 813 | CLA  | CMC-C2C-C1C | 2.40  | 128.78      | 125.03   |
| 11  | bA    | 802 | CLA  | CHD-C4C-NC  | 2.40  | 127.95      | 124.23   |
| 11  | cA    | 829 | CLA  | CMC-C2C-C1C | 2.40  | 128.78      | 125.03   |
| 11  | bA    | 823 | CLA  | CMC-C2C-C1C | 2.40  | 128.78      | 125.03   |
| 11  | cB    | 813 | CLA  | O2A-CGA-CBA | 2.40  | 119.15      | 111.83   |
| 11  | bA    | 806 | CLA  | CAA-C2A-C3A | -2.40 | 106.52      | 113.00   |
| 15  | aA    | 850 | BCR  | C15-C14-C13 | -2.40 | 123.91      | 127.28   |
| 11  | bB    | 804 | CLA  | O2A-CGA-CBA | 2.40  | 119.14      | 111.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cA    | 814 | CLA  | C4-C3-C5    | 2.40  | 119.39      | 115.23   |
| 11  | bA    | 838 | CLA  | O2D-CGD-O1D | -2.40 | 119.18      | 123.85   |
| 11  | bA    | 838 | CLA  | O2A-CGA-CBA | 2.40  | 119.14      | 111.83   |
| 11  | bA    | 841 | CLA  | CMC-C2C-C1C | 2.40  | 128.78      | 125.03   |
| 11  | aB    | 828 | CLA  | CMD-C2D-C3D | -2.40 | 122.20      | 127.69   |
| 15  | cA    | 847 | BCR  | C28-C27-C26 | -2.39 | 109.78      | 114.06   |
| 15  | bA    | 847 | BCR  | C28-C27-C26 | -2.39 | 109.79      | 114.06   |
| 11  | bB    | 807 | CLA  | CBC-CAC-C3C | -2.39 | 105.93      | 112.42   |
| 11  | cA    | 828 | CLA  | C1-C2-C3    | -2.39 | 122.28      | 126.20   |
| 11  | cB    | 806 | CLA  | CBC-CAC-C3C | -2.39 | 105.93      | 112.42   |
| 11  | aB    | 817 | CLA  | O2D-CGD-O1D | -2.39 | 119.19      | 123.85   |
| 11  | bB    | 828 | CLA  | CMD-C2D-C3D | -2.39 | 122.20      | 127.69   |
| 11  | bA    | 808 | CLA  | CHB-C4A-NA  | 2.39  | 127.85      | 124.40   |
| 11  | aB    | 807 | CLA  | CBC-CAC-C3C | -2.39 | 105.94      | 112.42   |
| 15  | aL    | 207 | BCR  | C11-C10-C9  | -2.39 | 123.92      | 127.28   |
| 11  | cA    | 841 | CLA  | CMC-C2C-C1C | 2.39  | 128.77      | 125.03   |
| 11  | bA    | 812 | CLA  | CHB-C4A-NA  | 2.39  | 127.85      | 124.40   |
| 11  | aA    | 824 | CLA  | C1-C2-C3    | -2.39 | 122.28      | 126.20   |
| 11  | bB    | 829 | CLA  | O2D-CGD-O1D | -2.39 | 119.19      | 123.85   |
| 11  | aA    | 803 | CLA  | C4-C3-C5    | 2.39  | 119.38      | 115.23   |
| 11  | bB    | 801 | CLA  | C4-C3-C5    | 2.39  | 119.38      | 115.23   |
| 11  | cB    | 820 | CLA  | C4C-C3C-C2C | -2.39 | 103.41      | 106.89   |
| 11  | aB    | 829 | CLA  | O2D-CGD-O1D | -2.39 | 119.20      | 123.85   |
| 11  | bA    | 813 | CLA  | CMC-C2C-C1C | 2.39  | 128.77      | 125.03   |
| 11  | bB    | 839 | CLA  | O2A-CGA-CBA | 2.39  | 119.12      | 111.83   |
| 11  | aL    | 204 | CLA  | O1D-CGD-CBD | -2.39 | 119.81      | 124.52   |
| 11  | aB    | 807 | CLA  | CHD-C4C-NC  | 2.39  | 127.93      | 124.23   |
| 11  | cB    | 825 | CLA  | O2D-CGD-O1D | -2.39 | 119.20      | 123.85   |
| 11  | aB    | 815 | CLA  | C4-C3-C5    | 2.39  | 119.37      | 115.23   |
| 11  | bB    | 825 | CLA  | O2D-CGD-O1D | -2.39 | 119.20      | 123.85   |
| 11  | cA    | 808 | CLA  | O2D-CGD-O1D | -2.39 | 119.20      | 123.85   |
| 11  | cB    | 814 | CLA  | O2D-CGD-O1D | -2.39 | 119.20      | 123.85   |
| 11  | bB    | 805 | CLA  | C4-C3-C5    | 2.39  | 119.37      | 115.23   |
| 11  | bB    | 813 | CLA  | O2A-CGA-CBA | 2.38  | 119.10      | 111.83   |
| 11  | bL    | 204 | CLA  | O1D-CGD-CBD | -2.38 | 119.82      | 124.52   |
| 11  | cB    | 827 | CLA  | CHD-C1D-ND  | -2.38 | 121.45      | 124.80   |
| 11  | bA    | 828 | CLA  | C1-C2-C3    | -2.38 | 122.29      | 126.20   |
| 12  | bA    | 844 | F6C  | CBC-CAC-C3C | -2.38 | 105.96      | 112.42   |
| 11  | cA    | 843 | CLA  | O2D-CGD-O1D | -2.38 | 119.21      | 123.85   |
| 11  | aB    | 820 | CLA  | C4C-C3C-C2C | -2.38 | 103.42      | 106.89   |
| 11  | cA    | 839 | CLA  | O2A-CGA-O1A | -2.38 | 117.67      | 123.63   |
| 11  | bB    | 814 | CLA  | O2D-CGD-O1D | -2.38 | 119.21      | 123.85   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bA    | 829 | CLA  | CMC-C2C-C1C | 2.38  | 128.75      | 125.03   |
| 11  | aB    | 801 | CLA  | C4-C3-C5    | 2.38  | 119.36      | 115.23   |
| 11  | bA    | 807 | CLA  | CHB-C4A-NA  | 2.38  | 127.84      | 124.40   |
| 12  | cA    | 844 | F6C  | CBC-CAC-C3C | -2.38 | 105.97      | 112.42   |
| 11  | bA    | 839 | CLA  | C4-C3-C5    | 2.38  | 119.36      | 115.23   |
| 15  | bL    | 207 | BCR  | C11-C10-C9  | -2.38 | 123.94      | 127.28   |
| 11  | aA    | 838 | CLA  | O2A-CGA-CBA | 2.38  | 119.09      | 111.83   |
| 11  | aA    | 834 | CLA  | CMC-C2C-C1C | 2.38  | 128.75      | 125.03   |
| 11  | cB    | 836 | CLA  | C1-C2-C3    | -2.38 | 122.30      | 126.20   |
| 11  | aB    | 804 | CLA  | O2A-CGA-CBA | 2.38  | 119.09      | 111.83   |
| 11  | cB    | 804 | CLA  | O2A-CGA-CBA | 2.38  | 119.09      | 111.83   |
| 11  | bB    | 826 | CLA  | O1D-CGD-CBD | -2.38 | 119.83      | 124.52   |
| 11  | bA    | 828 | CLA  | C4A-NA-C1A  | -2.38 | 105.59      | 106.68   |
| 15  | cA    | 851 | BCR  | C1-C6-C5    | -2.38 | 119.39      | 122.64   |
| 15  | bA    | 851 | BCR  | C24-C23-C22 | -2.38 | 122.72      | 126.23   |
| 15  | bL    | 208 | BCR  | C15-C14-C13 | -2.38 | 123.94      | 127.28   |
| 11  | cA    | 803 | CLA  | C4-C3-C5    | 2.38  | 119.35      | 115.23   |
| 11  | cL    | 204 | CLA  | O1D-CGD-CBD | -2.38 | 119.83      | 124.52   |
| 11  | aB    | 825 | CLA  | O2D-CGD-O1D | -2.38 | 119.22      | 123.85   |
| 11  | cB    | 839 | CLA  | C3B-C4B-NB  | 2.38  | 112.65      | 110.53   |
| 11  | aA    | 802 | CLA  | CHD-C4C-NC  | 2.38  | 127.92      | 124.23   |
| 11  | aB    | 839 | CLA  | O2A-CGA-CBA | 2.37  | 119.08      | 111.83   |
| 11  | bB    | 827 | CLA  | CHD-C1D-ND  | -2.37 | 121.46      | 124.80   |
| 11  | aA    | 836 | CLA  | CMC-C2C-C1C | 2.37  | 128.74      | 125.03   |
| 11  | aL    | 205 | CLA  | CMC-C2C-C1C | 2.37  | 128.74      | 125.03   |
| 11  | cB    | 836 | CLA  | O2D-CGD-O1D | -2.37 | 119.23      | 123.85   |
| 11  | cB    | 839 | CLA  | O2A-CGA-CBA | 2.37  | 119.07      | 111.83   |
| 11  | bA    | 808 | CLA  | O2D-CGD-O1D | -2.37 | 119.23      | 123.85   |
| 11  | cB    | 826 | CLA  | O1D-CGD-CBD | -2.37 | 119.84      | 124.52   |
| 11  | aA    | 807 | CLA  | C4-C3-C5    | 2.37  | 119.34      | 115.23   |
| 11  | aB    | 829 | CLA  | CHC-C1C-NC  | 2.37  | 127.88      | 124.31   |
| 15  | bM    | 101 | BCR  | C2-C1-C6    | 2.37  | 113.88      | 110.44   |
| 11  | aB    | 827 | CLA  | CHD-C1D-ND  | -2.37 | 121.47      | 124.80   |
| 15  | aL    | 207 | BCR  | C30-C25-C26 | -2.37 | 119.39      | 122.64   |
| 11  | bB    | 839 | CLA  | C3B-C4B-NB  | 2.37  | 112.65      | 110.53   |
| 11  | cA    | 836 | CLA  | CMC-C2C-C1C | 2.37  | 128.74      | 125.03   |
| 11  | cA    | 821 | CLA  | C4-C3-C5    | 2.37  | 119.34      | 115.23   |
| 11  | cB    | 829 | CLA  | O2D-CGD-O1D | -2.37 | 119.23      | 123.85   |
| 11  | bA    | 825 | CLA  | CMC-C2C-C1C | 2.37  | 128.74      | 125.03   |
| 11  | cL    | 205 | CLA  | CMC-C2C-C1C | 2.37  | 128.74      | 125.03   |
| 11  | cB    | 831 | CLA  | CBC-CAC-C3C | -2.37 | 106.00      | 112.42   |
| 11  | cB    | 805 | CLA  | C4-C3-C5    | 2.37  | 119.34      | 115.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cA    | 838 | CLA  | O2A-CGA-CBA | 2.37  | 119.06      | 111.83   |
| 11  | bA    | 834 | CLA  | CMC-C2C-C1C | 2.37  | 128.74      | 125.03   |
| 11  | bA    | 836 | CLA  | CMC-C2C-C1C | 2.37  | 128.74      | 125.03   |
| 11  | cA    | 823 | CLA  | CMC-C2C-C1C | 2.37  | 128.74      | 125.03   |
| 11  | bB    | 829 | CLA  | CHC-C1C-NC  | 2.37  | 127.88      | 124.31   |
| 11  | bB    | 806 | CLA  | CAC-C3C-C4C | 2.37  | 127.87      | 124.79   |
| 11  | cB    | 807 | CLA  | CHD-C4C-NC  | 2.37  | 127.90      | 124.23   |
| 15  | cL    | 207 | BCR  | C11-C10-C9  | -2.37 | 123.96      | 127.28   |
| 11  | bA    | 831 | CLA  | O2A-CGA-CBA | 2.37  | 119.05      | 111.83   |
| 11  | aB    | 826 | CLA  | O1D-CGD-CBD | -2.37 | 119.85      | 124.52   |
| 11  | aA    | 841 | CLA  | CMC-C2C-C1C | 2.37  | 128.73      | 125.03   |
| 11  | aA    | 831 | CLA  | O2A-CGA-CBA | 2.37  | 119.05      | 111.83   |
| 15  | aA    | 851 | BCR  | C24-C23-C22 | -2.37 | 122.73      | 126.23   |
| 11  | cA    | 814 | CLA  | CMC-C2C-C1C | 2.37  | 128.73      | 125.03   |
| 11  | aB    | 809 | CLA  | CBC-CAC-C3C | -2.37 | 106.01      | 112.42   |
| 11  | aA    | 807 | CLA  | CHB-C4A-NA  | 2.37  | 127.81      | 124.40   |
| 11  | bA    | 803 | CLA  | C4-C3-C5    | 2.37  | 119.33      | 115.23   |
| 11  | cB    | 831 | CLA  | CHB-C4A-NA  | 2.36  | 127.81      | 124.40   |
| 11  | cA    | 839 | CLA  | C4-C3-C5    | 2.36  | 119.33      | 115.23   |
| 11  | cA    | 831 | CLA  | O2A-CGA-CBA | 2.36  | 119.04      | 111.83   |
| 11  | aA    | 815 | CLA  | CBC-CAC-C3C | -2.36 | 106.01      | 112.42   |
| 11  | aB    | 831 | CLA  | CBC-CAC-C3C | -2.36 | 106.01      | 112.42   |
| 15  | cM    | 101 | BCR  | C15-C14-C13 | -2.36 | 123.96      | 127.28   |
| 11  | aA    | 829 | CLA  | CMC-C2C-C1C | 2.36  | 128.72      | 125.03   |
| 11  | bA    | 814 | CLA  | CMC-C2C-C1C | 2.36  | 128.72      | 125.03   |
| 11  | cA    | 825 | CLA  | CMC-C2C-C1C | 2.36  | 128.72      | 125.03   |
| 15  | aM    | 101 | BCR  | C15-C14-C13 | -2.36 | 123.97      | 127.28   |
| 11  | bB    | 809 | CLA  | CBC-CAC-C3C | -2.36 | 106.02      | 112.42   |
| 11  | aB    | 825 | CLA  | CAC-C3C-C4C | 2.36  | 127.86      | 124.79   |
| 11  | aA    | 821 | CLA  | CMC-C2C-C1C | 2.36  | 128.72      | 125.03   |
| 11  | bB    | 829 | CLA  | C3C-C4C-NC  | 2.36  | 113.45      | 110.43   |
| 11  | bB    | 820 | CLA  | C4C-C3C-C2C | -2.36 | 103.46      | 106.89   |
| 11  | cA    | 807 | CLA  | CHB-C4A-NA  | 2.36  | 127.80      | 124.40   |
| 11  | aA    | 828 | CLA  | C1-C2-C3    | -2.36 | 122.33      | 126.20   |
| 15  | bA    | 851 | BCR  | C1-C6-C5    | -2.36 | 119.42      | 122.64   |
| 11  | bA    | 834 | CLA  | CBC-CAC-C3C | -2.36 | 106.03      | 112.42   |
| 11  | aA    | 843 | CLA  | O2D-CGD-O1D | -2.36 | 119.26      | 123.85   |
| 15  | aM    | 101 | BCR  | C2-C1-C6    | 2.36  | 113.86      | 110.44   |
| 11  | bA    | 821 | CLA  | C4-C3-C5    | 2.36  | 119.32      | 115.23   |
| 15  | aK    | 102 | BCR  | C30-C25-C26 | -2.36 | 119.42      | 122.64   |
| 11  | bA    | 818 | CLA  | CAA-C2A-C3A | -2.36 | 106.63      | 113.00   |
| 11  | cB    | 806 | CLA  | CAC-C3C-C4C | 2.36  | 127.86      | 124.79   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bA    | 807 | CLA  | C4-C3-C5    | 2.36  | 119.32      | 115.23   |
| 11  | bB    | 807 | CLA  | CHD-C4C-NC  | 2.36  | 127.88      | 124.23   |
| 11  | cA    | 821 | CLA  | CMC-C2C-C1C | 2.36  | 128.72      | 125.03   |
| 11  | bA    | 838 | CLA  | C1-C2-C3    | -2.36 | 122.34      | 126.20   |
| 12  | cL    | 202 | F6C  | CHB-C1B-NB  | -2.36 | 120.58      | 124.23   |
| 11  | cA    | 818 | CLA  | CAA-C2A-C3A | -2.36 | 106.64      | 113.00   |
| 11  | cB    | 829 | CLA  | CHC-C1C-NC  | 2.36  | 127.86      | 124.31   |
| 11  | bL    | 205 | CLA  | CMC-C2C-C1C | 2.35  | 128.71      | 125.03   |
| 11  | bA    | 815 | CLA  | CBC-CAC-C3C | -2.35 | 106.04      | 112.42   |
| 11  | cL    | 204 | CLA  | CMC-C2C-C1C | 2.35  | 128.71      | 125.03   |
| 15  | cK    | 102 | BCR  | C30-C25-C26 | -2.35 | 119.42      | 122.64   |
| 11  | bB    | 831 | CLA  | CBC-CAC-C3C | -2.35 | 106.04      | 112.42   |
| 11  | aA    | 825 | CLA  | CMC-C2C-C1C | 2.35  | 128.71      | 125.03   |
| 12  | bA    | 832 | F6C  | CBC-CAC-C3C | -2.35 | 106.04      | 112.42   |
| 11  | bB    | 836 | CLA  | O2D-CGD-O1D | -2.35 | 119.27      | 123.85   |
| 11  | cA    | 833 | CLA  | O2D-CGD-O1D | -2.35 | 119.27      | 123.85   |
| 15  | aB    | 843 | BCR  | C33-C5-C6   | -2.35 | 121.92      | 124.48   |
| 12  | bL    | 202 | F6C  | CHB-C1B-NB  | -2.35 | 120.58      | 124.23   |
| 11  | bA    | 843 | CLA  | O2D-CGD-O1D | -2.35 | 119.27      | 123.85   |
| 15  | bL    | 207 | BCR  | C30-C25-C26 | -2.35 | 119.42      | 122.64   |
| 11  | aA    | 818 | CLA  | CAA-C2A-C3A | -2.35 | 106.64      | 113.00   |
| 11  | aA    | 821 | CLA  | C4-C3-C5    | 2.35  | 119.31      | 115.23   |
| 11  | aB    | 828 | CLA  | CBC-CAC-C3C | -2.35 | 106.05      | 112.42   |
| 12  | aA    | 832 | F6C  | CBC-CAC-C3C | -2.35 | 106.05      | 112.42   |
| 11  | aL    | 204 | CLA  | CBC-CAC-C3C | -2.35 | 106.05      | 112.42   |
| 11  | aA    | 808 | CLA  | O2D-CGD-O1D | -2.35 | 119.27      | 123.85   |
| 11  | bA    | 833 | CLA  | O2D-CGD-O1D | -2.35 | 119.27      | 123.85   |
| 12  | cA    | 832 | F6C  | CBC-CAC-C3C | -2.35 | 106.05      | 112.42   |
| 11  | cA    | 817 | CLA  | O2A-CGA-CBA | 2.35  | 119.00      | 111.83   |
| 10  | aA    | 801 | CL0  | C3D-C4D-ND  | 2.35  | 116.71      | 112.94   |
| 10  | cA    | 801 | CL0  | C3D-C4D-ND  | 2.35  | 116.71      | 112.94   |
| 12  | aB    | 824 | F6C  | O1D-CGD-CBD | -2.35 | 119.89      | 124.52   |
| 11  | cA    | 807 | CLA  | C4-C3-C5    | 2.35  | 119.30      | 115.23   |
| 11  | cB    | 809 | CLA  | CBC-CAC-C3C | -2.35 | 106.06      | 112.42   |
| 15  | cB    | 842 | BCR  | C27-C26-C25 | 2.35  | 125.88      | 122.70   |
| 11  | aB    | 836 | CLA  | O2D-CGD-O1D | -2.35 | 119.28      | 123.85   |
| 15  | cA    | 851 | BCR  | C24-C23-C22 | -2.35 | 122.76      | 126.23   |
| 11  | bB    | 807 | CLA  | CMA-C3A-C2A | -2.35 | 104.91      | 113.98   |
| 11  | aB    | 830 | CLA  | CHB-C4A-NA  | 2.35  | 127.79      | 124.40   |
| 11  | aA    | 839 | CLA  | C4-C3-C5    | 2.35  | 119.30      | 115.23   |
| 12  | aL    | 202 | F6C  | C4-C3-C5    | 2.35  | 119.30      | 115.23   |
| 11  | cA    | 834 | CLA  | CBC-CAC-C3C | -2.34 | 106.06      | 112.42   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aB    | 810 | CLA  | CMC-C2C-C1C | 2.34  | 128.70      | 125.03   |
| 11  | cA    | 834 | CLA  | CMC-C2C-C1C | 2.34  | 128.70      | 125.03   |
| 15  | cB    | 844 | BCR  | C15-C16-C17 | -2.34 | 118.72      | 123.52   |
| 11  | aB    | 802 | CLA  | CHA-C1A-NA  | -2.34 | 121.08      | 126.39   |
| 11  | bA    | 817 | CLA  | O2A-CGA-CBA | 2.34  | 118.98      | 111.83   |
| 11  | cA    | 815 | CLA  | CBC-CAC-C3C | -2.34 | 106.07      | 112.42   |
| 11  | aB    | 839 | CLA  | C3B-C4B-NB  | 2.34  | 112.62      | 110.53   |
| 11  | aA    | 834 | CLA  | CBC-CAC-C3C | -2.34 | 106.07      | 112.42   |
| 15  | bM    | 101 | BCR  | C15-C14-C13 | -2.34 | 123.99      | 127.28   |
| 11  | bA    | 843 | CLA  | CAA-C2A-C3A | -2.34 | 106.67      | 113.00   |
| 11  | bB    | 838 | CLA  | CHB-C4A-NA  | 2.34  | 127.78      | 124.40   |
| 11  | cB    | 829 | CLA  | C3C-C4C-NC  | 2.34  | 113.43      | 110.43   |
| 11  | cB    | 828 | CLA  | CBC-CAC-C3C | -2.34 | 106.07      | 112.42   |
| 11  | cA    | 838 | CLA  | C1-C2-C3    | -2.34 | 122.36      | 126.20   |
| 11  | aL    | 204 | CLA  | CMC-C2C-C1C | 2.34  | 128.69      | 125.03   |
| 11  | cA    | 843 | CLA  | CAA-C2A-C3A | -2.34 | 106.67      | 113.00   |
| 11  | aA    | 825 | CLA  | C4-C3-C5    | 2.34  | 119.29      | 115.23   |
| 11  | aA    | 838 | CLA  | C1-C2-C3    | -2.34 | 122.36      | 126.20   |
| 15  | bK    | 102 | BCR  | C30-C25-C26 | -2.34 | 119.44      | 122.64   |
| 15  | aB    | 842 | BCR  | C27-C26-C25 | 2.34  | 125.86      | 122.70   |
| 11  | bA    | 833 | CLA  | C4-C3-C5    | 2.34  | 119.29      | 115.23   |
| 11  | bB    | 828 | CLA  | CBC-CAC-C3C | -2.34 | 106.08      | 112.42   |
| 11  | cB    | 807 | CLA  | CMA-C3A-C2A | -2.34 | 104.94      | 113.98   |
| 11  | cL    | 204 | CLA  | CBC-CAC-C3C | -2.34 | 106.08      | 112.42   |
| 15  | bB    | 844 | BCR  | C15-C16-C17 | -2.34 | 118.73      | 123.52   |
| 11  | bB    | 809 | CLA  | O2D-CGD-O1D | -2.34 | 119.30      | 123.85   |
| 15  | bB    | 843 | BCR  | C33-C5-C6   | -2.34 | 121.93      | 124.48   |
| 11  | aB    | 807 | CLA  | CMA-C3A-C2A | -2.34 | 104.94      | 113.98   |
| 11  | aA    | 843 | CLA  | CAA-C2A-C3A | -2.34 | 106.68      | 113.00   |
| 11  | aA    | 825 | CLA  | CBC-CAC-C3C | -2.34 | 106.08      | 112.42   |
| 11  | aA    | 833 | CLA  | O2D-CGD-O1D | -2.34 | 119.30      | 123.85   |
| 11  | cB    | 810 | CLA  | CMC-C2C-C1C | 2.34  | 128.69      | 125.03   |
| 15  | bB    | 842 | BCR  | C27-C26-C25 | 2.34  | 125.86      | 122.70   |
| 11  | cA    | 825 | CLA  | CBC-CAC-C3C | -2.34 | 106.09      | 112.42   |
| 12  | cL    | 202 | F6C  | C4-C3-C5    | 2.34  | 119.28      | 115.23   |
| 11  | cB    | 817 | CLA  | C5-C3-C2    | -2.34 | 115.92      | 121.17   |
| 11  | bA    | 821 | CLA  | CMC-C2C-C1C | 2.34  | 128.68      | 125.03   |
| 11  | bA    | 825 | CLA  | C4-C3-C5    | 2.34  | 119.28      | 115.23   |
| 11  | bB    | 803 | CLA  | C4-C3-C5    | 2.33  | 119.28      | 115.23   |
| 12  | bL    | 202 | F6C  | C4-C3-C5    | 2.33  | 119.28      | 115.23   |
| 11  | bB    | 815 | CLA  | O2A-CGA-CBA | 2.33  | 118.95      | 111.83   |
| 11  | bL    | 204 | CLA  | CBC-CAC-C3C | -2.33 | 106.09      | 112.42   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 15  | aB    | 844 | BCR  | C15-C16-C17 | -2.33 | 118.74      | 123.52   |
| 11  | bB    | 825 | CLA  | CAC-C3C-C4C | 2.33  | 127.82      | 124.79   |
| 11  | aA    | 817 | CLA  | O2A-CGA-CBA | 2.33  | 118.94      | 111.83   |
| 11  | bA    | 825 | CLA  | CBC-CAC-C3C | -2.33 | 106.10      | 112.42   |
| 11  | bL    | 204 | CLA  | CMC-C2C-C1C | 2.33  | 128.68      | 125.03   |
| 15  | cM    | 101 | BCR  | C2-C1-C6    | 2.33  | 113.83      | 110.44   |
| 12  | bB    | 824 | F6C  | O1D-CGD-CBD | -2.33 | 119.92      | 124.52   |
| 11  | aA    | 804 | CLA  | CBC-CAC-C3C | -2.33 | 106.11      | 112.42   |
| 11  | bB    | 804 | CLA  | CMB-C2B-C1B | 2.33  | 128.97      | 125.42   |
| 11  | cB    | 825 | CLA  | CAC-C3C-C4C | 2.33  | 127.82      | 124.79   |
| 11  | cA    | 834 | CLA  | CMA-C3A-C2A | -2.33 | 104.98      | 113.98   |
| 11  | cA    | 824 | CLA  | CHB-C4A-NA  | 2.33  | 127.76      | 124.40   |
| 15  | bK    | 102 | BCR  | C38-C26-C27 | -2.33 | 108.63      | 113.60   |
| 11  | cB    | 803 | CLA  | C4-C3-C5    | 2.33  | 119.27      | 115.23   |
| 12  | aL    | 202 | F6C  | CHB-C1B-NB  | -2.33 | 120.62      | 124.23   |
| 11  | aA    | 834 | CLA  | CMA-C3A-C2A | -2.33 | 104.98      | 113.98   |
| 11  | aA    | 814 | CLA  | CMC-C2C-C1C | 2.33  | 128.67      | 125.03   |
| 16  | bA    | 852 | LHG  | C18-C17-C16 | -2.33 | 102.61      | 114.37   |
| 11  | cB    | 808 | CLA  | CHB-C4A-NA  | 2.33  | 127.76      | 124.40   |
| 11  | cB    | 837 | CLA  | CAA-C2A-C3A | -2.33 | 106.71      | 113.00   |
| 11  | aA    | 835 | CLA  | O2A-CGA-CBA | 2.33  | 118.93      | 111.83   |
| 11  | bB    | 802 | CLA  | CHA-C1A-NA  | -2.33 | 121.12      | 126.39   |
| 11  | aB    | 806 | CLA  | CAC-C3C-C4C | 2.33  | 127.82      | 124.79   |
| 11  | cA    | 825 | CLA  | C4-C3-C5    | 2.33  | 119.27      | 115.23   |
| 10  | bA    | 801 | CL0  | C3D-C4D-ND  | 2.33  | 116.67      | 112.94   |
| 11  | cA    | 833 | CLA  | C4-C3-C5    | 2.32  | 119.26      | 115.23   |
| 11  | aB    | 829 | CLA  | C3C-C4C-NC  | 2.32  | 113.41      | 110.43   |
| 11  | aB    | 815 | CLA  | O2A-CGA-CBA | 2.32  | 118.92      | 111.83   |
| 11  | bB    | 819 | CLA  | O2D-CGD-O1D | -2.32 | 119.33      | 123.85   |
| 16  | cA    | 852 | LHG  | C18-C17-C16 | -2.32 | 102.62      | 114.37   |
| 11  | cA    | 821 | CLA  | CHB-C4A-NA  | 2.32  | 127.75      | 124.40   |
| 11  | cA    | 804 | CLA  | CBC-CAC-C3C | -2.32 | 106.12      | 112.42   |
| 11  | bB    | 839 | CLA  | CAA-C2A-C3A | -2.32 | 106.72      | 113.00   |
| 11  | bA    | 825 | CLA  | CMB-C2B-C1B | 2.32  | 128.96      | 125.42   |
| 11  | bA    | 804 | CLA  | CBC-CAC-C3C | -2.32 | 106.12      | 112.42   |
| 16  | aA    | 852 | LHG  | C18-C17-C16 | -2.32 | 102.63      | 114.37   |
| 11  | aB    | 838 | CLA  | CHB-C4A-NA  | 2.32  | 127.75      | 124.40   |
| 11  | aB    | 837 | CLA  | CAA-C2A-C3A | -2.32 | 106.73      | 113.00   |
| 12  | cA    | 830 | F6C  | CMC-C2C-C1C | 2.32  | 128.95      | 125.42   |
| 12  | cA    | 830 | F6C  | CBC-CAC-C3C | -2.32 | 106.13      | 112.42   |
| 11  | aB    | 839 | CLA  | CAA-C2A-C3A | -2.32 | 106.73      | 113.00   |
| 12  | cB    | 824 | F6C  | O1D-CGD-CBD | -2.32 | 119.94      | 124.52   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bA    | 834 | CLA  | CMA-C3A-C2A | -2.32 | 105.01      | 113.98   |
| 11  | bB    | 835 | CLA  | O2D-CGD-O1D | -2.32 | 119.33      | 123.85   |
| 11  | aB    | 809 | CLA  | O2D-CGD-O1D | -2.32 | 119.33      | 123.85   |
| 15  | cB    | 843 | BCR  | C33-C5-C6   | -2.32 | 121.95      | 124.48   |
| 12  | aA    | 830 | F6C  | CBC-CAC-C3C | -2.32 | 106.14      | 112.42   |
| 11  | bA    | 835 | CLA  | O2A-CGA-CBA | 2.32  | 118.90      | 111.83   |
| 11  | bB    | 810 | CLA  | CMC-C2C-C1C | 2.32  | 128.66      | 125.03   |
| 11  | bB    | 837 | CLA  | CAA-C2A-C3A | -2.32 | 106.74      | 113.00   |
| 11  | cB    | 835 | CLA  | O2D-CGD-O1D | -2.32 | 119.34      | 123.85   |
| 11  | aL    | 204 | CLA  | C1-C2-C3    | -2.32 | 122.40      | 126.20   |
| 11  | cB    | 839 | CLA  | CAA-C2A-C3A | -2.32 | 106.74      | 113.00   |
| 11  | cB    | 809 | CLA  | O2D-CGD-O1D | -2.32 | 119.34      | 123.85   |
| 11  | aA    | 821 | CLA  | CHB-C4A-NA  | 2.32  | 127.74      | 124.40   |
| 11  | cB    | 802 | CLA  | CHA-C1A-NA  | -2.32 | 121.15      | 126.39   |
| 11  | cA    | 814 | CLA  | CMB-C2B-C1B | 2.32  | 128.94      | 125.42   |
| 11  | bB    | 830 | CLA  | CHB-C4A-NA  | 2.31  | 127.74      | 124.40   |
| 11  | cB    | 838 | CLA  | CHB-C4A-NA  | 2.31  | 127.74      | 124.40   |
| 11  | aB    | 803 | CLA  | C4-C3-C5    | 2.31  | 119.24      | 115.23   |
| 11  | aB    | 819 | CLA  | O2D-CGD-O1D | -2.31 | 119.35      | 123.85   |
| 15  | aB    | 846 | BCR  | C16-C15-C14 | -2.31 | 118.79      | 123.52   |
| 11  | cB    | 804 | CLA  | CMB-C2B-C1B | 2.31  | 128.94      | 125.42   |
| 18  | bB    | 847 | LMG  | O3-C3-C2    | -2.31 | 104.93      | 110.38   |
| 11  | cB    | 815 | CLA  | O2A-CGA-CBA | 2.31  | 118.88      | 111.83   |
| 12  | aA    | 830 | F6C  | CMC-C2C-C1C | 2.31  | 128.94      | 125.42   |
| 15  | aK    | 102 | BCR  | C38-C26-C27 | -2.31 | 108.67      | 113.60   |
| 11  | bA    | 837 | CLA  | CHB-C4A-NA  | 2.31  | 127.73      | 124.40   |
| 11  | cA    | 816 | CLA  | CHB-C4A-NA  | 2.31  | 127.73      | 124.40   |
| 11  | aB    | 817 | CLA  | C5-C3-C2    | -2.31 | 115.98      | 121.17   |
| 15  | aA    | 851 | BCR  | C7-C8-C9    | -2.31 | 122.82      | 126.23   |
| 11  | cB    | 837 | CLA  | C1-C2-C3    | -2.31 | 122.41      | 126.20   |
| 11  | aB    | 835 | CLA  | O2D-CGD-O1D | -2.31 | 119.35      | 123.85   |
| 15  | cL    | 207 | BCR  | C30-C25-C26 | -2.31 | 119.48      | 122.64   |
| 11  | aA    | 833 | CLA  | C4-C3-C5    | 2.31  | 119.23      | 115.23   |
| 15  | cL    | 207 | BCR  | C38-C26-C27 | -2.31 | 108.68      | 113.60   |
| 11  | aB    | 808 | CLA  | CHB-C4A-NA  | 2.31  | 127.73      | 124.40   |
| 11  | cB    | 819 | CLA  | O2D-CGD-O1D | -2.31 | 119.36      | 123.85   |
| 12  | bA    | 830 | F6C  | CMC-C2C-C1C | 2.31  | 128.93      | 125.42   |
| 12  | bA    | 830 | F6C  | CBC-CAC-C3C | -2.31 | 106.17      | 112.42   |
| 11  | aB    | 820 | CLA  | CHB-C4A-NA  | 2.31  | 127.73      | 124.40   |
| 15  | cA    | 847 | BCR  | C11-C10-C9  | -2.31 | 124.04      | 127.28   |
| 11  | bA    | 821 | CLA  | CHB-C4A-NA  | 2.31  | 127.73      | 124.40   |
| 11  | cA    | 835 | CLA  | O2A-CGA-CBA | 2.31  | 118.86      | 111.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 18  | cB    | 847 | LMG  | O3-C3-C2    | -2.30 | 104.94      | 110.38   |
| 11  | bB    | 817 | CLA  | C5-C3-C2    | -2.30 | 115.99      | 121.17   |
| 15  | bA    | 847 | BCR  | C11-C10-C9  | -2.30 | 124.05      | 127.28   |
| 15  | bB    | 843 | BCR  | C27-C26-C25 | 2.30  | 125.81      | 122.70   |
| 11  | aA    | 837 | CLA  | CHB-C4A-NA  | 2.30  | 127.72      | 124.40   |
| 15  | cB    | 846 | BCR  | C16-C15-C14 | -2.30 | 118.81      | 123.52   |
| 11  | bK    | 103 | CLA  | CHB-C4A-NA  | 2.30  | 127.72      | 124.40   |
| 11  | bL    | 204 | CLA  | C1-C2-C3    | -2.30 | 122.43      | 126.20   |
| 11  | bB    | 808 | CLA  | CHB-C4A-NA  | 2.30  | 127.72      | 124.40   |
| 11  | aA    | 839 | CLA  | O2A-CGA-CBA | 2.30  | 118.84      | 111.83   |
| 11  | aA    | 824 | CLA  | CHB-C4A-NA  | 2.30  | 127.72      | 124.40   |
| 15  | bB    | 845 | BCR  | C24-C23-C22 | -2.30 | 122.84      | 126.23   |
| 15  | bL    | 207 | BCR  | C38-C26-C27 | -2.30 | 108.70      | 113.60   |
| 15  | cB    | 845 | BCR  | C24-C23-C22 | -2.30 | 122.84      | 126.23   |
| 11  | bA    | 814 | CLA  | CMB-C2B-C1B | 2.30  | 128.91      | 125.42   |
| 18  | aB    | 847 | LMG  | O2-C2-C1    | -2.30 | 104.60      | 110.08   |
| 11  | bA    | 833 | CLA  | CMC-C2C-C1C | 2.30  | 128.62      | 125.03   |
| 11  | cB    | 830 | CLA  | CHB-C4A-NA  | 2.30  | 127.71      | 124.40   |
| 11  | aA    | 814 | CLA  | CMB-C2B-C1B | 2.29  | 128.91      | 125.42   |
| 11  | cL    | 204 | CLA  | C1-C2-C3    | -2.29 | 122.44      | 126.20   |
| 11  | bA    | 811 | CLA  | CMC-C2C-C1C | 2.29  | 128.62      | 125.03   |
| 15  | aL    | 207 | BCR  | C38-C26-C27 | -2.29 | 108.70      | 113.60   |
| 15  | aA    | 847 | BCR  | C24-C23-C22 | -2.29 | 122.84      | 126.23   |
| 11  | cA    | 820 | CLA  | CMC-C2C-C1C | 2.29  | 128.62      | 125.03   |
| 11  | bB    | 837 | CLA  | C1-C2-C3    | -2.29 | 122.44      | 126.20   |
| 15  | aM    | 101 | BCR  | C29-C30-C25 | 2.29  | 113.77      | 110.44   |
| 15  | bA    | 851 | BCR  | C7-C8-C9    | -2.29 | 122.84      | 126.23   |
| 18  | bB    | 847 | LMG  | O2-C2-C1    | -2.29 | 104.61      | 110.08   |
| 11  | aA    | 820 | CLA  | CMC-C2C-C1C | 2.29  | 128.61      | 125.03   |
| 15  | bA    | 847 | BCR  | C29-C30-C25 | 2.29  | 113.77      | 110.44   |
| 11  | bA    | 843 | CLA  | CMC-C2C-C1C | 2.29  | 128.61      | 125.03   |
| 11  | cA    | 843 | CLA  | CMC-C2C-C1C | 2.29  | 128.61      | 125.03   |
| 11  | bA    | 839 | CLA  | O2A-CGA-CBA | 2.29  | 118.81      | 111.83   |
| 11  | bB    | 820 | CLA  | O2D-CGD-O1D | -2.29 | 119.39      | 123.85   |
| 15  | bA    | 847 | BCR  | C24-C23-C22 | -2.29 | 122.85      | 126.23   |
| 18  | cB    | 847 | LMG  | O2-C2-C1    | -2.29 | 104.63      | 110.08   |
| 18  | aB    | 847 | LMG  | O3-C3-C2    | -2.29 | 104.99      | 110.38   |
| 11  | cA    | 837 | CLA  | CHB-C4A-NA  | 2.29  | 127.70      | 124.40   |
| 11  | aB    | 804 | CLA  | CMB-C2B-C1B | 2.29  | 128.90      | 125.42   |
| 11  | cB    | 826 | CLA  | CHA-C1A-NA  | -2.28 | 121.22      | 126.39   |
| 11  | aA    | 803 | CLA  | CHB-C1B-C2B | -2.28 | 120.79      | 127.43   |
| 15  | bB    | 846 | BCR  | C16-C15-C14 | -2.28 | 118.84      | 123.52   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cB    | 835 | CLA  | CBC-CAC-C3C | -2.28 | 106.23      | 112.42   |
| 12  | aA    | 830 | F6C  | O2D-CGD-O1D | -2.28 | 119.40      | 123.85   |
| 11  | aK    | 103 | CLA  | CHB-C4A-NA  | 2.28  | 127.70      | 124.40   |
| 11  | aA    | 833 | CLA  | CMC-C2C-C1C | 2.28  | 128.60      | 125.03   |
| 11  | aA    | 802 | CLA  | O2A-CGA-O1A | -2.28 | 117.92      | 123.63   |
| 15  | aA    | 847 | BCR  | C11-C10-C9  | -2.28 | 124.08      | 127.28   |
| 15  | cB    | 843 | BCR  | C27-C26-C25 | 2.28  | 125.79      | 122.70   |
| 11  | cA    | 840 | CLA  | CBC-CAC-C3C | -2.28 | 106.23      | 112.42   |
| 15  | aB    | 843 | BCR  | C27-C26-C25 | 2.28  | 125.79      | 122.70   |
| 15  | cK    | 102 | BCR  | C38-C26-C27 | -2.28 | 108.73      | 113.60   |
| 11  | bA    | 824 | CLA  | CHB-C4A-NA  | 2.28  | 127.69      | 124.40   |
| 11  | aA    | 825 | CLA  | CMB-C2B-C1B | 2.28  | 128.89      | 125.42   |
| 11  | cA    | 811 | CLA  | CMC-C2C-C1C | 2.28  | 128.60      | 125.03   |
| 11  | cA    | 839 | CLA  | O2A-CGA-CBA | 2.28  | 118.79      | 111.83   |
| 15  | cA    | 847 | BCR  | C24-C23-C22 | -2.28 | 122.86      | 126.23   |
| 11  | aB    | 820 | CLA  | O2D-CGD-O1D | -2.28 | 119.41      | 123.85   |
| 15  | aL    | 203 | BCR  | C33-C5-C6   | -2.28 | 122.00      | 124.48   |
| 11  | bA    | 820 | CLA  | CMC-C2C-C1C | 2.28  | 128.59      | 125.03   |
| 15  | cA    | 851 | BCR  | C7-C8-C9    | -2.28 | 122.87      | 126.23   |
| 11  | bB    | 820 | CLA  | CHB-C4A-NA  | 2.28  | 127.69      | 124.40   |
| 11  | aB    | 837 | CLA  | C1-C2-C3    | -2.28 | 122.47      | 126.20   |
| 12  | cA    | 830 | F6C  | O2D-CGD-O1D | -2.27 | 119.42      | 123.85   |
| 11  | bB    | 835 | CLA  | CBC-CAC-C3C | -2.27 | 106.25      | 112.42   |
| 11  | aA    | 811 | CLA  | CMC-C2C-C1C | 2.27  | 128.59      | 125.03   |
| 11  | aB    | 835 | CLA  | CBC-CAC-C3C | -2.27 | 106.25      | 112.42   |
| 15  | aB    | 845 | BCR  | C24-C23-C22 | -2.27 | 122.87      | 126.23   |
| 15  | cB    | 845 | BCR  | C11-C10-C9  | -2.27 | 124.09      | 127.28   |
| 11  | cA    | 833 | CLA  | CMC-C2C-C1C | 2.27  | 128.59      | 125.03   |
| 11  | aA    | 828 | CLA  | CHB-C4A-NA  | 2.27  | 127.68      | 124.40   |
| 11  | bA    | 840 | CLA  | CBC-CAC-C3C | -2.27 | 106.26      | 112.42   |
| 11  | cB    | 820 | CLA  | CHB-C4A-NA  | 2.27  | 127.68      | 124.40   |
| 12  | bA    | 832 | F6C  | C5-C3-C4    | 2.27  | 119.82      | 114.59   |
| 10  | cA    | 801 | CL0  | O2A-CGA-O1A | -2.27 | 117.95      | 123.63   |
| 11  | cK    | 103 | CLA  | CHB-C4A-NA  | 2.27  | 127.68      | 124.40   |
| 16  | aA    | 852 | LHG  | C20-C19-C18 | -2.27 | 102.89      | 114.37   |
| 16  | bA    | 852 | LHG  | C20-C19-C18 | -2.27 | 102.89      | 114.37   |
| 11  | cA    | 825 | CLA  | CMB-C2B-C1B | 2.27  | 128.88      | 125.42   |
| 12  | bA    | 830 | F6C  | O2D-CGD-O1D | -2.27 | 119.43      | 123.85   |
| 11  | aA    | 819 | CLA  | C3B-C4B-NB  | 2.27  | 112.56      | 110.53   |
| 11  | aB    | 840 | CLA  | CMC-C2C-C1C | 2.27  | 128.58      | 125.03   |
| 15  | aA    | 847 | BCR  | C29-C30-C25 | 2.27  | 113.74      | 110.44   |
| 11  | bA    | 816 | CLA  | CHB-C4A-NA  | 2.27  | 127.68      | 124.40   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bB    | 826 | CLA  | CHA-C1A-NA  | -2.27 | 121.25      | 126.39   |
| 11  | cA    | 802 | CLA  | O2A-CGA-O1A | -2.27 | 117.95      | 123.63   |
| 11  | bB    | 840 | CLA  | CMC-C2C-C1C | 2.27  | 128.58      | 125.03   |
| 11  | aA    | 840 | CLA  | CBC-CAC-C3C | -2.27 | 106.27      | 112.42   |
| 11  | cK    | 101 | CLA  | CHB-C4A-NA  | 2.27  | 127.67      | 124.40   |
| 10  | aA    | 801 | CL0  | C4-C3-C5    | 2.27  | 119.17      | 115.23   |
| 11  | bK    | 101 | CLA  | CMC-C2C-C1C | 2.27  | 128.58      | 125.03   |
| 11  | bA    | 819 | CLA  | C3B-C4B-NB  | 2.27  | 112.56      | 110.53   |
| 11  | aK    | 101 | CLA  | CMC-C2C-C1C | 2.27  | 128.58      | 125.03   |
| 11  | aA    | 814 | CLA  | O1D-CGD-CBD | -2.27 | 120.05      | 124.52   |
| 11  | aB    | 801 | CLA  | O2A-CGA-CBA | 2.27  | 118.75      | 111.83   |
| 11  | cB    | 823 | CLA  | CHB-C4A-NA  | 2.27  | 127.67      | 124.40   |
| 10  | aA    | 801 | CL0  | O2A-CGA-O1A | -2.27 | 117.96      | 123.63   |
| 16  | cA    | 852 | LHG  | C20-C19-C18 | -2.27 | 102.91      | 114.37   |
| 11  | aB    | 812 | CLA  | O2A-CGA-O1A | -2.27 | 117.96      | 123.63   |
| 15  | cA    | 847 | BCR  | C29-C30-C25 | 2.27  | 113.73      | 110.44   |
| 11  | cB    | 840 | CLA  | CMC-C2C-C1C | 2.27  | 128.57      | 125.03   |
| 12  | cA    | 832 | F6C  | C5-C3-C4    | 2.27  | 119.80      | 114.59   |
| 18  | bB    | 847 | LMG  | C42-C41-C40 | -2.26 | 102.92      | 114.37   |
| 11  | cB    | 821 | CLA  | CHB-C4A-NA  | 2.26  | 127.67      | 124.40   |
| 11  | cB    | 801 | CLA  | O2A-CGA-CBA | 2.26  | 118.74      | 111.83   |
| 11  | cA    | 803 | CLA  | CHB-C1B-C2B | -2.26 | 120.85      | 127.43   |
| 15  | aM    | 101 | BCR  | C7-C8-C9    | -2.26 | 122.89      | 126.23   |
| 11  | cB    | 823 | CLA  | O1D-CGD-CBD | -2.26 | 120.05      | 124.52   |
| 11  | bA    | 803 | CLA  | CHB-C1B-C2B | -2.26 | 120.86      | 127.43   |
| 11  | cA    | 809 | CLA  | CBA-CAA-C2A | 2.26  | 120.53      | 113.79   |
| 18  | cB    | 847 | LMG  | C42-C41-C40 | -2.26 | 102.93      | 114.37   |
| 11  | cB    | 820 | CLA  | O2D-CGD-O1D | -2.26 | 119.44      | 123.85   |
| 11  | bB    | 812 | CLA  | CHD-C4C-NC  | 2.26  | 127.74      | 124.23   |
| 11  | cA    | 824 | CLA  | O2D-CGD-O1D | -2.26 | 119.44      | 123.85   |
| 11  | aB    | 821 | CLA  | CHB-C4A-NA  | 2.26  | 127.67      | 124.40   |
| 12  | aL    | 202 | F6C  | CBC-CAC-C3C | -2.26 | 106.29      | 112.42   |
| 11  | aB    | 826 | CLA  | CHA-C1A-NA  | -2.26 | 121.27      | 126.39   |
| 11  | aB    | 823 | CLA  | CHB-C4A-NA  | 2.26  | 127.66      | 124.40   |
| 11  | bB    | 823 | CLA  | CHB-C4A-NA  | 2.26  | 127.66      | 124.40   |
| 11  | cA    | 842 | CLA  | CMB-C2B-C1B | 2.26  | 128.86      | 125.42   |
| 11  | bA    | 812 | CLA  | C4-C3-C5    | 2.26  | 119.15      | 115.23   |
| 11  | aA    | 828 | CLA  | C4A-NA-C1A  | -2.26 | 105.65      | 106.68   |
| 11  | aA    | 822 | CLA  | CAA-C2A-C3A | -2.26 | 106.89      | 113.00   |
| 11  | aA    | 821 | CLA  | CAA-C2A-C1A | 2.26  | 119.38      | 111.97   |
| 11  | bB    | 840 | CLA  | O2D-CGD-O1D | -2.26 | 119.45      | 123.85   |
| 11  | cA    | 825 | CLA  | CAA-C2A-C3A | -2.26 | 106.90      | 113.00   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cA    | 834 | CLA  | CMA-C3A-C4A | -2.26 | 105.70      | 111.77   |
| 11  | bA    | 814 | CLA  | O1D-CGD-CBD | -2.26 | 120.06      | 124.52   |
| 11  | aA    | 816 | CLA  | CHB-C4A-NA  | 2.26  | 127.66      | 124.40   |
| 11  | aA    | 843 | CLA  | CMC-C2C-C1C | 2.26  | 128.56      | 125.03   |
| 11  | aL    | 206 | CLA  | CMC-C2C-C1C | 2.26  | 128.56      | 125.03   |
| 15  | aB    | 845 | BCR  | C11-C10-C9  | -2.26 | 124.11      | 127.28   |
| 11  | bB    | 831 | CLA  | O2A-CGA-CBA | 2.26  | 118.72      | 111.83   |
| 11  | cA    | 812 | CLA  | C4-C3-C5    | 2.26  | 119.14      | 115.23   |
| 11  | bA    | 834 | CLA  | CMA-C3A-C4A | -2.26 | 105.71      | 111.77   |
| 15  | bM    | 101 | BCR  | C29-C30-C25 | 2.26  | 113.72      | 110.44   |
| 18  | aB    | 847 | LMG  | C42-C41-C40 | -2.26 | 102.97      | 114.37   |
| 11  | cA    | 822 | CLA  | O2A-CGA-CBA | 2.26  | 118.71      | 111.83   |
| 11  | bA    | 828 | CLA  | CHB-C4A-NA  | 2.26  | 127.66      | 124.40   |
| 10  | bA    | 801 | CL0  | O2A-CGA-O1A | -2.26 | 117.99      | 123.63   |
| 11  | aB    | 823 | CLA  | O1D-CGD-CBD | -2.26 | 120.07      | 124.52   |
| 11  | aK    | 101 | CLA  | CHB-C4A-NA  | 2.25  | 127.65      | 124.40   |
| 11  | cB    | 831 | CLA  | O2A-CGA-CBA | 2.25  | 118.71      | 111.83   |
| 11  | bA    | 825 | CLA  | CAA-C2A-C3A | -2.25 | 106.91      | 113.00   |
| 11  | bA    | 822 | CLA  | O2A-CGA-CBA | 2.25  | 118.71      | 111.83   |
| 11  | cA    | 841 | CLA  | CED-O2D-CGD | 2.25  | 121.03      | 115.92   |
| 11  | cK    | 101 | CLA  | CMC-C2C-C1C | 2.25  | 128.56      | 125.03   |
| 11  | bB    | 812 | CLA  | O2A-CGA-O1A | -2.25 | 117.99      | 123.63   |
| 10  | bA    | 801 | CL0  | C4-C3-C5    | 2.25  | 119.14      | 115.23   |
| 11  | cB    | 812 | CLA  | O2A-CGA-O1A | -2.25 | 117.99      | 123.63   |
| 11  | aA    | 834 | CLA  | CMA-C3A-C4A | -2.25 | 105.72      | 111.77   |
| 11  | bA    | 809 | CLA  | CBA-CAA-C2A | 2.25  | 120.49      | 113.79   |
| 11  | bB    | 815 | CLA  | CHB-C4A-NA  | 2.25  | 127.65      | 124.40   |
| 11  | cL    | 205 | CLA  | CHB-C4A-NA  | 2.25  | 127.65      | 124.40   |
| 11  | cB    | 817 | CLA  | C2A-C3A-C4A | -2.25 | 98.23       | 101.87   |
| 11  | aA    | 812 | CLA  | C4-C3-C5    | 2.25  | 119.14      | 115.23   |
| 11  | aL    | 205 | CLA  | CHB-C4A-NA  | 2.25  | 127.65      | 124.40   |
| 11  | bB    | 801 | CLA  | O2A-CGA-CBA | 2.25  | 118.70      | 111.83   |
| 11  | aB    | 812 | CLA  | CHD-C4C-NC  | 2.25  | 127.72      | 124.23   |
| 11  | bA    | 831 | CLA  | CHD-C4C-NC  | 2.25  | 127.72      | 124.23   |
| 11  | aB    | 810 | CLA  | O2D-CGD-O1D | -2.25 | 119.47      | 123.85   |
| 11  | cA    | 821 | CLA  | CAA-C2A-C1A | 2.25  | 119.35      | 111.97   |
| 11  | bB    | 823 | CLA  | O1D-CGD-CBD | -2.25 | 120.08      | 124.52   |
| 11  | bA    | 822 | CLA  | CAA-C2A-C3A | -2.25 | 106.92      | 113.00   |
| 11  | aB    | 831 | CLA  | O2A-CGA-CBA | 2.25  | 118.69      | 111.83   |
| 11  | bA    | 841 | CLA  | CED-O2D-CGD | 2.25  | 121.02      | 115.92   |
| 12  | aA    | 832 | F6C  | C5-C3-C4    | 2.25  | 119.76      | 114.59   |
| 11  | cB    | 804 | CLA  | CAA-C2A-C1A | 2.25  | 119.34      | 111.97   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12  | bL    | 202 | F6C  | CMC-C2C-C1C | 2.25  | 128.84      | 125.42   |
| 12  | cL    | 202 | F6C  | CBC-CAC-C3C | -2.25 | 106.33      | 112.42   |
| 11  | aB    | 815 | CLA  | CHB-C4A-NA  | 2.25  | 127.64      | 124.40   |
| 11  | aA    | 822 | CLA  | O2A-CGA-CBA | 2.25  | 118.69      | 111.83   |
| 11  | aA    | 842 | CLA  | CED-O2D-CGD | 2.25  | 121.01      | 115.92   |
| 11  | aB    | 804 | CLA  | CAA-C2A-C1A | 2.25  | 119.34      | 111.97   |
| 10  | cA    | 801 | CL0  | C4-C3-C5    | 2.25  | 119.13      | 115.23   |
| 15  | cM    | 101 | BCR  | C7-C8-C9    | -2.25 | 122.91      | 126.23   |
| 11  | cA    | 813 | CLA  | O2D-CGD-O1D | -2.25 | 119.48      | 123.85   |
| 11  | cA    | 814 | CLA  | O1D-CGD-CBD | -2.25 | 120.09      | 124.52   |
| 11  | bB    | 821 | CLA  | CHB-C4A-NA  | 2.25  | 127.64      | 124.40   |
| 11  | bA    | 802 | CLA  | O2A-CGA-O1A | -2.25 | 118.01      | 123.63   |
| 11  | aA    | 824 | CLA  | O2D-CGD-O1D | -2.24 | 119.48      | 123.85   |
| 11  | aA    | 809 | CLA  | CBA-CAA-C2A | 2.24  | 120.47      | 113.79   |
| 12  | aA    | 826 | F6C  | CMC-C2C-C3C | 2.24  | 130.38      | 125.62   |
| 11  | aB    | 833 | CLA  | CMC-C2C-C1C | 2.24  | 128.54      | 125.03   |
| 11  | bB    | 833 | CLA  | CMC-C2C-C1C | 2.24  | 128.54      | 125.03   |
| 11  | cA    | 822 | CLA  | CAA-C2A-C3A | -2.24 | 106.94      | 113.00   |
| 11  | cB    | 805 | CLA  | CAA-C2A-C3A | -2.24 | 106.94      | 113.00   |
| 15  | bB    | 845 | BCR  | C11-C10-C9  | -2.24 | 124.13      | 127.28   |
| 11  | aB    | 837 | CLA  | O2A-CGA-CBA | 2.24  | 118.68      | 111.83   |
| 11  | bB    | 838 | CLA  | CMC-C2C-C1C | 2.24  | 128.54      | 125.03   |
| 11  | bB    | 810 | CLA  | O2D-CGD-O1D | -2.24 | 119.48      | 123.85   |
| 11  | aA    | 835 | CLA  | CBC-CAC-C3C | -2.24 | 106.34      | 112.42   |
| 11  | cA    | 803 | CLA  | O2D-CGD-O1D | -2.24 | 119.48      | 123.85   |
| 11  | bA    | 825 | CLA  | O1D-CGD-CBD | -2.24 | 120.09      | 124.52   |
| 11  | bK    | 101 | CLA  | CHB-C4A-NA  | 2.24  | 127.64      | 124.40   |
| 11  | bL    | 206 | CLA  | CMC-C2C-C1C | 2.24  | 128.54      | 125.03   |
| 11  | aA    | 831 | CLA  | CHD-C4C-NC  | 2.24  | 127.71      | 124.23   |
| 11  | aA    | 841 | CLA  | CED-O2D-CGD | 2.24  | 121.00      | 115.92   |
| 11  | bB    | 837 | CLA  | O2A-CGA-CBA | 2.24  | 118.66      | 111.83   |
| 11  | bA    | 840 | CLA  | CHB-C4A-NA  | 2.24  | 127.63      | 124.40   |
| 11  | cA    | 828 | CLA  | CHB-C4A-NA  | 2.24  | 127.63      | 124.40   |
| 11  | cB    | 826 | CLA  | CHB-C4A-NA  | 2.24  | 127.63      | 124.40   |
| 11  | aA    | 825 | CLA  | CAA-C2A-C3A | -2.24 | 106.95      | 113.00   |
| 11  | aA    | 825 | CLA  | O2D-CGD-O1D | -2.24 | 119.49      | 123.85   |
| 11  | cB    | 840 | CLA  | O2D-CGD-O1D | -2.24 | 119.49      | 123.85   |
| 11  | aA    | 810 | CLA  | O2D-CGD-O1D | -2.24 | 119.49      | 123.85   |
| 11  | bA    | 821 | CLA  | CAA-C2A-C1A | 2.24  | 119.31      | 111.97   |
| 11  | bL    | 205 | CLA  | CHB-C4A-NA  | 2.24  | 127.63      | 124.40   |
| 11  | aB    | 805 | CLA  | CAA-C2A-C3A | -2.24 | 106.95      | 113.00   |
| 11  | bA    | 809 | CLA  | CAA-C2A-C3A | -2.24 | 106.95      | 113.00   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12  | cA    | 826 | F6C  | CMC-C2C-C3C | 2.24  | 130.37      | 125.62   |
| 11  | cB    | 837 | CLA  | O2A-CGA-CBA | 2.24  | 118.66      | 111.83   |
| 11  | aB    | 817 | CLA  | C2A-C3A-C4A | -2.24 | 98.26       | 101.87   |
| 12  | bA    | 826 | F6C  | CMC-C2C-C3C | 2.24  | 130.37      | 125.62   |
| 11  | aA    | 820 | CLA  | CBC-CAC-C3C | -2.24 | 106.36      | 112.42   |
| 12  | bL    | 202 | F6C  | CBC-CAC-C3C | -2.24 | 106.36      | 112.42   |
| 11  | bA    | 824 | CLA  | O2D-CGD-O1D | -2.24 | 119.50      | 123.85   |
| 11  | bA    | 823 | CLA  | C4A-NA-C1A  | -2.24 | 105.66      | 106.68   |
| 11  | cB    | 815 | CLA  | CHB-C4A-NA  | 2.24  | 127.63      | 124.40   |
| 11  | bA    | 825 | CLA  | CMA-C3A-C4A | -2.24 | 105.77      | 111.77   |
| 11  | cA    | 842 | CLA  | CED-O2D-CGD | 2.23  | 120.98      | 115.92   |
| 11  | cA    | 825 | CLA  | O1D-CGD-CBD | -2.23 | 120.11      | 124.52   |
| 11  | bA    | 803 | CLA  | O2D-CGD-O1D | -2.23 | 119.50      | 123.85   |
| 11  | cA    | 820 | CLA  | CBC-CAC-C3C | -2.23 | 106.36      | 112.42   |
| 11  | cB    | 822 | CLA  | CMC-C2C-C1C | 2.23  | 128.53      | 125.03   |
| 11  | cB    | 812 | CLA  | CHD-C4C-NC  | 2.23  | 127.69      | 124.23   |
| 11  | cA    | 819 | CLA  | C3B-C4B-NB  | 2.23  | 112.52      | 110.53   |
| 17  | aA    | 853 | LMT  | C3B-C4B-C5B | 2.23  | 114.28      | 110.23   |
| 11  | cB    | 810 | CLA  | O2D-CGD-O1D | -2.23 | 119.50      | 123.85   |
| 11  | aA    | 813 | CLA  | O2D-CGD-O1D | -2.23 | 119.50      | 123.85   |
| 11  | aA    | 819 | CLA  | O2D-CGD-O1D | -2.23 | 119.50      | 123.85   |
| 11  | cA    | 809 | CLA  | CAA-C2A-C3A | -2.23 | 106.97      | 113.00   |
| 11  | aA    | 804 | CLA  | CHB-C4A-NA  | 2.23  | 127.62      | 124.40   |
| 11  | bA    | 825 | CLA  | O2D-CGD-O1D | -2.23 | 119.50      | 123.85   |
| 11  | aA    | 837 | CLA  | O2A-CGA-CBA | 2.23  | 121.05      | 114.00   |
| 11  | bB    | 802 | CLA  | CMB-C2B-C3B | 2.23  | 131.80      | 126.55   |
| 11  | bA    | 819 | CLA  | O2D-CGD-O1D | -2.23 | 119.50      | 123.85   |
| 11  | bB    | 817 | CLA  | C2A-C3A-C4A | -2.23 | 98.27       | 101.87   |
| 11  | bB    | 805 | CLA  | CAA-C2A-C3A | -2.23 | 106.97      | 113.00   |
| 11  | bA    | 810 | CLA  | O2D-CGD-O1D | -2.23 | 119.51      | 123.85   |
| 11  | cA    | 835 | CLA  | CBC-CAC-C3C | -2.23 | 106.37      | 112.42   |
| 11  | aB    | 822 | CLA  | CMC-C2C-C1C | 2.23  | 128.52      | 125.03   |
| 11  | aB    | 840 | CLA  | O2D-CGD-O1D | -2.23 | 119.51      | 123.85   |
| 15  | bA    | 848 | BCR  | C33-C5-C6   | -2.23 | 122.05      | 124.48   |
| 11  | cA    | 831 | CLA  | CHD-C4C-NC  | 2.23  | 127.69      | 124.23   |
| 11  | cA    | 804 | CLA  | CHB-C4A-NA  | 2.23  | 127.62      | 124.40   |
| 11  | cB    | 833 | CLA  | CMC-C2C-C1C | 2.23  | 128.52      | 125.03   |
| 12  | cL    | 202 | F6C  | CMC-C2C-C1C | 2.23  | 128.81      | 125.42   |
| 11  | bA    | 813 | CLA  | O2D-CGD-O1D | -2.23 | 119.51      | 123.85   |
| 11  | bB    | 804 | CLA  | CAA-C2A-C1A | 2.23  | 119.27      | 111.97   |
| 11  | aA    | 803 | CLA  | O2D-CGD-O1D | -2.23 | 119.51      | 123.85   |
| 11  | aB    | 812 | CLA  | CMB-C2B-C1B | 2.23  | 128.81      | 125.42   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 15  | bK    | 102 | BCR  | C15-C16-C17 | -2.23 | 118.96      | 123.52   |
| 11  | cA    | 825 | CLA  | O2D-CGD-O1D | -2.23 | 119.52      | 123.85   |
| 11  | bA    | 837 | CLA  | O2A-CGA-CBA | 2.23  | 121.03      | 114.00   |
| 11  | aA    | 819 | CLA  | CHB-C4A-NA  | 2.23  | 127.61      | 124.40   |
| 11  | aB    | 825 | CLA  | CHB-C4A-NA  | 2.23  | 127.61      | 124.40   |
| 11  | aB    | 838 | CLA  | CMC-C2C-C1C | 2.22  | 128.51      | 125.03   |
| 11  | bB    | 822 | CLA  | CMC-C2C-C1C | 2.22  | 128.51      | 125.03   |
| 17  | bA    | 853 | LMT  | C3B-C4B-C5B | 2.22  | 114.27      | 110.23   |
| 15  | cM    | 101 | BCR  | C29-C30-C25 | 2.22  | 113.67      | 110.44   |
| 11  | bA    | 842 | CLA  | CED-O2D-CGD | 2.22  | 120.96      | 115.92   |
| 11  | bA    | 842 | CLA  | CMB-C2B-C1B | 2.22  | 128.81      | 125.42   |
| 11  | aB    | 820 | CLA  | CAC-C3C-C4C | 2.22  | 127.68      | 124.79   |
| 11  | bB    | 826 | CLA  | CHB-C4A-NA  | 2.22  | 127.61      | 124.40   |
| 11  | cA    | 820 | CLA  | C4-C3-C5    | 2.22  | 119.09      | 115.23   |
| 11  | aA    | 842 | CLA  | CMB-C2B-C1B | 2.22  | 128.80      | 125.42   |
| 11  | aA    | 809 | CLA  | CAA-C2A-C3A | -2.22 | 106.99      | 113.00   |
| 11  | aA    | 825 | CLA  | O1D-CGD-CBD | -2.22 | 120.13      | 124.52   |
| 11  | bA    | 836 | CLA  | CHB-C4A-NA  | 2.22  | 127.61      | 124.40   |
| 15  | cL    | 203 | BCR  | C33-C5-C6   | -2.22 | 122.06      | 124.48   |
| 11  | bA    | 820 | CLA  | CBC-CAC-C3C | -2.22 | 106.40      | 112.42   |
| 15  | cK    | 102 | BCR  | C15-C16-C17 | -2.22 | 118.98      | 123.52   |
| 11  | bA    | 835 | CLA  | CBC-CAC-C3C | -2.22 | 106.40      | 112.42   |
| 11  | aA    | 825 | CLA  | CMA-C3A-C4A | -2.22 | 105.81      | 111.77   |
| 11  | cB    | 838 | CLA  | CMC-C2C-C1C | 2.22  | 128.50      | 125.03   |
| 11  | bA    | 811 | CLA  | CED-O2D-CGD | 2.22  | 120.95      | 115.92   |
| 11  | aA    | 818 | CLA  | CBC-CAC-C3C | -2.22 | 106.41      | 112.42   |
| 15  | aK    | 102 | BCR  | C15-C16-C17 | -2.22 | 118.98      | 123.52   |
| 11  | bB    | 812 | CLA  | CHB-C4A-NA  | 2.22  | 127.60      | 124.40   |
| 11  | aB    | 831 | CLA  | CMC-C2C-C1C | 2.22  | 128.50      | 125.03   |
| 11  | bA    | 803 | CLA  | O2A-CGA-CBA | 2.22  | 118.59      | 111.83   |
| 11  | aB    | 826 | CLA  | CHB-C4A-NA  | 2.22  | 127.60      | 124.40   |
| 11  | bA    | 820 | CLA  | CMB-C2B-C1B | 2.22  | 128.79      | 125.42   |
| 11  | cA    | 837 | CLA  | O2A-CGA-CBA | 2.22  | 121.00      | 114.00   |
| 11  | bA    | 819 | CLA  | CHB-C4A-NA  | 2.22  | 127.60      | 124.40   |
| 11  | cA    | 803 | CLA  | O2A-CGA-CBA | 2.22  | 118.59      | 111.83   |
| 11  | cB    | 802 | CLA  | CMB-C2B-C3B | 2.22  | 131.76      | 126.55   |
| 11  | cA    | 820 | CLA  | CMB-C2B-C1B | 2.22  | 128.79      | 125.42   |
| 11  | bB    | 808 | CLA  | CHB-C1B-C2B | -2.22 | 121.00      | 127.43   |
| 11  | bB    | 818 | CLA  | C1-C2-C3    | -2.21 | 122.57      | 126.20   |
| 15  | bL    | 203 | BCR  | C33-C5-C6   | -2.21 | 122.07      | 124.48   |
| 11  | cB    | 820 | CLA  | CAC-C3C-C4C | 2.21  | 127.67      | 124.79   |
| 12  | aL    | 202 | F6C  | CMC-C2C-C1C | 2.21  | 128.79      | 125.42   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aA    | 810 | CLA  | CBC-CAC-C3C | -2.21 | 106.42      | 112.42   |
| 11  | aA    | 836 | CLA  | CHB-C4A-NA  | 2.21  | 127.59      | 124.40   |
| 11  | cA    | 839 | CLA  | CMC-C2C-C1C | 2.21  | 128.49      | 125.03   |
| 11  | cA    | 825 | CLA  | CMA-C3A-C4A | -2.21 | 105.83      | 111.77   |
| 11  | bL    | 206 | CLA  | CHB-C4A-NA  | 2.21  | 127.59      | 124.40   |
| 11  | aA    | 803 | CLA  | O2A-CGA-CBA | 2.21  | 118.58      | 111.83   |
| 11  | cB    | 831 | CLA  | CMC-C2C-C1C | 2.21  | 128.49      | 125.03   |
| 11  | cA    | 819 | CLA  | CHB-C4A-NA  | 2.21  | 127.59      | 124.40   |
| 11  | bA    | 810 | CLA  | CBC-CAC-C3C | -2.21 | 106.43      | 112.42   |
| 11  | cA    | 828 | CLA  | O1D-CGD-CBD | -2.21 | 120.16      | 124.52   |
| 11  | cB    | 818 | CLA  | C1-C2-C3    | -2.21 | 122.58      | 126.20   |
| 11  | bB    | 829 | CLA  | C4A-NA-C1A  | -2.21 | 105.67      | 106.68   |
| 11  | cA    | 818 | CLA  | CBC-CAC-C3C | -2.21 | 106.43      | 112.42   |
| 11  | aA    | 840 | CLA  | CHB-C4A-NA  | 2.21  | 127.59      | 124.40   |
| 11  | cA    | 840 | CLA  | CHB-C4A-NA  | 2.21  | 127.59      | 124.40   |
| 11  | bA    | 820 | CLA  | CHB-C1B-C2B | -2.21 | 121.01      | 127.43   |
| 11  | cA    | 809 | CLA  | O1D-CGD-CBD | -2.21 | 120.16      | 124.52   |
| 11  | bB    | 831 | CLA  | CMC-C2C-C1C | 2.21  | 128.49      | 125.03   |
| 15  | bM    | 101 | BCR  | C7-C8-C9    | -2.21 | 122.97      | 126.23   |
| 11  | aB    | 808 | CLA  | CHB-C1B-C2B | -2.21 | 121.02      | 127.43   |
| 11  | aB    | 802 | CLA  | CMB-C2B-C3B | 2.21  | 131.74      | 126.55   |
| 11  | bB    | 834 | CLA  | CHA-C1A-NA  | -2.21 | 121.39      | 126.39   |
| 11  | cA    | 810 | CLA  | CBC-CAC-C3C | -2.21 | 106.44      | 112.42   |
| 11  | bA    | 809 | CLA  | CMB-C2B-C1B | 2.21  | 128.78      | 125.42   |
| 11  | aA    | 828 | CLA  | CMB-C2B-C1B | 2.21  | 128.78      | 125.42   |
| 17  | cA    | 853 | LMT  | C3B-C4B-C5B | 2.21  | 114.23      | 110.23   |
| 11  | bA    | 828 | CLA  | O1D-CGD-CBD | -2.21 | 120.17      | 124.52   |
| 11  | aA    | 803 | CLA  | CBC-CAC-C3C | -2.21 | 106.44      | 112.42   |
| 11  | aL    | 206 | CLA  | CHB-C4A-NA  | 2.21  | 127.58      | 124.40   |
| 11  | bA    | 838 | CLA  | C1-O2A-CGA  | 2.21  | 121.99      | 116.65   |
| 11  | aA    | 820 | CLA  | CMB-C2B-C1B | 2.21  | 128.78      | 125.42   |
| 15  | cA    | 848 | BCR  | C33-C5-C6   | -2.20 | 122.08      | 124.48   |
| 11  | bA    | 806 | CLA  | CHC-C1C-NC  | 2.20  | 127.63      | 124.31   |
| 11  | cB    | 808 | CLA  | CHB-C1B-C2B | -2.20 | 121.03      | 127.43   |
| 15  | aA    | 848 | BCR  | C33-C5-C6   | -2.20 | 122.08      | 124.48   |
| 11  | bB    | 803 | CLA  | CED-O2D-CGD | 2.20  | 120.92      | 115.92   |
| 11  | bA    | 828 | CLA  | CMB-C2B-C1B | 2.20  | 128.78      | 125.42   |
| 10  | aA    | 801 | CL0  | CMB-C2B-C3B | 2.20  | 129.09      | 124.68   |
| 11  | cB    | 825 | CLA  | CHB-C4A-NA  | 2.20  | 127.58      | 124.40   |
| 11  | aA    | 820 | CLA  | C4-C3-C5    | 2.20  | 119.05      | 115.23   |
| 11  | aB    | 836 | CLA  | C3B-C4B-NB  | 2.20  | 112.50      | 110.53   |
| 11  | cA    | 819 | CLA  | O2D-CGD-O1D | -2.20 | 119.56      | 123.85   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bA    | 833 | CLA  | CHB-C4A-NA  | 2.20  | 127.58      | 124.40   |
| 11  | cA    | 828 | CLA  | CMB-C2B-C1B | 2.20  | 128.77      | 125.42   |
| 11  | aA    | 839 | CLA  | CMC-C2C-C1C | 2.20  | 128.48      | 125.03   |
| 11  | bA    | 839 | CLA  | CMC-C2C-C1C | 2.20  | 128.48      | 125.03   |
| 11  | cA    | 803 | CLA  | CBC-CAC-C3C | -2.20 | 106.45      | 112.42   |
| 11  | aB    | 802 | CLA  | C4-C3-C2    | -2.20 | 117.97      | 123.63   |
| 12  | aA    | 827 | F6C  | CMC-C2C-C1C | 2.20  | 128.77      | 125.42   |
| 11  | cL    | 206 | CLA  | CMC-C2C-C1C | 2.20  | 128.47      | 125.03   |
| 10  | cA    | 801 | CL0  | CMC-C2C-C1C | 2.20  | 128.69      | 124.73   |
| 11  | cB    | 834 | CLA  | CHA-C1A-NA  | -2.20 | 121.41      | 126.39   |
| 11  | aB    | 818 | CLA  | C1-C2-C3    | -2.20 | 122.59      | 126.20   |
| 10  | cA    | 801 | CL0  | CMB-C2B-C3B | 2.20  | 129.08      | 124.68   |
| 11  | bA    | 818 | CLA  | CBC-CAC-C3C | -2.20 | 106.45      | 112.42   |
| 11  | cB    | 807 | CLA  | O2A-CGA-CBA | 2.20  | 118.54      | 111.83   |
| 11  | aB    | 803 | CLA  | CED-O2D-CGD | 2.20  | 120.91      | 115.92   |
| 11  | cA    | 811 | CLA  | CED-O2D-CGD | 2.20  | 120.91      | 115.92   |
| 11  | aA    | 811 | CLA  | CED-O2D-CGD | 2.20  | 120.91      | 115.92   |
| 11  | cB    | 805 | CLA  | CMC-C2C-C1C | 2.20  | 128.47      | 125.03   |
| 11  | bA    | 803 | CLA  | CBC-CAC-C3C | -2.20 | 106.46      | 112.42   |
| 11  | bB    | 807 | CLA  | O2A-CGA-CBA | 2.20  | 118.54      | 111.83   |
| 11  | bA    | 802 | CLA  | C16-C15-C13 | -2.20 | 108.66      | 115.97   |
| 11  | cA    | 823 | CLA  | C4A-NA-C1A  | -2.20 | 105.68      | 106.68   |
| 11  | cA    | 810 | CLA  | O2D-CGD-O1D | -2.20 | 119.57      | 123.85   |
| 11  | aA    | 828 | CLA  | O1D-CGD-CBD | -2.20 | 120.18      | 124.52   |
| 11  | aB    | 837 | CLA  | CHB-C4A-NA  | 2.20  | 127.57      | 124.40   |
| 11  | cA    | 812 | CLA  | CAA-C2A-C3A | -2.20 | 107.06      | 113.00   |
| 11  | cB    | 834 | CLA  | CHB-C4A-NA  | 2.20  | 127.57      | 124.40   |
| 11  | aB    | 807 | CLA  | O2A-CGA-CBA | 2.20  | 118.53      | 111.83   |
| 15  | bB    | 842 | BCR  | C33-C5-C6   | -2.19 | 122.09      | 124.48   |
| 11  | cA    | 820 | CLA  | CHB-C1B-C2B | -2.19 | 121.06      | 127.43   |
| 11  | cA    | 816 | CLA  | O2D-CGD-O1D | -2.19 | 119.58      | 123.85   |
| 11  | cB    | 836 | CLA  | C3B-C4B-NB  | 2.19  | 112.49      | 110.53   |
| 11  | bB    | 802 | CLA  | C4-C3-C2    | -2.19 | 117.99      | 123.63   |
| 11  | cA    | 810 | CLA  | CMA-C3A-C4A | 2.19  | 117.67      | 111.77   |
| 15  | cB    | 848 | BCR  | C37-C22-C21 | -2.19 | 119.26      | 122.82   |
| 11  | aA    | 838 | CLA  | C1-O2A-CGA  | 2.19  | 121.96      | 116.65   |
| 11  | cA    | 802 | CLA  | C16-C15-C13 | -2.19 | 108.68      | 115.97   |
| 10  | bA    | 801 | CL0  | CMB-C2B-C3B | 2.19  | 129.06      | 124.68   |
| 10  | bA    | 801 | CL0  | CMC-C2C-C1C | 2.19  | 128.68      | 124.73   |
| 11  | bA    | 820 | CLA  | C4-C3-C5    | 2.19  | 119.03      | 115.23   |
| 11  | aA    | 820 | CLA  | CHB-C1B-C2B | -2.19 | 121.06      | 127.43   |
| 11  | cB    | 803 | CLA  | CED-O2D-CGD | 2.19  | 120.89      | 115.92   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 15  | bL    | 203 | BCR  | C15-C14-C13 | -2.19 | 124.20      | 127.28   |
| 11  | bB    | 803 | CLA  | C1-C2-C3    | -2.19 | 122.61      | 126.20   |
| 15  | aB    | 842 | BCR  | C33-C5-C6   | -2.19 | 122.09      | 124.48   |
| 15  | cL    | 203 | BCR  | C15-C14-C13 | -2.19 | 124.20      | 127.28   |
| 11  | bB    | 828 | CLA  | CHD-C4C-NC  | 2.19  | 127.63      | 124.23   |
| 11  | cB    | 801 | CLA  | C11-C12-C13 | -2.19 | 108.69      | 115.97   |
| 11  | aA    | 812 | CLA  | CAA-C2A-C3A | -2.19 | 107.08      | 113.00   |
| 12  | bB    | 824 | F6C  | C1-O2A-CGA  | 2.19  | 121.95      | 116.65   |
| 12  | aA    | 826 | F6C  | CMA-C3A-C2A | -2.19 | 120.23      | 126.15   |
| 11  | cB    | 802 | CLA  | C4-C3-C2    | -2.19 | 118.01      | 123.63   |
| 11  | bA    | 804 | CLA  | CHB-C4A-NA  | 2.19  | 127.56      | 124.40   |
| 11  | cA    | 817 | CLA  | CHB-C4A-NA  | 2.19  | 127.56      | 124.40   |
| 11  | bB    | 812 | CLA  | CMB-C2B-C1B | 2.19  | 128.75      | 125.42   |
| 12  | cA    | 826 | F6C  | CMA-C3A-C2A | -2.19 | 120.23      | 126.15   |
| 11  | cA    | 833 | CLA  | CHB-C4A-NA  | 2.19  | 127.56      | 124.40   |
| 11  | cA    | 829 | CLA  | O2D-CGD-O1D | -2.19 | 119.59      | 123.85   |
| 11  | cL    | 206 | CLA  | CHB-C4A-NA  | 2.19  | 127.56      | 124.40   |
| 11  | bB    | 836 | CLA  | C3B-C4B-NB  | 2.19  | 112.48      | 110.53   |
| 12  | bA    | 826 | F6C  | CMA-C3A-C2A | -2.19 | 120.24      | 126.15   |
| 15  | cA    | 848 | BCR  | C16-C15-C14 | -2.19 | 119.05      | 123.52   |
| 11  | aA    | 810 | CLA  | CMA-C3A-C4A | 2.18  | 117.64      | 111.77   |
| 11  | cB    | 812 | CLA  | CMB-C2B-C1B | 2.18  | 128.75      | 125.42   |
| 12  | cB    | 824 | F6C  | C1-O2A-CGA  | 2.18  | 121.94      | 116.65   |
| 11  | bB    | 801 | CLA  | C11-C12-C13 | -2.18 | 108.71      | 115.97   |
| 12  | cA    | 827 | F6C  | CMC-C2C-C1C | 2.18  | 128.74      | 125.42   |
| 11  | aA    | 802 | CLA  | C16-C15-C13 | -2.18 | 108.71      | 115.97   |
| 11  | bA    | 829 | CLA  | CMA-C3A-C2A | -2.18 | 105.55      | 113.98   |
| 11  | bA    | 829 | CLA  | O2D-CGD-O1D | -2.18 | 119.60      | 123.85   |
| 11  | cA    | 838 | CLA  | C1-O2A-CGA  | 2.18  | 121.93      | 116.65   |
| 15  | cB    | 842 | BCR  | C33-C5-C6   | -2.18 | 122.10      | 124.48   |
| 11  | aA    | 821 | CLA  | O1D-CGD-CBD | -2.18 | 120.22      | 124.52   |
| 11  | cA    | 821 | CLA  | O1D-CGD-CBD | -2.18 | 120.22      | 124.52   |
| 11  | cB    | 825 | CLA  | CMB-C2B-C1B | 2.18  | 128.74      | 125.42   |
| 12  | aB    | 824 | F6C  | C1-O2A-CGA  | 2.18  | 121.93      | 116.65   |
| 11  | aA    | 809 | CLA  | O1D-CGD-CBD | -2.18 | 120.22      | 124.52   |
| 10  | aA    | 801 | CL0  | CMC-C2C-C1C | 2.18  | 128.66      | 124.73   |
| 11  | aB    | 811 | CLA  | O2D-CGD-O1D | -2.18 | 119.61      | 123.85   |
| 11  | bA    | 816 | CLA  | O2D-CGD-O1D | -2.18 | 119.61      | 123.85   |
| 11  | bA    | 809 | CLA  | O1D-CGD-CBD | -2.18 | 120.22      | 124.52   |
| 11  | aB    | 801 | CLA  | C11-C12-C13 | -2.18 | 108.72      | 115.97   |
| 11  | aB    | 834 | CLA  | CHA-C1A-NA  | -2.18 | 121.46      | 126.39   |
| 15  | aL    | 203 | BCR  | C15-C14-C13 | -2.18 | 124.22      | 127.28   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aB    | 825 | CLA  | CMB-C2B-C1B | 2.18  | 128.73      | 125.42   |
| 12  | bA    | 827 | F6C  | CMC-C2C-C1C | 2.18  | 128.73      | 125.42   |
| 15  | aB    | 848 | BCR  | C37-C22-C21 | -2.18 | 119.29      | 122.82   |
| 11  | bB    | 825 | CLA  | CHB-C4A-NA  | 2.18  | 127.54      | 124.40   |
| 11  | bA    | 821 | CLA  | O1D-CGD-CBD | -2.18 | 120.22      | 124.52   |
| 11  | cA    | 837 | CLA  | CBA-CAA-C2A | 2.18  | 120.27      | 113.79   |
| 11  | aB    | 828 | CLA  | CHD-C4C-NC  | 2.18  | 127.61      | 124.23   |
| 11  | cA    | 829 | CLA  | CMA-C3A-C2A | -2.18 | 105.57      | 113.98   |
| 11  | cB    | 818 | CLA  | CHB-C4A-NA  | 2.18  | 127.54      | 124.40   |
| 11  | aL    | 206 | CLA  | C11-C10-C8  | -2.18 | 108.73      | 115.97   |
| 11  | bK    | 103 | CLA  | CHA-C1A-NA  | -2.17 | 121.47      | 126.39   |
| 11  | cB    | 827 | CLA  | O2D-CGD-O1D | -2.17 | 119.61      | 123.85   |
| 11  | aB    | 803 | CLA  | C1-C2-C3    | -2.17 | 122.63      | 126.20   |
| 11  | bB    | 834 | CLA  | CHB-C4A-NA  | 2.17  | 127.54      | 124.40   |
| 11  | aA    | 806 | CLA  | CHC-C1C-NC  | 2.17  | 127.59      | 124.31   |
| 15  | aB    | 846 | BCR  | C10-C11-C12 | -2.17 | 116.90      | 123.20   |
| 11  | cB    | 837 | CLA  | C4-C3-C5    | 2.17  | 119.00      | 115.23   |
| 11  | bB    | 805 | CLA  | CMC-C2C-C1C | 2.17  | 128.43      | 125.03   |
| 12  | aA    | 844 | F6C  | CMC-C2C-C1C | 2.17  | 128.73      | 125.42   |
| 11  | aB    | 812 | CLA  | CHB-C4A-NA  | 2.17  | 127.54      | 124.40   |
| 11  | aA    | 833 | CLA  | CHB-C4A-NA  | 2.17  | 127.53      | 124.40   |
| 11  | aB    | 835 | CLA  | CHB-C4A-NA  | 2.17  | 127.53      | 124.40   |
| 11  | aB    | 829 | CLA  | C4A-NA-C1A  | -2.17 | 105.69      | 106.68   |
| 11  | cA    | 813 | CLA  | C4-C3-C5    | 2.17  | 119.00      | 115.23   |
| 11  | aA    | 803 | CLA  | CMC-C2C-C1C | 2.17  | 128.43      | 125.03   |
| 11  | bA    | 810 | CLA  | CMA-C3A-C4A | 2.17  | 117.61      | 111.77   |
| 11  | cB    | 803 | CLA  | C1-C2-C3    | -2.17 | 122.64      | 126.20   |
| 11  | aA    | 816 | CLA  | O2D-CGD-O1D | -2.17 | 119.62      | 123.85   |
| 11  | bA    | 837 | CLA  | CBA-CAA-C2A | 2.17  | 120.25      | 113.79   |
| 11  | aA    | 837 | CLA  | CBA-CAA-C2A | 2.17  | 120.25      | 113.79   |
| 11  | cL    | 206 | CLA  | C11-C10-C8  | -2.17 | 108.75      | 115.97   |
| 11  | cA    | 836 | CLA  | CHB-C4A-NA  | 2.17  | 127.53      | 124.40   |
| 11  | bB    | 820 | CLA  | CAC-C3C-C4C | 2.17  | 127.61      | 124.79   |
| 12  | cA    | 844 | F6C  | O2D-CGD-O1D | -2.17 | 119.63      | 123.85   |
| 11  | aK    | 103 | CLA  | CHA-C1A-NA  | -2.17 | 121.48      | 126.39   |
| 11  | aB    | 804 | CLA  | O1D-CGD-CBD | -2.17 | 120.24      | 124.52   |
| 11  | aA    | 817 | CLA  | CHB-C4A-NA  | 2.17  | 127.53      | 124.40   |
| 11  | cA    | 803 | CLA  | CMC-C2C-C1C | 2.17  | 128.42      | 125.03   |
| 11  | bA    | 820 | CLA  | CAA-CBA-CGA | 2.17  | 119.36      | 113.21   |
| 11  | cA    | 820 | CLA  | CAA-CBA-CGA | 2.17  | 119.36      | 113.21   |
| 11  | cB    | 828 | CLA  | CHD-C4C-NC  | 2.17  | 127.59      | 124.23   |
| 15  | bB    | 848 | BCR  | C37-C22-C21 | -2.17 | 119.31      | 122.82   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aB    | 834 | CLA  | CHB-C4A-NA  | 2.16  | 127.52      | 124.40   |
| 11  | bA    | 812 | CLA  | CAA-C2A-C3A | -2.16 | 107.15      | 113.00   |
| 11  | cK    | 103 | CLA  | CHA-C1A-NA  | -2.16 | 121.49      | 126.39   |
| 15  | aA    | 848 | BCR  | C16-C15-C14 | -2.16 | 119.09      | 123.52   |
| 12  | bA    | 844 | F6C  | CMC-C2C-C1C | 2.16  | 128.71      | 125.42   |
| 11  | bL    | 206 | CLA  | C11-C10-C8  | -2.16 | 108.78      | 115.97   |
| 11  | aB    | 816 | CLA  | CED-O2D-CGD | 2.16  | 120.82      | 115.92   |
| 11  | cB    | 804 | CLA  | O1D-CGD-CBD | -2.16 | 120.25      | 124.52   |
| 11  | aB    | 837 | CLA  | C4-C3-C5    | 2.16  | 118.98      | 115.23   |
| 11  | bA    | 813 | CLA  | C4-C3-C5    | 2.16  | 118.98      | 115.23   |
| 11  | cB    | 812 | CLA  | CHB-C4A-NA  | 2.16  | 127.52      | 124.40   |
| 11  | aA    | 809 | CLA  | CMB-C2B-C1B | 2.16  | 128.71      | 125.42   |
| 11  | bB    | 811 | CLA  | O2D-CGD-O1D | -2.16 | 119.64      | 123.85   |
| 11  | aA    | 841 | CLA  | C5-C3-C4    | 2.16  | 119.56      | 114.59   |
| 11  | bB    | 837 | CLA  | CHB-C4A-NA  | 2.16  | 127.52      | 124.40   |
| 11  | bB    | 837 | CLA  | C4-C3-C5    | 2.16  | 118.98      | 115.23   |
| 11  | cB    | 814 | CLA  | CBC-CAC-C3C | -2.16 | 106.56      | 112.42   |
| 15  | bB    | 846 | BCR  | C10-C11-C12 | -2.16 | 116.94      | 123.20   |
| 11  | cA    | 842 | CLA  | CHB-C1B-C2B | -2.16 | 121.16      | 127.43   |
| 11  | cA    | 841 | CLA  | C5-C3-C4    | 2.16  | 119.56      | 114.59   |
| 11  | cA    | 806 | CLA  | CHC-C1C-NC  | 2.16  | 127.56      | 124.31   |
| 11  | aB    | 805 | CLA  | CMC-C2C-C1C | 2.16  | 128.41      | 125.03   |
| 11  | bA    | 841 | CLA  | C5-C3-C4    | 2.16  | 119.56      | 114.59   |
| 11  | aA    | 829 | CLA  | O2D-CGD-O1D | -2.16 | 119.65      | 123.85   |
| 11  | aA    | 829 | CLA  | CMA-C3A-C2A | -2.16 | 105.64      | 113.98   |
| 11  | bB    | 832 | CLA  | O2D-CGD-O1D | -2.16 | 119.65      | 123.85   |
| 15  | cL    | 208 | BCR  | C24-C23-C22 | -2.16 | 123.04      | 126.23   |
| 11  | aB    | 836 | CLA  | CHA-C1A-NA  | -2.16 | 121.51      | 126.39   |
| 11  | bA    | 817 | CLA  | CHB-C4A-NA  | 2.16  | 127.51      | 124.40   |
| 11  | cB    | 837 | CLA  | CHB-C4A-NA  | 2.16  | 127.51      | 124.40   |
| 12  | bA    | 844 | F6C  | O2D-CGD-O1D | -2.16 | 119.65      | 123.85   |
| 11  | cA    | 809 | CLA  | CMB-C2B-C1B | 2.16  | 128.70      | 125.42   |
| 15  | cL    | 203 | BCR  | C16-C15-C14 | -2.16 | 119.11      | 123.52   |
| 11  | bB    | 821 | CLA  | CAA-C2A-C3A | -2.16 | 107.17      | 113.00   |
| 15  | aB    | 848 | BCR  | C30-C25-C26 | -2.15 | 119.69      | 122.64   |
| 11  | bA    | 803 | CLA  | CMC-C2C-C1C | 2.15  | 128.40      | 125.03   |
| 11  | aB    | 813 | CLA  | CMC-C2C-C1C | 2.15  | 128.40      | 125.03   |
| 15  | aL    | 203 | BCR  | C16-C15-C14 | -2.15 | 119.11      | 123.52   |
| 15  | bA    | 847 | BCR  | C15-C16-C17 | -2.15 | 119.11      | 123.52   |
| 15  | cB    | 846 | BCR  | C10-C11-C12 | -2.15 | 116.96      | 123.20   |
| 15  | aI    | 101 | BCR  | C15-C14-C13 | -2.15 | 124.26      | 127.28   |
| 11  | aA    | 820 | CLA  | CAA-CBA-CGA | 2.15  | 119.32      | 113.21   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cA    | 807 | CLA  | CAC-C3C-C4C | 2.15  | 127.59      | 124.79   |
| 11  | cB    | 813 | CLA  | CMC-C2C-C1C | 2.15  | 128.39      | 125.03   |
| 11  | bB    | 827 | CLA  | O2D-CGD-O1D | -2.15 | 119.66      | 123.85   |
| 11  | bB    | 814 | CLA  | CBC-CAC-C3C | -2.15 | 106.59      | 112.42   |
| 15  | bA    | 848 | BCR  | C16-C15-C14 | -2.15 | 119.12      | 123.52   |
| 11  | bB    | 836 | CLA  | CHA-C1A-NA  | -2.15 | 121.53      | 126.39   |
| 11  | aA    | 813 | CLA  | C4-C3-C5    | 2.15  | 118.96      | 115.23   |
| 11  | bB    | 813 | CLA  | CMC-C2C-C1C | 2.15  | 128.39      | 125.03   |
| 11  | bB    | 827 | CLA  | CBC-CAC-C3C | -2.15 | 106.60      | 112.42   |
| 11  | aA    | 813 | CLA  | CHB-C4A-NA  | 2.15  | 127.50      | 124.40   |
| 11  | aA    | 842 | CLA  | CHB-C1B-C2B | -2.15 | 121.20      | 127.43   |
| 11  | aB    | 825 | CLA  | O1D-CGD-CBD | -2.15 | 120.28      | 124.52   |
| 15  | cB    | 848 | BCR  | C30-C25-C26 | -2.15 | 119.70      | 122.64   |
| 11  | cB    | 821 | CLA  | CAA-C2A-C3A | -2.15 | 107.20      | 113.00   |
| 11  | bB    | 816 | CLA  | CED-O2D-CGD | 2.15  | 120.78      | 115.92   |
| 11  | bB    | 815 | CLA  | CBC-CAC-C3C | -2.15 | 106.60      | 112.42   |
| 11  | bA    | 807 | CLA  | CAC-C3C-C4C | 2.15  | 127.58      | 124.79   |
| 11  | aB    | 840 | CLA  | CHB-C4A-NA  | 2.14  | 127.50      | 124.40   |
| 11  | cB    | 835 | CLA  | CMC-C2C-C1C | 2.14  | 128.38      | 125.03   |
| 11  | cB    | 840 | CLA  | CMB-C2B-C1B | 2.14  | 128.68      | 125.42   |
| 12  | cA    | 844 | F6C  | CMC-C2C-C1C | 2.14  | 128.68      | 125.42   |
| 11  | aB    | 835 | CLA  | CMC-C2C-C1C | 2.14  | 128.38      | 125.03   |
| 11  | aB    | 827 | CLA  | CBC-CAC-C3C | -2.14 | 106.61      | 112.42   |
| 11  | bB    | 835 | CLA  | CHB-C4A-NA  | 2.14  | 127.49      | 124.40   |
| 15  | cL    | 208 | BCR  | C7-C8-C9    | -2.14 | 123.07      | 126.23   |
| 12  | aA    | 844 | F6C  | CAA-CBA-CGA | -2.14 | 107.09      | 113.44   |
| 15  | cI    | 103 | BCR  | C15-C14-C13 | -2.14 | 124.28      | 127.28   |
| 11  | bB    | 835 | CLA  | CMC-C2C-C1C | 2.14  | 128.38      | 125.03   |
| 11  | aA    | 831 | CLA  | CHB-C4A-NA  | 2.14  | 127.49      | 124.40   |
| 11  | bK    | 101 | CLA  | CBC-CAC-C3C | -2.14 | 106.62      | 112.42   |
| 11  | cL    | 206 | CLA  | O2A-CGA-CBA | 2.14  | 118.36      | 111.83   |
| 11  | bB    | 833 | CLA  | CAA-C2A-C3A | -2.14 | 107.22      | 113.00   |
| 11  | aB    | 814 | CLA  | CBC-CAC-C3C | -2.14 | 106.62      | 112.42   |
| 11  | aB    | 827 | CLA  | O2D-CGD-O1D | -2.14 | 119.69      | 123.85   |
| 15  | aA    | 847 | BCR  | C15-C16-C17 | -2.14 | 119.14      | 123.52   |
| 15  | bI    | 101 | BCR  | C15-C14-C13 | -2.14 | 124.28      | 127.28   |
| 11  | bL    | 206 | CLA  | O2A-CGA-CBA | 2.14  | 118.35      | 111.83   |
| 11  | cK    | 101 | CLA  | CBC-CAC-C3C | -2.14 | 106.63      | 112.42   |
| 11  | aB    | 832 | CLA  | O2D-CGD-O1D | -2.14 | 119.69      | 123.85   |
| 12  | aA    | 844 | F6C  | O2D-CGD-O1D | -2.14 | 119.69      | 123.85   |
| 15  | bL    | 203 | BCR  | C16-C15-C14 | -2.14 | 119.15      | 123.52   |
| 15  | cA    | 847 | BCR  | C15-C16-C17 | -2.14 | 119.15      | 123.52   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aA    | 839 | CLA  | C6-C7-C8    | -2.13 | 108.87      | 115.97   |
| 11  | cB    | 833 | CLA  | CAA-C2A-C3A | -2.13 | 107.23      | 113.00   |
| 11  | bB    | 812 | CLA  | O1D-CGD-CBD | -2.13 | 120.31      | 124.52   |
| 11  | cB    | 835 | CLA  | CHB-C4A-NA  | 2.13  | 127.48      | 124.40   |
| 11  | cB    | 836 | CLA  | CHA-C1A-NA  | -2.13 | 121.56      | 126.39   |
| 15  | aL    | 208 | BCR  | C24-C23-C22 | -2.13 | 123.08      | 126.23   |
| 11  | cB    | 832 | CLA  | O2D-CGD-O1D | -2.13 | 119.70      | 123.85   |
| 11  | bA    | 842 | CLA  | CHB-C1B-C2B | -2.13 | 121.24      | 127.43   |
| 11  | aB    | 833 | CLA  | O2D-CGD-O1D | -2.13 | 119.70      | 123.85   |
| 11  | bB    | 804 | CLA  | O1D-CGD-CBD | -2.13 | 120.31      | 124.52   |
| 11  | cB    | 816 | CLA  | CED-O2D-CGD | 2.13  | 120.75      | 115.92   |
| 11  | cB    | 834 | CLA  | O2D-CGD-O1D | -2.13 | 119.70      | 123.85   |
| 11  | bA    | 828 | CLA  | OBD-CAD-C3D | -2.13 | 123.43      | 128.42   |
| 11  | bA    | 839 | CLA  | C6-C7-C8    | -2.13 | 108.88      | 115.97   |
| 11  | cB    | 827 | CLA  | CMC-C2C-C1C | 2.13  | 128.36      | 125.03   |
| 11  | aA    | 828 | CLA  | OBD-CAD-C3D | -2.13 | 123.44      | 128.42   |
| 12  | cA    | 844 | F6C  | CED-O2D-CGD | 2.13  | 120.75      | 115.92   |
| 11  | cB    | 811 | CLA  | O2D-CGD-O1D | -2.13 | 119.70      | 123.85   |
| 11  | aL    | 206 | CLA  | O2A-CGA-CBA | 2.13  | 118.33      | 111.83   |
| 11  | bB    | 827 | CLA  | CMC-C2C-C1C | 2.13  | 128.36      | 125.03   |
| 11  | bB    | 825 | CLA  | CMB-C2B-C1B | 2.13  | 128.66      | 125.42   |
| 11  | cA    | 825 | CLA  | C1-C2-C3    | -2.13 | 122.71      | 126.20   |
| 11  | bB    | 840 | CLA  | CHB-C4A-NA  | 2.13  | 127.47      | 124.40   |
| 11  | bB    | 840 | CLA  | CMB-C2B-C1B | 2.13  | 128.66      | 125.42   |
| 11  | aB    | 827 | CLA  | CMC-C2C-C1C | 2.13  | 128.36      | 125.03   |
| 11  | cA    | 815 | CLA  | CHA-C1A-NA  | -2.13 | 121.58      | 126.39   |
| 11  | bA    | 831 | CLA  | CHB-C4A-NA  | 2.13  | 127.47      | 124.40   |
| 11  | cA    | 810 | CLA  | CAA-C2A-C1A | 2.13  | 118.94      | 111.97   |
| 11  | cB    | 834 | CLA  | CMB-C2B-C1B | 2.13  | 128.66      | 125.42   |
| 11  | aB    | 833 | CLA  | CAA-C2A-C3A | -2.13 | 107.26      | 113.00   |
| 12  | bA    | 832 | F6C  | O2A-CGA-O1A | -2.13 | 118.31      | 123.63   |
| 12  | cA    | 832 | F6C  | O2A-CGA-O1A | -2.12 | 118.31      | 123.63   |
| 12  | bA    | 844 | F6C  | CAA-CBA-CGA | -2.12 | 107.14      | 113.44   |
| 11  | aA    | 815 | CLA  | CHA-C1A-NA  | -2.12 | 121.58      | 126.39   |
| 15  | bL    | 208 | BCR  | C24-C23-C22 | -2.12 | 123.09      | 126.23   |
| 11  | cB    | 812 | CLA  | O1D-CGD-CBD | -2.12 | 120.33      | 124.52   |
| 11  | bA    | 838 | CLA  | O1D-CGD-CBD | -2.12 | 120.33      | 124.52   |
| 11  | cB    | 832 | CLA  | O2A-CGA-CBA | 2.12  | 120.71      | 114.00   |
| 11  | bB    | 825 | CLA  | O1D-CGD-CBD | -2.12 | 120.33      | 124.52   |
| 11  | aB    | 840 | CLA  | CMB-C2B-C1B | 2.12  | 128.65      | 125.42   |
| 11  | cA    | 839 | CLA  | C6-C7-C8    | -2.12 | 108.91      | 115.97   |
| 11  | aB    | 834 | CLA  | O2D-CGD-O1D | -2.12 | 119.72      | 123.85   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cB    | 827 | CLA  | CBC-CAC-C3C | -2.12 | 106.67      | 112.42   |
| 11  | aB    | 818 | CLA  | CHB-C4A-NA  | 2.12  | 127.46      | 124.40   |
| 15  | aL    | 208 | BCR  | C7-C8-C9    | -2.12 | 123.10      | 126.23   |
| 11  | aB    | 812 | CLA  | O1D-CGD-CBD | -2.12 | 120.33      | 124.52   |
| 11  | cB    | 829 | CLA  | C4A-NA-C1A  | -2.12 | 105.71      | 106.68   |
| 11  | aB    | 828 | CLA  | CAA-C2A-C3A | -2.12 | 107.27      | 113.00   |
| 11  | aA    | 822 | CLA  | C6-C7-C8    | -2.12 | 108.92      | 115.97   |
| 11  | bA    | 810 | CLA  | CAA-C2A-C1A | 2.12  | 118.92      | 111.97   |
| 12  | cA    | 844 | F6C  | CAA-CBA-CGA | -2.12 | 107.15      | 113.44   |
| 11  | cB    | 819 | CLA  | CBA-CAA-C2A | 2.12  | 120.10      | 113.79   |
| 11  | aB    | 815 | CLA  | CBC-CAC-C3C | -2.12 | 106.67      | 112.42   |
| 11  | cA    | 831 | CLA  | CHB-C4A-NA  | 2.12  | 127.46      | 124.40   |
| 11  | bA    | 825 | CLA  | C1-C2-C3    | -2.12 | 122.72      | 126.20   |
| 11  | aK    | 101 | CLA  | CBC-CAC-C3C | -2.12 | 106.67      | 112.42   |
| 11  | aB    | 819 | CLA  | CBA-CAA-C2A | 2.12  | 120.09      | 113.79   |
| 11  | bB    | 826 | CLA  | C4-C3-C5    | 2.12  | 118.90      | 115.23   |
| 15  | bM    | 101 | BCR  | C31-C1-C6   | 2.12  | 113.56      | 110.24   |
| 15  | bA    | 847 | BCR  | C16-C15-C14 | -2.12 | 119.19      | 123.52   |
| 11  | aB    | 821 | CLA  | CAA-C2A-C3A | -2.12 | 107.28      | 113.00   |
| 11  | bA    | 805 | CLA  | CHB-C1B-C2B | -2.12 | 121.28      | 127.43   |
| 11  | aA    | 810 | CLA  | CAA-C2A-C1A | 2.12  | 118.91      | 111.97   |
| 11  | bB    | 832 | CLA  | O2A-CGA-CBA | 2.12  | 120.68      | 114.00   |
| 12  | bA    | 844 | F6C  | CED-O2D-CGD | 2.12  | 120.71      | 115.92   |
| 11  | cA    | 828 | CLA  | OBD-CAD-C3D | -2.12 | 123.47      | 128.42   |
| 12  | aA    | 832 | F6C  | O2A-CGA-O1A | -2.12 | 118.34      | 123.63   |
| 11  | aB    | 832 | CLA  | O2A-CGA-CBA | 2.12  | 120.68      | 114.00   |
| 11  | cB    | 825 | CLA  | O1D-CGD-CBD | -2.11 | 120.35      | 124.52   |
| 12  | bL    | 202 | F6C  | O1D-CGD-CBD | -2.11 | 120.35      | 124.52   |
| 11  | bB    | 819 | CLA  | CBA-CAA-C2A | 2.11  | 120.08      | 113.79   |
| 11  | aA    | 807 | CLA  | CAC-C3C-C4C | 2.11  | 127.54      | 124.79   |
| 11  | cB    | 815 | CLA  | CBC-CAC-C3C | -2.11 | 106.69      | 112.42   |
| 11  | cA    | 838 | CLA  | O1D-CGD-CBD | -2.11 | 120.35      | 124.52   |
| 11  | bA    | 815 | CLA  | CHA-C1A-NA  | -2.11 | 121.61      | 126.39   |
| 11  | cB    | 833 | CLA  | O2D-CGD-O1D | -2.11 | 119.73      | 123.85   |
| 11  | cA    | 842 | CLA  | CHB-C4A-NA  | 2.11  | 127.45      | 124.40   |
| 15  | aB    | 842 | BCR  | C29-C30-C25 | 2.11  | 113.51      | 110.44   |
| 11  | cA    | 803 | CLA  | CMA-C3A-C2A | -2.11 | 105.82      | 113.98   |
| 11  | cA    | 822 | CLA  | C6-C7-C8    | -2.11 | 108.95      | 115.97   |
| 15  | cA    | 847 | BCR  | C16-C15-C14 | -2.11 | 119.20      | 123.52   |
| 15  | bB    | 848 | BCR  | C30-C25-C26 | -2.11 | 119.75      | 122.64   |
| 15  | bB    | 842 | BCR  | C29-C30-C25 | 2.11  | 113.50      | 110.44   |
| 11  | aA    | 822 | CLA  | C1-C2-C3    | -2.11 | 122.74      | 126.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12  | aL    | 202 | F6C  | O1D-CGD-CBD | -2.11 | 120.36      | 124.52   |
| 11  | aB    | 834 | CLA  | CMB-C2B-C1B | 2.11  | 128.63      | 125.42   |
| 11  | bB    | 818 | CLA  | CHB-C4A-NA  | 2.11  | 127.44      | 124.40   |
| 11  | cB    | 828 | CLA  | CAA-C2A-C3A | -2.11 | 107.30      | 113.00   |
| 15  | aA    | 851 | BCR  | C11-C10-C9  | -2.11 | 124.32      | 127.28   |
| 11  | bB    | 834 | CLA  | O2D-CGD-O1D | -2.11 | 119.74      | 123.85   |
| 11  | cB    | 818 | CLA  | C1-O2A-CGA  | 2.11  | 121.75      | 116.65   |
| 11  | bA    | 842 | CLA  | CHB-C4A-NA  | 2.11  | 127.44      | 124.40   |
| 11  | aB    | 826 | CLA  | C4-C3-C5    | 2.11  | 118.89      | 115.23   |
| 11  | cA    | 813 | CLA  | CHB-C4A-NA  | 2.11  | 127.44      | 124.40   |
| 11  | aA    | 803 | CLA  | CMA-C3A-C2A | -2.11 | 105.83      | 113.98   |
| 11  | bB    | 828 | CLA  | CAA-C2A-C3A | -2.11 | 107.31      | 113.00   |
| 11  | cB    | 810 | CLA  | CHB-C4A-NA  | 2.11  | 127.44      | 124.40   |
| 11  | cB    | 840 | CLA  | CHB-C4A-NA  | 2.11  | 127.44      | 124.40   |
| 11  | aA    | 831 | CLA  | CBC-CAC-C3C | -2.11 | 106.71      | 112.42   |
| 11  | cB    | 806 | CLA  | CHB-C4A-NA  | 2.11  | 127.44      | 124.40   |
| 15  | cB    | 842 | BCR  | C29-C30-C25 | 2.11  | 113.50      | 110.44   |
| 11  | bB    | 801 | CLA  | C11-C10-C8  | -2.11 | 108.97      | 115.97   |
| 11  | bA    | 831 | CLA  | CBC-CAC-C3C | -2.11 | 106.71      | 112.42   |
| 11  | bB    | 840 | CLA  | CAA-C2A-C3A | -2.10 | 107.31      | 113.00   |
| 12  | aA    | 844 | F6C  | CED-O2D-CGD | 2.10  | 120.69      | 115.92   |
| 11  | bB    | 834 | CLA  | CMB-C2B-C1B | 2.10  | 128.62      | 125.42   |
| 15  | aA    | 847 | BCR  | C16-C15-C14 | -2.10 | 119.21      | 123.52   |
| 11  | bA    | 813 | CLA  | CHB-C4A-NA  | 2.10  | 127.44      | 124.40   |
| 11  | bB    | 839 | CLA  | O2A-CGA-O1A | -2.10 | 118.37      | 123.63   |
| 11  | bB    | 833 | CLA  | O2D-CGD-O1D | -2.10 | 119.75      | 123.85   |
| 11  | cB    | 826 | CLA  | C4-C3-C5    | 2.10  | 118.88      | 115.23   |
| 11  | cB    | 805 | CLA  | CBA-CAA-C2A | 2.10  | 120.04      | 113.79   |
| 11  | bB    | 817 | CLA  | CMC-C2C-C1C | 2.10  | 128.31      | 125.03   |
| 11  | bA    | 803 | CLA  | CMA-C3A-C2A | -2.10 | 105.86      | 113.98   |
| 15  | aM    | 101 | BCR  | C31-C1-C6   | 2.10  | 113.53      | 110.24   |
| 11  | bB    | 807 | CLA  | C1-C2-C3    | -2.10 | 122.76      | 126.20   |
| 11  | bA    | 807 | CLA  | O1D-CGD-CBD | -2.10 | 120.38      | 124.52   |
| 11  | cB    | 817 | CLA  | CMC-C2C-C1C | 2.10  | 128.31      | 125.03   |
| 11  | aK    | 101 | CLA  | OBD-CAD-C3D | -2.10 | 125.19      | 128.60   |
| 11  | aA    | 807 | CLA  | O1D-CGD-CBD | -2.10 | 120.38      | 124.52   |
| 11  | bA    | 841 | CLA  | CBC-CAC-C3C | -2.10 | 106.73      | 112.42   |
| 11  | bB    | 818 | CLA  | C1-O2A-CGA  | 2.10  | 121.73      | 116.65   |
| 11  | bA    | 843 | CLA  | CHB-C4A-NA  | 2.10  | 127.43      | 124.40   |
| 11  | bB    | 836 | CLA  | O2A-CGA-O1A | -2.10 | 118.38      | 123.63   |
| 11  | aA    | 841 | CLA  | CBC-CAC-C3C | -2.10 | 106.74      | 112.42   |
| 11  | bK    | 101 | CLA  | OBD-CAD-C3D | -2.10 | 125.19      | 128.60   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cA    | 841 | CLA  | CBC-CAC-C3C | -2.10 | 106.74      | 112.42   |
| 11  | aB    | 817 | CLA  | CMC-C2C-C1C | 2.10  | 128.31      | 125.03   |
| 11  | aA    | 842 | CLA  | CHB-C4A-NA  | 2.10  | 127.42      | 124.40   |
| 11  | cB    | 801 | CLA  | C11-C10-C8  | -2.10 | 109.00      | 115.97   |
| 11  | cA    | 805 | CLA  | CHB-C1B-C2B | -2.09 | 121.34      | 127.43   |
| 11  | bA    | 822 | CLA  | C1-C2-C3    | -2.09 | 122.77      | 126.20   |
| 11  | cB    | 840 | CLA  | CAA-C2A-C3A | -2.09 | 107.34      | 113.00   |
| 11  | cA    | 807 | CLA  | O1D-CGD-CBD | -2.09 | 120.39      | 124.52   |
| 11  | aA    | 825 | CLA  | C1-C2-C3    | -2.09 | 122.77      | 126.20   |
| 11  | bB    | 810 | CLA  | CHB-C4A-NA  | 2.09  | 127.42      | 124.40   |
| 16  | cA    | 852 | LHG  | C27-C26-C25 | -2.09 | 103.79      | 114.37   |
| 11  | aA    | 819 | CLA  | CHB-C1B-C2B | -2.09 | 121.35      | 127.43   |
| 11  | cB    | 816 | CLA  | CMC-C2C-C1C | 2.09  | 128.30      | 125.03   |
| 11  | aA    | 813 | CLA  | CAA-C2A-C3A | -2.09 | 107.35      | 113.00   |
| 11  | cA    | 831 | CLA  | CBC-CAC-C3C | -2.09 | 106.75      | 112.42   |
| 11  | aA    | 838 | CLA  | O1D-CGD-CBD | -2.09 | 120.40      | 124.52   |
| 11  | cB    | 836 | CLA  | O2A-CGA-O1A | -2.09 | 118.40      | 123.63   |
| 11  | aB    | 827 | CLA  | O2A-CGA-CBA | 2.09  | 118.21      | 111.83   |
| 11  | bA    | 822 | CLA  | C6-C7-C8    | -2.09 | 109.02      | 115.97   |
| 11  | aB    | 818 | CLA  | C1-O2A-CGA  | 2.09  | 121.71      | 116.65   |
| 11  | cA    | 843 | CLA  | CHB-C4A-NA  | 2.09  | 127.41      | 124.40   |
| 11  | bA    | 813 | CLA  | CAA-C2A-C3A | -2.09 | 107.36      | 113.00   |
| 11  | cB    | 802 | CLA  | CHB-C4A-NA  | 2.09  | 127.41      | 124.40   |
| 11  | aA    | 824 | CLA  | O2A-CGA-O1A | -2.09 | 118.41      | 123.63   |
| 11  | cA    | 806 | CLA  | CMA-C3A-C2A | -2.09 | 105.92      | 113.98   |
| 11  | aB    | 806 | CLA  | CHB-C4A-NA  | 2.09  | 127.41      | 124.40   |
| 11  | bA    | 819 | CLA  | CHB-C1B-C2B | -2.09 | 121.37      | 127.43   |
| 16  | aA    | 852 | LHG  | C27-C26-C25 | -2.09 | 103.83      | 114.37   |
| 11  | aB    | 840 | CLA  | CAA-C2A-C3A | -2.09 | 107.36      | 113.00   |
| 11  | cB    | 821 | CLA  | C1-C2-C3    | -2.08 | 122.78      | 126.20   |
| 11  | aB    | 801 | CLA  | C11-C10-C8  | -2.08 | 109.04      | 115.97   |
| 11  | cB    | 827 | CLA  | O2A-CGA-CBA | 2.08  | 118.19      | 111.83   |
| 16  | bA    | 852 | LHG  | C27-C26-C25 | -2.08 | 103.83      | 114.37   |
| 11  | aB    | 805 | CLA  | CBA-CAA-C2A | 2.08  | 119.99      | 113.79   |
| 11  | aB    | 816 | CLA  | CMC-C2C-C1C | 2.08  | 128.29      | 125.03   |
| 11  | cB    | 829 | CLA  | O1D-CGD-CBD | -2.08 | 120.41      | 124.52   |
| 11  | cB    | 807 | CLA  | C1-C2-C3    | -2.08 | 122.78      | 126.20   |
| 11  | cB    | 809 | CLA  | CHB-C4A-NA  | 2.08  | 127.41      | 124.40   |
| 12  | cL    | 202 | F6C  | O1D-CGD-CBD | -2.08 | 120.41      | 124.52   |
| 11  | aA    | 805 | CLA  | CHB-C1B-C2B | -2.08 | 121.38      | 127.43   |
| 11  | bB    | 805 | CLA  | CBA-CAA-C2A | 2.08  | 119.99      | 113.79   |
| 11  | bB    | 816 | CLA  | CMC-C2C-C1C | 2.08  | 128.28      | 125.03   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aB    | 828 | CLA  | O2A-CGA-O1A | -2.08 | 118.43      | 123.63   |
| 11  | cA    | 838 | CLA  | CHB-C4A-NA  | 2.08  | 127.40      | 124.40   |
| 11  | aA    | 843 | CLA  | CHB-C4A-NA  | 2.08  | 127.40      | 124.40   |
| 11  | aB    | 821 | CLA  | C1-C2-C3    | -2.08 | 122.79      | 126.20   |
| 11  | bA    | 806 | CLA  | CMA-C3A-C2A | -2.08 | 105.94      | 113.98   |
| 11  | aB    | 809 | CLA  | CHB-C4A-NA  | 2.08  | 127.40      | 124.40   |
| 11  | aB    | 839 | CLA  | O2A-CGA-O1A | -2.08 | 118.43      | 123.63   |
| 11  | bA    | 824 | CLA  | O2A-CGA-O1A | -2.08 | 118.43      | 123.63   |
| 11  | bB    | 815 | CLA  | CAA-C2A-C3A | -2.08 | 107.39      | 113.00   |
| 11  | cA    | 821 | CLA  | O2A-CGA-CBA | 2.08  | 118.17      | 111.83   |
| 11  | aA    | 821 | CLA  | CHA-C1A-NA  | -2.08 | 121.69      | 126.39   |
| 11  | aB    | 836 | CLA  | O2A-CGA-O1A | -2.08 | 118.43      | 123.63   |
| 11  | cB    | 822 | CLA  | CHB-C4A-NA  | 2.08  | 127.40      | 124.40   |
| 15  | bL    | 208 | BCR  | C7-C8-C9    | -2.08 | 123.16      | 126.23   |
| 11  | aA    | 806 | CLA  | CMA-C3A-C2A | -2.08 | 105.96      | 113.98   |
| 11  | cB    | 815 | CLA  | CAA-C2A-C3A | -2.08 | 107.39      | 113.00   |
| 11  | cA    | 821 | CLA  | CHA-C1A-NA  | -2.08 | 121.69      | 126.39   |
| 15  | cK    | 102 | BCR  | C7-C8-C9    | -2.08 | 123.17      | 126.23   |
| 11  | cA    | 813 | CLA  | CAA-C2A-C3A | -2.07 | 107.39      | 113.00   |
| 11  | bB    | 802 | CLA  | CHB-C4A-NA  | 2.07  | 127.39      | 124.40   |
| 11  | aA    | 821 | CLA  | O2A-CGA-CBA | 2.07  | 118.16      | 111.83   |
| 11  | bA    | 821 | CLA  | O2A-CGA-CBA | 2.07  | 118.16      | 111.83   |
| 11  | aB    | 816 | CLA  | O2D-CGD-O1D | -2.07 | 119.81      | 123.85   |
| 11  | aB    | 810 | CLA  | CHB-C4A-NA  | 2.07  | 127.39      | 124.40   |
| 15  | cM    | 101 | BCR  | C31-C1-C6   | 2.07  | 113.49      | 110.24   |
| 11  | aB    | 815 | CLA  | CAA-C2A-C3A | -2.07 | 107.40      | 113.00   |
| 11  | aA    | 829 | CLA  | CHB-C1B-C2B | -2.07 | 121.41      | 127.43   |
| 11  | cA    | 824 | CLA  | O2A-CGA-O1A | -2.07 | 118.44      | 123.63   |
| 11  | cB    | 828 | CLA  | O2A-CGA-O1A | -2.07 | 118.44      | 123.63   |
| 11  | cB    | 807 | CLA  | CHB-C4A-NA  | 2.07  | 127.39      | 124.40   |
| 11  | bB    | 827 | CLA  | O2A-CGA-CBA | 2.07  | 118.15      | 111.83   |
| 13  | cB    | 841 | PQN  | C11-C3-C4   | 2.07  | 120.76      | 118.58   |
| 11  | cB    | 823 | CLA  | CBC-CAC-C3C | -2.07 | 106.81      | 112.42   |
| 11  | bB    | 823 | CLA  | CBC-CAC-C3C | -2.07 | 106.81      | 112.42   |
| 11  | aA    | 838 | CLA  | CHB-C4A-NA  | 2.07  | 127.39      | 124.40   |
| 11  | cB    | 830 | CLA  | CBC-CAC-C3C | -2.07 | 106.81      | 112.42   |
| 11  | bB    | 821 | CLA  | C1-C2-C3    | -2.07 | 122.81      | 126.20   |
| 15  | aK    | 102 | BCR  | C7-C8-C9    | -2.07 | 123.18      | 126.23   |
| 11  | bA    | 821 | CLA  | CHA-C1A-NA  | -2.07 | 121.71      | 126.39   |
| 11  | cB    | 834 | CLA  | CED-O2D-CGD | 2.07  | 120.61      | 115.92   |
| 15  | bA    | 849 | BCR  | C24-C23-C22 | -2.07 | 123.18      | 126.23   |
| 11  | aB    | 832 | CLA  | CMC-C2C-C1C | 2.07  | 128.26      | 125.03   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | cA    | 836 | CLA  | CBC-CAC-C3C | -2.07 | 106.82      | 112.42   |
| 11  | cA    | 814 | CLA  | O2A-CGA-CBA | 2.07  | 118.14      | 111.83   |
| 11  | cA    | 819 | CLA  | CHB-C1B-C2B | -2.07 | 121.43      | 127.43   |
| 11  | bA    | 806 | CLA  | C6-C7-C8    | -2.07 | 109.10      | 115.97   |
| 11  | bB    | 806 | CLA  | CHB-C4A-NA  | 2.07  | 127.38      | 124.40   |
| 11  | aA    | 814 | CLA  | O2A-CGA-CBA | 2.06  | 118.13      | 111.83   |
| 11  | aL    | 205 | CLA  | CBC-CAC-C3C | -2.06 | 106.82      | 112.42   |
| 11  | bA    | 836 | CLA  | CBC-CAC-C3C | -2.06 | 106.82      | 112.42   |
| 11  | cK    | 101 | CLA  | OBD-CAD-C3D | -2.06 | 125.24      | 128.60   |
| 11  | cB    | 830 | CLA  | CHB-C1B-C2B | -2.06 | 121.44      | 127.43   |
| 11  | aB    | 807 | CLA  | C1-C2-C3    | -2.06 | 122.82      | 126.20   |
| 15  | cA    | 851 | BCR  | C11-C10-C9  | -2.06 | 124.38      | 127.28   |
| 11  | cB    | 816 | CLA  | CBC-CAC-C3C | -2.06 | 106.83      | 112.42   |
| 15  | bA    | 851 | BCR  | C11-C10-C9  | -2.06 | 124.39      | 127.28   |
| 11  | cB    | 813 | CLA  | C4-C3-C5    | 2.06  | 118.81      | 115.23   |
| 11  | cB    | 839 | CLA  | O2A-CGA-O1A | -2.06 | 118.47      | 123.63   |
| 11  | cB    | 816 | CLA  | O2D-CGD-O1D | -2.06 | 119.84      | 123.85   |
| 11  | cA    | 822 | CLA  | CHB-C4A-NA  | 2.06  | 127.37      | 124.40   |
| 11  | aA    | 843 | CLA  | CMB-C2B-C1B | 2.06  | 128.56      | 125.42   |
| 11  | aB    | 823 | CLA  | CBC-CAC-C3C | -2.06 | 106.83      | 112.42   |
| 11  | bA    | 828 | CLA  | CBC-CAC-C3C | -2.06 | 106.83      | 112.42   |
| 11  | cA    | 828 | CLA  | CBC-CAC-C3C | -2.06 | 106.84      | 112.42   |
| 12  | cA    | 827 | F6C  | CBC-CAC-C3C | -2.06 | 106.84      | 112.42   |
| 11  | aB    | 816 | CLA  | CBC-CAC-C3C | -2.06 | 106.84      | 112.42   |
| 11  | cB    | 829 | CLA  | O2A-CGA-CBA | 2.06  | 120.50      | 114.00   |
| 11  | aA    | 823 | CLA  | C4A-NA-C1A  | -2.06 | 105.74      | 106.68   |
| 11  | aA    | 828 | CLA  | CBC-CAC-C3C | -2.06 | 106.84      | 112.42   |
| 11  | aB    | 832 | CLA  | CAA-C2A-C3A | -2.06 | 107.44      | 113.00   |
| 11  | bB    | 807 | CLA  | CHB-C4A-NA  | 2.06  | 127.37      | 124.40   |
| 11  | aB    | 830 | CLA  | CHB-C1B-C2B | -2.06 | 121.45      | 127.43   |
| 11  | bA    | 829 | CLA  | CHB-C1B-C2B | -2.06 | 121.45      | 127.43   |
| 11  | aB    | 805 | CLA  | CHA-C1A-NA  | -2.06 | 121.73      | 126.39   |
| 11  | aA    | 806 | CLA  | C6-C7-C8    | -2.06 | 109.13      | 115.97   |
| 11  | cK    | 103 | CLA  | O2A-CGA-O1A | -2.06 | 118.48      | 123.63   |
| 11  | cA    | 843 | CLA  | CMB-C2B-C1B | 2.06  | 128.55      | 125.42   |
| 11  | bA    | 814 | CLA  | O2A-CGA-CBA | 2.06  | 118.10      | 111.83   |
| 11  | aB    | 829 | CLA  | O1D-CGD-CBD | -2.06 | 120.46      | 124.52   |
| 15  | cI    | 103 | BCR  | C1-C6-C5    | -2.06 | 119.83      | 122.64   |
| 11  | bA    | 840 | CLA  | O2A-CGA-O1A | -2.05 | 118.49      | 123.63   |
| 11  | aB    | 829 | CLA  | O2A-CGA-CBA | 2.05  | 120.49      | 114.00   |
| 11  | bK    | 103 | CLA  | O2A-CGA-O1A | -2.05 | 118.49      | 123.63   |
| 11  | cA    | 822 | CLA  | C1-C2-C3    | -2.05 | 122.83      | 126.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aB    | 810 | CLA  | CMB-C2B-C1B | 2.05  | 128.55      | 125.42   |
| 11  | aA    | 836 | CLA  | CBC-CAC-C3C | -2.05 | 106.85      | 112.42   |
| 12  | bA    | 827 | F6C  | CBC-CAC-C3C | -2.05 | 106.85      | 112.42   |
| 11  | cA    | 829 | CLA  | CHB-C1B-C2B | -2.05 | 121.46      | 127.43   |
| 11  | bB    | 834 | CLA  | CED-O2D-CGD | 2.05  | 120.58      | 115.92   |
| 11  | cA    | 806 | CLA  | C6-C7-C8    | -2.05 | 109.14      | 115.97   |
| 11  | cL    | 205 | CLA  | CBC-CAC-C3C | -2.05 | 106.85      | 112.42   |
| 11  | bB    | 828 | CLA  | O2A-CGA-O1A | -2.05 | 118.49      | 123.63   |
| 11  | bB    | 808 | CLA  | O1D-CGD-CBD | -2.05 | 120.47      | 124.52   |
| 11  | aA    | 819 | CLA  | CHA-C1A-NA  | -2.05 | 121.75      | 126.39   |
| 11  | bB    | 822 | CLA  | CHB-C4A-NA  | 2.05  | 127.36      | 124.40   |
| 11  | cB    | 832 | CLA  | CAA-C2A-C3A | -2.05 | 107.46      | 113.00   |
| 11  | bB    | 816 | CLA  | O2D-CGD-O1D | -2.05 | 119.86      | 123.85   |
| 15  | cL    | 207 | BCR  | C40-C30-C25 | 2.05  | 113.46      | 110.24   |
| 11  | bB    | 829 | CLA  | O2A-CGA-CBA | 2.05  | 120.48      | 114.00   |
| 11  | aB    | 819 | CLA  | CBC-CAC-C3C | -2.05 | 106.86      | 112.42   |
| 11  | bA    | 838 | CLA  | CHB-C4A-NA  | 2.05  | 127.36      | 124.40   |
| 11  | aA    | 802 | CLA  | C11-C10-C8  | -2.05 | 109.16      | 115.97   |
| 11  | bA    | 810 | CLA  | CHA-C1A-NA  | -2.05 | 121.75      | 126.39   |
| 11  | aB    | 830 | CLA  | CBC-CAC-C3C | -2.05 | 106.87      | 112.42   |
| 11  | aA    | 816 | CLA  | CMB-C2B-C1B | 2.05  | 128.54      | 125.42   |
| 11  | aB    | 802 | CLA  | CHB-C4A-NA  | 2.05  | 127.36      | 124.40   |
| 11  | cB    | 836 | CLA  | CHB-C4A-NA  | 2.05  | 127.36      | 124.40   |
| 11  | aB    | 823 | CLA  | O2A-CGA-CBA | 2.05  | 118.08      | 111.83   |
| 11  | cB    | 830 | CLA  | CHA-C1A-NA  | -2.05 | 121.76      | 126.39   |
| 11  | bB    | 819 | CLA  | CBC-CAC-C3C | -2.05 | 106.87      | 112.42   |
| 15  | aI    | 101 | BCR  | C1-C6-C5    | -2.05 | 119.84      | 122.64   |
| 11  | aA    | 822 | CLA  | O2D-CGD-O1D | -2.05 | 119.86      | 123.85   |
| 11  | bB    | 830 | CLA  | CBC-CAC-C3C | -2.05 | 106.87      | 112.42   |
| 11  | bB    | 829 | CLA  | O1D-CGD-CBD | -2.05 | 120.48      | 124.52   |
| 11  | cB    | 810 | CLA  | CMB-C2B-C1B | 2.05  | 128.53      | 125.42   |
| 11  | bB    | 830 | CLA  | CHB-C1B-C2B | -2.04 | 121.49      | 127.43   |
| 11  | aA    | 812 | CLA  | CBC-CAC-C3C | -2.04 | 106.88      | 112.42   |
| 11  | cA    | 812 | CLA  | CBC-CAC-C3C | -2.04 | 106.88      | 112.42   |
| 11  | cA    | 802 | CLA  | C11-C10-C8  | -2.04 | 109.17      | 115.97   |
| 11  | bB    | 816 | CLA  | CBC-CAC-C3C | -2.04 | 106.88      | 112.42   |
| 11  | aA    | 810 | CLA  | CHA-C1A-NA  | -2.04 | 121.77      | 126.39   |
| 11  | aB    | 834 | CLA  | CED-O2D-CGD | 2.04  | 120.55      | 115.92   |
| 11  | cB    | 808 | CLA  | O1D-CGD-CBD | -2.04 | 120.49      | 124.52   |
| 11  | bL    | 205 | CLA  | CBC-CAC-C3C | -2.04 | 106.88      | 112.42   |
| 11  | cA    | 810 | CLA  | CHA-C1A-NA  | -2.04 | 121.77      | 126.39   |
| 11  | bB    | 832 | CLA  | CAA-C2A-C3A | -2.04 | 107.48      | 113.00   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | bA    | 838 | CLA  | CHA-C1A-NA  | -2.04 | 121.77      | 126.39   |
| 12  | bA    | 827 | F6C  | O2A-CGA-O1A | -2.04 | 118.52      | 123.63   |
| 11  | aA    | 817 | CLA  | CHB-C1B-C2B | -2.04 | 121.50      | 127.43   |
| 11  | cA    | 817 | CLA  | CHB-C1B-C2B | -2.04 | 121.50      | 127.43   |
| 11  | aB    | 807 | CLA  | CHB-C4A-NA  | 2.04  | 127.34      | 124.40   |
| 11  | bA    | 817 | CLA  | CHB-C1B-C2B | -2.04 | 121.50      | 127.43   |
| 11  | aA    | 840 | CLA  | O2A-CGA-O1A | -2.04 | 118.52      | 123.63   |
| 11  | bA    | 822 | CLA  | CHB-C4A-NA  | 2.04  | 127.34      | 124.40   |
| 15  | bL    | 207 | BCR  | C40-C30-C25 | 2.04  | 113.44      | 110.24   |
| 11  | cB    | 817 | CLA  | CBC-CAC-C3C | -2.04 | 106.89      | 112.42   |
| 11  | bA    | 802 | CLA  | C11-C10-C8  | -2.04 | 109.19      | 115.97   |
| 15  | bK    | 102 | BCR  | C7-C8-C9    | -2.04 | 123.22      | 126.23   |
| 11  | aB    | 808 | CLA  | O1D-CGD-CBD | -2.04 | 120.50      | 124.52   |
| 11  | bB    | 810 | CLA  | CMB-C2B-C1B | 2.04  | 128.52      | 125.42   |
| 11  | cB    | 827 | CLA  | CMB-C2B-C1B | 2.04  | 128.52      | 125.42   |
| 11  | bA    | 840 | CLA  | CHA-C1A-NA  | -2.04 | 121.78      | 126.39   |
| 11  | cB    | 823 | CLA  | O2A-CGA-CBA | 2.04  | 118.05      | 111.83   |
| 12  | aA    | 827 | F6C  | O2A-CGA-O1A | -2.04 | 118.53      | 123.63   |
| 11  | bA    | 812 | CLA  | CBC-CAC-C3C | -2.04 | 106.90      | 112.42   |
| 11  | cA    | 840 | CLA  | O2A-CGA-O1A | -2.04 | 118.53      | 123.63   |
| 11  | aB    | 812 | CLA  | CHA-C1A-NA  | -2.04 | 121.78      | 126.39   |
| 11  | aB    | 836 | CLA  | CHB-C4A-NA  | 2.04  | 127.34      | 124.40   |
| 12  | bA    | 832 | F6C  | CMC-C2C-C1C | 2.04  | 128.52      | 125.42   |
| 15  | bK    | 102 | BCR  | C37-C22-C21 | -2.04 | 119.52      | 122.82   |
| 15  | bI    | 101 | BCR  | C1-C6-C5    | -2.03 | 119.86      | 122.64   |
| 11  | cB    | 819 | CLA  | CBC-CAC-C3C | -2.03 | 106.90      | 112.42   |
| 11  | bB    | 827 | CLA  | CMB-C2B-C1B | 2.03  | 128.52      | 125.42   |
| 11  | aK    | 103 | CLA  | O2A-CGA-O1A | -2.03 | 118.54      | 123.63   |
| 11  | aA    | 817 | CLA  | CHA-C1A-NA  | -2.03 | 121.78      | 126.39   |
| 15  | aA    | 849 | BCR  | C24-C23-C22 | -2.03 | 123.23      | 126.23   |
| 12  | aA    | 827 | F6C  | CBC-CAC-C3C | -2.03 | 106.91      | 112.42   |
| 15  | aA    | 850 | BCR  | C33-C5-C6   | -2.03 | 122.27      | 124.48   |
| 11  | cB    | 807 | CLA  | C4-C3-C5    | 2.03  | 118.76      | 115.23   |
| 11  | cB    | 805 | CLA  | CHA-C1A-NA  | -2.03 | 121.79      | 126.39   |
| 11  | aB    | 807 | CLA  | C4-C3-C5    | 2.03  | 118.75      | 115.23   |
| 11  | aB    | 822 | CLA  | CHB-C4A-NA  | 2.03  | 127.33      | 124.40   |
| 11  | aA    | 806 | CLA  | CBA-CAA-C2A | 2.03  | 119.84      | 113.79   |
| 11  | bB    | 823 | CLA  | O2A-CGA-CBA | 2.03  | 118.03      | 111.83   |
| 11  | cA    | 816 | CLA  | CMB-C2B-C1B | 2.03  | 128.51      | 125.42   |
| 11  | aB    | 829 | CLA  | CBA-CAA-C2A | 2.03  | 119.84      | 113.79   |
| 15  | aL    | 207 | BCR  | C40-C30-C25 | 2.03  | 113.43      | 110.24   |
| 11  | cB    | 816 | CLA  | CMB-C2B-C1B | 2.03  | 128.51      | 125.42   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 15  | cA    | 849 | BCR  | C24-C23-C22 | -2.03 | 123.23      | 126.23   |
| 11  | bB    | 829 | CLA  | CBA-CAA-C2A | 2.03  | 119.83      | 113.79   |
| 11  | bB    | 823 | CLA  | CAA-C2A-C1A | 2.03  | 118.63      | 111.97   |
| 11  | aB    | 823 | CLA  | CAA-C2A-C1A | 2.03  | 118.62      | 111.97   |
| 12  | cA    | 827 | F6C  | O2A-CGA-O1A | -2.03 | 118.55      | 123.63   |
| 15  | cB    | 844 | BCR  | C24-C23-C22 | -2.03 | 123.23      | 126.23   |
| 11  | bB    | 817 | CLA  | CBC-CAC-C3C | -2.03 | 106.92      | 112.42   |
| 11  | bB    | 813 | CLA  | C4-C3-C5    | 2.03  | 118.75      | 115.23   |
| 11  | bB    | 816 | CLA  | C4-C3-C5    | 2.03  | 118.75      | 115.23   |
| 11  | cA    | 840 | CLA  | CHA-C1A-NA  | -2.03 | 121.80      | 126.39   |
| 15  | aL    | 208 | BCR  | C16-C15-C14 | -2.03 | 119.37      | 123.52   |
| 11  | aB    | 827 | CLA  | CMB-C2B-C1B | 2.03  | 128.51      | 125.42   |
| 11  | cA    | 806 | CLA  | CBA-CAA-C2A | 2.03  | 119.82      | 113.79   |
| 11  | bA    | 817 | CLA  | CHA-C1A-NA  | -2.03 | 121.80      | 126.39   |
| 11  | bA    | 843 | CLA  | CMB-C2B-C1B | 2.03  | 128.50      | 125.42   |
| 11  | bB    | 805 | CLA  | CHA-C1A-NA  | -2.03 | 121.80      | 126.39   |
| 11  | bA    | 816 | CLA  | CMB-C2B-C1B | 2.03  | 128.50      | 125.42   |
| 11  | aA    | 840 | CLA  | CHB-C1B-C2B | -2.03 | 121.55      | 127.43   |
| 11  | cB    | 806 | CLA  | CHA-C1A-NA  | -2.03 | 121.80      | 126.39   |
| 11  | aB    | 813 | CLA  | C4-C3-C5    | 2.03  | 118.74      | 115.23   |
| 11  | bB    | 807 | CLA  | C4-C3-C5    | 2.03  | 118.74      | 115.23   |
| 11  | aA    | 816 | CLA  | O1D-CGD-CBD | -2.03 | 120.52      | 124.52   |
| 11  | cA    | 811 | CLA  | CMB-C2B-C1B | 2.03  | 128.50      | 125.42   |
| 12  | bA    | 830 | F6C  | CAA-CBA-CGA | -2.03 | 107.43      | 113.44   |
| 11  | cA    | 822 | CLA  | O2D-CGD-O1D | -2.03 | 119.91      | 123.85   |
| 15  | aK    | 102 | BCR  | C37-C22-C21 | -2.02 | 119.54      | 122.82   |
| 11  | bA    | 810 | CLA  | CAA-C2A-C3A | -2.02 | 107.53      | 113.00   |
| 11  | cA    | 817 | CLA  | CHA-C1A-NA  | -2.02 | 121.81      | 126.39   |
| 11  | cA    | 840 | CLA  | CHB-C1B-C2B | -2.02 | 121.55      | 127.43   |
| 11  | bB    | 809 | CLA  | CHB-C4A-NA  | 2.02  | 127.32      | 124.40   |
| 11  | bL    | 204 | CLA  | CHB-C4A-NA  | 2.02  | 127.32      | 124.40   |
| 11  | bB    | 830 | CLA  | CMC-C2C-C1C | 2.02  | 128.19      | 125.03   |
| 11  | bA    | 816 | CLA  | O1D-CGD-CBD | -2.02 | 120.53      | 124.52   |
| 11  | bB    | 831 | CLA  | CHA-C1A-NA  | -2.02 | 121.81      | 126.39   |
| 11  | aB    | 831 | CLA  | CHB-C1B-C2B | -2.02 | 121.56      | 127.43   |
| 11  | bA    | 840 | CLA  | CHB-C1B-C2B | -2.02 | 121.56      | 127.43   |
| 12  | cA    | 830 | F6C  | CAA-CBA-CGA | -2.02 | 107.44      | 113.44   |
| 11  | bB    | 809 | CLA  | CMB-C2B-C1B | 2.02  | 128.50      | 125.42   |
| 11  | cA    | 819 | CLA  | CHA-C1A-NA  | -2.02 | 121.81      | 126.39   |
| 15  | cL    | 203 | BCR  | C15-C16-C17 | -2.02 | 119.39      | 123.52   |
| 11  | cB    | 831 | CLA  | CHA-C1A-NA  | -2.02 | 121.82      | 126.39   |
| 11  | aA    | 807 | CLA  | C11-C12-C13 | -2.02 | 109.25      | 115.97   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aA    | 812 | CLA  | CHC-C1C-NC  | 2.02  | 127.35      | 124.31   |
| 15  | bA    | 850 | BCR  | C33-C5-C6   | -2.02 | 122.28      | 124.48   |
| 11  | aB    | 817 | CLA  | CBC-CAC-C3C | -2.02 | 106.95      | 112.42   |
| 11  | aB    | 825 | CLA  | O2A-CGA-O1A | -2.02 | 118.58      | 123.63   |
| 11  | bB    | 825 | CLA  | O2A-CGA-O1A | -2.02 | 118.58      | 123.63   |
| 11  | cB    | 823 | CLA  | CAA-C2A-C1A | 2.02  | 118.59      | 111.97   |
| 15  | cL    | 208 | BCR  | C16-C15-C14 | -2.02 | 119.39      | 123.52   |
| 11  | aA    | 838 | CLA  | CHA-C1A-NA  | -2.02 | 121.82      | 126.39   |
| 11  | cB    | 832 | CLA  | CMC-C2C-C1C | 2.02  | 128.19      | 125.03   |
| 11  | bA    | 815 | CLA  | O1D-CGD-CBD | -2.02 | 120.54      | 124.52   |
| 15  | bL    | 207 | BCR  | C29-C30-C25 | 2.02  | 113.37      | 110.44   |
| 11  | cB    | 829 | CLA  | CBA-CAA-C2A | 2.02  | 119.79      | 113.79   |
| 15  | bL    | 208 | BCR  | C16-C15-C14 | -2.02 | 119.39      | 123.52   |
| 11  | bA    | 819 | CLA  | CHA-C1A-NA  | -2.02 | 121.83      | 126.39   |
| 11  | cA    | 807 | CLA  | C11-C12-C13 | -2.02 | 109.27      | 115.97   |
| 13  | bB    | 841 | PQN  | C11-C3-C4   | 2.02  | 120.70      | 118.58   |
| 15  | cK    | 102 | BCR  | C37-C22-C21 | -2.02 | 119.55      | 122.82   |
| 11  | aA    | 840 | CLA  | CHA-C1A-NA  | -2.01 | 121.83      | 126.39   |
| 11  | bB    | 806 | CLA  | CHA-C1A-NA  | -2.01 | 121.83      | 126.39   |
| 11  | bA    | 811 | CLA  | CMB-C2B-C1B | 2.01  | 128.49      | 125.42   |
| 11  | cA    | 838 | CLA  | CHA-C1A-NA  | -2.01 | 121.83      | 126.39   |
| 15  | aL    | 207 | BCR  | C29-C30-C25 | 2.01  | 113.36      | 110.44   |
| 11  | aB    | 816 | CLA  | CMB-C2B-C1B | 2.01  | 128.49      | 125.42   |
| 11  | aA    | 817 | CLA  | CMB-C2B-C3B | 2.01  | 131.29      | 126.55   |
| 11  | bA    | 836 | CLA  | CHA-C1A-NA  | -2.01 | 121.83      | 126.39   |
| 11  | bA    | 807 | CLA  | O2A-CGA-O1A | -2.01 | 118.59      | 123.63   |
| 11  | bA    | 806 | CLA  | CBA-CAA-C2A | 2.01  | 119.78      | 113.79   |
| 11  | cA    | 819 | CLA  | O2A-CGA-O1A | -2.01 | 118.59      | 123.63   |
| 11  | aA    | 819 | CLA  | O2A-CGA-O1A | -2.01 | 118.60      | 123.63   |
| 11  | aA    | 843 | CLA  | CMA-C3A-C2A | -2.01 | 106.20      | 113.98   |
| 12  | aA    | 830 | F6C  | CAA-CBA-CGA | -2.01 | 107.47      | 113.44   |
| 11  | cL    | 204 | CLA  | CHB-C4A-NA  | 2.01  | 127.30      | 124.40   |
| 11  | cA    | 834 | CLA  | O2D-CGD-O1D | -2.01 | 119.93      | 123.85   |
| 11  | cA    | 815 | CLA  | O1D-CGD-CBD | -2.01 | 120.55      | 124.52   |
| 11  | bA    | 843 | CLA  | CHA-C1A-NA  | -2.01 | 121.84      | 126.39   |
| 11  | cB    | 812 | CLA  | CHA-C1A-NA  | -2.01 | 121.84      | 126.39   |
| 15  | aB    | 844 | BCR  | C24-C23-C22 | -2.01 | 123.26      | 126.23   |
| 15  | aL    | 203 | BCR  | C15-C16-C17 | -2.01 | 119.41      | 123.52   |
| 11  | bA    | 821 | CLA  | CBC-CAC-C3C | -2.01 | 106.97      | 112.42   |
| 11  | cB    | 831 | CLA  | CHB-C1B-C2B | -2.01 | 121.60      | 127.43   |
| 11  | bB    | 830 | CLA  | CHA-C1A-NA  | -2.01 | 121.84      | 126.39   |
| 11  | aL    | 206 | CLA  | CAA-C2A-C1A | -2.01 | 105.39      | 111.97   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | aB    | 830 | CLA  | O2A-CGA-CBA | 2.01  | 117.95      | 111.83   |
| 11  | aA    | 821 | CLA  | CBC-CAC-C3C | -2.01 | 106.98      | 112.42   |
| 11  | cA    | 836 | CLA  | CHA-C1A-NA  | -2.01 | 121.85      | 126.39   |
| 11  | cA    | 821 | CLA  | CBC-CAC-C3C | -2.01 | 106.98      | 112.42   |
| 11  | aA    | 823 | CLA  | O1D-CGD-CBD | -2.01 | 120.56      | 124.52   |
| 11  | bA    | 812 | CLA  | O2D-CGD-O1D | -2.01 | 119.94      | 123.85   |
| 15  | bB    | 844 | BCR  | C24-C23-C22 | -2.00 | 123.27      | 126.23   |
| 11  | bA    | 825 | CLA  | CHA-C1A-NA  | -2.00 | 121.85      | 126.39   |
| 11  | bB    | 816 | CLA  | CMB-C2B-C1B | 2.00  | 128.47      | 125.42   |
| 11  | bA    | 822 | CLA  | O2D-CGD-O1D | -2.00 | 119.95      | 123.85   |
| 11  | aA    | 807 | CLA  | O2A-CGA-O1A | -2.00 | 118.61      | 123.63   |
| 11  | bA    | 843 | CLA  | CMA-C3A-C2A | -2.00 | 106.24      | 113.98   |
| 11  | bA    | 819 | CLA  | O2A-CGA-O1A | -2.00 | 118.62      | 123.63   |
| 11  | aB    | 820 | CLA  | CAA-C2A-C3A | -2.00 | 107.59      | 113.00   |
| 11  | cA    | 811 | CLA  | CHB-C4A-NA  | 2.00  | 127.29      | 124.40   |
| 11  | aA    | 843 | CLA  | CHA-C1A-NA  | -2.00 | 121.86      | 126.39   |
| 11  | aA    | 810 | CLA  | CAA-C2A-C3A | -2.00 | 107.59      | 113.00   |
| 11  | aB    | 830 | CLA  | CMC-C2C-C1C | 2.00  | 128.16      | 125.03   |
| 11  | bB    | 816 | CLA  | CHB-C1B-C2B | -2.00 | 121.61      | 127.43   |
| 11  | bB    | 812 | CLA  | CHA-C1A-NA  | -2.00 | 121.86      | 126.39   |
| 11  | bB    | 832 | CLA  | CMC-C2C-C1C | 2.00  | 128.16      | 125.03   |
| 11  | bA    | 817 | CLA  | CMB-C2B-C3B | 2.00  | 131.25      | 126.55   |

All (273) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 10  | aA    | 801 | CL0  | NC   |
| 10  | aA    | 801 | CL0  | NA   |
| 10  | aA    | 801 | CL0  | ND   |
| 10  | bA    | 801 | CL0  | NC   |
| 10  | bA    | 801 | CL0  | NA   |
| 10  | bA    | 801 | CL0  | ND   |
| 10  | cA    | 801 | CL0  | NC   |
| 10  | cA    | 801 | CL0  | NA   |
| 10  | cA    | 801 | CL0  | ND   |
| 11  | aA    | 802 | CLA  | ND   |
| 11  | aA    | 803 | CLA  | ND   |
| 11  | aA    | 804 | CLA  | ND   |
| 11  | aA    | 805 | CLA  | ND   |
| 11  | aA    | 806 | CLA  | ND   |
| 11  | aA    | 807 | CLA  | ND   |
| 11  | aA    | 808 | CLA  | ND   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 11  | aA    | 809 | CLA  | ND   |
| 11  | aA    | 810 | CLA  | ND   |
| 11  | aA    | 811 | CLA  | ND   |
| 11  | aA    | 812 | CLA  | ND   |
| 11  | aA    | 813 | CLA  | ND   |
| 11  | aA    | 814 | CLA  | ND   |
| 11  | aA    | 815 | CLA  | ND   |
| 11  | aA    | 816 | CLA  | ND   |
| 11  | aA    | 817 | CLA  | ND   |
| 11  | aA    | 818 | CLA  | ND   |
| 11  | aA    | 819 | CLA  | ND   |
| 11  | aA    | 820 | CLA  | ND   |
| 11  | aA    | 821 | CLA  | ND   |
| 11  | aA    | 822 | CLA  | ND   |
| 11  | aA    | 823 | CLA  | ND   |
| 11  | aA    | 824 | CLA  | ND   |
| 11  | aA    | 825 | CLA  | ND   |
| 11  | aA    | 828 | CLA  | ND   |
| 11  | aA    | 829 | CLA  | ND   |
| 11  | aA    | 831 | CLA  | ND   |
| 11  | aA    | 833 | CLA  | ND   |
| 11  | aA    | 834 | CLA  | ND   |
| 11  | aA    | 835 | CLA  | ND   |
| 11  | aA    | 836 | CLA  | ND   |
| 11  | aA    | 837 | CLA  | ND   |
| 11  | aA    | 838 | CLA  | ND   |
| 11  | aA    | 839 | CLA  | ND   |
| 11  | aA    | 840 | CLA  | ND   |
| 11  | aA    | 841 | CLA  | ND   |
| 11  | aA    | 842 | CLA  | ND   |
| 11  | aA    | 843 | CLA  | ND   |
| 11  | aB    | 801 | CLA  | ND   |
| 11  | aB    | 802 | CLA  | ND   |
| 11  | aB    | 803 | CLA  | ND   |
| 11  | aB    | 804 | CLA  | ND   |
| 11  | aB    | 805 | CLA  | ND   |
| 11  | aB    | 806 | CLA  | ND   |
| 11  | aB    | 807 | CLA  | ND   |
| 11  | aB    | 808 | CLA  | ND   |
| 11  | aB    | 809 | CLA  | ND   |
| 11  | aB    | 810 | CLA  | ND   |
| 11  | aB    | 811 | CLA  | ND   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 11  | aB    | 812 | CLA  | ND   |
| 11  | aB    | 813 | CLA  | ND   |
| 11  | aB    | 814 | CLA  | ND   |
| 11  | aB    | 815 | CLA  | ND   |
| 11  | aB    | 816 | CLA  | ND   |
| 11  | aB    | 817 | CLA  | ND   |
| 11  | aB    | 818 | CLA  | ND   |
| 11  | aB    | 819 | CLA  | ND   |
| 11  | aB    | 820 | CLA  | ND   |
| 11  | aB    | 821 | CLA  | ND   |
| 11  | aB    | 823 | CLA  | ND   |
| 11  | aB    | 825 | CLA  | ND   |
| 11  | aB    | 826 | CLA  | ND   |
| 11  | aB    | 827 | CLA  | ND   |
| 11  | aB    | 828 | CLA  | ND   |
| 11  | aB    | 829 | CLA  | ND   |
| 11  | aB    | 830 | CLA  | ND   |
| 11  | aB    | 831 | CLA  | ND   |
| 11  | aB    | 832 | CLA  | ND   |
| 11  | aB    | 833 | CLA  | ND   |
| 11  | aB    | 834 | CLA  | ND   |
| 11  | aB    | 835 | CLA  | ND   |
| 11  | aB    | 836 | CLA  | ND   |
| 11  | aB    | 837 | CLA  | ND   |
| 11  | aB    | 838 | CLA  | ND   |
| 11  | aB    | 839 | CLA  | ND   |
| 11  | aB    | 840 | CLA  | ND   |
| 11  | aK    | 101 | CLA  | ND   |
| 11  | aL    | 204 | CLA  | ND   |
| 11  | aL    | 205 | CLA  | ND   |
| 11  | aL    | 206 | CLA  | ND   |
| 11  | bA    | 802 | CLA  | ND   |
| 11  | bA    | 803 | CLA  | ND   |
| 11  | bA    | 804 | CLA  | ND   |
| 11  | bA    | 805 | CLA  | ND   |
| 11  | bA    | 806 | CLA  | ND   |
| 11  | bA    | 807 | CLA  | ND   |
| 11  | bA    | 808 | CLA  | ND   |
| 11  | bA    | 809 | CLA  | ND   |
| 11  | bA    | 810 | CLA  | ND   |
| 11  | bA    | 811 | CLA  | ND   |
| 11  | bA    | 812 | CLA  | ND   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 11  | bA    | 813 | CLA  | ND   |
| 11  | bA    | 814 | CLA  | ND   |
| 11  | bA    | 815 | CLA  | ND   |
| 11  | bA    | 816 | CLA  | ND   |
| 11  | bA    | 817 | CLA  | ND   |
| 11  | bA    | 818 | CLA  | ND   |
| 11  | bA    | 819 | CLA  | ND   |
| 11  | bA    | 820 | CLA  | ND   |
| 11  | bA    | 821 | CLA  | ND   |
| 11  | bA    | 822 | CLA  | ND   |
| 11  | bA    | 823 | CLA  | ND   |
| 11  | bA    | 824 | CLA  | ND   |
| 11  | bA    | 825 | CLA  | ND   |
| 11  | bA    | 828 | CLA  | ND   |
| 11  | bA    | 829 | CLA  | ND   |
| 11  | bA    | 831 | CLA  | ND   |
| 11  | bA    | 833 | CLA  | ND   |
| 11  | bA    | 834 | CLA  | ND   |
| 11  | bA    | 835 | CLA  | ND   |
| 11  | bA    | 836 | CLA  | ND   |
| 11  | bA    | 837 | CLA  | ND   |
| 11  | bA    | 838 | CLA  | ND   |
| 11  | bA    | 839 | CLA  | ND   |
| 11  | bA    | 840 | CLA  | ND   |
| 11  | bA    | 841 | CLA  | ND   |
| 11  | bA    | 842 | CLA  | ND   |
| 11  | bA    | 843 | CLA  | ND   |
| 11  | bB    | 801 | CLA  | ND   |
| 11  | bB    | 802 | CLA  | ND   |
| 11  | bB    | 803 | CLA  | ND   |
| 11  | bB    | 804 | CLA  | ND   |
| 11  | bB    | 805 | CLA  | ND   |
| 11  | bB    | 806 | CLA  | ND   |
| 11  | bB    | 807 | CLA  | ND   |
| 11  | bB    | 808 | CLA  | ND   |
| 11  | bB    | 809 | CLA  | ND   |
| 11  | bB    | 810 | CLA  | ND   |
| 11  | bB    | 811 | CLA  | ND   |
| 11  | bB    | 812 | CLA  | ND   |
| 11  | bB    | 813 | CLA  | ND   |
| 11  | bB    | 814 | CLA  | ND   |
| 11  | bB    | 815 | CLA  | ND   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 11  | bB    | 816 | CLA  | ND   |
| 11  | bB    | 817 | CLA  | ND   |
| 11  | bB    | 818 | CLA  | ND   |
| 11  | bB    | 819 | CLA  | ND   |
| 11  | bB    | 820 | CLA  | ND   |
| 11  | bB    | 821 | CLA  | ND   |
| 11  | bB    | 823 | CLA  | ND   |
| 11  | bB    | 825 | CLA  | ND   |
| 11  | bB    | 826 | CLA  | ND   |
| 11  | bB    | 827 | CLA  | ND   |
| 11  | bB    | 828 | CLA  | ND   |
| 11  | bB    | 829 | CLA  | ND   |
| 11  | bB    | 830 | CLA  | ND   |
| 11  | bB    | 831 | CLA  | ND   |
| 11  | bB    | 832 | CLA  | ND   |
| 11  | bB    | 833 | CLA  | ND   |
| 11  | bB    | 834 | CLA  | ND   |
| 11  | bB    | 835 | CLA  | ND   |
| 11  | bB    | 836 | CLA  | ND   |
| 11  | bB    | 837 | CLA  | ND   |
| 11  | bB    | 838 | CLA  | ND   |
| 11  | bB    | 839 | CLA  | ND   |
| 11  | bB    | 840 | CLA  | ND   |
| 11  | bK    | 101 | CLA  | ND   |
| 11  | bL    | 204 | CLA  | ND   |
| 11  | bL    | 205 | CLA  | ND   |
| 11  | bL    | 206 | CLA  | ND   |
| 11  | cA    | 802 | CLA  | ND   |
| 11  | cA    | 803 | CLA  | ND   |
| 11  | cA    | 804 | CLA  | ND   |
| 11  | cA    | 805 | CLA  | ND   |
| 11  | cA    | 806 | CLA  | ND   |
| 11  | cA    | 807 | CLA  | ND   |
| 11  | cA    | 808 | CLA  | ND   |
| 11  | cA    | 809 | CLA  | ND   |
| 11  | cA    | 810 | CLA  | ND   |
| 11  | cA    | 811 | CLA  | ND   |
| 11  | cA    | 812 | CLA  | ND   |
| 11  | cA    | 813 | CLA  | ND   |
| 11  | cA    | 814 | CLA  | ND   |
| 11  | cA    | 815 | CLA  | ND   |
| 11  | cA    | 816 | CLA  | ND   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 11  | cA    | 817 | CLA  | ND   |
| 11  | cA    | 818 | CLA  | ND   |
| 11  | cA    | 819 | CLA  | ND   |
| 11  | cA    | 820 | CLA  | ND   |
| 11  | cA    | 821 | CLA  | ND   |
| 11  | cA    | 822 | CLA  | ND   |
| 11  | cA    | 823 | CLA  | ND   |
| 11  | cA    | 824 | CLA  | ND   |
| 11  | cA    | 825 | CLA  | ND   |
| 11  | cA    | 828 | CLA  | ND   |
| 11  | cA    | 829 | CLA  | ND   |
| 11  | cA    | 831 | CLA  | ND   |
| 11  | cA    | 833 | CLA  | ND   |
| 11  | cA    | 834 | CLA  | ND   |
| 11  | cA    | 835 | CLA  | ND   |
| 11  | cA    | 836 | CLA  | ND   |
| 11  | cA    | 837 | CLA  | ND   |
| 11  | cA    | 838 | CLA  | ND   |
| 11  | cA    | 839 | CLA  | ND   |
| 11  | cA    | 840 | CLA  | ND   |
| 11  | cA    | 841 | CLA  | ND   |
| 11  | cA    | 842 | CLA  | ND   |
| 11  | cA    | 843 | CLA  | ND   |
| 11  | cB    | 801 | CLA  | ND   |
| 11  | cB    | 802 | CLA  | ND   |
| 11  | cB    | 803 | CLA  | ND   |
| 11  | cB    | 804 | CLA  | ND   |
| 11  | cB    | 805 | CLA  | ND   |
| 11  | cB    | 806 | CLA  | ND   |
| 11  | cB    | 807 | CLA  | ND   |
| 11  | cB    | 808 | CLA  | ND   |
| 11  | cB    | 809 | CLA  | ND   |
| 11  | cB    | 810 | CLA  | ND   |
| 11  | cB    | 811 | CLA  | ND   |
| 11  | cB    | 812 | CLA  | ND   |
| 11  | cB    | 813 | CLA  | ND   |
| 11  | cB    | 814 | CLA  | ND   |
| 11  | cB    | 815 | CLA  | ND   |
| 11  | cB    | 816 | CLA  | ND   |
| 11  | cB    | 817 | CLA  | ND   |
| 11  | cB    | 818 | CLA  | ND   |
| 11  | cB    | 819 | CLA  | ND   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 11  | cB    | 820 | CLA  | ND   |
| 11  | cB    | 821 | CLA  | ND   |
| 11  | cB    | 823 | CLA  | ND   |
| 11  | cB    | 825 | CLA  | ND   |
| 11  | cB    | 826 | CLA  | ND   |
| 11  | cB    | 827 | CLA  | ND   |
| 11  | cB    | 828 | CLA  | ND   |
| 11  | cB    | 829 | CLA  | ND   |
| 11  | cB    | 830 | CLA  | ND   |
| 11  | cB    | 831 | CLA  | ND   |
| 11  | cB    | 832 | CLA  | ND   |
| 11  | cB    | 833 | CLA  | ND   |
| 11  | cB    | 834 | CLA  | ND   |
| 11  | cB    | 835 | CLA  | ND   |
| 11  | cB    | 836 | CLA  | ND   |
| 11  | cB    | 837 | CLA  | ND   |
| 11  | cB    | 838 | CLA  | ND   |
| 11  | cB    | 839 | CLA  | ND   |
| 11  | cB    | 840 | CLA  | ND   |
| 11  | cK    | 101 | CLA  | ND   |
| 11  | cL    | 204 | CLA  | ND   |
| 11  | cL    | 205 | CLA  | ND   |
| 11  | cL    | 206 | CLA  | ND   |
| 12  | aA    | 826 | F6C  | NA   |
| 12  | aA    | 827 | F6C  | C8   |
| 12  | aA    | 827 | F6C  | NA   |
| 12  | aA    | 830 | F6C  | NA   |
| 12  | aA    | 832 | F6C  | NA   |
| 12  | aA    | 844 | F6C  | NA   |
| 12  | aB    | 824 | F6C  | NA   |
| 12  | aL    | 202 | F6C  | NA   |
| 12  | bA    | 826 | F6C  | NA   |
| 12  | bA    | 827 | F6C  | C8   |
| 12  | bA    | 827 | F6C  | NA   |
| 12  | bA    | 830 | F6C  | NA   |
| 12  | bA    | 832 | F6C  | NA   |
| 12  | bA    | 844 | F6C  | NA   |
| 12  | bB    | 824 | F6C  | NA   |
| 12  | bL    | 202 | F6C  | NA   |
| 12  | cA    | 826 | F6C  | NA   |
| 12  | cA    | 827 | F6C  | C8   |
| 12  | cA    | 827 | F6C  | NA   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 12  | cA    | 830 | F6C  | NA   |
| 12  | cA    | 832 | F6C  | NA   |
| 12  | cA    | 844 | F6C  | NA   |
| 12  | cB    | 824 | F6C  | NA   |
| 12  | cL    | 202 | F6C  | NA   |

All (3142) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | aA    | 804 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aA    | 804 | CLA  | CHA-CBD-CGD-O1D |
| 11  | aA    | 804 | CLA  | CHA-CBD-CGD-O2D |
| 11  | aA    | 804 | CLA  | CBD-CGD-O2D-CED |
| 11  | aA    | 805 | CLA  | CAD-CBD-CGD-O2D |
| 11  | aA    | 806 | CLA  | C1A-C2A-CAA-CBA |
| 11  | aA    | 806 | CLA  | C3A-C2A-CAA-CBA |
| 11  | aA    | 806 | CLA  | CAD-CBD-CGD-O2D |
| 11  | aA    | 807 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aA    | 807 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aA    | 809 | CLA  | C3A-C2A-CAA-CBA |
| 11  | aA    | 809 | CLA  | CHA-CBD-CGD-O1D |
| 11  | aA    | 809 | CLA  | CHA-CBD-CGD-O2D |
| 11  | aA    | 812 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aA    | 818 | CLA  | CHA-CBD-CGD-O1D |
| 11  | aA    | 818 | CLA  | CHA-CBD-CGD-O2D |
| 11  | aA    | 819 | CLA  | C3A-C2A-CAA-CBA |
| 11  | aA    | 820 | CLA  | C1A-C2A-CAA-CBA |
| 11  | aA    | 820 | CLA  | C3A-C2A-CAA-CBA |
| 11  | aA    | 820 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aA    | 821 | CLA  | C1A-C2A-CAA-CBA |
| 11  | aA    | 823 | CLA  | C1A-C2A-CAA-CBA |
| 11  | aA    | 823 | CLA  | C3A-C2A-CAA-CBA |
| 11  | aA    | 823 | CLA  | CHA-CBD-CGD-O1D |
| 11  | aA    | 823 | CLA  | CHA-CBD-CGD-O2D |
| 11  | aA    | 824 | CLA  | O1A-CGA-O2A-C1  |
| 11  | aA    | 824 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aA    | 824 | CLA  | C2-C3-C5-C6     |
| 11  | aA    | 824 | CLA  | C4-C3-C5-C6     |
| 11  | aA    | 825 | CLA  | CBD-CGD-O2D-CED |
| 11  | aA    | 834 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aA    | 834 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aA    | 837 | CLA  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | aA    | 840 | CLA  | C1A-C2A-CAA-CBA |
| 11  | aA    | 842 | CLA  | CBD-CGD-O2D-CED |
| 11  | aB    | 801 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aB    | 802 | CLA  | C1A-C2A-CAA-CBA |
| 11  | aB    | 802 | CLA  | C3A-C2A-CAA-CBA |
| 11  | aB    | 804 | CLA  | C1A-C2A-CAA-CBA |
| 11  | aB    | 804 | CLA  | C3A-C2A-CAA-CBA |
| 11  | aB    | 805 | CLA  | C1A-C2A-CAA-CBA |
| 11  | aB    | 805 | CLA  | C3A-C2A-CAA-CBA |
| 11  | aB    | 805 | CLA  | CAD-CBD-CGD-O2D |
| 11  | aB    | 806 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aB    | 806 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aB    | 806 | CLA  | C11-C10-C8-C7   |
| 11  | aB    | 807 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aB    | 808 | CLA  | CHA-CBD-CGD-O2D |
| 11  | aB    | 809 | CLA  | C1A-C2A-CAA-CBA |
| 11  | aB    | 812 | CLA  | C1A-C2A-CAA-CBA |
| 11  | aB    | 812 | CLA  | C3A-C2A-CAA-CBA |
| 11  | aB    | 815 | CLA  | CBD-CGD-O2D-CED |
| 11  | aB    | 817 | CLA  | C1A-C2A-CAA-CBA |
| 11  | aB    | 818 | CLA  | CBD-CGD-O2D-CED |
| 11  | aB    | 819 | CLA  | C3A-C2A-CAA-CBA |
| 11  | aB    | 819 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aB    | 819 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aB    | 819 | CLA  | CHA-CBD-CGD-O2D |
| 11  | aB    | 820 | CLA  | CHA-CBD-CGD-O1D |
| 11  | aB    | 820 | CLA  | CHA-CBD-CGD-O2D |
| 11  | aB    | 822 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aB    | 822 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aB    | 823 | CLA  | CHA-CBD-CGD-O1D |
| 11  | aB    | 823 | CLA  | CHA-CBD-CGD-O2D |
| 11  | aB    | 826 | CLA  | C1A-C2A-CAA-CBA |
| 11  | aB    | 827 | CLA  | C1A-C2A-CAA-CBA |
| 11  | aB    | 827 | CLA  | C3A-C2A-CAA-CBA |
| 11  | aB    | 829 | CLA  | C3A-C2A-CAA-CBA |
| 11  | aB    | 829 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aB    | 829 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aB    | 832 | CLA  | C1A-C2A-CAA-CBA |
| 11  | aB    | 832 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aB    | 832 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aB    | 832 | CLA  | CBD-CGD-O2D-CED |
| 11  | aB    | 836 | CLA  | C2-C3-C5-C6     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | aL    | 205 | CLA  | C1A-C2A-CAA-CBA |
| 11  | aL    | 205 | CLA  | C3A-C2A-CAA-CBA |
| 11  | aL    | 205 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aL    | 205 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aL    | 205 | CLA  | C6-C7-C8-C9     |
| 11  | bA    | 804 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bA    | 804 | CLA  | CHA-CBD-CGD-O1D |
| 11  | bA    | 804 | CLA  | CHA-CBD-CGD-O2D |
| 11  | bA    | 804 | CLA  | CBD-CGD-O2D-CED |
| 11  | bA    | 805 | CLA  | CAD-CBD-CGD-O2D |
| 11  | bA    | 806 | CLA  | C1A-C2A-CAA-CBA |
| 11  | bA    | 806 | CLA  | C3A-C2A-CAA-CBA |
| 11  | bA    | 806 | CLA  | CAD-CBD-CGD-O2D |
| 11  | bA    | 807 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bA    | 807 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bA    | 809 | CLA  | C3A-C2A-CAA-CBA |
| 11  | bA    | 809 | CLA  | CHA-CBD-CGD-O1D |
| 11  | bA    | 809 | CLA  | CHA-CBD-CGD-O2D |
| 11  | bA    | 812 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bA    | 818 | CLA  | CHA-CBD-CGD-O1D |
| 11  | bA    | 818 | CLA  | CHA-CBD-CGD-O2D |
| 11  | bA    | 819 | CLA  | C3A-C2A-CAA-CBA |
| 11  | bA    | 820 | CLA  | C1A-C2A-CAA-CBA |
| 11  | bA    | 820 | CLA  | C3A-C2A-CAA-CBA |
| 11  | bA    | 820 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bA    | 821 | CLA  | C1A-C2A-CAA-CBA |
| 11  | bA    | 823 | CLA  | C1A-C2A-CAA-CBA |
| 11  | bA    | 823 | CLA  | C3A-C2A-CAA-CBA |
| 11  | bA    | 823 | CLA  | CHA-CBD-CGD-O1D |
| 11  | bA    | 823 | CLA  | CHA-CBD-CGD-O2D |
| 11  | bA    | 824 | CLA  | O1A-CGA-O2A-C1  |
| 11  | bA    | 824 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bA    | 824 | CLA  | C2-C3-C5-C6     |
| 11  | bA    | 824 | CLA  | C4-C3-C5-C6     |
| 11  | bA    | 825 | CLA  | CBD-CGD-O2D-CED |
| 11  | bA    | 834 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bA    | 834 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bA    | 837 | CLA  | C1A-C2A-CAA-CBA |
| 11  | bA    | 840 | CLA  | C1A-C2A-CAA-CBA |
| 11  | bA    | 842 | CLA  | CBD-CGD-O2D-CED |
| 11  | bB    | 801 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bB    | 802 | CLA  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | bB    | 802 | CLA  | C3A-C2A-CAA-CBA |
| 11  | bB    | 804 | CLA  | C1A-C2A-CAA-CBA |
| 11  | bB    | 804 | CLA  | C3A-C2A-CAA-CBA |
| 11  | bB    | 805 | CLA  | C1A-C2A-CAA-CBA |
| 11  | bB    | 805 | CLA  | C3A-C2A-CAA-CBA |
| 11  | bB    | 805 | CLA  | CAD-CBD-CGD-O2D |
| 11  | bB    | 806 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bB    | 806 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bB    | 806 | CLA  | C11-C10-C8-C7   |
| 11  | bB    | 807 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bB    | 808 | CLA  | CHA-CBD-CGD-O2D |
| 11  | bB    | 809 | CLA  | C1A-C2A-CAA-CBA |
| 11  | bB    | 812 | CLA  | C1A-C2A-CAA-CBA |
| 11  | bB    | 812 | CLA  | C3A-C2A-CAA-CBA |
| 11  | bB    | 815 | CLA  | CBD-CGD-O2D-CED |
| 11  | bB    | 817 | CLA  | C1A-C2A-CAA-CBA |
| 11  | bB    | 818 | CLA  | CBD-CGD-O2D-CED |
| 11  | bB    | 819 | CLA  | C3A-C2A-CAA-CBA |
| 11  | bB    | 819 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bB    | 819 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bB    | 819 | CLA  | CHA-CBD-CGD-O2D |
| 11  | bB    | 820 | CLA  | CHA-CBD-CGD-O1D |
| 11  | bB    | 820 | CLA  | CHA-CBD-CGD-O2D |
| 11  | bB    | 822 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bB    | 822 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bB    | 823 | CLA  | CHA-CBD-CGD-O1D |
| 11  | bB    | 823 | CLA  | CHA-CBD-CGD-O2D |
| 11  | bB    | 826 | CLA  | C1A-C2A-CAA-CBA |
| 11  | bB    | 827 | CLA  | C1A-C2A-CAA-CBA |
| 11  | bB    | 827 | CLA  | C3A-C2A-CAA-CBA |
| 11  | bB    | 829 | CLA  | C3A-C2A-CAA-CBA |
| 11  | bB    | 829 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bB    | 829 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bB    | 832 | CLA  | C1A-C2A-CAA-CBA |
| 11  | bB    | 832 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bB    | 832 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bB    | 832 | CLA  | CBD-CGD-O2D-CED |
| 11  | bB    | 836 | CLA  | C2-C3-C5-C6     |
| 11  | bL    | 205 | CLA  | C1A-C2A-CAA-CBA |
| 11  | bL    | 205 | CLA  | C3A-C2A-CAA-CBA |
| 11  | bL    | 205 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bL    | 205 | CLA  | C4B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | bL    | 205 | CLA  | C6-C7-C8-C9     |
| 11  | cA    | 804 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cA    | 804 | CLA  | CHA-CBD-CGD-O1D |
| 11  | cA    | 804 | CLA  | CHA-CBD-CGD-O2D |
| 11  | cA    | 804 | CLA  | CBD-CGD-O2D-CED |
| 11  | cA    | 805 | CLA  | CAD-CBD-CGD-O2D |
| 11  | cA    | 806 | CLA  | C1A-C2A-CAA-CBA |
| 11  | cA    | 806 | CLA  | C3A-C2A-CAA-CBA |
| 11  | cA    | 806 | CLA  | CAD-CBD-CGD-O2D |
| 11  | cA    | 807 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cA    | 807 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cA    | 809 | CLA  | C3A-C2A-CAA-CBA |
| 11  | cA    | 809 | CLA  | CHA-CBD-CGD-O1D |
| 11  | cA    | 809 | CLA  | CHA-CBD-CGD-O2D |
| 11  | cA    | 812 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cA    | 818 | CLA  | CHA-CBD-CGD-O1D |
| 11  | cA    | 818 | CLA  | CHA-CBD-CGD-O2D |
| 11  | cA    | 819 | CLA  | C3A-C2A-CAA-CBA |
| 11  | cA    | 820 | CLA  | C1A-C2A-CAA-CBA |
| 11  | cA    | 820 | CLA  | C3A-C2A-CAA-CBA |
| 11  | cA    | 820 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cA    | 821 | CLA  | C1A-C2A-CAA-CBA |
| 11  | cA    | 823 | CLA  | C1A-C2A-CAA-CBA |
| 11  | cA    | 823 | CLA  | C3A-C2A-CAA-CBA |
| 11  | cA    | 823 | CLA  | CHA-CBD-CGD-O1D |
| 11  | cA    | 823 | CLA  | CHA-CBD-CGD-O2D |
| 11  | cA    | 824 | CLA  | O1A-CGA-O2A-C1  |
| 11  | cA    | 824 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cA    | 824 | CLA  | C2-C3-C5-C6     |
| 11  | cA    | 824 | CLA  | C4-C3-C5-C6     |
| 11  | cA    | 825 | CLA  | CBD-CGD-O2D-CED |
| 11  | cA    | 834 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cA    | 834 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cA    | 837 | CLA  | C1A-C2A-CAA-CBA |
| 11  | cA    | 840 | CLA  | C1A-C2A-CAA-CBA |
| 11  | cA    | 842 | CLA  | CBD-CGD-O2D-CED |
| 11  | cB    | 801 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cB    | 802 | CLA  | C1A-C2A-CAA-CBA |
| 11  | cB    | 802 | CLA  | C3A-C2A-CAA-CBA |
| 11  | cB    | 804 | CLA  | C1A-C2A-CAA-CBA |
| 11  | cB    | 804 | CLA  | C3A-C2A-CAA-CBA |
| 11  | cB    | 805 | CLA  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | cB    | 805 | CLA  | C3A-C2A-CAA-CBA |
| 11  | cB    | 805 | CLA  | CAD-CBD-CGD-O2D |
| 11  | cB    | 806 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cB    | 806 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cB    | 806 | CLA  | C11-C10-C8-C7   |
| 11  | cB    | 807 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cB    | 808 | CLA  | CHA-CBD-CGD-O2D |
| 11  | cB    | 809 | CLA  | C1A-C2A-CAA-CBA |
| 11  | cB    | 812 | CLA  | C1A-C2A-CAA-CBA |
| 11  | cB    | 812 | CLA  | C3A-C2A-CAA-CBA |
| 11  | cB    | 815 | CLA  | CBD-CGD-O2D-CED |
| 11  | cB    | 817 | CLA  | C1A-C2A-CAA-CBA |
| 11  | cB    | 818 | CLA  | CBD-CGD-O2D-CED |
| 11  | cB    | 819 | CLA  | C3A-C2A-CAA-CBA |
| 11  | cB    | 819 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cB    | 819 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cB    | 819 | CLA  | CHA-CBD-CGD-O2D |
| 11  | cB    | 820 | CLA  | CHA-CBD-CGD-O1D |
| 11  | cB    | 820 | CLA  | CHA-CBD-CGD-O2D |
| 11  | cB    | 822 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cB    | 822 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cB    | 823 | CLA  | CHA-CBD-CGD-O1D |
| 11  | cB    | 823 | CLA  | CHA-CBD-CGD-O2D |
| 11  | cB    | 826 | CLA  | C1A-C2A-CAA-CBA |
| 11  | cB    | 827 | CLA  | C1A-C2A-CAA-CBA |
| 11  | cB    | 827 | CLA  | C3A-C2A-CAA-CBA |
| 11  | cB    | 829 | CLA  | C3A-C2A-CAA-CBA |
| 11  | cB    | 829 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cB    | 829 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cB    | 832 | CLA  | C1A-C2A-CAA-CBA |
| 11  | cB    | 832 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cB    | 832 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cB    | 832 | CLA  | CBD-CGD-O2D-CED |
| 11  | cB    | 836 | CLA  | C2-C3-C5-C6     |
| 11  | cL    | 205 | CLA  | C1A-C2A-CAA-CBA |
| 11  | cL    | 205 | CLA  | C3A-C2A-CAA-CBA |
| 11  | cL    | 205 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cL    | 205 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cL    | 205 | CLA  | C6-C7-C8-C9     |
| 12  | aA    | 826 | F6C  | C2C-C3C-CAC-CBC |
| 12  | aA    | 826 | F6C  | CHA-CBD-CGD-O1D |
| 12  | aA    | 826 | F6C  | CHA-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 12  | aA    | 830 | F6C  | C3A-C2A-CAA-CBA |
| 12  | aA    | 832 | F6C  | C3B-C2B-CMB-OMB |
| 12  | aA    | 844 | F6C  | C2A-CAA-CBA-CGA |
| 12  | aB    | 824 | F6C  | C1A-C2A-CAA-CBA |
| 12  | aB    | 824 | F6C  | C3A-C2A-CAA-CBA |
| 12  | aB    | 824 | F6C  | CHA-CBD-CGD-O1D |
| 12  | aB    | 824 | F6C  | CHA-CBD-CGD-O2D |
| 12  | aB    | 824 | F6C  | C1B-C2B-CMB-OMB |
| 12  | aB    | 824 | F6C  | C3B-C2B-CMB-OMB |
| 12  | aL    | 202 | F6C  | C3B-C2B-CMB-OMB |
| 12  | bA    | 826 | F6C  | C2C-C3C-CAC-CBC |
| 12  | bA    | 826 | F6C  | CHA-CBD-CGD-O1D |
| 12  | bA    | 826 | F6C  | CHA-CBD-CGD-O2D |
| 12  | bA    | 830 | F6C  | C3A-C2A-CAA-CBA |
| 12  | bA    | 832 | F6C  | C3B-C2B-CMB-OMB |
| 12  | bA    | 844 | F6C  | C2A-CAA-CBA-CGA |
| 12  | bB    | 824 | F6C  | C1A-C2A-CAA-CBA |
| 12  | bB    | 824 | F6C  | C3A-C2A-CAA-CBA |
| 12  | bB    | 824 | F6C  | CHA-CBD-CGD-O1D |
| 12  | bB    | 824 | F6C  | CHA-CBD-CGD-O2D |
| 12  | bB    | 824 | F6C  | C1B-C2B-CMB-OMB |
| 12  | bB    | 824 | F6C  | C3B-C2B-CMB-OMB |
| 12  | bL    | 202 | F6C  | C3B-C2B-CMB-OMB |
| 12  | cA    | 826 | F6C  | C2C-C3C-CAC-CBC |
| 12  | cA    | 826 | F6C  | CHA-CBD-CGD-O1D |
| 12  | cA    | 826 | F6C  | CHA-CBD-CGD-O2D |
| 12  | cA    | 830 | F6C  | C3A-C2A-CAA-CBA |
| 12  | cA    | 832 | F6C  | C3B-C2B-CMB-OMB |
| 12  | cA    | 844 | F6C  | C2A-CAA-CBA-CGA |
| 12  | cB    | 824 | F6C  | C1A-C2A-CAA-CBA |
| 12  | cB    | 824 | F6C  | C3A-C2A-CAA-CBA |
| 12  | cB    | 824 | F6C  | CHA-CBD-CGD-O1D |
| 12  | cB    | 824 | F6C  | CHA-CBD-CGD-O2D |
| 12  | cB    | 824 | F6C  | C1B-C2B-CMB-OMB |
| 12  | cB    | 824 | F6C  | C3B-C2B-CMB-OMB |
| 12  | cL    | 202 | F6C  | C3B-C2B-CMB-OMB |
| 15  | aA    | 847 | BCR  | C37-C22-C23-C24 |
| 15  | aA    | 848 | BCR  | C6-C7-C8-C9     |
| 15  | aA    | 848 | BCR  | C7-C8-C9-C34    |
| 15  | aA    | 848 | BCR  | C20-C21-C22-C23 |
| 15  | aA    | 848 | BCR  | C20-C21-C22-C37 |
| 15  | aA    | 848 | BCR  | C37-C22-C23-C24 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 15  | aA    | 849 | BCR  | C7-C8-C9-C34    |
| 15  | aA    | 849 | BCR  | C20-C21-C22-C37 |
| 15  | aA    | 849 | BCR  | C21-C22-C23-C24 |
| 15  | aA    | 849 | BCR  | C22-C23-C24-C25 |
| 15  | aA    | 850 | BCR  | C22-C23-C24-C25 |
| 15  | aA    | 851 | BCR  | C6-C7-C8-C9     |
| 15  | aA    | 851 | BCR  | C18-C19-C20-C21 |
| 15  | aA    | 851 | BCR  | C20-C21-C22-C23 |
| 15  | aA    | 851 | BCR  | C20-C21-C22-C37 |
| 15  | aA    | 851 | BCR  | C21-C22-C23-C24 |
| 15  | aA    | 851 | BCR  | C22-C23-C24-C25 |
| 15  | aB    | 842 | BCR  | C6-C7-C8-C9     |
| 15  | aB    | 842 | BCR  | C7-C8-C9-C10    |
| 15  | aB    | 842 | BCR  | C37-C22-C23-C24 |
| 15  | aB    | 843 | BCR  | C7-C8-C9-C10    |
| 15  | aB    | 843 | BCR  | C7-C8-C9-C34    |
| 15  | aB    | 843 | BCR  | C21-C22-C23-C24 |
| 15  | aB    | 843 | BCR  | C37-C22-C23-C24 |
| 15  | aB    | 845 | BCR  | C6-C7-C8-C9     |
| 15  | aB    | 845 | BCR  | C10-C11-C12-C13 |
| 15  | aB    | 845 | BCR  | C18-C19-C20-C21 |
| 15  | aB    | 846 | BCR  | C7-C8-C9-C10    |
| 15  | aB    | 846 | BCR  | C18-C19-C20-C21 |
| 15  | aB    | 846 | BCR  | C20-C21-C22-C23 |
| 15  | aB    | 846 | BCR  | C20-C21-C22-C37 |
| 15  | aB    | 848 | BCR  | C7-C8-C9-C34    |
| 15  | aB    | 848 | BCR  | C16-C17-C18-C19 |
| 15  | aB    | 848 | BCR  | C16-C17-C18-C36 |
| 15  | aB    | 848 | BCR  | C20-C21-C22-C23 |
| 15  | aB    | 848 | BCR  | C20-C21-C22-C37 |
| 15  | aB    | 848 | BCR  | C37-C22-C23-C24 |
| 15  | aB    | 848 | BCR  | C22-C23-C24-C25 |
| 15  | aB    | 848 | BCR  | C23-C24-C25-C26 |
| 15  | aB    | 848 | BCR  | C23-C24-C25-C30 |
| 15  | aI    | 101 | BCR  | C7-C8-C9-C10    |
| 15  | aI    | 101 | BCR  | C7-C8-C9-C34    |
| 15  | aI    | 101 | BCR  | C20-C21-C22-C23 |
| 15  | aI    | 101 | BCR  | C21-C22-C23-C24 |
| 15  | aI    | 101 | BCR  | C37-C22-C23-C24 |
| 15  | aK    | 102 | BCR  | C7-C8-C9-C10    |
| 15  | aK    | 102 | BCR  | C7-C8-C9-C34    |
| 15  | aK    | 102 | BCR  | C21-C22-C23-C24 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 15  | aK    | 102 | BCR  | C37-C22-C23-C24 |
| 15  | aM    | 101 | BCR  | C22-C23-C24-C25 |
| 15  | bA    | 847 | BCR  | C37-C22-C23-C24 |
| 15  | bA    | 848 | BCR  | C6-C7-C8-C9     |
| 15  | bA    | 848 | BCR  | C7-C8-C9-C34    |
| 15  | bA    | 848 | BCR  | C20-C21-C22-C23 |
| 15  | bA    | 848 | BCR  | C20-C21-C22-C37 |
| 15  | bA    | 848 | BCR  | C37-C22-C23-C24 |
| 15  | bA    | 849 | BCR  | C7-C8-C9-C34    |
| 15  | bA    | 849 | BCR  | C20-C21-C22-C37 |
| 15  | bA    | 849 | BCR  | C21-C22-C23-C24 |
| 15  | bA    | 849 | BCR  | C22-C23-C24-C25 |
| 15  | bA    | 850 | BCR  | C22-C23-C24-C25 |
| 15  | bA    | 851 | BCR  | C6-C7-C8-C9     |
| 15  | bA    | 851 | BCR  | C18-C19-C20-C21 |
| 15  | bA    | 851 | BCR  | C20-C21-C22-C23 |
| 15  | bA    | 851 | BCR  | C20-C21-C22-C37 |
| 15  | bA    | 851 | BCR  | C21-C22-C23-C24 |
| 15  | bA    | 851 | BCR  | C22-C23-C24-C25 |
| 15  | bB    | 842 | BCR  | C6-C7-C8-C9     |
| 15  | bB    | 842 | BCR  | C7-C8-C9-C10    |
| 15  | bB    | 842 | BCR  | C37-C22-C23-C24 |
| 15  | bB    | 843 | BCR  | C7-C8-C9-C10    |
| 15  | bB    | 843 | BCR  | C7-C8-C9-C34    |
| 15  | bB    | 843 | BCR  | C21-C22-C23-C24 |
| 15  | bB    | 843 | BCR  | C37-C22-C23-C24 |
| 15  | bB    | 845 | BCR  | C6-C7-C8-C9     |
| 15  | bB    | 845 | BCR  | C10-C11-C12-C13 |
| 15  | bB    | 845 | BCR  | C18-C19-C20-C21 |
| 15  | bB    | 846 | BCR  | C7-C8-C9-C10    |
| 15  | bB    | 846 | BCR  | C18-C19-C20-C21 |
| 15  | bB    | 846 | BCR  | C20-C21-C22-C23 |
| 15  | bB    | 846 | BCR  | C20-C21-C22-C37 |
| 15  | bB    | 848 | BCR  | C7-C8-C9-C34    |
| 15  | bB    | 848 | BCR  | C16-C17-C18-C19 |
| 15  | bB    | 848 | BCR  | C16-C17-C18-C36 |
| 15  | bB    | 848 | BCR  | C20-C21-C22-C23 |
| 15  | bB    | 848 | BCR  | C20-C21-C22-C37 |
| 15  | bB    | 848 | BCR  | C37-C22-C23-C24 |
| 15  | bB    | 848 | BCR  | C22-C23-C24-C25 |
| 15  | bB    | 848 | BCR  | C23-C24-C25-C26 |
| 15  | bB    | 848 | BCR  | C23-C24-C25-C30 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 15  | bI    | 101 | BCR  | C7-C8-C9-C10    |
| 15  | bI    | 101 | BCR  | C7-C8-C9-C34    |
| 15  | bI    | 101 | BCR  | C20-C21-C22-C23 |
| 15  | bI    | 101 | BCR  | C21-C22-C23-C24 |
| 15  | bI    | 101 | BCR  | C37-C22-C23-C24 |
| 15  | bK    | 102 | BCR  | C7-C8-C9-C10    |
| 15  | bK    | 102 | BCR  | C7-C8-C9-C34    |
| 15  | bK    | 102 | BCR  | C21-C22-C23-C24 |
| 15  | bK    | 102 | BCR  | C37-C22-C23-C24 |
| 15  | bM    | 101 | BCR  | C22-C23-C24-C25 |
| 15  | cA    | 847 | BCR  | C37-C22-C23-C24 |
| 15  | cA    | 848 | BCR  | C6-C7-C8-C9     |
| 15  | cA    | 848 | BCR  | C7-C8-C9-C34    |
| 15  | cA    | 848 | BCR  | C20-C21-C22-C23 |
| 15  | cA    | 848 | BCR  | C20-C21-C22-C37 |
| 15  | cA    | 848 | BCR  | C37-C22-C23-C24 |
| 15  | cA    | 849 | BCR  | C7-C8-C9-C34    |
| 15  | cA    | 849 | BCR  | C20-C21-C22-C37 |
| 15  | cA    | 849 | BCR  | C21-C22-C23-C24 |
| 15  | cA    | 849 | BCR  | C22-C23-C24-C25 |
| 15  | cA    | 850 | BCR  | C22-C23-C24-C25 |
| 15  | cA    | 851 | BCR  | C6-C7-C8-C9     |
| 15  | cA    | 851 | BCR  | C18-C19-C20-C21 |
| 15  | cA    | 851 | BCR  | C20-C21-C22-C23 |
| 15  | cA    | 851 | BCR  | C20-C21-C22-C37 |
| 15  | cA    | 851 | BCR  | C21-C22-C23-C24 |
| 15  | cA    | 851 | BCR  | C22-C23-C24-C25 |
| 15  | cB    | 842 | BCR  | C6-C7-C8-C9     |
| 15  | cB    | 842 | BCR  | C7-C8-C9-C10    |
| 15  | cB    | 842 | BCR  | C37-C22-C23-C24 |
| 15  | cB    | 843 | BCR  | C7-C8-C9-C10    |
| 15  | cB    | 843 | BCR  | C7-C8-C9-C34    |
| 15  | cB    | 843 | BCR  | C21-C22-C23-C24 |
| 15  | cB    | 843 | BCR  | C37-C22-C23-C24 |
| 15  | cB    | 845 | BCR  | C6-C7-C8-C9     |
| 15  | cB    | 845 | BCR  | C10-C11-C12-C13 |
| 15  | cB    | 845 | BCR  | C18-C19-C20-C21 |
| 15  | cB    | 846 | BCR  | C7-C8-C9-C10    |
| 15  | cB    | 846 | BCR  | C18-C19-C20-C21 |
| 15  | cB    | 846 | BCR  | C20-C21-C22-C23 |
| 15  | cB    | 846 | BCR  | C20-C21-C22-C37 |
| 15  | cB    | 848 | BCR  | C7-C8-C9-C34    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 15  | cB    | 848 | BCR  | C16-C17-C18-C19 |
| 15  | cB    | 848 | BCR  | C16-C17-C18-C36 |
| 15  | cB    | 848 | BCR  | C20-C21-C22-C23 |
| 15  | cB    | 848 | BCR  | C20-C21-C22-C37 |
| 15  | cB    | 848 | BCR  | C37-C22-C23-C24 |
| 15  | cB    | 848 | BCR  | C22-C23-C24-C25 |
| 15  | cB    | 848 | BCR  | C23-C24-C25-C26 |
| 15  | cB    | 848 | BCR  | C23-C24-C25-C30 |
| 15  | cI    | 103 | BCR  | C7-C8-C9-C10    |
| 15  | cI    | 103 | BCR  | C7-C8-C9-C34    |
| 15  | cI    | 103 | BCR  | C20-C21-C22-C23 |
| 15  | cI    | 103 | BCR  | C21-C22-C23-C24 |
| 15  | cI    | 103 | BCR  | C37-C22-C23-C24 |
| 15  | cK    | 102 | BCR  | C7-C8-C9-C10    |
| 15  | cK    | 102 | BCR  | C7-C8-C9-C34    |
| 15  | cK    | 102 | BCR  | C21-C22-C23-C24 |
| 15  | cK    | 102 | BCR  | C37-C22-C23-C24 |
| 15  | cM    | 101 | BCR  | C22-C23-C24-C25 |
| 16  | aA    | 852 | LHG  | C3-O3-P-O4      |
| 16  | aA    | 852 | LHG  | C3-O3-P-O6      |
| 16  | bA    | 852 | LHG  | C3-O3-P-O4      |
| 16  | bA    | 852 | LHG  | C3-O3-P-O6      |
| 16  | cA    | 852 | LHG  | C3-O3-P-O4      |
| 16  | cA    | 852 | LHG  | C3-O3-P-O6      |
| 11  | aA    | 810 | CLA  | CBD-CGD-O2D-CED |
| 11  | aA    | 817 | CLA  | CBD-CGD-O2D-CED |
| 11  | aA    | 818 | CLA  | CBD-CGD-O2D-CED |
| 11  | aA    | 822 | CLA  | CBD-CGD-O2D-CED |
| 11  | aA    | 824 | CLA  | CBD-CGD-O2D-CED |
| 11  | aA    | 836 | CLA  | CBD-CGD-O2D-CED |
| 11  | aB    | 806 | CLA  | CBD-CGD-O2D-CED |
| 11  | bA    | 810 | CLA  | CBD-CGD-O2D-CED |
| 11  | bA    | 817 | CLA  | CBD-CGD-O2D-CED |
| 11  | bA    | 818 | CLA  | CBD-CGD-O2D-CED |
| 11  | bA    | 822 | CLA  | CBD-CGD-O2D-CED |
| 11  | bA    | 824 | CLA  | CBD-CGD-O2D-CED |
| 11  | bA    | 836 | CLA  | CBD-CGD-O2D-CED |
| 11  | bB    | 806 | CLA  | CBD-CGD-O2D-CED |
| 11  | cA    | 810 | CLA  | CBD-CGD-O2D-CED |
| 11  | cA    | 817 | CLA  | CBD-CGD-O2D-CED |
| 11  | cA    | 818 | CLA  | CBD-CGD-O2D-CED |
| 11  | cA    | 822 | CLA  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | cA    | 824 | CLA  | CBD-CGD-O2D-CED |
| 11  | cA    | 836 | CLA  | CBD-CGD-O2D-CED |
| 11  | cB    | 806 | CLA  | CBD-CGD-O2D-CED |
| 11  | aA    | 821 | CLA  | O1A-CGA-O2A-C1  |
| 11  | bA    | 821 | CLA  | O1A-CGA-O2A-C1  |
| 11  | cA    | 821 | CLA  | O1A-CGA-O2A-C1  |
| 11  | aB    | 806 | CLA  | O1D-CGD-O2D-CED |
| 11  | bB    | 806 | CLA  | O1D-CGD-O2D-CED |
| 11  | cB    | 806 | CLA  | O1D-CGD-O2D-CED |
| 11  | aA    | 806 | CLA  | CBD-CGD-O2D-CED |
| 11  | aA    | 822 | CLA  | O1A-CGA-O2A-C1  |
| 11  | aA    | 829 | CLA  | O1A-CGA-O2A-C1  |
| 11  | bA    | 822 | CLA  | O1A-CGA-O2A-C1  |
| 11  | bA    | 829 | CLA  | O1A-CGA-O2A-C1  |
| 11  | cA    | 822 | CLA  | O1A-CGA-O2A-C1  |
| 11  | cA    | 829 | CLA  | O1A-CGA-O2A-C1  |
| 12  | aL    | 202 | F6C  | O1A-CGA-O2A-C1  |
| 12  | bL    | 202 | F6C  | O1A-CGA-O2A-C1  |
| 12  | cL    | 202 | F6C  | O1A-CGA-O2A-C1  |
| 12  | aA    | 826 | F6C  | C4C-C3C-CAC-CBC |
| 12  | bA    | 826 | F6C  | C4C-C3C-CAC-CBC |
| 12  | cA    | 826 | F6C  | C4C-C3C-CAC-CBC |
| 11  | aB    | 818 | CLA  | O1D-CGD-O2D-CED |
| 11  | bB    | 818 | CLA  | O1D-CGD-O2D-CED |
| 11  | cB    | 818 | CLA  | O1D-CGD-O2D-CED |
| 11  | aA    | 804 | CLA  | O1D-CGD-O2D-CED |
| 11  | aA    | 842 | CLA  | O1D-CGD-O2D-CED |
| 11  | aB    | 815 | CLA  | O1D-CGD-O2D-CED |
| 11  | aB    | 832 | CLA  | O1D-CGD-O2D-CED |
| 11  | bA    | 804 | CLA  | O1D-CGD-O2D-CED |
| 11  | bA    | 842 | CLA  | O1D-CGD-O2D-CED |
| 11  | bB    | 815 | CLA  | O1D-CGD-O2D-CED |
| 11  | bB    | 832 | CLA  | O1D-CGD-O2D-CED |
| 11  | cA    | 804 | CLA  | O1D-CGD-O2D-CED |
| 11  | cA    | 842 | CLA  | O1D-CGD-O2D-CED |
| 11  | cB    | 815 | CLA  | O1D-CGD-O2D-CED |
| 11  | cB    | 832 | CLA  | O1D-CGD-O2D-CED |
| 11  | aA    | 812 | CLA  | CBD-CGD-O2D-CED |
| 11  | aA    | 816 | CLA  | CBD-CGD-O2D-CED |
| 11  | bA    | 806 | CLA  | CBD-CGD-O2D-CED |
| 11  | bA    | 812 | CLA  | CBD-CGD-O2D-CED |
| 11  | bA    | 816 | CLA  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | cA    | 806 | CLA  | CBD-CGD-O2D-CED |
| 11  | cA    | 816 | CLA  | CBD-CGD-O2D-CED |
| 11  | aB    | 802 | CLA  | O1A-CGA-O2A-C1  |
| 11  | bB    | 802 | CLA  | O1A-CGA-O2A-C1  |
| 11  | cB    | 802 | CLA  | O1A-CGA-O2A-C1  |
| 11  | aA    | 803 | CLA  | C3-C5-C6-C7     |
| 11  | aA    | 807 | CLA  | C3-C5-C6-C7     |
| 11  | aA    | 819 | CLA  | C3-C5-C6-C7     |
| 11  | aA    | 828 | CLA  | C3-C5-C6-C7     |
| 11  | aA    | 829 | CLA  | C3-C5-C6-C7     |
| 11  | aA    | 833 | CLA  | C3-C5-C6-C7     |
| 11  | aA    | 839 | CLA  | C3-C5-C6-C7     |
| 11  | aB    | 802 | CLA  | C3-C5-C6-C7     |
| 11  | aB    | 806 | CLA  | C3-C5-C6-C7     |
| 11  | aB    | 813 | CLA  | C3-C5-C6-C7     |
| 11  | aB    | 831 | CLA  | C3-C5-C6-C7     |
| 11  | aB    | 839 | CLA  | C3-C5-C6-C7     |
| 11  | bA    | 803 | CLA  | C3-C5-C6-C7     |
| 11  | bA    | 807 | CLA  | C3-C5-C6-C7     |
| 11  | bA    | 819 | CLA  | C3-C5-C6-C7     |
| 11  | bA    | 828 | CLA  | C3-C5-C6-C7     |
| 11  | bA    | 829 | CLA  | C3-C5-C6-C7     |
| 11  | bA    | 833 | CLA  | C3-C5-C6-C7     |
| 11  | bA    | 839 | CLA  | C3-C5-C6-C7     |
| 11  | bB    | 802 | CLA  | C3-C5-C6-C7     |
| 11  | bB    | 806 | CLA  | C3-C5-C6-C7     |
| 11  | bB    | 813 | CLA  | C3-C5-C6-C7     |
| 11  | bB    | 831 | CLA  | C3-C5-C6-C7     |
| 11  | bB    | 839 | CLA  | C3-C5-C6-C7     |
| 11  | cA    | 803 | CLA  | C3-C5-C6-C7     |
| 11  | cA    | 807 | CLA  | C3-C5-C6-C7     |
| 11  | cA    | 819 | CLA  | C3-C5-C6-C7     |
| 11  | cA    | 828 | CLA  | C3-C5-C6-C7     |
| 11  | cA    | 829 | CLA  | C3-C5-C6-C7     |
| 11  | cA    | 833 | CLA  | C3-C5-C6-C7     |
| 11  | cA    | 839 | CLA  | C3-C5-C6-C7     |
| 11  | cB    | 802 | CLA  | C3-C5-C6-C7     |
| 11  | cB    | 806 | CLA  | C3-C5-C6-C7     |
| 11  | cB    | 813 | CLA  | C3-C5-C6-C7     |
| 11  | cB    | 831 | CLA  | C3-C5-C6-C7     |
| 11  | cB    | 839 | CLA  | C3-C5-C6-C7     |
| 11  | aA    | 820 | CLA  | CBA-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | aA    | 821 | CLA  | CBA-CGA-O2A-C1  |
| 11  | aA    | 822 | CLA  | CBA-CGA-O2A-C1  |
| 11  | aA    | 824 | CLA  | CBA-CGA-O2A-C1  |
| 11  | bA    | 820 | CLA  | CBA-CGA-O2A-C1  |
| 11  | bA    | 821 | CLA  | CBA-CGA-O2A-C1  |
| 11  | bA    | 822 | CLA  | CBA-CGA-O2A-C1  |
| 11  | bA    | 824 | CLA  | CBA-CGA-O2A-C1  |
| 11  | cA    | 820 | CLA  | CBA-CGA-O2A-C1  |
| 11  | cA    | 821 | CLA  | CBA-CGA-O2A-C1  |
| 11  | cA    | 822 | CLA  | CBA-CGA-O2A-C1  |
| 11  | cA    | 824 | CLA  | CBA-CGA-O2A-C1  |
| 11  | aA    | 807 | CLA  | CBD-CGD-O2D-CED |
| 11  | aA    | 835 | CLA  | CBD-CGD-O2D-CED |
| 11  | aA    | 840 | CLA  | CBD-CGD-O2D-CED |
| 11  | aB    | 809 | CLA  | CBD-CGD-O2D-CED |
| 11  | aB    | 810 | CLA  | CBD-CGD-O2D-CED |
| 11  | aB    | 820 | CLA  | CBD-CGD-O2D-CED |
| 11  | aB    | 826 | CLA  | CBD-CGD-O2D-CED |
| 11  | bA    | 807 | CLA  | CBD-CGD-O2D-CED |
| 11  | bA    | 835 | CLA  | CBD-CGD-O2D-CED |
| 11  | bA    | 840 | CLA  | CBD-CGD-O2D-CED |
| 11  | bB    | 809 | CLA  | CBD-CGD-O2D-CED |
| 11  | bB    | 810 | CLA  | CBD-CGD-O2D-CED |
| 11  | bB    | 820 | CLA  | CBD-CGD-O2D-CED |
| 11  | bB    | 826 | CLA  | CBD-CGD-O2D-CED |
| 11  | cA    | 807 | CLA  | CBD-CGD-O2D-CED |
| 11  | cA    | 812 | CLA  | CBD-CGD-O2D-CED |
| 11  | cA    | 835 | CLA  | CBD-CGD-O2D-CED |
| 11  | cA    | 840 | CLA  | CBD-CGD-O2D-CED |
| 11  | cB    | 809 | CLA  | CBD-CGD-O2D-CED |
| 11  | cB    | 810 | CLA  | CBD-CGD-O2D-CED |
| 11  | cB    | 820 | CLA  | CBD-CGD-O2D-CED |
| 11  | cB    | 826 | CLA  | CBD-CGD-O2D-CED |
| 11  | aA    | 833 | CLA  | C4-C3-C5-C6     |
| 11  | aB    | 817 | CLA  | C4-C3-C5-C6     |
| 11  | aB    | 821 | CLA  | C4-C3-C5-C6     |
| 11  | bA    | 833 | CLA  | C4-C3-C5-C6     |
| 11  | bB    | 817 | CLA  | C4-C3-C5-C6     |
| 11  | bB    | 821 | CLA  | C4-C3-C5-C6     |
| 11  | cA    | 833 | CLA  | C4-C3-C5-C6     |
| 11  | cB    | 817 | CLA  | C4-C3-C5-C6     |
| 11  | cB    | 821 | CLA  | C4-C3-C5-C6     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 12  | aL    | 202 | F6C  | C4-C3-C5-C6     |
| 12  | bL    | 202 | F6C  | C4-C3-C5-C6     |
| 12  | cL    | 202 | F6C  | C4-C3-C5-C6     |
| 11  | aB    | 817 | CLA  | C2-C3-C5-C6     |
| 11  | aB    | 821 | CLA  | C2-C3-C5-C6     |
| 11  | bB    | 817 | CLA  | C2-C3-C5-C6     |
| 11  | bB    | 821 | CLA  | C2-C3-C5-C6     |
| 11  | cB    | 817 | CLA  | C2-C3-C5-C6     |
| 11  | cB    | 821 | CLA  | C2-C3-C5-C6     |
| 12  | aL    | 202 | F6C  | C2-C3-C5-C6     |
| 12  | bL    | 202 | F6C  | C2-C3-C5-C6     |
| 12  | cL    | 202 | F6C  | C2-C3-C5-C6     |
| 11  | aA    | 843 | CLA  | CBD-CGD-O2D-CED |
| 11  | bA    | 843 | CLA  | CBD-CGD-O2D-CED |
| 11  | bB    | 801 | CLA  | CBD-CGD-O2D-CED |
| 11  | cA    | 843 | CLA  | CBD-CGD-O2D-CED |
| 11  | cB    | 801 | CLA  | CBD-CGD-O2D-CED |
| 11  | aA    | 825 | CLA  | O1D-CGD-O2D-CED |
| 11  | bA    | 825 | CLA  | O1D-CGD-O2D-CED |
| 11  | cA    | 825 | CLA  | O1D-CGD-O2D-CED |
| 11  | aB    | 821 | CLA  | C2A-CAA-CBA-CGA |
| 11  | bB    | 821 | CLA  | C2A-CAA-CBA-CGA |
| 11  | cB    | 821 | CLA  | C2A-CAA-CBA-CGA |
| 11  | aA    | 818 | CLA  | C3-C5-C6-C7     |
| 11  | aA    | 820 | CLA  | C3-C5-C6-C7     |
| 11  | aA    | 831 | CLA  | C3-C5-C6-C7     |
| 11  | aB    | 808 | CLA  | C3-C5-C6-C7     |
| 11  | aB    | 817 | CLA  | C3-C5-C6-C7     |
| 11  | bA    | 818 | CLA  | C3-C5-C6-C7     |
| 11  | bA    | 820 | CLA  | C3-C5-C6-C7     |
| 11  | bA    | 831 | CLA  | C3-C5-C6-C7     |
| 11  | bB    | 808 | CLA  | C3-C5-C6-C7     |
| 11  | bB    | 817 | CLA  | C3-C5-C6-C7     |
| 11  | cA    | 818 | CLA  | C3-C5-C6-C7     |
| 11  | cA    | 820 | CLA  | C3-C5-C6-C7     |
| 11  | cA    | 831 | CLA  | C3-C5-C6-C7     |
| 11  | cB    | 808 | CLA  | C3-C5-C6-C7     |
| 11  | cB    | 817 | CLA  | C3-C5-C6-C7     |
| 11  | aA    | 829 | CLA  | CBA-CGA-O2A-C1  |
| 11  | aA    | 838 | CLA  | CBA-CGA-O2A-C1  |
| 11  | aB    | 804 | CLA  | CBA-CGA-O2A-C1  |
| 11  | bA    | 829 | CLA  | CBA-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | bA    | 838 | CLA  | CBA-CGA-O2A-C1  |
| 11  | bB    | 804 | CLA  | CBA-CGA-O2A-C1  |
| 11  | bB    | 828 | CLA  | CBA-CGA-O2A-C1  |
| 11  | cA    | 829 | CLA  | CBA-CGA-O2A-C1  |
| 11  | cA    | 838 | CLA  | CBA-CGA-O2A-C1  |
| 11  | cB    | 804 | CLA  | CBA-CGA-O2A-C1  |
| 12  | aL    | 202 | F6C  | CBA-CGA-O2A-C1  |
| 12  | bL    | 202 | F6C  | CBA-CGA-O2A-C1  |
| 12  | cL    | 202 | F6C  | CBA-CGA-O2A-C1  |
| 15  | aA    | 851 | BCR  | C19-C20-C21-C22 |
| 15  | aB    | 848 | BCR  | C19-C20-C21-C22 |
| 15  | bA    | 851 | BCR  | C19-C20-C21-C22 |
| 15  | bB    | 848 | BCR  | C19-C20-C21-C22 |
| 15  | cA    | 851 | BCR  | C19-C20-C21-C22 |
| 15  | cB    | 848 | BCR  | C19-C20-C21-C22 |
| 11  | aA    | 838 | CLA  | O1A-CGA-O2A-C1  |
| 11  | bA    | 838 | CLA  | O1A-CGA-O2A-C1  |
| 11  | cA    | 838 | CLA  | O1A-CGA-O2A-C1  |
| 12  | aA    | 844 | F6C  | O1A-CGA-O2A-C1  |
| 12  | bA    | 844 | F6C  | O1A-CGA-O2A-C1  |
| 12  | cA    | 844 | F6C  | O1A-CGA-O2A-C1  |
| 12  | aA    | 826 | F6C  | C1A-C2A-CAA-CBA |
| 12  | aA    | 827 | F6C  | C1A-C2A-CAA-CBA |
| 12  | aL    | 202 | F6C  | C1A-C2A-CAA-CBA |
| 12  | bA    | 826 | F6C  | C1A-C2A-CAA-CBA |
| 12  | bA    | 827 | F6C  | C1A-C2A-CAA-CBA |
| 12  | bL    | 202 | F6C  | C1A-C2A-CAA-CBA |
| 12  | cA    | 826 | F6C  | C1A-C2A-CAA-CBA |
| 12  | cA    | 827 | F6C  | C1A-C2A-CAA-CBA |
| 12  | cL    | 202 | F6C  | C1A-C2A-CAA-CBA |
| 11  | aA    | 824 | CLA  | O1D-CGD-O2D-CED |
| 11  | bA    | 824 | CLA  | O1D-CGD-O2D-CED |
| 11  | cA    | 824 | CLA  | O1D-CGD-O2D-CED |
| 12  | aB    | 824 | F6C  | C3-C5-C6-C7     |
| 12  | bB    | 824 | F6C  | C3-C5-C6-C7     |
| 12  | cB    | 824 | F6C  | C3-C5-C6-C7     |
| 11  | aA    | 809 | CLA  | CBD-CGD-O2D-CED |
| 11  | aA    | 815 | CLA  | CBD-CGD-O2D-CED |
| 11  | aB    | 801 | CLA  | CBD-CGD-O2D-CED |
| 11  | aB    | 822 | CLA  | CBD-CGD-O2D-CED |
| 11  | bA    | 809 | CLA  | CBD-CGD-O2D-CED |
| 11  | bA    | 815 | CLA  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | bB    | 822 | CLA  | CBD-CGD-O2D-CED |
| 11  | cA    | 809 | CLA  | CBD-CGD-O2D-CED |
| 11  | cA    | 815 | CLA  | CBD-CGD-O2D-CED |
| 11  | cB    | 822 | CLA  | CBD-CGD-O2D-CED |
| 11  | aA    | 817 | CLA  | O1D-CGD-O2D-CED |
| 11  | bA    | 817 | CLA  | O1D-CGD-O2D-CED |
| 11  | cA    | 817 | CLA  | O1D-CGD-O2D-CED |
| 11  | aA    | 840 | CLA  | CBA-CGA-O2A-C1  |
| 11  | aB    | 821 | CLA  | CBA-CGA-O2A-C1  |
| 11  | aB    | 828 | CLA  | CBA-CGA-O2A-C1  |
| 11  | bA    | 840 | CLA  | CBA-CGA-O2A-C1  |
| 11  | bB    | 821 | CLA  | CBA-CGA-O2A-C1  |
| 11  | cA    | 840 | CLA  | CBA-CGA-O2A-C1  |
| 11  | cB    | 821 | CLA  | CBA-CGA-O2A-C1  |
| 11  | cB    | 828 | CLA  | CBA-CGA-O2A-C1  |
| 12  | aA    | 844 | F6C  | CBA-CGA-O2A-C1  |
| 12  | bA    | 844 | F6C  | CBA-CGA-O2A-C1  |
| 12  | cA    | 844 | F6C  | CBA-CGA-O2A-C1  |
| 11  | aA    | 820 | CLA  | O1A-CGA-O2A-C1  |
| 11  | aB    | 804 | CLA  | O1A-CGA-O2A-C1  |
| 11  | bA    | 820 | CLA  | O1A-CGA-O2A-C1  |
| 11  | bB    | 804 | CLA  | O1A-CGA-O2A-C1  |
| 11  | cA    | 820 | CLA  | O1A-CGA-O2A-C1  |
| 11  | cB    | 804 | CLA  | O1A-CGA-O2A-C1  |
| 11  | aA    | 836 | CLA  | O1D-CGD-O2D-CED |
| 11  | bA    | 836 | CLA  | O1D-CGD-O2D-CED |
| 11  | cA    | 836 | CLA  | O1D-CGD-O2D-CED |
| 11  | aA    | 810 | CLA  | O1D-CGD-O2D-CED |
| 11  | bA    | 810 | CLA  | O1D-CGD-O2D-CED |
| 11  | cA    | 810 | CLA  | O1D-CGD-O2D-CED |
| 11  | aB    | 802 | CLA  | CBA-CGA-O2A-C1  |
| 11  | bB    | 802 | CLA  | CBA-CGA-O2A-C1  |
| 11  | cB    | 802 | CLA  | CBA-CGA-O2A-C1  |
| 11  | aB    | 827 | CLA  | C4-C3-C5-C6     |
| 11  | bB    | 827 | CLA  | C4-C3-C5-C6     |
| 11  | cB    | 827 | CLA  | C4-C3-C5-C6     |
| 11  | aA    | 833 | CLA  | C2-C3-C5-C6     |
| 11  | aB    | 827 | CLA  | C2-C3-C5-C6     |
| 11  | bA    | 833 | CLA  | C2-C3-C5-C6     |
| 11  | bB    | 827 | CLA  | C2-C3-C5-C6     |
| 11  | cA    | 833 | CLA  | C2-C3-C5-C6     |
| 11  | cB    | 827 | CLA  | C2-C3-C5-C6     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | aB    | 821 | CLA  | O1A-CGA-O2A-C1  |
| 11  | aB    | 828 | CLA  | O1A-CGA-O2A-C1  |
| 11  | bB    | 821 | CLA  | O1A-CGA-O2A-C1  |
| 11  | cB    | 821 | CLA  | O1A-CGA-O2A-C1  |
| 12  | aA    | 830 | F6C  | C2A-CAA-CBA-CGA |
| 12  | bA    | 830 | F6C  | C2A-CAA-CBA-CGA |
| 12  | cA    | 830 | F6C  | C2A-CAA-CBA-CGA |
| 11  | aA    | 818 | CLA  | O1D-CGD-O2D-CED |
| 11  | bA    | 818 | CLA  | O1D-CGD-O2D-CED |
| 11  | cA    | 818 | CLA  | O1D-CGD-O2D-CED |
| 11  | bB    | 828 | CLA  | O1A-CGA-O2A-C1  |
| 11  | cB    | 828 | CLA  | O1A-CGA-O2A-C1  |
| 17  | aA    | 853 | LMT  | O5'-C1'-O1'-C1  |
| 17  | bA    | 853 | LMT  | O5'-C1'-O1'-C1  |
| 17  | cA    | 853 | LMT  | O5'-C1'-O1'-C1  |
| 11  | aB    | 830 | CLA  | CBD-CGD-O2D-CED |
| 11  | aB    | 838 | CLA  | CBD-CGD-O2D-CED |
| 11  | bB    | 830 | CLA  | CBD-CGD-O2D-CED |
| 11  | bB    | 838 | CLA  | CBD-CGD-O2D-CED |
| 11  | cB    | 830 | CLA  | CBD-CGD-O2D-CED |
| 11  | cB    | 838 | CLA  | CBD-CGD-O2D-CED |
| 11  | aA    | 840 | CLA  | O1A-CGA-O2A-C1  |
| 11  | bA    | 840 | CLA  | O1A-CGA-O2A-C1  |
| 11  | cA    | 840 | CLA  | O1A-CGA-O2A-C1  |
| 11  | aA    | 806 | CLA  | O1D-CGD-O2D-CED |
| 11  | bA    | 806 | CLA  | O1D-CGD-O2D-CED |
| 11  | cA    | 806 | CLA  | O1D-CGD-O2D-CED |
| 11  | aB    | 814 | CLA  | CBD-CGD-O2D-CED |
| 11  | bB    | 814 | CLA  | CBD-CGD-O2D-CED |
| 11  | cB    | 814 | CLA  | CBD-CGD-O2D-CED |
| 11  | aA    | 812 | CLA  | O1D-CGD-O2D-CED |
| 11  | bA    | 812 | CLA  | O1D-CGD-O2D-CED |
| 11  | cA    | 812 | CLA  | O1D-CGD-O2D-CED |
| 11  | aA    | 812 | CLA  | CBA-CGA-O2A-C1  |
| 11  | aA    | 817 | CLA  | CBA-CGA-O2A-C1  |
| 11  | aA    | 828 | CLA  | CBA-CGA-O2A-C1  |
| 11  | aB    | 817 | CLA  | CBA-CGA-O2A-C1  |
| 11  | aB    | 830 | CLA  | CBA-CGA-O2A-C1  |
| 11  | bA    | 812 | CLA  | CBA-CGA-O2A-C1  |
| 11  | bA    | 817 | CLA  | CBA-CGA-O2A-C1  |
| 11  | bA    | 828 | CLA  | CBA-CGA-O2A-C1  |
| 11  | bB    | 817 | CLA  | CBA-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | bB    | 830 | CLA  | CBA-CGA-O2A-C1  |
| 11  | cA    | 812 | CLA  | CBA-CGA-O2A-C1  |
| 11  | cA    | 817 | CLA  | CBA-CGA-O2A-C1  |
| 11  | cA    | 828 | CLA  | CBA-CGA-O2A-C1  |
| 11  | cB    | 817 | CLA  | CBA-CGA-O2A-C1  |
| 11  | cB    | 830 | CLA  | CBA-CGA-O2A-C1  |
| 11  | aA    | 816 | CLA  | O1D-CGD-O2D-CED |
| 11  | aA    | 822 | CLA  | O1D-CGD-O2D-CED |
| 11  | bA    | 816 | CLA  | O1D-CGD-O2D-CED |
| 11  | bA    | 822 | CLA  | O1D-CGD-O2D-CED |
| 11  | cA    | 816 | CLA  | O1D-CGD-O2D-CED |
| 11  | cA    | 822 | CLA  | O1D-CGD-O2D-CED |
| 11  | aB    | 821 | CLA  | C3-C5-C6-C7     |
| 11  | bB    | 821 | CLA  | C3-C5-C6-C7     |
| 11  | cB    | 821 | CLA  | C3-C5-C6-C7     |
| 11  | aA    | 814 | CLA  | C11-C12-C13-C14 |
| 11  | aA    | 822 | CLA  | C11-C10-C8-C9   |
| 11  | aA    | 825 | CLA  | C11-C12-C13-C14 |
| 11  | aA    | 833 | CLA  | C6-C7-C8-C9     |
| 11  | aA    | 833 | CLA  | C14-C13-C15-C16 |
| 11  | aA    | 840 | CLA  | C14-C13-C15-C16 |
| 11  | aB    | 812 | CLA  | C11-C12-C13-C14 |
| 11  | bA    | 814 | CLA  | C11-C12-C13-C14 |
| 11  | bA    | 822 | CLA  | C11-C10-C8-C9   |
| 11  | bA    | 825 | CLA  | C11-C12-C13-C14 |
| 11  | bA    | 833 | CLA  | C6-C7-C8-C9     |
| 11  | bA    | 833 | CLA  | C14-C13-C15-C16 |
| 11  | bA    | 840 | CLA  | C14-C13-C15-C16 |
| 11  | bB    | 812 | CLA  | C11-C12-C13-C14 |
| 11  | cA    | 814 | CLA  | C11-C12-C13-C14 |
| 11  | cA    | 822 | CLA  | C11-C10-C8-C9   |
| 11  | cA    | 825 | CLA  | C11-C12-C13-C14 |
| 11  | cA    | 833 | CLA  | C6-C7-C8-C9     |
| 11  | cA    | 833 | CLA  | C14-C13-C15-C16 |
| 11  | cA    | 840 | CLA  | C14-C13-C15-C16 |
| 11  | cB    | 812 | CLA  | C11-C12-C13-C14 |
| 12  | aA    | 844 | F6C  | C11-C12-C13-C14 |
| 12  | cA    | 844 | F6C  | C11-C12-C13-C14 |
| 17  | aA    | 853 | LMT  | C2'-C1'-O1'-C1  |
| 17  | bA    | 853 | LMT  | C2'-C1'-O1'-C1  |
| 17  | cA    | 853 | LMT  | C2'-C1'-O1'-C1  |
| 18  | aB    | 847 | LMG  | C28-C29-C30-C31 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 18  | cB    | 847 | LMG  | C28-C29-C30-C31 |
| 11  | aA    | 828 | CLA  | O1A-CGA-O2A-C1  |
| 11  | aB    | 830 | CLA  | O1A-CGA-O2A-C1  |
| 11  | bA    | 828 | CLA  | O1A-CGA-O2A-C1  |
| 11  | bB    | 830 | CLA  | O1A-CGA-O2A-C1  |
| 11  | cA    | 828 | CLA  | O1A-CGA-O2A-C1  |
| 11  | cB    | 830 | CLA  | O1A-CGA-O2A-C1  |
| 15  | aA    | 848 | BCR  | C11-C12-C13-C35 |
| 15  | aA    | 849 | BCR  | C37-C22-C23-C24 |
| 15  | aB    | 842 | BCR  | C7-C8-C9-C34    |
| 15  | aB    | 844 | BCR  | C37-C22-C23-C24 |
| 15  | aB    | 845 | BCR  | C11-C12-C13-C35 |
| 15  | aL    | 208 | BCR  | C7-C8-C9-C34    |
| 15  | aM    | 101 | BCR  | C7-C8-C9-C34    |
| 15  | bA    | 848 | BCR  | C11-C12-C13-C35 |
| 15  | bA    | 849 | BCR  | C37-C22-C23-C24 |
| 15  | bB    | 842 | BCR  | C7-C8-C9-C34    |
| 15  | bB    | 844 | BCR  | C37-C22-C23-C24 |
| 15  | bB    | 845 | BCR  | C11-C12-C13-C35 |
| 15  | bL    | 208 | BCR  | C7-C8-C9-C34    |
| 15  | bM    | 101 | BCR  | C7-C8-C9-C34    |
| 15  | cA    | 848 | BCR  | C11-C12-C13-C35 |
| 15  | cA    | 849 | BCR  | C37-C22-C23-C24 |
| 15  | cB    | 842 | BCR  | C7-C8-C9-C34    |
| 15  | cB    | 844 | BCR  | C37-C22-C23-C24 |
| 15  | cB    | 845 | BCR  | C11-C12-C13-C35 |
| 15  | cL    | 208 | BCR  | C7-C8-C9-C34    |
| 15  | cM    | 101 | BCR  | C7-C8-C9-C34    |
| 12  | aA    | 832 | F6C  | C3A-C2A-CAA-CBA |
| 12  | bA    | 832 | F6C  | C3A-C2A-CAA-CBA |
| 12  | cA    | 832 | F6C  | C3A-C2A-CAA-CBA |
| 15  | aA    | 847 | BCR  | C21-C22-C23-C24 |
| 15  | aB    | 842 | BCR  | C21-C22-C23-C24 |
| 15  | aL    | 207 | BCR  | C21-C22-C23-C24 |
| 15  | bA    | 847 | BCR  | C21-C22-C23-C24 |
| 15  | bB    | 842 | BCR  | C21-C22-C23-C24 |
| 15  | bL    | 207 | BCR  | C21-C22-C23-C24 |
| 15  | cA    | 847 | BCR  | C21-C22-C23-C24 |
| 15  | cB    | 842 | BCR  | C21-C22-C23-C24 |
| 15  | cL    | 207 | BCR  | C21-C22-C23-C24 |
| 18  | bB    | 847 | LMG  | C28-C29-C30-C31 |
| 11  | aA    | 831 | CLA  | CBA-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | bA    | 831 | CLA  | CBA-CGA-O2A-C1  |
| 11  | cA    | 831 | CLA  | CBA-CGA-O2A-C1  |
| 11  | aA    | 807 | CLA  | O1D-CGD-O2D-CED |
| 11  | aB    | 809 | CLA  | O1D-CGD-O2D-CED |
| 11  | bA    | 807 | CLA  | O1D-CGD-O2D-CED |
| 11  | bB    | 809 | CLA  | O1D-CGD-O2D-CED |
| 11  | cA    | 807 | CLA  | O1D-CGD-O2D-CED |
| 11  | cB    | 809 | CLA  | O1D-CGD-O2D-CED |
| 11  | aB    | 827 | CLA  | C5-C6-C7-C8     |
| 11  | bB    | 827 | CLA  | C5-C6-C7-C8     |
| 11  | cB    | 827 | CLA  | C5-C6-C7-C8     |
| 11  | aB    | 820 | CLA  | O1D-CGD-O2D-CED |
| 11  | bB    | 820 | CLA  | O1D-CGD-O2D-CED |
| 11  | cB    | 820 | CLA  | O1D-CGD-O2D-CED |
| 11  | aB    | 806 | CLA  | C15-C16-C17-C18 |
| 11  | bB    | 806 | CLA  | C15-C16-C17-C18 |
| 11  | cB    | 806 | CLA  | C15-C16-C17-C18 |
| 11  | aA    | 841 | CLA  | CBD-CGD-O2D-CED |
| 11  | aB    | 828 | CLA  | CBD-CGD-O2D-CED |
| 11  | bA    | 841 | CLA  | CBD-CGD-O2D-CED |
| 11  | bB    | 828 | CLA  | CBD-CGD-O2D-CED |
| 11  | cA    | 841 | CLA  | CBD-CGD-O2D-CED |
| 11  | cB    | 828 | CLA  | CBD-CGD-O2D-CED |
| 11  | aB    | 806 | CLA  | C4-C3-C5-C6     |
| 11  | bB    | 806 | CLA  | C4-C3-C5-C6     |
| 11  | cB    | 806 | CLA  | C4-C3-C5-C6     |
| 11  | bA    | 825 | CLA  | C10-C11-C12-C13 |
| 11  | cA    | 825 | CLA  | C10-C11-C12-C13 |
| 11  | aA    | 825 | CLA  | C10-C11-C12-C13 |
| 11  | aA    | 831 | CLA  | C13-C15-C16-C17 |
| 11  | bA    | 831 | CLA  | C13-C15-C16-C17 |
| 11  | cA    | 831 | CLA  | C13-C15-C16-C17 |
| 11  | aA    | 812 | CLA  | O1A-CGA-O2A-C1  |
| 11  | bA    | 812 | CLA  | O1A-CGA-O2A-C1  |
| 11  | cA    | 812 | CLA  | O1A-CGA-O2A-C1  |
| 11  | aB    | 810 | CLA  | O1D-CGD-O2D-CED |
| 11  | bB    | 810 | CLA  | O1D-CGD-O2D-CED |
| 11  | cB    | 810 | CLA  | O1D-CGD-O2D-CED |
| 11  | aA    | 814 | CLA  | C5-C6-C7-C8     |
| 11  | aA    | 814 | CLA  | C15-C16-C17-C18 |
| 11  | aA    | 833 | CLA  | C5-C6-C7-C8     |
| 11  | aA    | 834 | CLA  | C5-C6-C7-C8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | aB    | 808 | CLA  | C10-C11-C12-C13 |
| 11  | aB    | 812 | CLA  | C15-C16-C17-C18 |
| 11  | bA    | 814 | CLA  | C5-C6-C7-C8     |
| 11  | bA    | 814 | CLA  | C15-C16-C17-C18 |
| 11  | bA    | 833 | CLA  | C5-C6-C7-C8     |
| 11  | bA    | 834 | CLA  | C5-C6-C7-C8     |
| 11  | bB    | 808 | CLA  | C10-C11-C12-C13 |
| 11  | bB    | 812 | CLA  | C15-C16-C17-C18 |
| 11  | cA    | 814 | CLA  | C5-C6-C7-C8     |
| 11  | cA    | 814 | CLA  | C15-C16-C17-C18 |
| 11  | cA    | 833 | CLA  | C5-C6-C7-C8     |
| 11  | cA    | 834 | CLA  | C5-C6-C7-C8     |
| 11  | cB    | 808 | CLA  | C10-C11-C12-C13 |
| 11  | cB    | 812 | CLA  | C15-C16-C17-C18 |
| 12  | aA    | 827 | F6C  | C5-C6-C7-C8     |
| 12  | aL    | 202 | F6C  | C15-C16-C17-C18 |
| 12  | bA    | 827 | F6C  | C5-C6-C7-C8     |
| 12  | bL    | 202 | F6C  | C15-C16-C17-C18 |
| 12  | cA    | 827 | F6C  | C5-C6-C7-C8     |
| 12  | cL    | 202 | F6C  | C15-C16-C17-C18 |
| 11  | aA    | 812 | CLA  | C2A-CAA-CBA-CGA |
| 11  | aB    | 811 | CLA  | C2A-CAA-CBA-CGA |
| 11  | aB    | 829 | CLA  | C2A-CAA-CBA-CGA |
| 11  | aB    | 839 | CLA  | C2A-CAA-CBA-CGA |
| 11  | bA    | 812 | CLA  | C2A-CAA-CBA-CGA |
| 11  | bB    | 811 | CLA  | C2A-CAA-CBA-CGA |
| 11  | bB    | 829 | CLA  | C2A-CAA-CBA-CGA |
| 11  | bB    | 839 | CLA  | C2A-CAA-CBA-CGA |
| 11  | cA    | 812 | CLA  | C2A-CAA-CBA-CGA |
| 11  | cB    | 811 | CLA  | C2A-CAA-CBA-CGA |
| 11  | cB    | 829 | CLA  | C2A-CAA-CBA-CGA |
| 11  | cB    | 839 | CLA  | C2A-CAA-CBA-CGA |
| 15  | aM    | 101 | BCR  | C18-C19-C20-C21 |
| 15  | bM    | 101 | BCR  | C18-C19-C20-C21 |
| 15  | cM    | 101 | BCR  | C18-C19-C20-C21 |
| 11  | aA    | 812 | CLA  | C8-C10-C11-C12  |
| 11  | aL    | 204 | CLA  | C13-C15-C16-C17 |
| 11  | aL    | 205 | CLA  | C8-C10-C11-C12  |
| 11  | bL    | 204 | CLA  | C13-C15-C16-C17 |
| 11  | bL    | 205 | CLA  | C8-C10-C11-C12  |
| 11  | cL    | 204 | CLA  | C13-C15-C16-C17 |
| 11  | cL    | 205 | CLA  | C8-C10-C11-C12  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | aB    | 840 | CLA  | CBD-CGD-O2D-CED |
| 11  | bB    | 840 | CLA  | CBD-CGD-O2D-CED |
| 11  | cB    | 840 | CLA  | CBD-CGD-O2D-CED |
| 11  | aA    | 840 | CLA  | O1D-CGD-O2D-CED |
| 11  | bA    | 840 | CLA  | O1D-CGD-O2D-CED |
| 11  | aA    | 840 | CLA  | C13-C15-C16-C17 |
| 11  | aL    | 206 | CLA  | C5-C6-C7-C8     |
| 11  | bA    | 812 | CLA  | C8-C10-C11-C12  |
| 11  | bA    | 840 | CLA  | C13-C15-C16-C17 |
| 11  | bL    | 206 | CLA  | C5-C6-C7-C8     |
| 11  | cA    | 812 | CLA  | C8-C10-C11-C12  |
| 11  | cA    | 840 | CLA  | C13-C15-C16-C17 |
| 11  | cL    | 206 | CLA  | C5-C6-C7-C8     |
| 16  | aA    | 852 | LHG  | O2-C2-C3-O3     |
| 16  | bA    | 852 | LHG  | O2-C2-C3-O3     |
| 16  | cA    | 852 | LHG  | O2-C2-C3-O3     |
| 11  | aA    | 817 | CLA  | O1A-CGA-O2A-C1  |
| 11  | aB    | 817 | CLA  | O1A-CGA-O2A-C1  |
| 11  | bA    | 817 | CLA  | O1A-CGA-O2A-C1  |
| 11  | bB    | 817 | CLA  | O1A-CGA-O2A-C1  |
| 11  | cA    | 817 | CLA  | O1A-CGA-O2A-C1  |
| 11  | cB    | 817 | CLA  | O1A-CGA-O2A-C1  |
| 11  | bA    | 843 | CLA  | O1D-CGD-O2D-CED |
| 11  | bB    | 822 | CLA  | O1D-CGD-O2D-CED |
| 11  | cA    | 843 | CLA  | O1D-CGD-O2D-CED |
| 11  | aA    | 843 | CLA  | O1D-CGD-O2D-CED |
| 11  | aB    | 822 | CLA  | O1D-CGD-O2D-CED |
| 11  | bA    | 835 | CLA  | O1D-CGD-O2D-CED |
| 11  | cA    | 835 | CLA  | O1D-CGD-O2D-CED |
| 11  | cB    | 822 | CLA  | O1D-CGD-O2D-CED |
| 11  | aA    | 840 | CLA  | C10-C11-C12-C13 |
| 11  | aB    | 805 | CLA  | C15-C16-C17-C18 |
| 11  | aB    | 806 | CLA  | C5-C6-C7-C8     |
| 11  | aL    | 204 | CLA  | C10-C11-C12-C13 |
| 11  | aL    | 204 | CLA  | C15-C16-C17-C18 |
| 11  | bA    | 840 | CLA  | C10-C11-C12-C13 |
| 11  | bB    | 805 | CLA  | C15-C16-C17-C18 |
| 11  | bB    | 806 | CLA  | C5-C6-C7-C8     |
| 11  | bL    | 204 | CLA  | C10-C11-C12-C13 |
| 11  | bL    | 204 | CLA  | C15-C16-C17-C18 |
| 11  | cA    | 840 | CLA  | C10-C11-C12-C13 |
| 11  | cB    | 805 | CLA  | C15-C16-C17-C18 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | cB    | 806 | CLA  | C5-C6-C7-C8     |
| 11  | cL    | 204 | CLA  | C10-C11-C12-C13 |
| 11  | cL    | 204 | CLA  | C15-C16-C17-C18 |
| 11  | aA    | 831 | CLA  | O1A-CGA-O2A-C1  |
| 11  | bA    | 831 | CLA  | O1A-CGA-O2A-C1  |
| 11  | cA    | 831 | CLA  | O1A-CGA-O2A-C1  |
| 11  | aA    | 835 | CLA  | O1D-CGD-O2D-CED |
| 11  | cA    | 840 | CLA  | O1D-CGD-O2D-CED |
| 11  | aL    | 206 | CLA  | C15-C16-C17-C18 |
| 11  | bL    | 206 | CLA  | C15-C16-C17-C18 |
| 11  | cL    | 206 | CLA  | C15-C16-C17-C18 |
| 12  | aA    | 832 | F6C  | CBA-CGA-O2A-C1  |
| 12  | bA    | 832 | F6C  | CBA-CGA-O2A-C1  |
| 12  | cA    | 832 | F6C  | CBA-CGA-O2A-C1  |
| 11  | aB    | 826 | CLA  | O1D-CGD-O2D-CED |
| 11  | bB    | 826 | CLA  | O1D-CGD-O2D-CED |
| 11  | cB    | 826 | CLA  | O1D-CGD-O2D-CED |
| 11  | aA    | 834 | CLA  | C3-C5-C6-C7     |
| 11  | bA    | 834 | CLA  | C3-C5-C6-C7     |
| 11  | cA    | 834 | CLA  | C3-C5-C6-C7     |
| 16  | aA    | 852 | LHG  | C1-C2-C3-O3     |
| 16  | bA    | 852 | LHG  | C1-C2-C3-O3     |
| 16  | cA    | 852 | LHG  | C1-C2-C3-O3     |
| 11  | aA    | 808 | CLA  | CBA-CGA-O2A-C1  |
| 11  | aB    | 826 | CLA  | CBA-CGA-O2A-C1  |
| 11  | bA    | 808 | CLA  | CBA-CGA-O2A-C1  |
| 11  | bB    | 826 | CLA  | CBA-CGA-O2A-C1  |
| 11  | cA    | 808 | CLA  | CBA-CGA-O2A-C1  |
| 11  | cB    | 826 | CLA  | CBA-CGA-O2A-C1  |
| 11  | aA    | 803 | CLA  | C5-C6-C7-C8     |
| 11  | aA    | 840 | CLA  | C15-C16-C17-C18 |
| 11  | bA    | 803 | CLA  | C5-C6-C7-C8     |
| 11  | bA    | 840 | CLA  | C15-C16-C17-C18 |
| 11  | cA    | 803 | CLA  | C5-C6-C7-C8     |
| 11  | cA    | 840 | CLA  | C15-C16-C17-C18 |
| 11  | aB    | 802 | CLA  | C5-C6-C7-C8     |
| 11  | aB    | 808 | CLA  | C13-C15-C16-C17 |
| 11  | cB    | 802 | CLA  | C5-C6-C7-C8     |
| 11  | aA    | 839 | CLA  | C15-C16-C17-C18 |
| 11  | aB    | 812 | CLA  | C10-C11-C12-C13 |
| 11  | bA    | 839 | CLA  | C15-C16-C17-C18 |
| 11  | bB    | 802 | CLA  | C5-C6-C7-C8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | bB    | 808 | CLA  | C13-C15-C16-C17 |
| 11  | bB    | 812 | CLA  | C10-C11-C12-C13 |
| 11  | cA    | 839 | CLA  | C15-C16-C17-C18 |
| 11  | cB    | 808 | CLA  | C13-C15-C16-C17 |
| 11  | cB    | 812 | CLA  | C10-C11-C12-C13 |
| 11  | aL    | 205 | CLA  | C3-C5-C6-C7     |
| 11  | bL    | 205 | CLA  | C3-C5-C6-C7     |
| 11  | cL    | 205 | CLA  | C3-C5-C6-C7     |
| 11  | aL    | 206 | CLA  | C14-C13-C15-C16 |
| 11  | bL    | 206 | CLA  | C14-C13-C15-C16 |
| 12  | bA    | 844 | F6C  | C11-C12-C13-C14 |
| 11  | aA    | 809 | CLA  | O1D-CGD-O2D-CED |
| 11  | bA    | 809 | CLA  | O1D-CGD-O2D-CED |
| 11  | bB    | 801 | CLA  | O1D-CGD-O2D-CED |
| 11  | cA    | 809 | CLA  | O1D-CGD-O2D-CED |
| 11  | cB    | 801 | CLA  | O1D-CGD-O2D-CED |
| 11  | aB    | 801 | CLA  | O1D-CGD-O2D-CED |
| 11  | aB    | 809 | CLA  | CBA-CGA-O2A-C1  |
| 11  | bB    | 809 | CLA  | CBA-CGA-O2A-C1  |
| 11  | cB    | 809 | CLA  | CBA-CGA-O2A-C1  |
| 15  | aA    | 847 | BCR  | C20-C21-C22-C37 |
| 15  | aB    | 843 | BCR  | C20-C21-C22-C37 |
| 15  | aB    | 846 | BCR  | C11-C10-C9-C34  |
| 15  | aI    | 101 | BCR  | C20-C21-C22-C37 |
| 15  | aL    | 208 | BCR  | C20-C21-C22-C37 |
| 15  | bA    | 847 | BCR  | C20-C21-C22-C37 |
| 15  | bB    | 843 | BCR  | C20-C21-C22-C37 |
| 15  | bB    | 846 | BCR  | C11-C10-C9-C34  |
| 15  | bI    | 101 | BCR  | C20-C21-C22-C37 |
| 15  | bL    | 208 | BCR  | C20-C21-C22-C37 |
| 15  | cA    | 847 | BCR  | C20-C21-C22-C37 |
| 15  | cB    | 843 | BCR  | C20-C21-C22-C37 |
| 15  | cB    | 846 | BCR  | C11-C10-C9-C34  |
| 15  | cI    | 103 | BCR  | C20-C21-C22-C37 |
| 15  | cL    | 208 | BCR  | C20-C21-C22-C37 |
| 15  | aA    | 851 | BCR  | C37-C22-C23-C24 |
| 15  | aB    | 844 | BCR  | C11-C12-C13-C35 |
| 15  | aL    | 207 | BCR  | C37-C22-C23-C24 |
| 15  | bA    | 851 | BCR  | C37-C22-C23-C24 |
| 15  | bB    | 844 | BCR  | C11-C12-C13-C35 |
| 15  | bL    | 207 | BCR  | C37-C22-C23-C24 |
| 15  | cA    | 851 | BCR  | C37-C22-C23-C24 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 15  | cB    | 844 | BCR  | C11-C12-C13-C35 |
| 15  | cL    | 207 | BCR  | C37-C22-C23-C24 |
| 15  | aL    | 207 | BCR  | C7-C8-C9-C10    |
| 15  | bL    | 207 | BCR  | C7-C8-C9-C10    |
| 15  | cL    | 207 | BCR  | C7-C8-C9-C10    |
| 11  | aA    | 802 | CLA  | C2A-CAA-CBA-CGA |
| 11  | aA    | 809 | CLA  | C2A-CAA-CBA-CGA |
| 11  | aB    | 809 | CLA  | C2A-CAA-CBA-CGA |
| 11  | bA    | 802 | CLA  | C2A-CAA-CBA-CGA |
| 11  | bA    | 809 | CLA  | C2A-CAA-CBA-CGA |
| 11  | bB    | 809 | CLA  | C2A-CAA-CBA-CGA |
| 11  | cA    | 802 | CLA  | C2A-CAA-CBA-CGA |
| 11  | cA    | 809 | CLA  | C2A-CAA-CBA-CGA |
| 11  | cB    | 809 | CLA  | C2A-CAA-CBA-CGA |
| 11  | aA    | 822 | CLA  | C8-C10-C11-C12  |
| 11  | bA    | 822 | CLA  | C8-C10-C11-C12  |
| 11  | cA    | 822 | CLA  | C8-C10-C11-C12  |
| 11  | aA    | 815 | CLA  | O1D-CGD-O2D-CED |
| 11  | bA    | 815 | CLA  | O1D-CGD-O2D-CED |
| 11  | cA    | 815 | CLA  | O1D-CGD-O2D-CED |
| 12  | aA    | 832 | F6C  | O1A-CGA-O2A-C1  |
| 12  | bA    | 832 | F6C  | O1A-CGA-O2A-C1  |
| 12  | cA    | 832 | F6C  | O1A-CGA-O2A-C1  |
| 15  | aA    | 847 | BCR  | C16-C17-C18-C19 |
| 15  | aA    | 849 | BCR  | C20-C21-C22-C23 |
| 15  | aB    | 848 | BCR  | C11-C10-C9-C8   |
| 15  | aK    | 102 | BCR  | C20-C21-C22-C23 |
| 15  | aL    | 203 | BCR  | C20-C21-C22-C23 |
| 15  | aL    | 208 | BCR  | C20-C21-C22-C23 |
| 15  | bA    | 847 | BCR  | C16-C17-C18-C19 |
| 15  | bA    | 849 | BCR  | C20-C21-C22-C23 |
| 15  | bB    | 848 | BCR  | C11-C10-C9-C8   |
| 15  | bK    | 102 | BCR  | C20-C21-C22-C23 |
| 15  | bL    | 203 | BCR  | C20-C21-C22-C23 |
| 15  | bL    | 208 | BCR  | C20-C21-C22-C23 |
| 15  | cA    | 847 | BCR  | C16-C17-C18-C19 |
| 15  | cA    | 849 | BCR  | C20-C21-C22-C23 |
| 15  | cB    | 848 | BCR  | C11-C10-C9-C8   |
| 15  | cK    | 102 | BCR  | C20-C21-C22-C23 |
| 15  | cL    | 203 | BCR  | C20-C21-C22-C23 |
| 15  | cL    | 208 | BCR  | C20-C21-C22-C23 |
| 11  | aA    | 821 | CLA  | C2-C1-O2A-CGA   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | aB    | 802 | CLA  | C2-C1-O2A-CGA   |
| 11  | bA    | 821 | CLA  | C2-C1-O2A-CGA   |
| 11  | bB    | 802 | CLA  | C2-C1-O2A-CGA   |
| 11  | cA    | 821 | CLA  | C2-C1-O2A-CGA   |
| 11  | cB    | 802 | CLA  | C2-C1-O2A-CGA   |
| 12  | aA    | 826 | F6C  | C2-C1-O2A-CGA   |
| 12  | bA    | 826 | F6C  | C2-C1-O2A-CGA   |
| 12  | cA    | 826 | F6C  | C2-C1-O2A-CGA   |
| 11  | aB    | 837 | CLA  | C6-C7-C8-C10    |
| 11  | bB    | 837 | CLA  | C6-C7-C8-C10    |
| 11  | cB    | 837 | CLA  | C6-C7-C8-C10    |
| 11  | aB    | 826 | CLA  | O1A-CGA-O2A-C1  |
| 11  | bA    | 808 | CLA  | O1A-CGA-O2A-C1  |
| 11  | bB    | 826 | CLA  | O1A-CGA-O2A-C1  |
| 11  | cA    | 808 | CLA  | O1A-CGA-O2A-C1  |
| 11  | cB    | 826 | CLA  | O1A-CGA-O2A-C1  |
| 11  | aA    | 822 | CLA  | C13-C15-C16-C17 |
| 11  | bA    | 822 | CLA  | C13-C15-C16-C17 |
| 15  | aB    | 842 | BCR  | C14-C15-C16-C17 |
| 15  | aB    | 848 | BCR  | C14-C15-C16-C17 |
| 15  | bB    | 842 | BCR  | C14-C15-C16-C17 |
| 15  | bB    | 848 | BCR  | C14-C15-C16-C17 |
| 15  | cB    | 842 | BCR  | C14-C15-C16-C17 |
| 15  | cB    | 848 | BCR  | C14-C15-C16-C17 |
| 18  | aB    | 847 | LMG  | C29-C30-C31-C32 |
| 18  | bB    | 847 | LMG  | C29-C30-C31-C32 |
| 18  | cB    | 847 | LMG  | C29-C30-C31-C32 |
| 11  | aA    | 831 | CLA  | C8-C10-C11-C12  |
| 11  | bA    | 831 | CLA  | C8-C10-C11-C12  |
| 11  | cA    | 822 | CLA  | C13-C15-C16-C17 |
| 11  | cA    | 831 | CLA  | C8-C10-C11-C12  |
| 11  | aA    | 808 | CLA  | O1A-CGA-O2A-C1  |
| 11  | aA    | 807 | CLA  | CBA-CGA-O2A-C1  |
| 11  | aB    | 831 | CLA  | CBA-CGA-O2A-C1  |
| 11  | bA    | 807 | CLA  | CBA-CGA-O2A-C1  |
| 11  | bB    | 831 | CLA  | CBA-CGA-O2A-C1  |
| 11  | cA    | 807 | CLA  | CBA-CGA-O2A-C1  |
| 11  | cB    | 831 | CLA  | CBA-CGA-O2A-C1  |
| 11  | aA    | 810 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aA    | 811 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aA    | 814 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aA    | 822 | CLA  | C4B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | aA    | 823 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aA    | 825 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aA    | 835 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aA    | 836 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aA    | 841 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aB    | 815 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aB    | 816 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aB    | 820 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aB    | 830 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aB    | 835 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aB    | 837 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bA    | 810 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bA    | 811 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bA    | 814 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bA    | 822 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bA    | 823 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bA    | 825 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bA    | 835 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bA    | 836 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bA    | 841 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bB    | 815 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bB    | 816 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bB    | 820 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bB    | 830 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bB    | 834 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bB    | 835 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bB    | 837 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cA    | 810 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cA    | 811 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cA    | 814 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cA    | 822 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cA    | 823 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cA    | 825 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cA    | 835 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cA    | 836 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cA    | 841 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cB    | 815 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cB    | 816 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cB    | 820 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cB    | 830 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cB    | 834 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cB    | 835 | CLA  | C4B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | cB    | 837 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aA    | 813 | CLA  | C2A-CAA-CBA-CGA |
| 11  | aB    | 826 | CLA  | C2A-CAA-CBA-CGA |
| 11  | bB    | 826 | CLA  | C2A-CAA-CBA-CGA |
| 11  | cA    | 813 | CLA  | C2A-CAA-CBA-CGA |
| 11  | cB    | 826 | CLA  | C2A-CAA-CBA-CGA |
| 11  | aB    | 806 | CLA  | C13-C15-C16-C17 |
| 11  | aA    | 814 | CLA  | C12-C13-C15-C16 |
| 11  | aB    | 816 | CLA  | C11-C10-C8-C7   |
| 11  | aL    | 205 | CLA  | C11-C12-C13-C15 |
| 11  | bA    | 814 | CLA  | C12-C13-C15-C16 |
| 11  | bB    | 816 | CLA  | C11-C10-C8-C7   |
| 11  | bL    | 205 | CLA  | C11-C12-C13-C15 |
| 11  | cA    | 814 | CLA  | C12-C13-C15-C16 |
| 11  | cB    | 816 | CLA  | C11-C10-C8-C7   |
| 11  | cL    | 205 | CLA  | C11-C12-C13-C15 |
| 11  | aL    | 206 | CLA  | C8-C10-C11-C12  |
| 11  | bB    | 806 | CLA  | C13-C15-C16-C17 |
| 11  | bL    | 206 | CLA  | C8-C10-C11-C12  |
| 11  | cB    | 806 | CLA  | C13-C15-C16-C17 |
| 11  | cL    | 206 | CLA  | C8-C10-C11-C12  |
| 11  | cB    | 823 | CLA  | C5-C6-C7-C8     |
| 11  | aB    | 809 | CLA  | O1A-CGA-O2A-C1  |
| 11  | bB    | 809 | CLA  | O1A-CGA-O2A-C1  |
| 11  | cB    | 809 | CLA  | O1A-CGA-O2A-C1  |
| 11  | aA    | 802 | CLA  | C3A-C2A-CAA-CBA |
| 11  | aA    | 804 | CLA  | C3A-C2A-CAA-CBA |
| 11  | aA    | 814 | CLA  | C3A-C2A-CAA-CBA |
| 11  | aA    | 821 | CLA  | C3A-C2A-CAA-CBA |
| 11  | aA    | 837 | CLA  | C3A-C2A-CAA-CBA |
| 11  | aA    | 838 | CLA  | C3A-C2A-CAA-CBA |
| 11  | aB    | 825 | CLA  | C3A-C2A-CAA-CBA |
| 11  | aB    | 826 | CLA  | C3A-C2A-CAA-CBA |
| 11  | aB    | 836 | CLA  | C3A-C2A-CAA-CBA |
| 11  | bA    | 802 | CLA  | C3A-C2A-CAA-CBA |
| 11  | bA    | 804 | CLA  | C3A-C2A-CAA-CBA |
| 11  | bA    | 814 | CLA  | C3A-C2A-CAA-CBA |
| 11  | bA    | 821 | CLA  | C3A-C2A-CAA-CBA |
| 11  | bA    | 837 | CLA  | C3A-C2A-CAA-CBA |
| 11  | bA    | 838 | CLA  | C3A-C2A-CAA-CBA |
| 11  | bB    | 825 | CLA  | C3A-C2A-CAA-CBA |
| 11  | bB    | 826 | CLA  | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | bB    | 836 | CLA  | C3A-C2A-CAA-CBA |
| 11  | cA    | 802 | CLA  | C3A-C2A-CAA-CBA |
| 11  | cA    | 804 | CLA  | C3A-C2A-CAA-CBA |
| 11  | cA    | 814 | CLA  | C3A-C2A-CAA-CBA |
| 11  | cA    | 821 | CLA  | C3A-C2A-CAA-CBA |
| 11  | cA    | 837 | CLA  | C3A-C2A-CAA-CBA |
| 11  | cA    | 838 | CLA  | C3A-C2A-CAA-CBA |
| 11  | cB    | 825 | CLA  | C3A-C2A-CAA-CBA |
| 11  | cB    | 826 | CLA  | C3A-C2A-CAA-CBA |
| 11  | cB    | 836 | CLA  | C3A-C2A-CAA-CBA |
| 11  | aB    | 823 | CLA  | C5-C6-C7-C8     |
| 11  | bB    | 823 | CLA  | C5-C6-C7-C8     |
| 18  | aB    | 847 | LMG  | C39-C40-C41-C42 |
| 11  | aB    | 806 | CLA  | C2-C3-C5-C6     |
| 11  | bB    | 806 | CLA  | C2-C3-C5-C6     |
| 11  | cB    | 806 | CLA  | C2-C3-C5-C6     |
| 17  | aA    | 853 | LMT  | C1-C2-C3-C4     |
| 17  | bA    | 853 | LMT  | C1-C2-C3-C4     |
| 17  | cA    | 853 | LMT  | C1-C2-C3-C4     |
| 18  | bB    | 847 | LMG  | C39-C40-C41-C42 |
| 18  | cB    | 847 | LMG  | C39-C40-C41-C42 |
| 11  | cB    | 806 | CLA  | C10-C11-C12-C13 |
| 11  | aB    | 806 | CLA  | C10-C11-C12-C13 |
| 11  | bB    | 806 | CLA  | C10-C11-C12-C13 |
| 11  | aB    | 836 | CLA  | CBA-CGA-O2A-C1  |
| 11  | bB    | 836 | CLA  | CBA-CGA-O2A-C1  |
| 11  | cB    | 836 | CLA  | CBA-CGA-O2A-C1  |
| 16  | aA    | 852 | LHG  | C32-C33-C34-C35 |
| 16  | bA    | 852 | LHG  | C28-C29-C30-C31 |
| 16  | bA    | 852 | LHG  | C32-C33-C34-C35 |
| 16  | bA    | 852 | LHG  | C34-C35-C36-C37 |
| 16  | cA    | 852 | LHG  | C32-C33-C34-C35 |
| 16  | aA    | 852 | LHG  | C28-C29-C30-C31 |
| 16  | aA    | 852 | LHG  | C34-C35-C36-C37 |
| 16  | cA    | 852 | LHG  | C28-C29-C30-C31 |
| 16  | cA    | 852 | LHG  | C34-C35-C36-C37 |
| 17  | aA    | 853 | LMT  | C2-C3-C4-C5     |
| 17  | bA    | 853 | LMT  | C2-C3-C4-C5     |
| 17  | cA    | 853 | LMT  | C2-C3-C4-C5     |
| 18  | bB    | 847 | LMG  | C41-C42-C43-C44 |
| 18  | cB    | 847 | LMG  | C41-C42-C43-C44 |
| 18  | aB    | 847 | LMG  | C41-C42-C43-C44 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | bB    | 838 | CLA  | O1D-CGD-O2D-CED |
| 16  | aA    | 852 | LHG  | C27-C28-C29-C30 |
| 16  | bA    | 852 | LHG  | C27-C28-C29-C30 |
| 16  | cA    | 852 | LHG  | C27-C28-C29-C30 |
| 18  | aB    | 847 | LMG  | C35-C36-C37-C38 |
| 11  | aB    | 837 | CLA  | C6-C7-C8-C9     |
| 11  | bB    | 837 | CLA  | C6-C7-C8-C9     |
| 11  | cB    | 837 | CLA  | C6-C7-C8-C9     |
| 11  | aA    | 804 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aA    | 812 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aA    | 820 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aA    | 824 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aA    | 825 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aA    | 841 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aB    | 801 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aB    | 807 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aB    | 811 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aB    | 815 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aB    | 816 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aB    | 830 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aB    | 831 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aB    | 834 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aB    | 835 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aB    | 839 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aB    | 840 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aK    | 101 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aK    | 103 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bA    | 804 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bA    | 812 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bA    | 820 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bA    | 824 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bA    | 825 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bA    | 841 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bB    | 801 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bB    | 807 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bB    | 811 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bB    | 815 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bB    | 816 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bB    | 830 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bB    | 831 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bB    | 834 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bB    | 835 | CLA  | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | bB    | 839 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bB    | 840 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bK    | 103 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cA    | 804 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cA    | 812 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cA    | 820 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cA    | 824 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cA    | 825 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cA    | 841 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cB    | 801 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cB    | 807 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cB    | 811 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cB    | 815 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cB    | 816 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cB    | 830 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cB    | 831 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cB    | 834 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cB    | 835 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cB    | 839 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cB    | 840 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cK    | 103 | CLA  | C2B-C3B-CAB-CBB |
| 15  | aA    | 848 | BCR  | C1-C6-C7-C8     |
| 15  | aA    | 848 | BCR  | C5-C6-C7-C8     |
| 15  | aB    | 843 | BCR  | C1-C6-C7-C8     |
| 15  | aB    | 843 | BCR  | C5-C6-C7-C8     |
| 15  | aB    | 845 | BCR  | C23-C24-C25-C26 |
| 15  | aB    | 845 | BCR  | C23-C24-C25-C30 |
| 15  | bA    | 848 | BCR  | C1-C6-C7-C8     |
| 15  | bA    | 848 | BCR  | C5-C6-C7-C8     |
| 15  | bB    | 843 | BCR  | C1-C6-C7-C8     |
| 15  | bB    | 843 | BCR  | C5-C6-C7-C8     |
| 15  | bB    | 845 | BCR  | C23-C24-C25-C26 |
| 15  | bB    | 845 | BCR  | C23-C24-C25-C30 |
| 15  | cA    | 848 | BCR  | C1-C6-C7-C8     |
| 15  | cA    | 848 | BCR  | C5-C6-C7-C8     |
| 15  | cB    | 843 | BCR  | C1-C6-C7-C8     |
| 15  | cB    | 843 | BCR  | C5-C6-C7-C8     |
| 15  | cB    | 845 | BCR  | C23-C24-C25-C26 |
| 15  | cB    | 845 | BCR  | C23-C24-C25-C30 |
| 18  | bB    | 847 | LMG  | C35-C36-C37-C38 |
| 18  | cB    | 847 | LMG  | C35-C36-C37-C38 |
| 11  | aA    | 819 | CLA  | CBA-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | aA    | 833 | CLA  | CBA-CGA-O2A-C1  |
| 11  | aB    | 812 | CLA  | CBA-CGA-O2A-C1  |
| 11  | bA    | 819 | CLA  | CBA-CGA-O2A-C1  |
| 11  | bA    | 833 | CLA  | CBA-CGA-O2A-C1  |
| 11  | bB    | 812 | CLA  | CBA-CGA-O2A-C1  |
| 11  | cA    | 819 | CLA  | CBA-CGA-O2A-C1  |
| 11  | cA    | 833 | CLA  | CBA-CGA-O2A-C1  |
| 11  | cB    | 812 | CLA  | CBA-CGA-O2A-C1  |
| 10  | aA    | 801 | CL0  | C15-C16-C17-C18 |
| 10  | bA    | 801 | CL0  | C15-C16-C17-C18 |
| 10  | cA    | 801 | CL0  | C15-C16-C17-C18 |
| 12  | aL    | 202 | F6C  | C13-C15-C16-C17 |
| 12  | bL    | 202 | F6C  | C13-C15-C16-C17 |
| 12  | cL    | 202 | F6C  | C13-C15-C16-C17 |
| 11  | aB    | 818 | CLA  | C3-C5-C6-C7     |
| 11  | aL    | 206 | CLA  | C3-C5-C6-C7     |
| 11  | bB    | 818 | CLA  | C3-C5-C6-C7     |
| 11  | bL    | 206 | CLA  | C3-C5-C6-C7     |
| 11  | cB    | 818 | CLA  | C3-C5-C6-C7     |
| 11  | cL    | 206 | CLA  | C3-C5-C6-C7     |
| 11  | aB    | 838 | CLA  | O1D-CGD-O2D-CED |
| 11  | cB    | 838 | CLA  | O1D-CGD-O2D-CED |
| 11  | aB    | 827 | CLA  | C2A-CAA-CBA-CGA |
| 11  | bA    | 813 | CLA  | C2A-CAA-CBA-CGA |
| 11  | bB    | 827 | CLA  | C2A-CAA-CBA-CGA |
| 11  | cB    | 827 | CLA  | C2A-CAA-CBA-CGA |
| 11  | aA    | 807 | CLA  | O1A-CGA-O2A-C1  |
| 11  | aB    | 831 | CLA  | O1A-CGA-O2A-C1  |
| 11  | bA    | 807 | CLA  | O1A-CGA-O2A-C1  |
| 11  | bB    | 831 | CLA  | O1A-CGA-O2A-C1  |
| 11  | cA    | 807 | CLA  | O1A-CGA-O2A-C1  |
| 11  | cB    | 831 | CLA  | O1A-CGA-O2A-C1  |
| 11  | aA    | 822 | CLA  | C4-C3-C5-C6     |
| 11  | aB    | 823 | CLA  | C4-C3-C5-C6     |
| 11  | bA    | 822 | CLA  | C4-C3-C5-C6     |
| 11  | bB    | 823 | CLA  | C4-C3-C5-C6     |
| 11  | cA    | 822 | CLA  | C4-C3-C5-C6     |
| 11  | cB    | 823 | CLA  | C4-C3-C5-C6     |
| 15  | aB    | 842 | BCR  | C10-C11-C12-C13 |
| 15  | aB    | 848 | BCR  | C18-C19-C20-C21 |
| 15  | bB    | 842 | BCR  | C10-C11-C12-C13 |
| 15  | bB    | 848 | BCR  | C18-C19-C20-C21 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 15  | cB    | 842 | BCR  | C10-C11-C12-C13 |
| 15  | cB    | 848 | BCR  | C18-C19-C20-C21 |
| 11  | aA    | 803 | CLA  | C6-C7-C8-C9     |
| 11  | aB    | 805 | CLA  | C6-C7-C8-C9     |
| 11  | bA    | 803 | CLA  | C6-C7-C8-C9     |
| 11  | bB    | 805 | CLA  | C6-C7-C8-C9     |
| 11  | cB    | 805 | CLA  | C6-C7-C8-C9     |
| 11  | cL    | 206 | CLA  | C14-C13-C15-C16 |
| 11  | bB    | 803 | CLA  | C10-C11-C12-C13 |
| 11  | cB    | 803 | CLA  | C10-C11-C12-C13 |
| 15  | aA    | 849 | BCR  | C6-C7-C8-C9     |
| 15  | aB    | 846 | BCR  | C22-C23-C24-C25 |
| 15  | bA    | 849 | BCR  | C6-C7-C8-C9     |
| 15  | bB    | 846 | BCR  | C22-C23-C24-C25 |
| 15  | cA    | 849 | BCR  | C6-C7-C8-C9     |
| 15  | cB    | 846 | BCR  | C22-C23-C24-C25 |
| 11  | aB    | 803 | CLA  | C10-C11-C12-C13 |
| 10  | aA    | 801 | CL0  | C3-C5-C6-C7     |
| 10  | bA    | 801 | CL0  | C3-C5-C6-C7     |
| 10  | cA    | 801 | CL0  | C3-C5-C6-C7     |
| 12  | aA    | 844 | F6C  | C3-C5-C6-C7     |
| 12  | bA    | 844 | F6C  | C3-C5-C6-C7     |
| 12  | cA    | 844 | F6C  | C3-C5-C6-C7     |
| 16  | aA    | 852 | LHG  | C8-C7-O7-C5     |
| 16  | bA    | 852 | LHG  | C8-C7-O7-C5     |
| 16  | cA    | 852 | LHG  | C8-C7-O7-C5     |
| 12  | aA    | 844 | F6C  | C1A-C2A-CAA-CBA |
| 12  | bA    | 844 | F6C  | C1A-C2A-CAA-CBA |
| 12  | cA    | 844 | F6C  | C1A-C2A-CAA-CBA |
| 11  | bB    | 804 | CLA  | CBD-CGD-O2D-CED |
| 11  | cB    | 804 | CLA  | CBD-CGD-O2D-CED |
| 15  | aA    | 851 | BCR  | C36-C18-C19-C20 |
| 15  | bA    | 851 | BCR  | C36-C18-C19-C20 |
| 15  | cA    | 851 | BCR  | C36-C18-C19-C20 |
| 11  | aA    | 822 | CLA  | C16-C17-C18-C19 |
| 11  | bA    | 822 | CLA  | C16-C17-C18-C19 |
| 11  | cA    | 822 | CLA  | C16-C17-C18-C19 |
| 11  | aA    | 834 | CLA  | CBD-CGD-O2D-CED |
| 11  | aB    | 804 | CLA  | CBD-CGD-O2D-CED |
| 11  | aA    | 806 | CLA  | C4-C3-C5-C6     |
| 11  | aA    | 818 | CLA  | C4-C3-C5-C6     |
| 11  | bA    | 806 | CLA  | C4-C3-C5-C6     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | bA    | 818 | CLA  | C4-C3-C5-C6     |
| 11  | cA    | 806 | CLA  | C4-C3-C5-C6     |
| 11  | cA    | 818 | CLA  | C4-C3-C5-C6     |
| 11  | aL    | 206 | CLA  | C13-C15-C16-C17 |
| 11  | bL    | 206 | CLA  | C13-C15-C16-C17 |
| 11  | cL    | 206 | CLA  | C13-C15-C16-C17 |
| 11  | bA    | 834 | CLA  | CBD-CGD-O2D-CED |
| 11  | cA    | 834 | CLA  | CBD-CGD-O2D-CED |
| 11  | aB    | 836 | CLA  | O1A-CGA-O2A-C1  |
| 11  | bB    | 836 | CLA  | O1A-CGA-O2A-C1  |
| 11  | cB    | 836 | CLA  | O1A-CGA-O2A-C1  |
| 11  | aA    | 835 | CLA  | C13-C15-C16-C17 |
| 11  | cA    | 835 | CLA  | C13-C15-C16-C17 |
| 11  | bA    | 835 | CLA  | C13-C15-C16-C17 |
| 11  | aB    | 839 | CLA  | C13-C15-C16-C17 |
| 11  | cB    | 839 | CLA  | C13-C15-C16-C17 |
| 11  | bA    | 818 | CLA  | C5-C6-C7-C8     |
| 11  | cA    | 818 | CLA  | C5-C6-C7-C8     |
| 11  | aA    | 818 | CLA  | C5-C6-C7-C8     |
| 11  | aB    | 805 | CLA  | CBA-CGA-O2A-C1  |
| 11  | bB    | 805 | CLA  | CBA-CGA-O2A-C1  |
| 11  | cB    | 805 | CLA  | CBA-CGA-O2A-C1  |
| 11  | bB    | 839 | CLA  | C13-C15-C16-C17 |
| 11  | aA    | 829 | CLA  | C2-C1-O2A-CGA   |
| 11  | bA    | 829 | CLA  | C2-C1-O2A-CGA   |
| 11  | cA    | 829 | CLA  | C2-C1-O2A-CGA   |
| 11  | aB    | 815 | CLA  | C4-C3-C5-C6     |
| 11  | bB    | 815 | CLA  | C4-C3-C5-C6     |
| 11  | cB    | 815 | CLA  | C4-C3-C5-C6     |
| 11  | aA    | 824 | CLA  | C2A-CAA-CBA-CGA |
| 11  | aB    | 815 | CLA  | C2A-CAA-CBA-CGA |
| 11  | aL    | 206 | CLA  | C2A-CAA-CBA-CGA |
| 11  | bA    | 824 | CLA  | C2A-CAA-CBA-CGA |
| 11  | bB    | 815 | CLA  | C2A-CAA-CBA-CGA |
| 11  | bL    | 206 | CLA  | C2A-CAA-CBA-CGA |
| 11  | cA    | 824 | CLA  | C2A-CAA-CBA-CGA |
| 11  | cB    | 815 | CLA  | C2A-CAA-CBA-CGA |
| 11  | cL    | 206 | CLA  | C2A-CAA-CBA-CGA |
| 11  | aA    | 805 | CLA  | CBD-CGD-O2D-CED |
| 11  | bA    | 805 | CLA  | CBD-CGD-O2D-CED |
| 11  | cA    | 805 | CLA  | CBD-CGD-O2D-CED |
| 11  | aA    | 819 | CLA  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | aA    | 833 | CLA  | O1A-CGA-O2A-C1  |
| 11  | bA    | 819 | CLA  | O1A-CGA-O2A-C1  |
| 11  | bA    | 833 | CLA  | O1A-CGA-O2A-C1  |
| 11  | cA    | 819 | CLA  | O1A-CGA-O2A-C1  |
| 11  | cA    | 833 | CLA  | O1A-CGA-O2A-C1  |
| 11  | cB    | 812 | CLA  | O1A-CGA-O2A-C1  |
| 11  | aA    | 840 | CLA  | C3-C5-C6-C7     |
| 11  | bA    | 840 | CLA  | C3-C5-C6-C7     |
| 11  | cA    | 840 | CLA  | C3-C5-C6-C7     |
| 11  | aA    | 804 | CLA  | C1A-C2A-CAA-CBA |
| 11  | aA    | 808 | CLA  | C1A-C2A-CAA-CBA |
| 11  | aA    | 809 | CLA  | C1A-C2A-CAA-CBA |
| 11  | aA    | 814 | CLA  | C1A-C2A-CAA-CBA |
| 11  | aA    | 817 | CLA  | C1A-C2A-CAA-CBA |
| 11  | aA    | 819 | CLA  | C1A-C2A-CAA-CBA |
| 11  | aA    | 833 | CLA  | C1A-C2A-CAA-CBA |
| 11  | aA    | 838 | CLA  | C1A-C2A-CAA-CBA |
| 11  | aB    | 810 | CLA  | C1A-C2A-CAA-CBA |
| 11  | aB    | 814 | CLA  | C1A-C2A-CAA-CBA |
| 11  | aB    | 818 | CLA  | C1A-C2A-CAA-CBA |
| 11  | aB    | 819 | CLA  | C1A-C2A-CAA-CBA |
| 11  | aB    | 825 | CLA  | C1A-C2A-CAA-CBA |
| 11  | aB    | 829 | CLA  | C1A-C2A-CAA-CBA |
| 11  | aB    | 836 | CLA  | C1A-C2A-CAA-CBA |
| 11  | aB    | 838 | CLA  | C1A-C2A-CAA-CBA |
| 11  | bA    | 804 | CLA  | C1A-C2A-CAA-CBA |
| 11  | bA    | 808 | CLA  | C1A-C2A-CAA-CBA |
| 11  | bA    | 809 | CLA  | C1A-C2A-CAA-CBA |
| 11  | bA    | 814 | CLA  | C1A-C2A-CAA-CBA |
| 11  | bA    | 817 | CLA  | C1A-C2A-CAA-CBA |
| 11  | bA    | 819 | CLA  | C1A-C2A-CAA-CBA |
| 11  | bA    | 833 | CLA  | C1A-C2A-CAA-CBA |
| 11  | bA    | 838 | CLA  | C1A-C2A-CAA-CBA |
| 11  | bB    | 810 | CLA  | C1A-C2A-CAA-CBA |
| 11  | bB    | 814 | CLA  | C1A-C2A-CAA-CBA |
| 11  | bB    | 818 | CLA  | C1A-C2A-CAA-CBA |
| 11  | bB    | 819 | CLA  | C1A-C2A-CAA-CBA |
| 11  | bB    | 825 | CLA  | C1A-C2A-CAA-CBA |
| 11  | bB    | 829 | CLA  | C1A-C2A-CAA-CBA |
| 11  | bB    | 836 | CLA  | C1A-C2A-CAA-CBA |
| 11  | bB    | 838 | CLA  | C1A-C2A-CAA-CBA |
| 11  | cA    | 804 | CLA  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | cA    | 808 | CLA  | C1A-C2A-CAA-CBA |
| 11  | cA    | 809 | CLA  | C1A-C2A-CAA-CBA |
| 11  | cA    | 814 | CLA  | C1A-C2A-CAA-CBA |
| 11  | cA    | 817 | CLA  | C1A-C2A-CAA-CBA |
| 11  | cA    | 819 | CLA  | C1A-C2A-CAA-CBA |
| 11  | cA    | 833 | CLA  | C1A-C2A-CAA-CBA |
| 11  | cA    | 838 | CLA  | C1A-C2A-CAA-CBA |
| 11  | cB    | 810 | CLA  | C1A-C2A-CAA-CBA |
| 11  | cB    | 814 | CLA  | C1A-C2A-CAA-CBA |
| 11  | cB    | 818 | CLA  | C1A-C2A-CAA-CBA |
| 11  | cB    | 819 | CLA  | C1A-C2A-CAA-CBA |
| 11  | cB    | 825 | CLA  | C1A-C2A-CAA-CBA |
| 11  | cB    | 829 | CLA  | C1A-C2A-CAA-CBA |
| 11  | cB    | 836 | CLA  | C1A-C2A-CAA-CBA |
| 11  | cB    | 838 | CLA  | C1A-C2A-CAA-CBA |
| 11  | aB    | 812 | CLA  | O1A-CGA-O2A-C1  |
| 11  | bB    | 812 | CLA  | O1A-CGA-O2A-C1  |
| 18  | bB    | 847 | LMG  | C36-C37-C38-C39 |
| 18  | aB    | 847 | LMG  | C36-C37-C38-C39 |
| 18  | cB    | 847 | LMG  | C36-C37-C38-C39 |
| 11  | aA    | 825 | CLA  | C11-C12-C13-C15 |
| 11  | aA    | 840 | CLA  | C12-C13-C15-C16 |
| 11  | aB    | 812 | CLA  | C11-C12-C13-C15 |
| 11  | aB    | 825 | CLA  | C11-C12-C13-C15 |
| 11  | bA    | 825 | CLA  | C11-C12-C13-C15 |
| 11  | bA    | 840 | CLA  | C12-C13-C15-C16 |
| 11  | bB    | 812 | CLA  | C11-C12-C13-C15 |
| 11  | bB    | 825 | CLA  | C11-C12-C13-C15 |
| 11  | cA    | 825 | CLA  | C11-C12-C13-C15 |
| 11  | cA    | 840 | CLA  | C12-C13-C15-C16 |
| 11  | cB    | 812 | CLA  | C11-C12-C13-C15 |
| 11  | cB    | 825 | CLA  | C11-C12-C13-C15 |
| 11  | bK    | 103 | CLA  | CBA-CGA-O2A-C1  |
| 11  | aA    | 838 | CLA  | C2A-CAA-CBA-CGA |
| 11  | aB    | 819 | CLA  | C2A-CAA-CBA-CGA |
| 11  | bA    | 838 | CLA  | C2A-CAA-CBA-CGA |
| 11  | bB    | 819 | CLA  | C2A-CAA-CBA-CGA |
| 11  | cA    | 838 | CLA  | C2A-CAA-CBA-CGA |
| 11  | cB    | 819 | CLA  | C2A-CAA-CBA-CGA |
| 11  | aB    | 812 | CLA  | C14-C13-C15-C16 |
| 11  | aL    | 205 | CLA  | C11-C12-C13-C14 |
| 11  | bB    | 812 | CLA  | C14-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | bL    | 205 | CLA  | C11-C12-C13-C14 |
| 11  | cA    | 803 | CLA  | C6-C7-C8-C9     |
| 11  | cB    | 812 | CLA  | C14-C13-C15-C16 |
| 11  | cL    | 205 | CLA  | C11-C12-C13-C14 |
| 13  | aB    | 841 | PQN  | C16-C17-C18-C19 |
| 13  | bB    | 841 | PQN  | C16-C17-C18-C19 |
| 13  | cB    | 841 | PQN  | C16-C17-C18-C19 |
| 18  | aB    | 847 | LMG  | C38-C39-C40-C41 |
| 18  | bB    | 847 | LMG  | C38-C39-C40-C41 |
| 18  | cB    | 847 | LMG  | C38-C39-C40-C41 |
| 11  | bB    | 830 | CLA  | O1D-CGD-O2D-CED |
| 11  | aB    | 816 | CLA  | CBA-CGA-O2A-C1  |
| 11  | aK    | 103 | CLA  | CBA-CGA-O2A-C1  |
| 11  | bB    | 816 | CLA  | CBA-CGA-O2A-C1  |
| 11  | cB    | 816 | CLA  | CBA-CGA-O2A-C1  |
| 11  | cK    | 103 | CLA  | CBA-CGA-O2A-C1  |
| 11  | aB    | 830 | CLA  | O1D-CGD-O2D-CED |
| 11  | cB    | 830 | CLA  | O1D-CGD-O2D-CED |
| 11  | aB    | 808 | CLA  | C15-C16-C17-C18 |
| 11  | bB    | 808 | CLA  | C15-C16-C17-C18 |
| 11  | cB    | 808 | CLA  | C15-C16-C17-C18 |
| 13  | aA    | 845 | PQN  | C23-C25-C26-C27 |
| 13  | bA    | 845 | PQN  | C23-C25-C26-C27 |
| 13  | cA    | 845 | PQN  | C23-C25-C26-C27 |
| 17  | aA    | 853 | LMT  | O5B-C5B-C6B-O6B |
| 17  | bA    | 853 | LMT  | O5B-C5B-C6B-O6B |
| 17  | cA    | 853 | LMT  | O5B-C5B-C6B-O6B |
| 16  | aA    | 852 | LHG  | C29-C30-C31-C32 |
| 16  | cA    | 852 | LHG  | C29-C30-C31-C32 |
| 16  | bA    | 852 | LHG  | C29-C30-C31-C32 |
| 15  | aB    | 844 | BCR  | C20-C21-C22-C37 |
| 15  | bB    | 844 | BCR  | C20-C21-C22-C37 |
| 15  | cB    | 844 | BCR  | C20-C21-C22-C37 |
| 11  | aK    | 103 | CLA  | O1A-CGA-O2A-C1  |
| 11  | bK    | 103 | CLA  | O1A-CGA-O2A-C1  |
| 11  | cK    | 103 | CLA  | O1A-CGA-O2A-C1  |
| 11  | aA    | 806 | CLA  | C2-C3-C5-C6     |
| 11  | aB    | 815 | CLA  | C2-C3-C5-C6     |
| 11  | bA    | 806 | CLA  | C2-C3-C5-C6     |
| 11  | bB    | 815 | CLA  | C2-C3-C5-C6     |
| 11  | cA    | 806 | CLA  | C2-C3-C5-C6     |
| 11  | cB    | 815 | CLA  | C2-C3-C5-C6     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | aA    | 814 | CLA  | C10-C11-C12-C13 |
| 11  | bA    | 814 | CLA  | C10-C11-C12-C13 |
| 15  | cB    | 845 | BCR  | C7-C8-C9-C34    |
| 15  | aA    | 848 | BCR  | C21-C22-C23-C24 |
| 15  | bA    | 848 | BCR  | C21-C22-C23-C24 |
| 15  | cA    | 848 | BCR  | C21-C22-C23-C24 |
| 11  | aA    | 840 | CLA  | C5-C6-C7-C8     |
| 11  | aB    | 816 | CLA  | C8-C10-C11-C12  |
| 11  | bA    | 840 | CLA  | C5-C6-C7-C8     |
| 11  | bB    | 816 | CLA  | C8-C10-C11-C12  |
| 11  | cA    | 814 | CLA  | C10-C11-C12-C13 |
| 11  | cA    | 840 | CLA  | C5-C6-C7-C8     |
| 11  | cB    | 816 | CLA  | C8-C10-C11-C12  |
| 15  | aL    | 207 | BCR  | C10-C11-C12-C13 |
| 15  | bL    | 207 | BCR  | C10-C11-C12-C13 |
| 15  | cL    | 207 | BCR  | C10-C11-C12-C13 |
| 15  | aB    | 846 | BCR  | C11-C10-C9-C8   |
| 15  | aL    | 207 | BCR  | C20-C21-C22-C23 |
| 15  | bB    | 846 | BCR  | C11-C10-C9-C8   |
| 15  | bL    | 207 | BCR  | C20-C21-C22-C23 |
| 15  | cB    | 846 | BCR  | C11-C10-C9-C8   |
| 15  | cL    | 207 | BCR  | C20-C21-C22-C23 |
| 11  | aA    | 806 | CLA  | CBA-CGA-O2A-C1  |
| 11  | bA    | 806 | CLA  | CBA-CGA-O2A-C1  |
| 11  | cA    | 806 | CLA  | CBA-CGA-O2A-C1  |
| 17  | aA    | 853 | LMT  | C3-C4-C5-C6     |
| 17  | bA    | 853 | LMT  | C3-C4-C5-C6     |
| 17  | cA    | 853 | LMT  | C3-C4-C5-C6     |
| 12  | aL    | 202 | F6C  | C3-C5-C6-C7     |
| 11  | aA    | 818 | CLA  | C6-C7-C8-C9     |
| 11  | bA    | 818 | CLA  | C6-C7-C8-C9     |
| 11  | cA    | 818 | CLA  | C6-C7-C8-C9     |
| 16  | aA    | 852 | LHG  | O7-C5-C6-O8     |
| 16  | bA    | 852 | LHG  | O7-C5-C6-O8     |
| 16  | cA    | 852 | LHG  | O7-C5-C6-O8     |
| 16  | bA    | 852 | LHG  | C35-C36-C37-C38 |
| 16  | cA    | 852 | LHG  | C35-C36-C37-C38 |
| 11  | aB    | 815 | CLA  | CAA-CBA-CGA-O2A |
| 11  | bB    | 815 | CLA  | CAA-CBA-CGA-O2A |
| 11  | cB    | 815 | CLA  | CAA-CBA-CGA-O2A |
| 12  | bL    | 202 | F6C  | C3-C5-C6-C7     |
| 12  | cL    | 202 | F6C  | C3-C5-C6-C7     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 16  | aA    | 852 | LHG  | C35-C36-C37-C38 |
| 11  | aB    | 805 | CLA  | C13-C15-C16-C17 |
| 11  | aB    | 825 | CLA  | C8-C10-C11-C12  |
| 11  | bB    | 805 | CLA  | C13-C15-C16-C17 |
| 11  | bB    | 825 | CLA  | C8-C10-C11-C12  |
| 11  | cB    | 805 | CLA  | C13-C15-C16-C17 |
| 11  | cB    | 825 | CLA  | C8-C10-C11-C12  |
| 11  | cB    | 814 | CLA  | O1D-CGD-O2D-CED |
| 12  | aA    | 826 | F6C  | CBA-CGA-O2A-C1  |
| 12  | bA    | 826 | F6C  | CBA-CGA-O2A-C1  |
| 12  | cA    | 826 | F6C  | CBA-CGA-O2A-C1  |
| 11  | aB    | 814 | CLA  | O1D-CGD-O2D-CED |
| 11  | aA    | 829 | CLA  | CBD-CGD-O2D-CED |
| 11  | aB    | 813 | CLA  | CBD-CGD-O2D-CED |
| 11  | bA    | 829 | CLA  | CBD-CGD-O2D-CED |
| 11  | bB    | 813 | CLA  | CBD-CGD-O2D-CED |
| 11  | cA    | 829 | CLA  | CBD-CGD-O2D-CED |
| 11  | cB    | 813 | CLA  | CBD-CGD-O2D-CED |
| 11  | aB    | 840 | CLA  | O1D-CGD-O2D-CED |
| 11  | cB    | 828 | CLA  | O1D-CGD-O2D-CED |
| 11  | cB    | 840 | CLA  | O1D-CGD-O2D-CED |
| 11  | aA    | 833 | CLA  | C10-C11-C12-C13 |
| 11  | bA    | 833 | CLA  | C10-C11-C12-C13 |
| 11  | cA    | 833 | CLA  | C10-C11-C12-C13 |
| 11  | aB    | 828 | CLA  | O1D-CGD-O2D-CED |
| 11  | bB    | 814 | CLA  | O1D-CGD-O2D-CED |
| 11  | bB    | 828 | CLA  | O1D-CGD-O2D-CED |
| 11  | bB    | 840 | CLA  | O1D-CGD-O2D-CED |
| 11  | aA    | 835 | CLA  | C2-C3-C5-C6     |
| 11  | bA    | 835 | CLA  | C2-C3-C5-C6     |
| 11  | cA    | 835 | CLA  | C2-C3-C5-C6     |
| 11  | aB    | 837 | CLA  | C5-C6-C7-C8     |
| 11  | bB    | 837 | CLA  | C5-C6-C7-C8     |
| 11  | cB    | 837 | CLA  | C5-C6-C7-C8     |
| 11  | aA    | 814 | CLA  | C14-C13-C15-C16 |
| 11  | aA    | 821 | CLA  | C6-C7-C8-C9     |
| 11  | aA    | 833 | CLA  | C11-C10-C8-C9   |
| 11  | aA    | 839 | CLA  | C6-C7-C8-C9     |
| 11  | aB    | 806 | CLA  | C6-C7-C8-C9     |
| 11  | aB    | 825 | CLA  | C11-C12-C13-C14 |
| 11  | aL    | 206 | CLA  | C11-C10-C8-C9   |
| 11  | bA    | 814 | CLA  | C14-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | bA    | 821 | CLA  | C6-C7-C8-C9     |
| 11  | bA    | 833 | CLA  | C11-C10-C8-C9   |
| 11  | bA    | 839 | CLA  | C6-C7-C8-C9     |
| 11  | bB    | 806 | CLA  | C6-C7-C8-C9     |
| 11  | bB    | 825 | CLA  | C11-C12-C13-C14 |
| 11  | bL    | 206 | CLA  | C11-C10-C8-C9   |
| 11  | cA    | 814 | CLA  | C14-C13-C15-C16 |
| 11  | cA    | 821 | CLA  | C6-C7-C8-C9     |
| 11  | cA    | 833 | CLA  | C11-C10-C8-C9   |
| 11  | cA    | 839 | CLA  | C6-C7-C8-C9     |
| 11  | cB    | 806 | CLA  | C6-C7-C8-C9     |
| 11  | cB    | 825 | CLA  | C11-C12-C13-C14 |
| 11  | cL    | 206 | CLA  | C11-C10-C8-C9   |
| 11  | aB    | 806 | CLA  | C8-C10-C11-C12  |
| 11  | bB    | 806 | CLA  | C8-C10-C11-C12  |
| 16  | aA    | 852 | LHG  | C2-C3-O3-P      |
| 16  | bA    | 852 | LHG  | C2-C3-O3-P      |
| 16  | cA    | 852 | LHG  | C2-C3-O3-P      |
| 11  | aB    | 816 | CLA  | O1A-CGA-O2A-C1  |
| 11  | bB    | 816 | CLA  | O1A-CGA-O2A-C1  |
| 11  | cB    | 816 | CLA  | O1A-CGA-O2A-C1  |
| 11  | aA    | 808 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aB    | 803 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aB    | 809 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aB    | 810 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aB    | 811 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aB    | 823 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aB    | 826 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aB    | 827 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aB    | 831 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aB    | 834 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aB    | 839 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aB    | 840 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aK    | 101 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aK    | 103 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aL    | 206 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bA    | 808 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bB    | 803 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bB    | 809 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bB    | 810 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bB    | 811 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bB    | 823 | CLA  | C4B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | bB    | 826 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bB    | 827 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bB    | 831 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bB    | 839 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bB    | 840 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bK    | 101 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bK    | 103 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bL    | 206 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cA    | 808 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cB    | 803 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cB    | 809 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cB    | 810 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cB    | 811 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cB    | 823 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cB    | 826 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cB    | 827 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cB    | 831 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cB    | 839 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cB    | 840 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cK    | 101 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cK    | 103 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cL    | 206 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bA    | 841 | CLA  | O1D-CGD-O2D-CED |
| 11  | aA    | 807 | CLA  | C5-C6-C7-C8     |
| 11  | bA    | 807 | CLA  | C5-C6-C7-C8     |
| 11  | cA    | 807 | CLA  | C5-C6-C7-C8     |
| 11  | cB    | 806 | CLA  | C8-C10-C11-C12  |
| 11  | aA    | 841 | CLA  | O1D-CGD-O2D-CED |
| 17  | aA    | 853 | LMT  | C5'-C4'-O1B-C1B |
| 17  | bA    | 853 | LMT  | C5'-C4'-O1B-C1B |
| 17  | cA    | 853 | LMT  | C5'-C4'-O1B-C1B |
| 11  | aA    | 821 | CLA  | C6-C7-C8-C10    |
| 11  | aA    | 825 | CLA  | C11-C10-C8-C7   |
| 11  | aA    | 828 | CLA  | C6-C7-C8-C10    |
| 11  | aA    | 833 | CLA  | C11-C10-C8-C7   |
| 11  | aA    | 833 | CLA  | C12-C13-C15-C16 |
| 11  | aA    | 839 | CLA  | C6-C7-C8-C10    |
| 11  | aA    | 839 | CLA  | C12-C13-C15-C16 |
| 11  | aB    | 806 | CLA  | C6-C7-C8-C10    |
| 11  | aB    | 812 | CLA  | C12-C13-C15-C16 |
| 11  | aL    | 206 | CLA  | C11-C10-C8-C7   |
| 11  | bA    | 821 | CLA  | C6-C7-C8-C10    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | bA    | 825 | CLA  | C11-C10-C8-C7   |
| 11  | bA    | 828 | CLA  | C6-C7-C8-C10    |
| 11  | bA    | 833 | CLA  | C11-C10-C8-C7   |
| 11  | bA    | 833 | CLA  | C12-C13-C15-C16 |
| 11  | bA    | 839 | CLA  | C6-C7-C8-C10    |
| 11  | bA    | 839 | CLA  | C12-C13-C15-C16 |
| 11  | bB    | 806 | CLA  | C6-C7-C8-C10    |
| 11  | bB    | 812 | CLA  | C12-C13-C15-C16 |
| 11  | bL    | 206 | CLA  | C11-C10-C8-C7   |
| 11  | cA    | 821 | CLA  | C6-C7-C8-C10    |
| 11  | cA    | 825 | CLA  | C11-C10-C8-C7   |
| 11  | cA    | 828 | CLA  | C6-C7-C8-C10    |
| 11  | cA    | 833 | CLA  | C11-C10-C8-C7   |
| 11  | cA    | 833 | CLA  | C12-C13-C15-C16 |
| 11  | cA    | 839 | CLA  | C6-C7-C8-C10    |
| 11  | cA    | 839 | CLA  | C12-C13-C15-C16 |
| 11  | cB    | 806 | CLA  | C6-C7-C8-C10    |
| 11  | cB    | 812 | CLA  | C12-C13-C15-C16 |
| 11  | cL    | 206 | CLA  | C11-C10-C8-C7   |
| 13  | aB    | 841 | PQN  | C16-C17-C18-C20 |
| 13  | bB    | 841 | PQN  | C16-C17-C18-C20 |
| 13  | cB    | 841 | PQN  | C16-C17-C18-C20 |
| 11  | aA    | 835 | CLA  | C5-C6-C7-C8     |
| 11  | bA    | 835 | CLA  | C5-C6-C7-C8     |
| 11  | cA    | 835 | CLA  | C5-C6-C7-C8     |
| 11  | bB    | 816 | CLA  | C11-C12-C13-C14 |
| 11  | cB    | 816 | CLA  | C11-C12-C13-C14 |
| 11  | cA    | 841 | CLA  | O1D-CGD-O2D-CED |
| 11  | aB    | 816 | CLA  | C11-C12-C13-C14 |
| 11  | aA    | 807 | CLA  | C4-C3-C5-C6     |
| 11  | aA    | 812 | CLA  | C3A-C2A-CAA-CBA |
| 11  | aA    | 813 | CLA  | C3A-C2A-CAA-CBA |
| 11  | aA    | 829 | CLA  | C3A-C2A-CAA-CBA |
| 11  | aA    | 834 | CLA  | C4-C3-C5-C6     |
| 11  | aA    | 843 | CLA  | C3A-C2A-CAA-CBA |
| 11  | aB    | 815 | CLA  | C3A-C2A-CAA-CBA |
| 11  | aB    | 832 | CLA  | C3A-C2A-CAA-CBA |
| 11  | aB    | 833 | CLA  | C3A-C2A-CAA-CBA |
| 11  | bA    | 807 | CLA  | C4-C3-C5-C6     |
| 11  | bA    | 812 | CLA  | C3A-C2A-CAA-CBA |
| 11  | bA    | 813 | CLA  | C3A-C2A-CAA-CBA |
| 11  | bA    | 829 | CLA  | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | bA    | 834 | CLA  | C4-C3-C5-C6     |
| 11  | bA    | 843 | CLA  | C3A-C2A-CAA-CBA |
| 11  | bB    | 815 | CLA  | C3A-C2A-CAA-CBA |
| 11  | bB    | 832 | CLA  | C3A-C2A-CAA-CBA |
| 11  | bB    | 833 | CLA  | C3A-C2A-CAA-CBA |
| 11  | cA    | 807 | CLA  | C4-C3-C5-C6     |
| 11  | cA    | 812 | CLA  | C3A-C2A-CAA-CBA |
| 11  | cA    | 813 | CLA  | C3A-C2A-CAA-CBA |
| 11  | cA    | 829 | CLA  | C3A-C2A-CAA-CBA |
| 11  | cA    | 834 | CLA  | C4-C3-C5-C6     |
| 11  | cA    | 843 | CLA  | C3A-C2A-CAA-CBA |
| 11  | cB    | 815 | CLA  | C3A-C2A-CAA-CBA |
| 11  | cB    | 832 | CLA  | C3A-C2A-CAA-CBA |
| 11  | cB    | 833 | CLA  | C3A-C2A-CAA-CBA |
| 12  | aA    | 830 | F6C  | C4-C3-C5-C6     |
| 12  | bA    | 830 | F6C  | C4-C3-C5-C6     |
| 12  | cA    | 830 | F6C  | C4-C3-C5-C6     |
| 11  | aB    | 805 | CLA  | O1A-CGA-O2A-C1  |
| 11  | bB    | 805 | CLA  | O1A-CGA-O2A-C1  |
| 11  | cB    | 805 | CLA  | O1A-CGA-O2A-C1  |
| 15  | aB    | 848 | BCR  | C15-C16-C17-C18 |
| 15  | aL    | 207 | BCR  | C9-C10-C11-C12  |
| 15  | bB    | 848 | BCR  | C15-C16-C17-C18 |
| 15  | bL    | 207 | BCR  | C9-C10-C11-C12  |
| 15  | cB    | 848 | BCR  | C15-C16-C17-C18 |
| 15  | cL    | 207 | BCR  | C9-C10-C11-C12  |
| 15  | aB    | 845 | BCR  | C7-C8-C9-C34    |
| 15  | aB    | 846 | BCR  | C7-C8-C9-C34    |
| 15  | bB    | 845 | BCR  | C7-C8-C9-C34    |
| 15  | bB    | 846 | BCR  | C7-C8-C9-C34    |
| 15  | cB    | 846 | BCR  | C7-C8-C9-C34    |
| 11  | aB    | 836 | CLA  | C4-C3-C5-C6     |
| 11  | bB    | 836 | CLA  | C4-C3-C5-C6     |
| 11  | cB    | 836 | CLA  | C4-C3-C5-C6     |
| 11  | aB    | 803 | CLA  | C8-C10-C11-C12  |
| 11  | bB    | 803 | CLA  | C8-C10-C11-C12  |
| 11  | cB    | 803 | CLA  | C8-C10-C11-C12  |
| 11  | aA    | 811 | CLA  | C2A-CAA-CBA-CGA |
| 11  | bA    | 811 | CLA  | C2A-CAA-CBA-CGA |
| 11  | cA    | 811 | CLA  | C2A-CAA-CBA-CGA |
| 16  | aA    | 852 | LHG  | C15-C16-C17-C18 |
| 16  | cA    | 852 | LHG  | C15-C16-C17-C18 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 16  | bA    | 852 | LHG  | C15-C16-C17-C18 |
| 11  | aA    | 803 | CLA  | C4-C3-C5-C6     |
| 11  | aA    | 835 | CLA  | C4-C3-C5-C6     |
| 11  | bA    | 803 | CLA  | C4-C3-C5-C6     |
| 11  | bA    | 835 | CLA  | C4-C3-C5-C6     |
| 11  | cA    | 803 | CLA  | C4-C3-C5-C6     |
| 11  | cA    | 835 | CLA  | C4-C3-C5-C6     |
| 11  | aA    | 834 | CLA  | C2-C3-C5-C6     |
| 11  | cA    | 834 | CLA  | C2-C3-C5-C6     |
| 12  | aA    | 830 | F6C  | C2-C3-C5-C6     |
| 12  | bA    | 830 | F6C  | C2-C3-C5-C6     |
| 12  | cA    | 830 | F6C  | C2-C3-C5-C6     |
| 11  | aB    | 818 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bB    | 818 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bK    | 101 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cB    | 818 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cK    | 101 | CLA  | C2B-C3B-CAB-CBB |
| 15  | aA    | 847 | BCR  | C1-C6-C7-C8     |
| 15  | aA    | 847 | BCR  | C23-C24-C25-C30 |
| 15  | aA    | 848 | BCR  | C23-C24-C25-C30 |
| 15  | aA    | 849 | BCR  | C1-C6-C7-C8     |
| 15  | aA    | 850 | BCR  | C1-C6-C7-C8     |
| 15  | aB    | 842 | BCR  | C1-C6-C7-C8     |
| 15  | aB    | 844 | BCR  | C1-C6-C7-C8     |
| 15  | aB    | 848 | BCR  | C1-C6-C7-C8     |
| 15  | aI    | 101 | BCR  | C1-C6-C7-C8     |
| 15  | aK    | 102 | BCR  | C1-C6-C7-C8     |
| 15  | aL    | 203 | BCR  | C1-C6-C7-C8     |
| 15  | aL    | 203 | BCR  | C5-C6-C7-C8     |
| 15  | aL    | 203 | BCR  | C23-C24-C25-C30 |
| 15  | aL    | 207 | BCR  | C1-C6-C7-C8     |
| 15  | aM    | 101 | BCR  | C1-C6-C7-C8     |
| 15  | bA    | 847 | BCR  | C1-C6-C7-C8     |
| 15  | bA    | 847 | BCR  | C23-C24-C25-C30 |
| 15  | bA    | 848 | BCR  | C23-C24-C25-C30 |
| 15  | bA    | 849 | BCR  | C1-C6-C7-C8     |
| 15  | bA    | 850 | BCR  | C1-C6-C7-C8     |
| 15  | bB    | 842 | BCR  | C1-C6-C7-C8     |
| 15  | bB    | 844 | BCR  | C1-C6-C7-C8     |
| 15  | bB    | 848 | BCR  | C1-C6-C7-C8     |
| 15  | bI    | 101 | BCR  | C1-C6-C7-C8     |
| 15  | bK    | 102 | BCR  | C1-C6-C7-C8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 15  | bL    | 203 | BCR  | C1-C6-C7-C8     |
| 15  | bL    | 203 | BCR  | C5-C6-C7-C8     |
| 15  | bL    | 203 | BCR  | C23-C24-C25-C30 |
| 15  | bL    | 207 | BCR  | C1-C6-C7-C8     |
| 15  | bM    | 101 | BCR  | C1-C6-C7-C8     |
| 15  | cA    | 847 | BCR  | C1-C6-C7-C8     |
| 15  | cA    | 847 | BCR  | C23-C24-C25-C30 |
| 15  | cA    | 848 | BCR  | C23-C24-C25-C30 |
| 15  | cA    | 849 | BCR  | C1-C6-C7-C8     |
| 15  | cA    | 850 | BCR  | C1-C6-C7-C8     |
| 15  | cB    | 842 | BCR  | C1-C6-C7-C8     |
| 15  | cB    | 844 | BCR  | C1-C6-C7-C8     |
| 15  | cB    | 848 | BCR  | C1-C6-C7-C8     |
| 15  | cI    | 103 | BCR  | C1-C6-C7-C8     |
| 15  | cK    | 102 | BCR  | C1-C6-C7-C8     |
| 15  | cL    | 203 | BCR  | C1-C6-C7-C8     |
| 15  | cL    | 203 | BCR  | C5-C6-C7-C8     |
| 15  | cL    | 203 | BCR  | C23-C24-C25-C30 |
| 15  | cL    | 207 | BCR  | C1-C6-C7-C8     |
| 15  | cM    | 101 | BCR  | C1-C6-C7-C8     |
| 11  | aA    | 813 | CLA  | C6-C7-C8-C9     |
| 11  | bA    | 813 | CLA  | C6-C7-C8-C9     |
| 11  | cA    | 813 | CLA  | C6-C7-C8-C9     |
| 11  | aA    | 831 | CLA  | C5-C6-C7-C8     |
| 11  | bA    | 831 | CLA  | C5-C6-C7-C8     |
| 11  | cA    | 831 | CLA  | C5-C6-C7-C8     |
| 12  | aA    | 827 | F6C  | C3A-C2A-CAA-CBA |
| 12  | bA    | 827 | F6C  | C3A-C2A-CAA-CBA |
| 12  | cA    | 827 | F6C  | C3A-C2A-CAA-CBA |
| 11  | aA    | 843 | CLA  | CAA-CBA-CGA-O2A |
| 11  | bA    | 843 | CLA  | CAA-CBA-CGA-O2A |
| 11  | cA    | 843 | CLA  | CAA-CBA-CGA-O2A |
| 11  | aB    | 831 | CLA  | C2A-CAA-CBA-CGA |
| 11  | bB    | 831 | CLA  | C2A-CAA-CBA-CGA |
| 11  | cB    | 831 | CLA  | C2A-CAA-CBA-CGA |
| 11  | aA    | 819 | CLA  | C6-C7-C8-C9     |
| 11  | cA    | 819 | CLA  | C6-C7-C8-C9     |
| 12  | bL    | 202 | F6C  | CBD-CGD-O2D-CED |
| 12  | cL    | 202 | F6C  | CBD-CGD-O2D-CED |
| 11  | bA    | 819 | CLA  | C6-C7-C8-C9     |
| 17  | aA    | 853 | LMT  | C3'-C4'-O1B-C1B |
| 17  | bA    | 853 | LMT  | C3'-C4'-O1B-C1B |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 17  | cA    | 853 | LMT  | C3'-C4'-O1B-C1B |
| 11  | aA    | 803 | CLA  | C2-C3-C5-C6     |
| 11  | aA    | 807 | CLA  | C2-C3-C5-C6     |
| 11  | bA    | 803 | CLA  | C2-C3-C5-C6     |
| 11  | bA    | 807 | CLA  | C2-C3-C5-C6     |
| 11  | bA    | 834 | CLA  | C2-C3-C5-C6     |
| 11  | cA    | 803 | CLA  | C2-C3-C5-C6     |
| 11  | cA    | 807 | CLA  | C2-C3-C5-C6     |
| 11  | aA    | 825 | CLA  | C11-C10-C8-C9   |
| 11  | aA    | 831 | CLA  | C14-C13-C15-C16 |
| 11  | aA    | 835 | CLA  | C14-C13-C15-C16 |
| 11  | aB    | 839 | CLA  | C14-C13-C15-C16 |
| 11  | bA    | 825 | CLA  | C11-C10-C8-C9   |
| 11  | bA    | 831 | CLA  | C14-C13-C15-C16 |
| 11  | bA    | 835 | CLA  | C14-C13-C15-C16 |
| 11  | bB    | 839 | CLA  | C14-C13-C15-C16 |
| 11  | cA    | 825 | CLA  | C11-C10-C8-C9   |
| 11  | cA    | 831 | CLA  | C14-C13-C15-C16 |
| 11  | cA    | 835 | CLA  | C14-C13-C15-C16 |
| 11  | cB    | 839 | CLA  | C14-C13-C15-C16 |
| 18  | aB    | 847 | LMG  | O6-C1-O1-C7     |
| 18  | bB    | 847 | LMG  | O6-C1-O1-C7     |
| 18  | cB    | 847 | LMG  | O6-C1-O1-C7     |
| 12  | aL    | 202 | F6C  | CBD-CGD-O2D-CED |
| 11  | aA    | 835 | CLA  | C2A-CAA-CBA-CGA |
| 11  | bA    | 835 | CLA  | C2A-CAA-CBA-CGA |
| 11  | cA    | 835 | CLA  | C2A-CAA-CBA-CGA |
| 16  | aA    | 852 | LHG  | O1-C1-C2-O2     |
| 16  | bA    | 852 | LHG  | O1-C1-C2-O2     |
| 16  | cA    | 852 | LHG  | O1-C1-C2-O2     |
| 15  | aB    | 842 | BCR  | C15-C16-C17-C18 |
| 15  | bB    | 842 | BCR  | C15-C16-C17-C18 |
| 15  | cB    | 842 | BCR  | C15-C16-C17-C18 |
| 11  | aA    | 822 | CLA  | C15-C16-C17-C18 |
| 11  | bA    | 822 | CLA  | C15-C16-C17-C18 |
| 11  | cA    | 834 | CLA  | O1D-CGD-O2D-CED |
| 11  | cA    | 822 | CLA  | C15-C16-C17-C18 |
| 12  | aA    | 830 | F6C  | C5-C6-C7-C8     |
| 12  | cA    | 830 | F6C  | C5-C6-C7-C8     |
| 15  | aB    | 842 | BCR  | C16-C17-C18-C36 |
| 15  | bB    | 842 | BCR  | C16-C17-C18-C36 |
| 15  | cB    | 842 | BCR  | C16-C17-C18-C36 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | aB    | 815 | CLA  | C3-C5-C6-C7     |
| 11  | bB    | 815 | CLA  | C3-C5-C6-C7     |
| 11  | cB    | 815 | CLA  | C3-C5-C6-C7     |
| 12  | bA    | 827 | F6C  | C3-C5-C6-C7     |
| 11  | bA    | 834 | CLA  | O1D-CGD-O2D-CED |
| 12  | bA    | 830 | F6C  | C5-C6-C7-C8     |
| 11  | cA    | 822 | CLA  | C16-C17-C18-C20 |
| 11  | aB    | 812 | CLA  | C8-C10-C11-C12  |
| 15  | aA    | 851 | BCR  | C7-C8-C9-C34    |
| 15  | aL    | 207 | BCR  | C7-C8-C9-C34    |
| 15  | bA    | 851 | BCR  | C7-C8-C9-C34    |
| 15  | bL    | 207 | BCR  | C7-C8-C9-C34    |
| 15  | cA    | 851 | BCR  | C7-C8-C9-C34    |
| 15  | cL    | 207 | BCR  | C7-C8-C9-C34    |
| 11  | aA    | 807 | CLA  | C12-C13-C15-C16 |
| 11  | aA    | 812 | CLA  | C6-C7-C8-C10    |
| 11  | aA    | 831 | CLA  | C12-C13-C15-C16 |
| 11  | aA    | 835 | CLA  | C12-C13-C15-C16 |
| 11  | aA    | 840 | CLA  | C6-C7-C8-C10    |
| 11  | aB    | 839 | CLA  | C12-C13-C15-C16 |
| 11  | bA    | 807 | CLA  | C12-C13-C15-C16 |
| 11  | bA    | 812 | CLA  | C6-C7-C8-C10    |
| 11  | bA    | 831 | CLA  | C12-C13-C15-C16 |
| 11  | bA    | 835 | CLA  | C12-C13-C15-C16 |
| 11  | bA    | 840 | CLA  | C6-C7-C8-C10    |
| 11  | bB    | 839 | CLA  | C12-C13-C15-C16 |
| 11  | cA    | 807 | CLA  | C12-C13-C15-C16 |
| 11  | cA    | 812 | CLA  | C6-C7-C8-C10    |
| 11  | cA    | 831 | CLA  | C12-C13-C15-C16 |
| 11  | cA    | 835 | CLA  | C12-C13-C15-C16 |
| 11  | cA    | 840 | CLA  | C6-C7-C8-C10    |
| 11  | cB    | 839 | CLA  | C12-C13-C15-C16 |
| 12  | aA    | 827 | F6C  | C3-C5-C6-C7     |
| 12  | cA    | 827 | F6C  | C3-C5-C6-C7     |
| 11  | aA    | 825 | CLA  | C8-C10-C11-C12  |
| 11  | bA    | 825 | CLA  | C8-C10-C11-C12  |
| 11  | bB    | 812 | CLA  | C8-C10-C11-C12  |
| 11  | cA    | 825 | CLA  | C8-C10-C11-C12  |
| 11  | cB    | 812 | CLA  | C8-C10-C11-C12  |
| 15  | aB    | 848 | BCR  | C7-C8-C9-C10    |
| 15  | bB    | 848 | BCR  | C7-C8-C9-C10    |
| 15  | cB    | 848 | BCR  | C7-C8-C9-C10    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | aA    | 834 | CLA  | O1D-CGD-O2D-CED |
| 11  | aB    | 803 | CLA  | C2A-CAA-CBA-CGA |
| 11  | bB    | 803 | CLA  | C2A-CAA-CBA-CGA |
| 11  | cB    | 803 | CLA  | C2A-CAA-CBA-CGA |
| 11  | aA    | 822 | CLA  | C16-C17-C18-C20 |
| 11  | bA    | 822 | CLA  | C16-C17-C18-C20 |
| 12  | aA    | 826 | F6C  | O1A-CGA-O2A-C1  |
| 12  | bA    | 826 | F6C  | O1A-CGA-O2A-C1  |
| 12  | cA    | 826 | F6C  | O1A-CGA-O2A-C1  |
| 12  | aA    | 827 | F6C  | C2B-C3B-CAB-CBB |
| 12  | aA    | 832 | F6C  | C2B-C3B-CAB-CBB |
| 12  | bA    | 827 | F6C  | C2B-C3B-CAB-CBB |
| 12  | bA    | 832 | F6C  | C2B-C3B-CAB-CBB |
| 12  | cA    | 827 | F6C  | C2B-C3B-CAB-CBB |
| 12  | cA    | 832 | F6C  | C2B-C3B-CAB-CBB |
| 11  | aB    | 817 | CLA  | CBD-CGD-O2D-CED |
| 10  | aA    | 801 | CL0  | C13-C15-C16-C17 |
| 10  | bA    | 801 | CL0  | C13-C15-C16-C17 |
| 10  | cA    | 801 | CL0  | C13-C15-C16-C17 |
| 11  | bB    | 817 | CLA  | CBD-CGD-O2D-CED |
| 11  | cB    | 817 | CLA  | CBD-CGD-O2D-CED |
| 11  | aA    | 822 | CLA  | C2-C3-C5-C6     |
| 11  | bA    | 822 | CLA  | C2-C3-C5-C6     |
| 11  | cA    | 822 | CLA  | C2-C3-C5-C6     |
| 11  | aB    | 805 | CLA  | C10-C11-C12-C13 |
| 11  | bB    | 805 | CLA  | C10-C11-C12-C13 |
| 11  | cB    | 805 | CLA  | C10-C11-C12-C13 |
| 11  | aA    | 840 | CLA  | C16-C17-C18-C19 |
| 11  | bA    | 840 | CLA  | C16-C17-C18-C19 |
| 11  | cA    | 840 | CLA  | C16-C17-C18-C19 |
| 11  | aL    | 206 | CLA  | C10-C11-C12-C13 |
| 11  | bL    | 206 | CLA  | C10-C11-C12-C13 |
| 11  | aA    | 806 | CLA  | O1A-CGA-O2A-C1  |
| 11  | bA    | 806 | CLA  | O1A-CGA-O2A-C1  |
| 11  | cA    | 806 | CLA  | O1A-CGA-O2A-C1  |
| 18  | aB    | 847 | LMG  | C11-C12-C13-C14 |
| 18  | bB    | 847 | LMG  | C11-C12-C13-C14 |
| 18  | cB    | 847 | LMG  | C11-C12-C13-C14 |
| 11  | aB    | 817 | CLA  | C2-C1-O2A-CGA   |
| 11  | bB    | 817 | CLA  | C2-C1-O2A-CGA   |
| 11  | cB    | 817 | CLA  | C2-C1-O2A-CGA   |
| 12  | aL    | 202 | F6C  | C2-C1-O2A-CGA   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 12  | bL    | 202 | F6C  | C2-C1-O2A-CGA   |
| 12  | cL    | 202 | F6C  | C2-C1-O2A-CGA   |
| 11  | aB    | 827 | CLA  | CBA-CGA-O2A-C1  |
| 11  | bB    | 827 | CLA  | CBA-CGA-O2A-C1  |
| 11  | cB    | 827 | CLA  | CBA-CGA-O2A-C1  |
| 11  | cB    | 808 | CLA  | C5-C6-C7-C8     |
| 11  | cL    | 206 | CLA  | C10-C11-C12-C13 |
| 17  | bA    | 853 | LMT  | O1'-C1-C2-C3    |
| 11  | aA    | 828 | CLA  | C4-C3-C5-C6     |
| 11  | aA    | 829 | CLA  | C4-C3-C5-C6     |
| 11  | bA    | 828 | CLA  | C4-C3-C5-C6     |
| 11  | bA    | 829 | CLA  | C4-C3-C5-C6     |
| 11  | cA    | 828 | CLA  | C4-C3-C5-C6     |
| 11  | cA    | 829 | CLA  | C4-C3-C5-C6     |
| 11  | aB    | 808 | CLA  | C5-C6-C7-C8     |
| 11  | bB    | 808 | CLA  | C5-C6-C7-C8     |
| 17  | aA    | 853 | LMT  | O1'-C1-C2-C3    |
| 17  | cA    | 853 | LMT  | O1'-C1-C2-C3    |
| 11  | aA    | 843 | CLA  | C2A-CAA-CBA-CGA |
| 11  | bA    | 843 | CLA  | C2A-CAA-CBA-CGA |
| 11  | bL    | 205 | CLA  | C2A-CAA-CBA-CGA |
| 11  | cA    | 843 | CLA  | C2A-CAA-CBA-CGA |
| 17  | aA    | 853 | LMT  | C9-C10-C11-C12  |
| 17  | bA    | 853 | LMT  | C9-C10-C11-C12  |
| 17  | cA    | 853 | LMT  | C9-C10-C11-C12  |
| 11  | bB    | 819 | CLA  | CBD-CGD-O2D-CED |
| 11  | cB    | 819 | CLA  | CBD-CGD-O2D-CED |
| 11  | cB    | 812 | CLA  | C13-C15-C16-C17 |
| 17  | bA    | 853 | LMT  | C4-C5-C6-C7     |
| 16  | bA    | 852 | LHG  | C24-C23-O8-C6   |
| 17  | aA    | 853 | LMT  | C4-C5-C6-C7     |
| 17  | cA    | 853 | LMT  | C4-C5-C6-C7     |
| 11  | aA    | 819 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aA    | 839 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aA    | 842 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aA    | 843 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aB    | 814 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aB    | 818 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aB    | 821 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aB    | 833 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aB    | 836 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aK    | 103 | CLA  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | bA    | 819 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bA    | 839 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bA    | 842 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bA    | 843 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bB    | 814 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bB    | 818 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bB    | 821 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bB    | 833 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bB    | 836 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bK    | 103 | CLA  | C1A-C2A-CAA-CBA |
| 11  | cA    | 819 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cA    | 839 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cA    | 842 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cA    | 843 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cB    | 814 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cB    | 818 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cB    | 821 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cB    | 833 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cB    | 836 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cK    | 103 | CLA  | C1A-C2A-CAA-CBA |
| 16  | aA    | 852 | LHG  | C24-C23-O8-C6   |
| 16  | cA    | 852 | LHG  | C24-C23-O8-C6   |
| 12  | aB    | 824 | F6C  | C4-C3-C5-C6     |
| 12  | bB    | 824 | F6C  | C4-C3-C5-C6     |
| 12  | cB    | 824 | F6C  | C4-C3-C5-C6     |
| 11  | aB    | 812 | CLA  | C13-C15-C16-C17 |
| 11  | bB    | 812 | CLA  | C13-C15-C16-C17 |
| 11  | aL    | 205 | CLA  | C2A-CAA-CBA-CGA |
| 11  | cL    | 205 | CLA  | C2A-CAA-CBA-CGA |
| 11  | aB    | 819 | CLA  | CBD-CGD-O2D-CED |
| 11  | aA    | 821 | CLA  | C11-C10-C8-C7   |
| 11  | aB    | 803 | CLA  | C11-C10-C8-C7   |
| 11  | bA    | 821 | CLA  | C11-C10-C8-C7   |
| 11  | bB    | 803 | CLA  | C11-C10-C8-C7   |
| 11  | cA    | 821 | CLA  | C11-C10-C8-C7   |
| 11  | cB    | 803 | CLA  | C11-C10-C8-C7   |
| 12  | aA    | 826 | F6C  | C11-C10-C8-C7   |
| 12  | aA    | 844 | F6C  | C12-C13-C15-C16 |
| 12  | aL    | 202 | F6C  | C11-C10-C8-C7   |
| 12  | bA    | 826 | F6C  | C11-C10-C8-C7   |
| 12  | bA    | 844 | F6C  | C12-C13-C15-C16 |
| 12  | bL    | 202 | F6C  | C11-C10-C8-C7   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 12  | cA    | 826 | F6C  | C11-C10-C8-C7   |
| 12  | cA    | 844 | F6C  | C12-C13-C15-C16 |
| 12  | cL    | 202 | F6C  | C11-C10-C8-C7   |
| 11  | aB    | 801 | CLA  | CBA-CGA-O2A-C1  |
| 11  | bB    | 801 | CLA  | CBA-CGA-O2A-C1  |
| 11  | cB    | 801 | CLA  | CBA-CGA-O2A-C1  |
| 11  | aB    | 805 | CLA  | C16-C17-C18-C19 |
| 11  | bB    | 805 | CLA  | C16-C17-C18-C19 |
| 11  | cB    | 805 | CLA  | C16-C17-C18-C19 |
| 11  | aA    | 812 | CLA  | C6-C7-C8-C9     |
| 11  | aB    | 806 | CLA  | C14-C13-C15-C16 |
| 11  | bA    | 812 | CLA  | C6-C7-C8-C9     |
| 11  | bB    | 806 | CLA  | C14-C13-C15-C16 |
| 11  | cA    | 812 | CLA  | C6-C7-C8-C9     |
| 11  | cB    | 806 | CLA  | C14-C13-C15-C16 |
| 11  | aB    | 827 | CLA  | O1A-CGA-O2A-C1  |
| 11  | bB    | 827 | CLA  | O1A-CGA-O2A-C1  |
| 11  | cB    | 827 | CLA  | O1A-CGA-O2A-C1  |
| 11  | aB    | 830 | CLA  | C1-C2-C3-C4     |
| 11  | bB    | 830 | CLA  | C1-C2-C3-C4     |
| 11  | cB    | 830 | CLA  | C1-C2-C3-C4     |
| 12  | aA    | 832 | F6C  | C1B-C2B-CMB-OMB |
| 12  | aL    | 202 | F6C  | C1B-C2B-CMB-OMB |
| 12  | bA    | 832 | F6C  | C1B-C2B-CMB-OMB |
| 12  | bL    | 202 | F6C  | C1B-C2B-CMB-OMB |
| 12  | cA    | 832 | F6C  | C1B-C2B-CMB-OMB |
| 12  | cL    | 202 | F6C  | C1B-C2B-CMB-OMB |
| 12  | aA    | 827 | F6C  | O1A-CGA-O2A-C1  |
| 12  | bA    | 827 | F6C  | O1A-CGA-O2A-C1  |
| 12  | cA    | 827 | F6C  | O1A-CGA-O2A-C1  |
| 11  | aA    | 820 | CLA  | C4-C3-C5-C6     |
| 11  | bA    | 820 | CLA  | C4-C3-C5-C6     |
| 11  | cA    | 820 | CLA  | C4-C3-C5-C6     |
| 16  | aA    | 852 | LHG  | C11-C12-C13-C14 |
| 16  | bA    | 852 | LHG  | C11-C12-C13-C14 |
| 11  | aB    | 802 | CLA  | CAD-CBD-CGD-O2D |
| 11  | bB    | 802 | CLA  | CAD-CBD-CGD-O2D |
| 11  | cB    | 802 | CLA  | CAD-CBD-CGD-O2D |
| 11  | aA    | 829 | CLA  | O1D-CGD-O2D-CED |
| 11  | cA    | 829 | CLA  | O1D-CGD-O2D-CED |
| 11  | bA    | 829 | CLA  | O1D-CGD-O2D-CED |
| 12  | aA    | 827 | F6C  | CBA-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 12  | bA    | 827 | F6C  | CBA-CGA-O2A-C1  |
| 12  | cA    | 827 | F6C  | CBA-CGA-O2A-C1  |
| 16  | cA    | 852 | LHG  | C11-C12-C13-C14 |
| 11  | aB    | 801 | CLA  | O1A-CGA-O2A-C1  |
| 11  | cB    | 801 | CLA  | O1A-CGA-O2A-C1  |
| 10  | aA    | 801 | CL0  | CHA-CBD-CGD-O2D |
| 10  | bA    | 801 | CL0  | CHA-CBD-CGD-O2D |
| 10  | cA    | 801 | CL0  | CHA-CBD-CGD-O2D |
| 11  | aA    | 805 | CLA  | CAD-CBD-CGD-O1D |
| 11  | aA    | 806 | CLA  | CAD-CBD-CGD-O1D |
| 11  | aB    | 802 | CLA  | CAD-CBD-CGD-O1D |
| 11  | aB    | 804 | CLA  | CHA-CBD-CGD-O1D |
| 11  | aB    | 804 | CLA  | CHA-CBD-CGD-O2D |
| 11  | aB    | 805 | CLA  | CAD-CBD-CGD-O1D |
| 11  | aB    | 808 | CLA  | CHA-CBD-CGD-O1D |
| 11  | aB    | 813 | CLA  | CHA-CBD-CGD-O1D |
| 11  | aB    | 813 | CLA  | CHA-CBD-CGD-O2D |
| 11  | aB    | 814 | CLA  | CHA-CBD-CGD-O1D |
| 11  | aB    | 814 | CLA  | CHA-CBD-CGD-O2D |
| 11  | aB    | 819 | CLA  | CHA-CBD-CGD-O1D |
| 11  | aB    | 836 | CLA  | CHA-CBD-CGD-O1D |
| 11  | aB    | 836 | CLA  | CHA-CBD-CGD-O2D |
| 11  | bA    | 805 | CLA  | CAD-CBD-CGD-O1D |
| 11  | bA    | 806 | CLA  | CAD-CBD-CGD-O1D |
| 11  | bB    | 802 | CLA  | CAD-CBD-CGD-O1D |
| 11  | bB    | 804 | CLA  | CHA-CBD-CGD-O1D |
| 11  | bB    | 804 | CLA  | CHA-CBD-CGD-O2D |
| 11  | bB    | 805 | CLA  | CAD-CBD-CGD-O1D |
| 11  | bB    | 808 | CLA  | CHA-CBD-CGD-O1D |
| 11  | bB    | 813 | CLA  | CHA-CBD-CGD-O1D |
| 11  | bB    | 813 | CLA  | CHA-CBD-CGD-O2D |
| 11  | bB    | 814 | CLA  | CHA-CBD-CGD-O1D |
| 11  | bB    | 814 | CLA  | CHA-CBD-CGD-O2D |
| 11  | bB    | 819 | CLA  | CHA-CBD-CGD-O1D |
| 11  | bB    | 836 | CLA  | CHA-CBD-CGD-O1D |
| 11  | bB    | 836 | CLA  | CHA-CBD-CGD-O2D |
| 11  | cA    | 805 | CLA  | CAD-CBD-CGD-O1D |
| 11  | cA    | 806 | CLA  | CAD-CBD-CGD-O1D |
| 11  | cB    | 802 | CLA  | CAD-CBD-CGD-O1D |
| 11  | cB    | 804 | CLA  | CHA-CBD-CGD-O1D |
| 11  | cB    | 804 | CLA  | CHA-CBD-CGD-O2D |
| 11  | cB    | 805 | CLA  | CAD-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | cB    | 808 | CLA  | CHA-CBD-CGD-O1D |
| 11  | cB    | 813 | CLA  | CHA-CBD-CGD-O1D |
| 11  | cB    | 813 | CLA  | CHA-CBD-CGD-O2D |
| 11  | cB    | 814 | CLA  | CHA-CBD-CGD-O1D |
| 11  | cB    | 814 | CLA  | CHA-CBD-CGD-O2D |
| 11  | cB    | 819 | CLA  | CHA-CBD-CGD-O1D |
| 11  | cB    | 836 | CLA  | CHA-CBD-CGD-O1D |
| 11  | cB    | 836 | CLA  | CHA-CBD-CGD-O2D |
| 12  | aA    | 832 | F6C  | CHA-CBD-CGD-O1D |
| 12  | aA    | 832 | F6C  | CHA-CBD-CGD-O2D |
| 12  | bA    | 832 | F6C  | CHA-CBD-CGD-O1D |
| 12  | bA    | 832 | F6C  | CHA-CBD-CGD-O2D |
| 12  | cA    | 832 | F6C  | CHA-CBD-CGD-O1D |
| 12  | cA    | 832 | F6C  | CHA-CBD-CGD-O2D |
| 15  | aA    | 848 | BCR  | C19-C20-C21-C22 |
| 15  | bA    | 848 | BCR  | C19-C20-C21-C22 |
| 15  | cA    | 848 | BCR  | C19-C20-C21-C22 |
| 11  | bB    | 801 | CLA  | O1A-CGA-O2A-C1  |
| 11  | aA    | 806 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aA    | 810 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aA    | 811 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aA    | 814 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aA    | 816 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aA    | 819 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aA    | 822 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aA    | 823 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aA    | 835 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aA    | 836 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aA    | 839 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aB    | 820 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aB    | 821 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aB    | 837 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bA    | 806 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bA    | 810 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bA    | 811 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bA    | 814 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bA    | 816 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bA    | 819 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bA    | 822 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bA    | 823 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bA    | 835 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bA    | 836 | CLA  | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | bA    | 839 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bB    | 820 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bB    | 821 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bB    | 837 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cA    | 806 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cA    | 810 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cA    | 811 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cA    | 814 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cA    | 816 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cA    | 819 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cA    | 822 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cA    | 823 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cA    | 835 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cA    | 836 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cA    | 839 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cB    | 820 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cB    | 821 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cB    | 837 | CLA  | C2B-C3B-CAB-CBB |
| 15  | aB    | 845 | BCR  | C1-C6-C7-C8     |
| 15  | aL    | 208 | BCR  | C23-C24-C25-C30 |
| 15  | bB    | 845 | BCR  | C1-C6-C7-C8     |
| 15  | bL    | 208 | BCR  | C23-C24-C25-C30 |
| 15  | cB    | 845 | BCR  | C1-C6-C7-C8     |
| 15  | cL    | 208 | BCR  | C23-C24-C25-C30 |
| 11  | aB    | 825 | CLA  | C10-C11-C12-C13 |
| 11  | cB    | 825 | CLA  | C10-C11-C12-C13 |
| 11  | bB    | 825 | CLA  | C10-C11-C12-C13 |
| 18  | aB    | 847 | LMG  | C37-C38-C39-C40 |
| 18  | bB    | 847 | LMG  | C37-C38-C39-C40 |
| 18  | cB    | 847 | LMG  | C37-C38-C39-C40 |
| 11  | aA    | 821 | CLA  | C5-C6-C7-C8     |
| 11  | bA    | 821 | CLA  | C5-C6-C7-C8     |
| 11  | cA    | 821 | CLA  | C5-C6-C7-C8     |
| 11  | cA    | 802 | CLA  | C8-C10-C11-C12  |
| 11  | aA    | 802 | CLA  | C8-C10-C11-C12  |
| 11  | bA    | 802 | CLA  | C8-C10-C11-C12  |
| 11  | aA    | 818 | CLA  | C2-C3-C5-C6     |
| 11  | bA    | 818 | CLA  | C2-C3-C5-C6     |
| 11  | cA    | 818 | CLA  | C2-C3-C5-C6     |
| 11  | aA    | 807 | CLA  | C14-C13-C15-C16 |
| 11  | aA    | 828 | CLA  | C6-C7-C8-C9     |
| 11  | aA    | 840 | CLA  | C6-C7-C8-C9     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | aB    | 803 | CLA  | C11-C10-C8-C9   |
| 11  | aB    | 816 | CLA  | C11-C10-C8-C9   |
| 11  | bA    | 807 | CLA  | C14-C13-C15-C16 |
| 11  | bA    | 828 | CLA  | C6-C7-C8-C9     |
| 11  | bA    | 840 | CLA  | C6-C7-C8-C9     |
| 11  | bB    | 803 | CLA  | C11-C10-C8-C9   |
| 11  | bB    | 816 | CLA  | C11-C10-C8-C9   |
| 11  | cA    | 807 | CLA  | C14-C13-C15-C16 |
| 11  | cA    | 828 | CLA  | C6-C7-C8-C9     |
| 11  | cA    | 840 | CLA  | C6-C7-C8-C9     |
| 11  | cB    | 803 | CLA  | C11-C10-C8-C9   |
| 11  | cB    | 816 | CLA  | C11-C10-C8-C9   |
| 12  | aA    | 844 | F6C  | C14-C13-C15-C16 |
| 12  | bA    | 844 | F6C  | C14-C13-C15-C16 |
| 11  | cA    | 813 | CLA  | C4-C3-C5-C6     |
| 11  | aB    | 823 | CLA  | C2-C3-C5-C6     |
| 11  | bB    | 823 | CLA  | C2-C3-C5-C6     |
| 11  | cB    | 823 | CLA  | C2-C3-C5-C6     |
| 11  | bA    | 813 | CLA  | CAA-CBA-CGA-O2A |
| 11  | aB    | 808 | CLA  | C4-C3-C5-C6     |
| 11  | aB    | 813 | CLA  | C4-C3-C5-C6     |
| 11  | bB    | 808 | CLA  | C4-C3-C5-C6     |
| 11  | bB    | 813 | CLA  | C4-C3-C5-C6     |
| 11  | cB    | 808 | CLA  | C4-C3-C5-C6     |
| 11  | cB    | 813 | CLA  | C4-C3-C5-C6     |
| 11  | aA    | 813 | CLA  | CAA-CBA-CGA-O2A |
| 11  | cA    | 813 | CLA  | CAA-CBA-CGA-O2A |
| 18  | aB    | 847 | LMG  | O1-C7-C8-C9     |
| 18  | bB    | 847 | LMG  | O1-C7-C8-C9     |
| 18  | cB    | 847 | LMG  | O1-C7-C8-C9     |
| 11  | bA    | 828 | CLA  | C5-C6-C7-C8     |
| 11  | aA    | 828 | CLA  | C5-C6-C7-C8     |
| 11  | bA    | 822 | CLA  | C10-C11-C12-C13 |
| 11  | cA    | 828 | CLA  | C5-C6-C7-C8     |
| 11  | aA    | 822 | CLA  | C10-C11-C12-C13 |
| 11  | cA    | 822 | CLA  | C10-C11-C12-C13 |
| 18  | aB    | 847 | LMG  | C30-C31-C32-C33 |
| 18  | bB    | 847 | LMG  | C30-C31-C32-C33 |
| 11  | aA    | 819 | CLA  | C2A-CAA-CBA-CGA |
| 11  | bA    | 819 | CLA  | C2A-CAA-CBA-CGA |
| 11  | cA    | 819 | CLA  | C2A-CAA-CBA-CGA |
| 16  | aA    | 852 | LHG  | C25-C26-C27-C28 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 18  | cB    | 847 | LMG  | C30-C31-C32-C33 |
| 11  | aA    | 813 | CLA  | C4-C3-C5-C6     |
| 11  | bA    | 813 | CLA  | C4-C3-C5-C6     |
| 12  | aA    | 827 | F6C  | C4-C3-C5-C6     |
| 12  | bA    | 827 | F6C  | C4-C3-C5-C6     |
| 12  | cA    | 827 | F6C  | C4-C3-C5-C6     |
| 11  | aA    | 828 | CLA  | C2-C3-C5-C6     |
| 16  | bA    | 852 | LHG  | C25-C26-C27-C28 |
| 16  | cA    | 852 | LHG  | C25-C26-C27-C28 |
| 11  | aB    | 801 | CLA  | C8-C10-C11-C12  |
| 11  | bB    | 801 | CLA  | C8-C10-C11-C12  |
| 11  | aB    | 801 | CLA  | CAA-CBA-CGA-O2A |
| 11  | bB    | 801 | CLA  | CAA-CBA-CGA-O2A |
| 11  | cB    | 801 | CLA  | CAA-CBA-CGA-O2A |
| 12  | cA    | 844 | F6C  | C14-C13-C15-C16 |
| 11  | cB    | 801 | CLA  | C8-C10-C11-C12  |
| 11  | aA    | 805 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aA    | 806 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aA    | 816 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aB    | 812 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bA    | 805 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bA    | 806 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bA    | 816 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bB    | 812 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cA    | 805 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cA    | 806 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cA    | 816 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cB    | 812 | CLA  | C4B-C3B-CAB-CBB |
| 16  | aA    | 852 | LHG  | C31-C32-C33-C34 |
| 11  | aB    | 825 | CLA  | C16-C17-C18-C20 |
| 11  | bB    | 825 | CLA  | C16-C17-C18-C20 |
| 11  | cB    | 825 | CLA  | C16-C17-C18-C20 |
| 16  | cA    | 852 | LHG  | C31-C32-C33-C34 |
| 11  | aA    | 806 | CLA  | C15-C16-C17-C18 |
| 11  | bA    | 806 | CLA  | C15-C16-C17-C18 |
| 11  | cA    | 806 | CLA  | C15-C16-C17-C18 |
| 11  | aB    | 840 | CLA  | C2A-CAA-CBA-CGA |
| 11  | bB    | 840 | CLA  | C2A-CAA-CBA-CGA |
| 11  | cB    | 840 | CLA  | C2A-CAA-CBA-CGA |
| 11  | aB    | 808 | CLA  | C2-C3-C5-C6     |
| 11  | aB    | 813 | CLA  | C2-C3-C5-C6     |
| 11  | bA    | 828 | CLA  | C2-C3-C5-C6     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | bB    | 808 | CLA  | C2-C3-C5-C6     |
| 11  | bB    | 813 | CLA  | C2-C3-C5-C6     |
| 11  | cA    | 828 | CLA  | C2-C3-C5-C6     |
| 11  | cB    | 808 | CLA  | C2-C3-C5-C6     |
| 11  | cB    | 813 | CLA  | C2-C3-C5-C6     |
| 12  | aB    | 824 | F6C  | C2-C3-C5-C6     |
| 12  | bB    | 824 | F6C  | C2-C3-C5-C6     |
| 12  | cB    | 824 | F6C  | C2-C3-C5-C6     |
| 11  | aB    | 815 | CLA  | CAA-CBA-CGA-O1A |
| 11  | bB    | 815 | CLA  | CAA-CBA-CGA-O1A |
| 16  | cA    | 852 | LHG  | C26-C27-C28-C29 |
| 16  | bA    | 852 | LHG  | C31-C32-C33-C34 |
| 16  | aA    | 852 | LHG  | C26-C27-C28-C29 |
| 11  | cB    | 815 | CLA  | CAA-CBA-CGA-O1A |
| 16  | bA    | 852 | LHG  | C26-C27-C28-C29 |
| 11  | aL    | 206 | CLA  | C11-C12-C13-C15 |
| 11  | bL    | 206 | CLA  | C11-C12-C13-C15 |
| 11  | cL    | 206 | CLA  | C11-C12-C13-C15 |
| 11  | aA    | 815 | CLA  | C3A-C2A-CAA-CBA |
| 11  | aB    | 812 | CLA  | C4-C3-C5-C6     |
| 11  | aB    | 817 | CLA  | C3A-C2A-CAA-CBA |
| 11  | bA    | 815 | CLA  | C3A-C2A-CAA-CBA |
| 11  | bB    | 812 | CLA  | C4-C3-C5-C6     |
| 11  | bB    | 817 | CLA  | C3A-C2A-CAA-CBA |
| 11  | cA    | 815 | CLA  | C3A-C2A-CAA-CBA |
| 11  | cB    | 812 | CLA  | C4-C3-C5-C6     |
| 11  | cB    | 817 | CLA  | C3A-C2A-CAA-CBA |
| 11  | aA    | 820 | CLA  | C2-C3-C5-C6     |
| 11  | cA    | 820 | CLA  | C2-C3-C5-C6     |
| 15  | aA    | 851 | BCR  | C11-C10-C9-C34  |
| 15  | bA    | 851 | BCR  | C11-C10-C9-C34  |
| 15  | cA    | 851 | BCR  | C11-C10-C9-C34  |
| 11  | cA    | 819 | CLA  | O1D-CGD-O2D-CED |
| 11  | aB    | 834 | CLA  | CAA-CBA-CGA-O2A |
| 11  | bA    | 819 | CLA  | O1D-CGD-O2D-CED |
| 11  | aA    | 819 | CLA  | O1D-CGD-O2D-CED |
| 10  | aA    | 801 | CL0  | CAA-CBA-CGA-O2A |
| 10  | bA    | 801 | CL0  | CAA-CBA-CGA-O2A |
| 10  | cA    | 801 | CL0  | CAA-CBA-CGA-O2A |
| 11  | bA    | 820 | CLA  | C2-C3-C5-C6     |
| 11  | aA    | 822 | CLA  | C2A-CAA-CBA-CGA |
| 11  | bA    | 822 | CLA  | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | cA    | 822 | CLA  | C2A-CAA-CBA-CGA |
| 11  | bB    | 834 | CLA  | CAA-CBA-CGA-O2A |
| 11  | cB    | 834 | CLA  | CAA-CBA-CGA-O2A |
| 11  | cB    | 819 | CLA  | O1D-CGD-O2D-CED |
| 11  | aB    | 834 | CLA  | CAA-CBA-CGA-O1A |
| 11  | bB    | 834 | CLA  | CAA-CBA-CGA-O1A |
| 11  | cB    | 834 | CLA  | CAA-CBA-CGA-O1A |
| 11  | aB    | 806 | CLA  | C11-C10-C8-C9   |
| 11  | aL    | 206 | CLA  | C11-C12-C13-C14 |
| 11  | bB    | 806 | CLA  | C11-C10-C8-C9   |
| 11  | bL    | 206 | CLA  | C11-C12-C13-C14 |
| 11  | cB    | 806 | CLA  | C11-C10-C8-C9   |
| 11  | cL    | 206 | CLA  | C11-C12-C13-C14 |
| 18  | aB    | 847 | LMG  | C32-C33-C34-C35 |
| 18  | bB    | 847 | LMG  | C32-C33-C34-C35 |
| 18  | cB    | 847 | LMG  | C32-C33-C34-C35 |
| 11  | aA    | 840 | CLA  | C4-C3-C5-C6     |
| 11  | bA    | 840 | CLA  | C4-C3-C5-C6     |
| 11  | cA    | 840 | CLA  | C4-C3-C5-C6     |
| 11  | aB    | 812 | CLA  | C2-C3-C5-C6     |
| 11  | bB    | 812 | CLA  | C2-C3-C5-C6     |
| 11  | cB    | 812 | CLA  | C2-C3-C5-C6     |
| 11  | aB    | 813 | CLA  | O1D-CGD-O2D-CED |
| 11  | aB    | 819 | CLA  | O1D-CGD-O2D-CED |
| 12  | aA    | 832 | F6C  | C1A-C2A-CAA-CBA |
| 12  | bA    | 832 | F6C  | C1A-C2A-CAA-CBA |
| 12  | cA    | 832 | F6C  | C1A-C2A-CAA-CBA |
| 11  | aA    | 802 | CLA  | C1A-C2A-CAA-CBA |
| 11  | aA    | 812 | CLA  | C1A-C2A-CAA-CBA |
| 11  | aA    | 813 | CLA  | C1A-C2A-CAA-CBA |
| 11  | aA    | 843 | CLA  | C1A-C2A-CAA-CBA |
| 11  | aB    | 815 | CLA  | C1A-C2A-CAA-CBA |
| 11  | aB    | 816 | CLA  | C1A-C2A-CAA-CBA |
| 11  | aB    | 834 | CLA  | C1A-C2A-CAA-CBA |
| 11  | bA    | 802 | CLA  | C1A-C2A-CAA-CBA |
| 11  | bA    | 812 | CLA  | C1A-C2A-CAA-CBA |
| 11  | bA    | 813 | CLA  | C1A-C2A-CAA-CBA |
| 11  | bA    | 843 | CLA  | C1A-C2A-CAA-CBA |
| 11  | bB    | 815 | CLA  | C1A-C2A-CAA-CBA |
| 11  | bB    | 816 | CLA  | C1A-C2A-CAA-CBA |
| 11  | bB    | 833 | CLA  | C1A-C2A-CAA-CBA |
| 11  | bB    | 834 | CLA  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | cA    | 802 | CLA  | C1A-C2A-CAA-CBA |
| 11  | cA    | 812 | CLA  | C1A-C2A-CAA-CBA |
| 11  | cA    | 813 | CLA  | C1A-C2A-CAA-CBA |
| 11  | cA    | 843 | CLA  | C1A-C2A-CAA-CBA |
| 11  | cB    | 815 | CLA  | C1A-C2A-CAA-CBA |
| 11  | cB    | 816 | CLA  | C1A-C2A-CAA-CBA |
| 11  | cB    | 834 | CLA  | C1A-C2A-CAA-CBA |
| 15  | aA    | 851 | BCR  | C11-C10-C9-C8   |
| 15  | aA    | 851 | BCR  | C16-C17-C18-C19 |
| 15  | aB    | 844 | BCR  | C11-C10-C9-C8   |
| 15  | aB    | 844 | BCR  | C20-C21-C22-C23 |
| 15  | aB    | 846 | BCR  | C12-C13-C14-C15 |
| 15  | bA    | 851 | BCR  | C11-C10-C9-C8   |
| 15  | bA    | 851 | BCR  | C16-C17-C18-C19 |
| 15  | bB    | 844 | BCR  | C11-C10-C9-C8   |
| 15  | bB    | 844 | BCR  | C20-C21-C22-C23 |
| 15  | bB    | 846 | BCR  | C12-C13-C14-C15 |
| 15  | cA    | 851 | BCR  | C11-C10-C9-C8   |
| 15  | cA    | 851 | BCR  | C16-C17-C18-C19 |
| 15  | cB    | 844 | BCR  | C11-C10-C9-C8   |
| 15  | cB    | 844 | BCR  | C20-C21-C22-C23 |
| 15  | cB    | 846 | BCR  | C12-C13-C14-C15 |
| 11  | aA    | 805 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aA    | 808 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aA    | 842 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aA    | 843 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aB    | 809 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aB    | 810 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aB    | 812 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aB    | 814 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aB    | 817 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aB    | 833 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aB    | 836 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aL    | 206 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bA    | 805 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bA    | 808 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bA    | 842 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bA    | 843 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bB    | 809 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bB    | 810 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bB    | 812 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bB    | 814 | CLA  | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | bB    | 817 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bB    | 833 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bB    | 836 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bL    | 206 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cA    | 805 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cA    | 808 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cA    | 842 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cA    | 843 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cB    | 809 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cB    | 810 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cB    | 812 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cB    | 814 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cB    | 833 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cB    | 836 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cL    | 206 | CLA  | C2B-C3B-CAB-CBB |
| 15  | aA    | 847 | BCR  | C5-C6-C7-C8     |
| 15  | aA    | 847 | BCR  | C23-C24-C25-C26 |
| 15  | aA    | 848 | BCR  | C23-C24-C25-C26 |
| 15  | aA    | 849 | BCR  | C5-C6-C7-C8     |
| 15  | aA    | 849 | BCR  | C23-C24-C25-C30 |
| 15  | aA    | 850 | BCR  | C5-C6-C7-C8     |
| 15  | aA    | 850 | BCR  | C23-C24-C25-C30 |
| 15  | aA    | 851 | BCR  | C23-C24-C25-C30 |
| 15  | aB    | 842 | BCR  | C5-C6-C7-C8     |
| 15  | aB    | 842 | BCR  | C23-C24-C25-C30 |
| 15  | aB    | 844 | BCR  | C5-C6-C7-C8     |
| 15  | aB    | 845 | BCR  | C5-C6-C7-C8     |
| 15  | aB    | 846 | BCR  | C1-C6-C7-C8     |
| 15  | aB    | 846 | BCR  | C23-C24-C25-C30 |
| 15  | aB    | 848 | BCR  | C5-C6-C7-C8     |
| 15  | aI    | 101 | BCR  | C5-C6-C7-C8     |
| 15  | aI    | 101 | BCR  | C23-C24-C25-C30 |
| 15  | aK    | 102 | BCR  | C5-C6-C7-C8     |
| 15  | aL    | 203 | BCR  | C23-C24-C25-C26 |
| 15  | aL    | 207 | BCR  | C5-C6-C7-C8     |
| 15  | aL    | 208 | BCR  | C23-C24-C25-C26 |
| 15  | aM    | 101 | BCR  | C5-C6-C7-C8     |
| 15  | aM    | 101 | BCR  | C23-C24-C25-C30 |
| 15  | bA    | 847 | BCR  | C5-C6-C7-C8     |
| 15  | bA    | 847 | BCR  | C23-C24-C25-C26 |
| 15  | bA    | 848 | BCR  | C23-C24-C25-C26 |
| 15  | bA    | 849 | BCR  | C5-C6-C7-C8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 15  | bA    | 849 | BCR  | C23-C24-C25-C30 |
| 15  | bA    | 850 | BCR  | C5-C6-C7-C8     |
| 15  | bA    | 850 | BCR  | C23-C24-C25-C30 |
| 15  | bA    | 851 | BCR  | C23-C24-C25-C30 |
| 15  | bB    | 842 | BCR  | C5-C6-C7-C8     |
| 15  | bB    | 842 | BCR  | C23-C24-C25-C30 |
| 15  | bB    | 844 | BCR  | C5-C6-C7-C8     |
| 15  | bB    | 845 | BCR  | C5-C6-C7-C8     |
| 15  | bB    | 846 | BCR  | C1-C6-C7-C8     |
| 15  | bB    | 846 | BCR  | C23-C24-C25-C30 |
| 15  | bB    | 848 | BCR  | C5-C6-C7-C8     |
| 15  | bI    | 101 | BCR  | C5-C6-C7-C8     |
| 15  | bI    | 101 | BCR  | C23-C24-C25-C30 |
| 15  | bK    | 102 | BCR  | C5-C6-C7-C8     |
| 15  | bL    | 203 | BCR  | C23-C24-C25-C26 |
| 15  | bL    | 207 | BCR  | C5-C6-C7-C8     |
| 15  | bL    | 208 | BCR  | C23-C24-C25-C26 |
| 15  | bM    | 101 | BCR  | C5-C6-C7-C8     |
| 15  | bM    | 101 | BCR  | C23-C24-C25-C30 |
| 15  | cA    | 847 | BCR  | C5-C6-C7-C8     |
| 15  | cA    | 847 | BCR  | C23-C24-C25-C26 |
| 15  | cA    | 848 | BCR  | C23-C24-C25-C26 |
| 15  | cA    | 849 | BCR  | C5-C6-C7-C8     |
| 15  | cA    | 849 | BCR  | C23-C24-C25-C26 |
| 15  | cA    | 849 | BCR  | C23-C24-C25-C30 |
| 15  | cA    | 850 | BCR  | C5-C6-C7-C8     |
| 15  | cA    | 850 | BCR  | C23-C24-C25-C30 |
| 15  | cA    | 851 | BCR  | C23-C24-C25-C30 |
| 15  | cB    | 842 | BCR  | C5-C6-C7-C8     |
| 15  | cB    | 842 | BCR  | C23-C24-C25-C30 |
| 15  | cB    | 844 | BCR  | C5-C6-C7-C8     |
| 15  | cB    | 845 | BCR  | C5-C6-C7-C8     |
| 15  | cB    | 846 | BCR  | C1-C6-C7-C8     |
| 15  | cB    | 846 | BCR  | C23-C24-C25-C30 |
| 15  | cB    | 848 | BCR  | C5-C6-C7-C8     |
| 15  | cI    | 103 | BCR  | C5-C6-C7-C8     |
| 15  | cI    | 103 | BCR  | C23-C24-C25-C30 |
| 15  | cK    | 102 | BCR  | C5-C6-C7-C8     |
| 15  | cL    | 203 | BCR  | C23-C24-C25-C26 |
| 15  | cL    | 207 | BCR  | C5-C6-C7-C8     |
| 15  | cL    | 208 | BCR  | C23-C24-C25-C26 |
| 15  | cM    | 101 | BCR  | C5-C6-C7-C8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 15  | cM    | 101 | BCR  | C23-C24-C25-C30 |
| 11  | aB    | 835 | CLA  | CAA-CBA-CGA-O1A |
| 11  | cB    | 835 | CLA  | CAA-CBA-CGA-O1A |
| 11  | aB    | 813 | CLA  | CBA-CGA-O2A-C1  |
| 11  | bB    | 813 | CLA  | CBA-CGA-O2A-C1  |
| 11  | cB    | 813 | CLA  | CBA-CGA-O2A-C1  |
| 11  | bB    | 819 | CLA  | O1D-CGD-O2D-CED |
| 11  | bB    | 835 | CLA  | CAA-CBA-CGA-O1A |
| 11  | aB    | 839 | CLA  | C4-C3-C5-C6     |
| 11  | bB    | 839 | CLA  | C4-C3-C5-C6     |
| 11  | cB    | 839 | CLA  | C4-C3-C5-C6     |
| 11  | aA    | 820 | CLA  | C11-C12-C13-C15 |
| 11  | aA    | 822 | CLA  | C6-C7-C8-C10    |
| 11  | aA    | 833 | CLA  | C6-C7-C8-C10    |
| 11  | aL    | 205 | CLA  | C12-C13-C15-C16 |
| 11  | bA    | 820 | CLA  | C11-C12-C13-C15 |
| 11  | bA    | 822 | CLA  | C6-C7-C8-C10    |
| 11  | bA    | 833 | CLA  | C6-C7-C8-C10    |
| 11  | bL    | 205 | CLA  | C12-C13-C15-C16 |
| 11  | cA    | 820 | CLA  | C11-C12-C13-C15 |
| 11  | cA    | 822 | CLA  | C6-C7-C8-C10    |
| 11  | cA    | 833 | CLA  | C6-C7-C8-C10    |
| 11  | cL    | 205 | CLA  | C12-C13-C15-C16 |
| 11  | aA    | 823 | CLA  | C2A-CAA-CBA-CGA |
| 11  | bA    | 823 | CLA  | C2A-CAA-CBA-CGA |
| 11  | cA    | 823 | CLA  | C2A-CAA-CBA-CGA |
| 11  | aB    | 832 | CLA  | CAA-CBA-CGA-O1A |
| 11  | bB    | 832 | CLA  | CAA-CBA-CGA-O1A |
| 11  | cB    | 832 | CLA  | CAA-CBA-CGA-O1A |
| 11  | aL    | 205 | CLA  | C13-C15-C16-C17 |
| 11  | bL    | 205 | CLA  | C13-C15-C16-C17 |
| 11  | cL    | 205 | CLA  | C13-C15-C16-C17 |
| 11  | aA    | 802 | CLA  | C3-C5-C6-C7     |
| 11  | bA    | 802 | CLA  | C3-C5-C6-C7     |
| 11  | cA    | 802 | CLA  | C3-C5-C6-C7     |
| 11  | bB    | 813 | CLA  | O1D-CGD-O2D-CED |
| 11  | aB    | 839 | CLA  | C2-C3-C5-C6     |
| 11  | bB    | 839 | CLA  | C2-C3-C5-C6     |
| 11  | cB    | 839 | CLA  | C2-C3-C5-C6     |
| 11  | cB    | 813 | CLA  | O1D-CGD-O2D-CED |
| 11  | aB    | 835 | CLA  | CAA-CBA-CGA-O2A |
| 11  | bB    | 835 | CLA  | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | cB    | 835 | CLA  | CAA-CBA-CGA-O2A |
| 11  | aA    | 829 | CLA  | C16-C17-C18-C19 |
| 11  | bA    | 829 | CLA  | C16-C17-C18-C19 |
| 11  | cA    | 829 | CLA  | C16-C17-C18-C19 |
| 11  | aB    | 808 | CLA  | C8-C10-C11-C12  |
| 11  | bB    | 808 | CLA  | C8-C10-C11-C12  |
| 11  | cA    | 831 | CLA  | C10-C11-C12-C13 |
| 15  | aI    | 101 | BCR  | C6-C7-C8-C9     |
| 15  | aK    | 102 | BCR  | C22-C23-C24-C25 |
| 15  | bI    | 101 | BCR  | C6-C7-C8-C9     |
| 15  | cI    | 103 | BCR  | C6-C7-C8-C9     |
| 15  | cK    | 102 | BCR  | C22-C23-C24-C25 |
| 11  | aB    | 815 | CLA  | C5-C6-C7-C8     |
| 11  | bA    | 831 | CLA  | C10-C11-C12-C13 |
| 11  | cB    | 808 | CLA  | C8-C10-C11-C12  |
| 11  | cB    | 815 | CLA  | C5-C6-C7-C8     |
| 11  | aB    | 810 | CLA  | CAA-CBA-CGA-O2A |
| 11  | bB    | 810 | CLA  | CAA-CBA-CGA-O2A |
| 11  | cB    | 810 | CLA  | CAA-CBA-CGA-O2A |
| 15  | aL    | 203 | BCR  | C14-C15-C16-C17 |
| 15  | bL    | 203 | BCR  | C14-C15-C16-C17 |
| 15  | cL    | 203 | BCR  | C14-C15-C16-C17 |
| 11  | aA    | 831 | CLA  | C10-C11-C12-C13 |
| 11  | bB    | 815 | CLA  | C5-C6-C7-C8     |
| 11  | aB    | 832 | CLA  | CAA-CBA-CGA-O2A |
| 11  | bB    | 832 | CLA  | CAA-CBA-CGA-O2A |
| 11  | cB    | 832 | CLA  | CAA-CBA-CGA-O2A |
| 11  | aA    | 842 | CLA  | CAA-CBA-CGA-O2A |
| 11  | bA    | 836 | CLA  | CAA-CBA-CGA-O1A |
| 11  | bA    | 836 | CLA  | CAA-CBA-CGA-O2A |
| 11  | bA    | 842 | CLA  | CAA-CBA-CGA-O2A |
| 11  | cA    | 842 | CLA  | CAA-CBA-CGA-O2A |
| 11  | aB    | 826 | CLA  | CAA-CBA-CGA-O2A |
| 11  | bB    | 826 | CLA  | CAA-CBA-CGA-O2A |
| 11  | cB    | 826 | CLA  | CAA-CBA-CGA-O2A |
| 11  | aA    | 828 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aB    | 817 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bA    | 828 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bB    | 817 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cA    | 828 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cB    | 817 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aB    | 813 | CLA  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | bB    | 813 | CLA  | O1A-CGA-O2A-C1  |
| 11  | cB    | 813 | CLA  | O1A-CGA-O2A-C1  |
| 11  | aA    | 836 | CLA  | CAA-CBA-CGA-O1A |
| 11  | cA    | 836 | CLA  | CAA-CBA-CGA-O1A |
| 11  | aA    | 819 | CLA  | CAA-CBA-CGA-O2A |
| 11  | bA    | 819 | CLA  | CAA-CBA-CGA-O2A |
| 11  | cA    | 819 | CLA  | CAA-CBA-CGA-O2A |
| 11  | aA    | 836 | CLA  | CAA-CBA-CGA-O2A |
| 11  | bA    | 819 | CLA  | CBD-CGD-O2D-CED |
| 10  | aA    | 801 | CL0  | CHA-CBD-CGD-O1D |
| 10  | bA    | 801 | CL0  | CHA-CBD-CGD-O1D |
| 10  | cA    | 801 | CL0  | CHA-CBD-CGD-O1D |
| 15  | aA    | 847 | BCR  | C16-C17-C18-C36 |
| 15  | aA    | 850 | BCR  | C16-C17-C18-C36 |
| 15  | aA    | 851 | BCR  | C16-C17-C18-C36 |
| 15  | aB    | 842 | BCR  | C20-C21-C22-C37 |
| 15  | aB    | 844 | BCR  | C11-C10-C9-C34  |
| 15  | aL    | 203 | BCR  | C20-C21-C22-C37 |
| 15  | aL    | 208 | BCR  | C35-C13-C14-C15 |
| 15  | bA    | 847 | BCR  | C16-C17-C18-C36 |
| 15  | bA    | 850 | BCR  | C16-C17-C18-C36 |
| 15  | bA    | 851 | BCR  | C16-C17-C18-C36 |
| 15  | bB    | 842 | BCR  | C20-C21-C22-C37 |
| 15  | bB    | 844 | BCR  | C11-C10-C9-C34  |
| 15  | bL    | 203 | BCR  | C20-C21-C22-C37 |
| 15  | bL    | 208 | BCR  | C35-C13-C14-C15 |
| 15  | cA    | 847 | BCR  | C16-C17-C18-C36 |
| 15  | cA    | 850 | BCR  | C16-C17-C18-C36 |
| 15  | cA    | 851 | BCR  | C16-C17-C18-C36 |
| 15  | cB    | 842 | BCR  | C20-C21-C22-C37 |
| 15  | cB    | 844 | BCR  | C11-C10-C9-C34  |
| 15  | cL    | 203 | BCR  | C20-C21-C22-C37 |
| 15  | cL    | 208 | BCR  | C35-C13-C14-C15 |
| 11  | aA    | 807 | CLA  | C15-C16-C17-C18 |
| 11  | bA    | 807 | CLA  | C15-C16-C17-C18 |
| 11  | cA    | 807 | CLA  | C15-C16-C17-C18 |
| 11  | aA    | 804 | CLA  | C2A-CAA-CBA-CGA |
| 11  | bA    | 804 | CLA  | C2A-CAA-CBA-CGA |
| 11  | cA    | 804 | CLA  | C2A-CAA-CBA-CGA |
| 11  | aB    | 810 | CLA  | CAA-CBA-CGA-O1A |
| 11  | cA    | 836 | CLA  | CAA-CBA-CGA-O2A |
| 11  | aB    | 825 | CLA  | C15-C16-C17-C18 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | bB    | 825 | CLA  | C15-C16-C17-C18 |
| 11  | cB    | 825 | CLA  | C15-C16-C17-C18 |
| 11  | cA    | 819 | CLA  | CBD-CGD-O2D-CED |
| 11  | aA    | 822 | CLA  | C11-C10-C8-C7   |
| 11  | aL    | 205 | CLA  | C6-C7-C8-C10    |
| 11  | bA    | 822 | CLA  | C11-C10-C8-C7   |
| 11  | bL    | 205 | CLA  | C6-C7-C8-C10    |
| 11  | cA    | 822 | CLA  | C11-C10-C8-C7   |
| 11  | cL    | 205 | CLA  | C6-C7-C8-C10    |
| 11  | aA    | 804 | CLA  | CAA-CBA-CGA-O2A |
| 11  | bA    | 804 | CLA  | CAA-CBA-CGA-O2A |
| 11  | bB    | 810 | CLA  | CAA-CBA-CGA-O1A |
| 11  | cA    | 804 | CLA  | CAA-CBA-CGA-O2A |
| 15  | aA    | 851 | BCR  | C13-C14-C15-C16 |
| 15  | bA    | 851 | BCR  | C13-C14-C15-C16 |
| 15  | cA    | 851 | BCR  | C13-C14-C15-C16 |
| 11  | aA    | 842 | CLA  | CAA-CBA-CGA-O1A |
| 11  | bA    | 842 | CLA  | CAA-CBA-CGA-O1A |
| 11  | cA    | 842 | CLA  | CAA-CBA-CGA-O1A |
| 11  | cB    | 810 | CLA  | CAA-CBA-CGA-O1A |
| 11  | aA    | 831 | CLA  | C11-C10-C8-C9   |
| 11  | aB    | 825 | CLA  | C14-C13-C15-C16 |
| 11  | bA    | 831 | CLA  | C11-C10-C8-C9   |
| 11  | bB    | 825 | CLA  | C14-C13-C15-C16 |
| 11  | cA    | 831 | CLA  | C11-C10-C8-C9   |
| 11  | cB    | 825 | CLA  | C14-C13-C15-C16 |
| 12  | aL    | 202 | F6C  | C6-C7-C8-C9     |
| 12  | bL    | 202 | F6C  | C6-C7-C8-C9     |
| 12  | cL    | 202 | F6C  | C6-C7-C8-C9     |
| 10  | bA    | 801 | CL0  | C16-C17-C18-C20 |
| 10  | cA    | 801 | CL0  | C16-C17-C18-C20 |
| 11  | aA    | 819 | CLA  | CBD-CGD-O2D-CED |
| 11  | aB    | 809 | CLA  | C3A-C2A-CAA-CBA |
| 11  | aB    | 834 | CLA  | C3A-C2A-CAA-CBA |
| 11  | bB    | 809 | CLA  | C3A-C2A-CAA-CBA |
| 11  | bB    | 834 | CLA  | C3A-C2A-CAA-CBA |
| 11  | cB    | 809 | CLA  | C3A-C2A-CAA-CBA |
| 11  | cB    | 834 | CLA  | C3A-C2A-CAA-CBA |
| 11  | aA    | 813 | CLA  | C2-C3-C5-C6     |
| 11  | bA    | 813 | CLA  | C2-C3-C5-C6     |
| 11  | cA    | 813 | CLA  | C2-C3-C5-C6     |
| 11  | cB    | 819 | CLA  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 10  | aA    | 801 | CL0  | C16-C17-C18-C20 |
| 11  | aB    | 819 | CLA  | O1A-CGA-O2A-C1  |
| 11  | bB    | 819 | CLA  | O1A-CGA-O2A-C1  |
| 11  | bB    | 804 | CLA  | O1D-CGD-O2D-CED |
| 11  | aB    | 804 | CLA  | O1D-CGD-O2D-CED |
| 11  | cB    | 804 | CLA  | O1D-CGD-O2D-CED |
| 11  | aA    | 804 | CLA  | CAA-CBA-CGA-O1A |
| 11  | bA    | 804 | CLA  | CAA-CBA-CGA-O1A |
| 11  | cA    | 804 | CLA  | CAA-CBA-CGA-O1A |
| 12  | aA    | 826 | F6C  | C3-C5-C6-C7     |
| 12  | bA    | 826 | F6C  | C3-C5-C6-C7     |
| 12  | cA    | 826 | F6C  | C3-C5-C6-C7     |
| 15  | bK    | 102 | BCR  | C22-C23-C24-C25 |
| 16  | aA    | 852 | LHG  | C4-C5-C6-O8     |
| 16  | bA    | 852 | LHG  | C4-C5-C6-O8     |
| 16  | cA    | 852 | LHG  | C4-C5-C6-O8     |
| 12  | aA    | 827 | F6C  | C4B-C3B-CAB-CBB |
| 12  | aA    | 832 | F6C  | C4B-C3B-CAB-CBB |
| 12  | bA    | 827 | F6C  | C4B-C3B-CAB-CBB |
| 12  | bA    | 832 | F6C  | C4B-C3B-CAB-CBB |
| 12  | cA    | 827 | F6C  | C4B-C3B-CAB-CBB |
| 12  | cA    | 832 | F6C  | C4B-C3B-CAB-CBB |
| 12  | aA    | 832 | F6C  | C2A-CAA-CBA-CGA |
| 12  | bA    | 832 | F6C  | C2A-CAA-CBA-CGA |
| 12  | cA    | 832 | F6C  | C2A-CAA-CBA-CGA |
| 11  | aB    | 823 | CLA  | C2A-CAA-CBA-CGA |
| 11  | bB    | 823 | CLA  | C2A-CAA-CBA-CGA |
| 11  | aB    | 822 | CLA  | CAA-CBA-CGA-O1A |
| 11  | bB    | 822 | CLA  | CAA-CBA-CGA-O1A |
| 11  | cB    | 822 | CLA  | CAA-CBA-CGA-O1A |
| 18  | aB    | 847 | LMG  | O7-C8-C9-O8     |
| 18  | bB    | 847 | LMG  | O7-C8-C9-O8     |
| 18  | cB    | 847 | LMG  | O7-C8-C9-O8     |
| 11  | aB    | 822 | CLA  | CAA-CBA-CGA-O2A |
| 11  | bB    | 822 | CLA  | CAA-CBA-CGA-O2A |
| 11  | cB    | 822 | CLA  | CAA-CBA-CGA-O2A |
| 11  | aA    | 821 | CLA  | C11-C10-C8-C9   |
| 11  | aB    | 817 | CLA  | C6-C7-C8-C9     |
| 11  | bA    | 821 | CLA  | C11-C10-C8-C9   |
| 11  | bB    | 817 | CLA  | C6-C7-C8-C9     |
| 11  | cA    | 821 | CLA  | C11-C10-C8-C9   |
| 11  | cB    | 817 | CLA  | C6-C7-C8-C9     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 12  | aA    | 826 | F6C  | C11-C10-C8-C9   |
| 12  | aL    | 202 | F6C  | C11-C10-C8-C9   |
| 12  | bA    | 826 | F6C  | C11-C10-C8-C9   |
| 12  | bL    | 202 | F6C  | C11-C10-C8-C9   |
| 12  | cA    | 826 | F6C  | C11-C10-C8-C9   |
| 12  | cL    | 202 | F6C  | C11-C10-C8-C9   |
| 11  | aA    | 843 | CLA  | CAA-CBA-CGA-O1A |
| 11  | bA    | 843 | CLA  | CAA-CBA-CGA-O1A |
| 11  | cA    | 843 | CLA  | CAA-CBA-CGA-O1A |
| 15  | aB    | 848 | BCR  | C17-C18-C19-C20 |
| 15  | bB    | 848 | BCR  | C17-C18-C19-C20 |
| 15  | cB    | 848 | BCR  | C17-C18-C19-C20 |
| 11  | aB    | 816 | CLA  | C10-C11-C12-C13 |
| 11  | bB    | 816 | CLA  | C10-C11-C12-C13 |
| 11  | cB    | 816 | CLA  | C10-C11-C12-C13 |
| 11  | aA    | 802 | CLA  | C4-C3-C5-C6     |
| 11  | bA    | 802 | CLA  | C4-C3-C5-C6     |
| 11  | cA    | 802 | CLA  | C4-C3-C5-C6     |
| 11  | aB    | 817 | CLA  | O1D-CGD-O2D-CED |
| 12  | bA    | 827 | F6C  | C2-C3-C5-C6     |
| 11  | cB    | 823 | CLA  | C2A-CAA-CBA-CGA |
| 11  | aA    | 814 | CLA  | C11-C12-C13-C15 |
| 11  | aA    | 822 | CLA  | C11-C12-C13-C15 |
| 11  | aA    | 831 | CLA  | C11-C10-C8-C7   |
| 11  | aB    | 825 | CLA  | C12-C13-C15-C16 |
| 11  | aL    | 205 | CLA  | C11-C10-C8-C7   |
| 11  | bA    | 814 | CLA  | C11-C12-C13-C15 |
| 11  | bA    | 822 | CLA  | C11-C12-C13-C15 |
| 11  | bA    | 831 | CLA  | C11-C10-C8-C7   |
| 11  | bB    | 825 | CLA  | C12-C13-C15-C16 |
| 11  | bL    | 205 | CLA  | C11-C10-C8-C7   |
| 11  | cA    | 814 | CLA  | C11-C12-C13-C15 |
| 11  | cA    | 822 | CLA  | C11-C12-C13-C15 |
| 11  | cA    | 831 | CLA  | C11-C10-C8-C7   |
| 11  | cB    | 825 | CLA  | C12-C13-C15-C16 |
| 11  | cL    | 205 | CLA  | C11-C10-C8-C7   |
| 11  | aA    | 821 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aA    | 828 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aB    | 803 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aB    | 823 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aB    | 826 | CLA  | C2B-C3B-CAB-CBB |
| 11  | aB    | 827 | CLA  | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | bA    | 821 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bB    | 803 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bB    | 823 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bB    | 826 | CLA  | C2B-C3B-CAB-CBB |
| 11  | bB    | 827 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cA    | 821 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cA    | 828 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cB    | 803 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cB    | 817 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cB    | 823 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cB    | 826 | CLA  | C2B-C3B-CAB-CBB |
| 11  | cB    | 827 | CLA  | C2B-C3B-CAB-CBB |
| 15  | aA    | 849 | BCR  | C23-C24-C25-C26 |
| 15  | aA    | 850 | BCR  | C23-C24-C25-C26 |
| 15  | aA    | 851 | BCR  | C23-C24-C25-C26 |
| 15  | aB    | 842 | BCR  | C23-C24-C25-C26 |
| 15  | aB    | 846 | BCR  | C23-C24-C25-C26 |
| 15  | aI    | 101 | BCR  | C23-C24-C25-C26 |
| 15  | bA    | 849 | BCR  | C23-C24-C25-C26 |
| 15  | bA    | 850 | BCR  | C23-C24-C25-C26 |
| 15  | bA    | 851 | BCR  | C23-C24-C25-C26 |
| 15  | bB    | 842 | BCR  | C23-C24-C25-C26 |
| 15  | bB    | 843 | BCR  | C23-C24-C25-C26 |
| 15  | bB    | 843 | BCR  | C23-C24-C25-C30 |
| 15  | bI    | 101 | BCR  | C23-C24-C25-C26 |
| 15  | cA    | 850 | BCR  | C23-C24-C25-C26 |
| 15  | cA    | 851 | BCR  | C23-C24-C25-C26 |
| 15  | cB    | 842 | BCR  | C23-C24-C25-C26 |
| 15  | cB    | 843 | BCR  | C23-C24-C25-C26 |
| 15  | cB    | 846 | BCR  | C23-C24-C25-C26 |
| 15  | cI    | 103 | BCR  | C23-C24-C25-C26 |
| 11  | aA    | 807 | CLA  | C2-C1-O2A-CGA   |
| 11  | bA    | 807 | CLA  | C2-C1-O2A-CGA   |
| 11  | cA    | 807 | CLA  | C2-C1-O2A-CGA   |
| 12  | aA    | 832 | F6C  | C2-C1-O2A-CGA   |
| 12  | bA    | 832 | F6C  | C2-C1-O2A-CGA   |
| 12  | cA    | 832 | F6C  | C2-C1-O2A-CGA   |
| 11  | aA    | 817 | CLA  | O2A-C1-C2-C3    |
| 11  | bA    | 817 | CLA  | O2A-C1-C2-C3    |
| 11  | cA    | 817 | CLA  | O2A-C1-C2-C3    |
| 11  | bB    | 817 | CLA  | O1D-CGD-O2D-CED |
| 11  | cB    | 817 | CLA  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | cB    | 819 | CLA  | CBA-CGA-O2A-C1  |
| 11  | bB    | 837 | CLA  | C4-C3-C5-C6     |
| 11  | aB    | 828 | CLA  | C2-C3-C5-C6     |
| 11  | bB    | 828 | CLA  | C2-C3-C5-C6     |
| 11  | cB    | 828 | CLA  | C2-C3-C5-C6     |
| 16  | bA    | 852 | LHG  | O8-C23-C24-C25  |
| 11  | bB    | 818 | CLA  | C10-C11-C12-C13 |
| 11  | aB    | 819 | CLA  | CBA-CGA-O2A-C1  |
| 11  | bB    | 819 | CLA  | CBA-CGA-O2A-C1  |
| 11  | aA    | 828 | CLA  | CAA-CBA-CGA-O2A |
| 11  | cA    | 828 | CLA  | CAA-CBA-CGA-O2A |
| 11  | cB    | 837 | CLA  | CAA-CBA-CGA-O2A |
| 16  | aA    | 852 | LHG  | O8-C23-C24-C25  |
| 16  | cA    | 852 | LHG  | O8-C23-C24-C25  |
| 11  | aB    | 837 | CLA  | C4-C3-C5-C6     |
| 11  | cB    | 837 | CLA  | C4-C3-C5-C6     |
| 12  | aA    | 844 | F6C  | C3A-C2A-CAA-CBA |
| 12  | bA    | 844 | F6C  | C3A-C2A-CAA-CBA |
| 12  | cA    | 844 | F6C  | C3A-C2A-CAA-CBA |
| 11  | aB    | 837 | CLA  | CAA-CBA-CGA-O2A |
| 11  | bA    | 828 | CLA  | CAA-CBA-CGA-O2A |
| 11  | bB    | 837 | CLA  | CAA-CBA-CGA-O2A |
| 12  | aA    | 827 | F6C  | C2-C3-C5-C6     |
| 12  | cA    | 827 | F6C  | C2-C3-C5-C6     |
| 11  | aA    | 803 | CLA  | C2A-CAA-CBA-CGA |
| 11  | aB    | 813 | CLA  | C2A-CAA-CBA-CGA |
| 11  | bB    | 813 | CLA  | C2A-CAA-CBA-CGA |
| 11  | cA    | 803 | CLA  | C2A-CAA-CBA-CGA |
| 11  | cB    | 813 | CLA  | C2A-CAA-CBA-CGA |
| 18  | aB    | 847 | LMG  | C31-C32-C33-C34 |
| 18  | bB    | 847 | LMG  | C31-C32-C33-C34 |
| 18  | cB    | 847 | LMG  | C31-C32-C33-C34 |
| 11  | aB    | 818 | CLA  | C10-C11-C12-C13 |
| 11  | cB    | 818 | CLA  | C10-C11-C12-C13 |
| 11  | bA    | 834 | CLA  | O1A-CGA-O2A-C1  |
| 11  | cA    | 834 | CLA  | O1A-CGA-O2A-C1  |
| 11  | aL    | 205 | CLA  | C14-C13-C15-C16 |
| 11  | bL    | 205 | CLA  | C14-C13-C15-C16 |
| 11  | cL    | 205 | CLA  | C14-C13-C15-C16 |
| 11  | bB    | 806 | CLA  | CAA-CBA-CGA-O2A |
| 11  | aA    | 834 | CLA  | O1A-CGA-O2A-C1  |
| 11  | aA    | 809 | CLA  | C4B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | aA    | 821 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aA    | 829 | CLA  | C1A-C2A-CAA-CBA |
| 11  | aB    | 833 | CLA  | C1A-C2A-CAA-CBA |
| 11  | aB    | 838 | CLA  | C4B-C3B-CAB-CBB |
| 11  | aL    | 206 | CLA  | C1A-C2A-CAA-CBA |
| 11  | bA    | 821 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bA    | 829 | CLA  | C1A-C2A-CAA-CBA |
| 11  | bB    | 838 | CLA  | C4B-C3B-CAB-CBB |
| 11  | bL    | 206 | CLA  | C1A-C2A-CAA-CBA |
| 11  | cA    | 809 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cA    | 821 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cA    | 829 | CLA  | C1A-C2A-CAA-CBA |
| 11  | cB    | 833 | CLA  | C1A-C2A-CAA-CBA |
| 11  | cB    | 838 | CLA  | C4B-C3B-CAB-CBB |
| 11  | cL    | 206 | CLA  | C1A-C2A-CAA-CBA |
| 11  | cA    | 825 | CLA  | CAA-CBA-CGA-O2A |
| 15  | aA    | 848 | BCR  | C7-C8-C9-C10    |
| 15  | aA    | 849 | BCR  | C7-C8-C9-C10    |
| 15  | aB    | 844 | BCR  | C17-C18-C19-C20 |
| 15  | aL    | 203 | BCR  | C7-C8-C9-C10    |
| 15  | bA    | 848 | BCR  | C7-C8-C9-C10    |
| 15  | bA    | 849 | BCR  | C7-C8-C9-C10    |
| 15  | bB    | 844 | BCR  | C17-C18-C19-C20 |
| 15  | bL    | 203 | BCR  | C7-C8-C9-C10    |
| 15  | cA    | 848 | BCR  | C7-C8-C9-C10    |
| 15  | cA    | 849 | BCR  | C7-C8-C9-C10    |
| 15  | cB    | 844 | BCR  | C17-C18-C19-C20 |
| 15  | cL    | 203 | BCR  | C7-C8-C9-C10    |
| 15  | aA    | 851 | BCR  | C15-C16-C17-C18 |
| 15  | bA    | 851 | BCR  | C15-C16-C17-C18 |
| 15  | cA    | 851 | BCR  | C15-C16-C17-C18 |
| 12  | aA    | 830 | F6C  | C16-C17-C18-C19 |
| 12  | bA    | 830 | F6C  | C16-C17-C18-C19 |
| 12  | cA    | 830 | F6C  | C16-C17-C18-C19 |
| 11  | aB    | 820 | CLA  | CAA-CBA-CGA-O2A |
| 11  | bB    | 820 | CLA  | CAA-CBA-CGA-O2A |
| 11  | cB    | 820 | CLA  | CAA-CBA-CGA-O2A |
| 11  | aA    | 825 | CLA  | CAA-CBA-CGA-O2A |
| 11  | aA    | 838 | CLA  | CAA-CBA-CGA-O2A |
| 11  | aB    | 806 | CLA  | CAA-CBA-CGA-O2A |
| 11  | bA    | 825 | CLA  | CAA-CBA-CGA-O2A |
| 11  | bA    | 838 | CLA  | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | cA    | 838 | CLA  | CAA-CBA-CGA-O2A |
| 11  | cB    | 806 | CLA  | CAA-CBA-CGA-O2A |
| 12  | aA    | 844 | F6C  | CAA-CBA-CGA-O2A |
| 12  | bA    | 844 | F6C  | CAA-CBA-CGA-O2A |
| 12  | cA    | 844 | F6C  | CAA-CBA-CGA-O2A |
| 11  | aA    | 818 | CLA  | C2A-CAA-CBA-CGA |
| 11  | aA    | 821 | CLA  | C2A-CAA-CBA-CGA |
| 11  | bA    | 803 | CLA  | C2A-CAA-CBA-CGA |
| 11  | bA    | 818 | CLA  | C2A-CAA-CBA-CGA |
| 11  | bA    | 821 | CLA  | C2A-CAA-CBA-CGA |
| 11  | cA    | 818 | CLA  | C2A-CAA-CBA-CGA |
| 11  | cA    | 821 | CLA  | C2A-CAA-CBA-CGA |
| 18  | aB    | 847 | LMG  | C2-C1-O1-C7     |
| 18  | bB    | 847 | LMG  | C2-C1-O1-C7     |
| 11  | bA    | 821 | CLA  | CAA-CBA-CGA-O2A |
| 11  | cA    | 821 | CLA  | CAA-CBA-CGA-O2A |
| 11  | aA    | 817 | CLA  | C2-C1-O2A-CGA   |
| 11  | aB    | 813 | CLA  | C2-C1-O2A-CGA   |
| 11  | aB    | 830 | CLA  | C2-C1-O2A-CGA   |
| 11  | bA    | 817 | CLA  | C2-C1-O2A-CGA   |
| 11  | bB    | 813 | CLA  | C2-C1-O2A-CGA   |
| 11  | bB    | 830 | CLA  | C2-C1-O2A-CGA   |
| 11  | cA    | 817 | CLA  | C2-C1-O2A-CGA   |
| 11  | cB    | 813 | CLA  | C2-C1-O2A-CGA   |
| 11  | cB    | 830 | CLA  | C2-C1-O2A-CGA   |
| 11  | aA    | 821 | CLA  | CAA-CBA-CGA-O2A |
| 11  | aB    | 816 | CLA  | C6-C7-C8-C10    |
| 11  | bB    | 816 | CLA  | C6-C7-C8-C10    |
| 11  | cB    | 816 | CLA  | C6-C7-C8-C10    |
| 11  | aB    | 813 | CLA  | C5-C6-C7-C8     |
| 11  | cB    | 813 | CLA  | C5-C6-C7-C8     |
| 11  | bB    | 813 | CLA  | C5-C6-C7-C8     |
| 11  | aB    | 812 | CLA  | C2A-CAA-CBA-CGA |
| 11  | bB    | 812 | CLA  | C2A-CAA-CBA-CGA |
| 11  | cB    | 812 | CLA  | C2A-CAA-CBA-CGA |
| 13  | cA    | 845 | PQN  | C18-C20-C21-C22 |
| 11  | cA    | 814 | CLA  | C13-C15-C16-C17 |
| 11  | aA    | 814 | CLA  | C13-C15-C16-C17 |
| 11  | bA    | 814 | CLA  | C13-C15-C16-C17 |
| 13  | aA    | 845 | PQN  | C18-C20-C21-C22 |
| 13  | bA    | 845 | PQN  | C18-C20-C21-C22 |
| 11  | aB    | 838 | CLA  | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | aL    | 204 | CLA  | CAA-CBA-CGA-O2A |
| 11  | bB    | 838 | CLA  | CAA-CBA-CGA-O2A |
| 11  | bL    | 204 | CLA  | CAA-CBA-CGA-O2A |
| 11  | cA    | 807 | CLA  | CAA-CBA-CGA-O2A |
| 11  | cB    | 838 | CLA  | CAA-CBA-CGA-O2A |
| 11  | cL    | 204 | CLA  | CAA-CBA-CGA-O2A |
| 11  | cA    | 805 | CLA  | CAA-CBA-CGA-O2A |
| 18  | aB    | 847 | LMG  | C4-C5-C6-O5     |
| 18  | bB    | 847 | LMG  | C4-C5-C6-O5     |
| 11  | aA    | 807 | CLA  | CAA-CBA-CGA-O2A |
| 11  | aB    | 821 | CLA  | CAA-CBA-CGA-O2A |
| 11  | bA    | 807 | CLA  | CAA-CBA-CGA-O2A |
| 11  | bB    | 821 | CLA  | CAA-CBA-CGA-O2A |
| 11  | cB    | 821 | CLA  | CAA-CBA-CGA-O2A |
| 11  | aA    | 805 | CLA  | CAA-CBA-CGA-O2A |
| 11  | bA    | 805 | CLA  | CAA-CBA-CGA-O2A |
| 11  | bA    | 814 | CLA  | O1A-CGA-O2A-C1  |
| 11  | cA    | 814 | CLA  | O1A-CGA-O2A-C1  |
| 11  | bB    | 837 | CLA  | CAA-CBA-CGA-O1A |
| 11  | cB    | 837 | CLA  | CAA-CBA-CGA-O1A |
| 18  | cB    | 847 | LMG  | C4-C5-C6-O5     |
| 11  | aA    | 820 | CLA  | C11-C12-C13-C14 |
| 11  | cA    | 820 | CLA  | C11-C12-C13-C14 |
| 11  | aB    | 837 | CLA  | CAA-CBA-CGA-O1A |
| 11  | aA    | 814 | CLA  | O1A-CGA-O2A-C1  |
| 11  | aB    | 817 | CLA  | CAA-CBA-CGA-O2A |
| 11  | cB    | 817 | CLA  | CAA-CBA-CGA-O2A |
| 16  | cA    | 852 | LHG  | O9-C7-C8-C9     |
| 11  | bB    | 817 | CLA  | CAA-CBA-CGA-O2A |
| 11  | aA    | 829 | CLA  | C16-C17-C18-C20 |
| 11  | bA    | 829 | CLA  | C16-C17-C18-C20 |
| 11  | cA    | 829 | CLA  | C16-C17-C18-C20 |
| 11  | aA    | 838 | CLA  | CBD-CGD-O2D-CED |
| 11  | bA    | 838 | CLA  | CBD-CGD-O2D-CED |
| 11  | cA    | 838 | CLA  | CBD-CGD-O2D-CED |
| 11  | aA    | 825 | CLA  | CAA-CBA-CGA-O1A |
| 11  | bA    | 825 | CLA  | CAA-CBA-CGA-O1A |
| 11  | cA    | 825 | CLA  | CAA-CBA-CGA-O1A |
| 16  | aA    | 852 | LHG  | O9-C7-C8-C9     |
| 16  | bA    | 852 | LHG  | O9-C7-C8-C9     |
| 18  | aB    | 847 | LMG  | O1-C7-C8-O7     |
| 18  | bB    | 847 | LMG  | O1-C7-C8-O7     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 18  | cB    | 847 | LMG  | O1-C7-C8-O7     |
| 11  | aB    | 820 | CLA  | CAA-CBA-CGA-O1A |
| 11  | bB    | 820 | CLA  | CAA-CBA-CGA-O1A |
| 11  | cA    | 837 | CLA  | CAA-CBA-CGA-O1A |
| 11  | cB    | 820 | CLA  | CAA-CBA-CGA-O1A |
| 18  | cB    | 847 | LMG  | C2-C1-O1-C7     |
| 11  | aB    | 805 | CLA  | CAA-CBA-CGA-O2A |
| 11  | cB    | 805 | CLA  | CAA-CBA-CGA-O2A |
| 11  | aA    | 837 | CLA  | CAA-CBA-CGA-O1A |
| 11  | bA    | 823 | CLA  | CAA-CBA-CGA-O2A |
| 11  | bA    | 837 | CLA  | CAA-CBA-CGA-O1A |
| 11  | cA    | 823 | CLA  | CAA-CBA-CGA-O2A |
| 11  | aB    | 818 | CLA  | C15-C16-C17-C18 |
| 11  | bB    | 818 | CLA  | C15-C16-C17-C18 |
| 11  | cB    | 818 | CLA  | C15-C16-C17-C18 |
| 11  | aA    | 829 | CLA  | CAA-CBA-CGA-O2A |
| 11  | bA    | 829 | CLA  | CAA-CBA-CGA-O2A |
| 11  | bB    | 805 | CLA  | CAA-CBA-CGA-O2A |
| 11  | cA    | 829 | CLA  | CAA-CBA-CGA-O2A |
| 11  | aA    | 823 | CLA  | CAA-CBA-CGA-O2A |
| 11  | aA    | 828 | CLA  | CAA-CBA-CGA-O1A |
| 11  | bA    | 828 | CLA  | CAA-CBA-CGA-O1A |
| 11  | cA    | 828 | CLA  | CAA-CBA-CGA-O1A |
| 11  | aA    | 824 | CLA  | CAD-CBD-CGD-O2D |
| 11  | aA    | 831 | CLA  | CAD-CBD-CGD-O2D |
| 11  | aB    | 829 | CLA  | CAD-CBD-CGD-O2D |
| 11  | aB    | 839 | CLA  | CAD-CBD-CGD-O2D |
| 11  | bA    | 824 | CLA  | CAD-CBD-CGD-O2D |
| 11  | bA    | 831 | CLA  | CAD-CBD-CGD-O2D |
| 11  | bB    | 829 | CLA  | CAD-CBD-CGD-O2D |
| 11  | bB    | 835 | CLA  | CAD-CBD-CGD-O2D |
| 11  | bB    | 839 | CLA  | CAD-CBD-CGD-O2D |
| 11  | cA    | 824 | CLA  | CAD-CBD-CGD-O2D |
| 11  | cA    | 831 | CLA  | CAD-CBD-CGD-O2D |
| 11  | cB    | 829 | CLA  | CAD-CBD-CGD-O2D |
| 11  | cB    | 835 | CLA  | CAD-CBD-CGD-O2D |
| 11  | cB    | 839 | CLA  | CAD-CBD-CGD-O2D |
| 11  | aA    | 824 | CLA  | CAA-CBA-CGA-O2A |
| 11  | aB    | 816 | CLA  | CAA-CBA-CGA-O2A |
| 11  | bB    | 816 | CLA  | CAA-CBA-CGA-O2A |
| 11  | cB    | 816 | CLA  | CAA-CBA-CGA-O2A |
| 11  | aB    | 811 | CLA  | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | bB    | 811 | CLA  | CAA-CBA-CGA-O2A |
| 11  | cB    | 811 | CLA  | CAA-CBA-CGA-O2A |
| 11  | bA    | 821 | CLA  | CAA-CBA-CGA-O1A |
| 11  | cA    | 821 | CLA  | CAA-CBA-CGA-O1A |
| 12  | aA    | 844 | F6C  | CAA-CBA-CGA-O1A |
| 11  | aA    | 807 | CLA  | C8-C10-C11-C12  |
| 11  | bA    | 807 | CLA  | C8-C10-C11-C12  |
| 11  | cA    | 807 | CLA  | C8-C10-C11-C12  |
| 11  | aA    | 812 | CLA  | C2-C1-O2A-CGA   |
| 11  | bA    | 812 | CLA  | C2-C1-O2A-CGA   |
| 11  | cA    | 812 | CLA  | C2-C1-O2A-CGA   |
| 11  | aA    | 823 | CLA  | CAA-CBA-CGA-O1A |
| 11  | aB    | 811 | CLA  | CAA-CBA-CGA-O1A |
| 11  | cA    | 823 | CLA  | CAA-CBA-CGA-O1A |
| 11  | aA    | 821 | CLA  | CAA-CBA-CGA-O1A |
| 12  | bA    | 844 | F6C  | CAA-CBA-CGA-O1A |
| 12  | cA    | 844 | F6C  | CAA-CBA-CGA-O1A |
| 11  | aA    | 840 | CLA  | CAA-CBA-CGA-O2A |
| 11  | bA    | 824 | CLA  | CAA-CBA-CGA-O2A |
| 11  | bA    | 840 | CLA  | CAA-CBA-CGA-O2A |
| 11  | cA    | 824 | CLA  | CAA-CBA-CGA-O2A |
| 11  | cA    | 840 | CLA  | CAA-CBA-CGA-O2A |
| 11  | bA    | 823 | CLA  | CAA-CBA-CGA-O1A |
| 11  | cK    | 103 | CLA  | CAA-CBA-CGA-O2A |
| 11  | bB    | 811 | CLA  | CAA-CBA-CGA-O1A |
| 11  | aA    | 840 | CLA  | C16-C17-C18-C20 |
| 11  | bA    | 840 | CLA  | C16-C17-C18-C20 |
| 11  | aA    | 807 | CLA  | CAA-CBA-CGA-O1A |
| 11  | aB    | 821 | CLA  | CAA-CBA-CGA-O1A |
| 11  | aL    | 204 | CLA  | CAA-CBA-CGA-O1A |
| 11  | bL    | 204 | CLA  | CAA-CBA-CGA-O1A |
| 11  | cA    | 807 | CLA  | CAA-CBA-CGA-O1A |
| 11  | aA    | 814 | CLA  | CAA-CBA-CGA-O2A |
| 11  | aK    | 103 | CLA  | CAA-CBA-CGA-O2A |
| 11  | bA    | 814 | CLA  | CAA-CBA-CGA-O2A |
| 11  | bK    | 103 | CLA  | CAA-CBA-CGA-O2A |
| 11  | cA    | 814 | CLA  | CAA-CBA-CGA-O2A |
| 11  | cB    | 811 | CLA  | CAA-CBA-CGA-O1A |
| 11  | bA    | 807 | CLA  | CAA-CBA-CGA-O1A |
| 11  | bB    | 806 | CLA  | CAA-CBA-CGA-O1A |
| 11  | bB    | 821 | CLA  | CAA-CBA-CGA-O1A |
| 11  | cB    | 806 | CLA  | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | cL    | 204 | CLA  | CAA-CBA-CGA-O1A |

There are no ring outliers.

240 monomers are involved in 402 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 15  | aK    | 102 | BCR  | 2       | 0            |
| 11  | cA    | 823 | CLA  | 1       | 0            |
| 15  | aA    | 851 | BCR  | 7       | 0            |
| 11  | bB    | 802 | CLA  | 4       | 0            |
| 15  | aB    | 844 | BCR  | 1       | 0            |
| 11  | aB    | 825 | CLA  | 1       | 0            |
| 11  | bB    | 828 | CLA  | 2       | 0            |
| 13  | bA    | 845 | PQN  | 1       | 0            |
| 11  | cA    | 834 | CLA  | 1       | 0            |
| 11  | aA    | 819 | CLA  | 1       | 0            |
| 11  | bB    | 821 | CLA  | 1       | 0            |
| 11  | bB    | 812 | CLA  | 3       | 0            |
| 17  | cA    | 853 | LMT  | 2       | 0            |
| 11  | aL    | 206 | CLA  | 2       | 0            |
| 11  | aA    | 843 | CLA  | 2       | 0            |
| 11  | bA    | 814 | CLA  | 3       | 0            |
| 13  | aB    | 841 | PQN  | 3       | 0            |
| 11  | cA    | 840 | CLA  | 2       | 0            |
| 11  | aA    | 812 | CLA  | 1       | 0            |
| 11  | cB    | 834 | CLA  | 1       | 0            |
| 11  | aB    | 836 | CLA  | 2       | 0            |
| 11  | bB    | 826 | CLA  | 1       | 0            |
| 12  | cB    | 824 | F6C  | 1       | 0            |
| 11  | cB    | 807 | CLA  | 1       | 0            |
| 11  | cA    | 813 | CLA  | 2       | 0            |
| 11  | aB    | 805 | CLA  | 2       | 0            |
| 11  | aB    | 817 | CLA  | 2       | 0            |
| 11  | bA    | 836 | CLA  | 2       | 0            |
| 11  | cB    | 813 | CLA  | 1       | 0            |
| 11  | aA    | 802 | CLA  | 1       | 0            |
| 11  | cB    | 829 | CLA  | 1       | 0            |
| 15  | cK    | 102 | BCR  | 2       | 0            |
| 11  | cB    | 801 | CLA  | 2       | 0            |
| 15  | aL    | 203 | BCR  | 2       | 0            |
| 11  | cB    | 810 | CLA  | 1       | 0            |
| 11  | bB    | 808 | CLA  | 4       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 11  | cA    | 821 | CLA  | 2       | 0            |
| 11  | cA    | 818 | CLA  | 2       | 0            |
| 15  | bL    | 207 | BCR  | 2       | 0            |
| 11  | bA    | 820 | CLA  | 3       | 0            |
| 15  | bL    | 203 | BCR  | 3       | 0            |
| 11  | aA    | 825 | CLA  | 3       | 0            |
| 11  | aB    | 815 | CLA  | 3       | 0            |
| 18  | cB    | 847 | LMG  | 1       | 0            |
| 11  | aA    | 813 | CLA  | 3       | 0            |
| 15  | bA    | 851 | BCR  | 7       | 0            |
| 11  | aK    | 103 | CLA  | 1       | 0            |
| 11  | bB    | 823 | CLA  | 4       | 0            |
| 11  | aB    | 812 | CLA  | 3       | 0            |
| 11  | cB    | 821 | CLA  | 1       | 0            |
| 11  | aB    | 832 | CLA  | 1       | 0            |
| 11  | cA    | 802 | CLA  | 1       | 0            |
| 11  | bA    | 822 | CLA  | 4       | 0            |
| 11  | cB    | 828 | CLA  | 3       | 0            |
| 11  | bA    | 810 | CLA  | 1       | 0            |
| 11  | aB    | 823 | CLA  | 6       | 0            |
| 11  | cA    | 814 | CLA  | 3       | 0            |
| 11  | cB    | 838 | CLA  | 2       | 0            |
| 11  | aA    | 829 | CLA  | 3       | 0            |
| 11  | bA    | 806 | CLA  | 5       | 0            |
| 18  | bB    | 847 | LMG  | 1       | 0            |
| 11  | cB    | 818 | CLA  | 1       | 0            |
| 11  | aA    | 806 | CLA  | 4       | 0            |
| 11  | bA    | 823 | CLA  | 2       | 0            |
| 11  | bB    | 819 | CLA  | 1       | 0            |
| 11  | cL    | 204 | CLA  | 1       | 0            |
| 11  | cA    | 804 | CLA  | 1       | 0            |
| 13  | bB    | 841 | PQN  | 2       | 0            |
| 15  | bA    | 850 | BCR  | 1       | 0            |
| 11  | cL    | 205 | CLA  | 3       | 0            |
| 15  | bB    | 845 | BCR  | 1       | 0            |
| 11  | aB    | 813 | CLA  | 1       | 0            |
| 11  | bA    | 819 | CLA  | 2       | 0            |
| 11  | cA    | 838 | CLA  | 2       | 0            |
| 11  | bA    | 821 | CLA  | 2       | 0            |
| 11  | cB    | 812 | CLA  | 5       | 0            |
| 11  | aA    | 840 | CLA  | 3       | 0            |
| 11  | cB    | 832 | CLA  | 1       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 11  | cA    | 809 | CLA  | 2       | 0            |
| 11  | aB    | 834 | CLA  | 1       | 0            |
| 11  | bB    | 815 | CLA  | 1       | 0            |
| 11  | cB    | 833 | CLA  | 1       | 0            |
| 11  | cB    | 802 | CLA  | 3       | 0            |
| 11  | aA    | 820 | CLA  | 3       | 0            |
| 11  | bB    | 805 | CLA  | 3       | 0            |
| 13  | cA    | 845 | PQN  | 1       | 0            |
| 18  | aB    | 847 | LMG  | 1       | 0            |
| 11  | bA    | 818 | CLA  | 2       | 0            |
| 11  | bA    | 825 | CLA  | 2       | 0            |
| 11  | cB    | 804 | CLA  | 4       | 0            |
| 15  | bB    | 843 | BCR  | 1       | 0            |
| 11  | bK    | 103 | CLA  | 1       | 0            |
| 11  | aB    | 840 | CLA  | 1       | 0            |
| 11  | cA    | 807 | CLA  | 1       | 0            |
| 15  | cB    | 848 | BCR  | 3       | 0            |
| 11  | aB    | 810 | CLA  | 1       | 0            |
| 11  | aB    | 806 | CLA  | 3       | 0            |
| 11  | cA    | 820 | CLA  | 4       | 0            |
| 16  | cA    | 852 | LHG  | 1       | 0            |
| 17  | aA    | 853 | LMT  | 2       | 0            |
| 11  | cA    | 819 | CLA  | 3       | 0            |
| 11  | bB    | 832 | CLA  | 1       | 0            |
| 15  | aB    | 846 | BCR  | 2       | 0            |
| 11  | aA    | 833 | CLA  | 2       | 0            |
| 15  | cB    | 845 | BCR  | 2       | 0            |
| 11  | aA    | 824 | CLA  | 2       | 0            |
| 11  | bA    | 804 | CLA  | 1       | 0            |
| 11  | cL    | 206 | CLA  | 1       | 0            |
| 11  | bA    | 828 | CLA  | 1       | 0            |
| 15  | bA    | 848 | BCR  | 3       | 0            |
| 11  | bL    | 205 | CLA  | 3       | 0            |
| 11  | cB    | 840 | CLA  | 1       | 0            |
| 11  | aB    | 828 | CLA  | 2       | 0            |
| 11  | cA    | 839 | CLA  | 3       | 0            |
| 15  | cA    | 849 | BCR  | 2       | 0            |
| 11  | aB    | 827 | CLA  | 3       | 0            |
| 15  | aB    | 843 | BCR  | 1       | 0            |
| 15  | aA    | 848 | BCR  | 3       | 0            |
| 12  | aB    | 824 | F6C  | 1       | 0            |
| 15  | aL    | 208 | BCR  | 3       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 15  | aL    | 207 | BCR  | 2       | 0            |
| 15  | aB    | 842 | BCR  | 1       | 0            |
| 15  | cL    | 207 | BCR  | 2       | 0            |
| 11  | bB    | 813 | CLA  | 1       | 0            |
| 11  | bB    | 829 | CLA  | 1       | 0            |
| 11  | cB    | 825 | CLA  | 1       | 0            |
| 15  | aB    | 845 | BCR  | 2       | 0            |
| 15  | bB    | 844 | BCR  | 1       | 0            |
| 11  | aB    | 801 | CLA  | 3       | 0            |
| 11  | bA    | 839 | CLA  | 3       | 0            |
| 11  | aA    | 804 | CLA  | 1       | 0            |
| 11  | aB    | 826 | CLA  | 1       | 0            |
| 11  | bB    | 834 | CLA  | 1       | 0            |
| 16  | bA    | 852 | LHG  | 1       | 0            |
| 11  | cA    | 822 | CLA  | 5       | 0            |
| 11  | aA    | 809 | CLA  | 2       | 0            |
| 11  | bB    | 806 | CLA  | 3       | 0            |
| 11  | cA    | 803 | CLA  | 2       | 0            |
| 15  | cA    | 851 | BCR  | 7       | 0            |
| 11  | aA    | 838 | CLA  | 2       | 0            |
| 15  | aA    | 850 | BCR  | 1       | 0            |
| 15  | aI    | 101 | BCR  | 2       | 0            |
| 11  | aB    | 807 | CLA  | 1       | 0            |
| 11  | cB    | 827 | CLA  | 3       | 0            |
| 11  | aA    | 818 | CLA  | 2       | 0            |
| 11  | bB    | 836 | CLA  | 2       | 0            |
| 11  | bB    | 840 | CLA  | 1       | 0            |
| 15  | aA    | 847 | BCR  | 3       | 0            |
| 11  | cB    | 805 | CLA  | 3       | 0            |
| 11  | aB    | 804 | CLA  | 4       | 0            |
| 11  | cA    | 835 | CLA  | 1       | 0            |
| 11  | aA    | 822 | CLA  | 4       | 0            |
| 11  | bA    | 840 | CLA  | 2       | 0            |
| 11  | aB    | 837 | CLA  | 2       | 0            |
| 15  | aB    | 848 | BCR  | 2       | 0            |
| 11  | cA    | 833 | CLA  | 2       | 0            |
| 11  | aB    | 838 | CLA  | 2       | 0            |
| 11  | cB    | 803 | CLA  | 1       | 0            |
| 11  | cB    | 826 | CLA  | 1       | 0            |
| 15  | bB    | 846 | BCR  | 1       | 0            |
| 11  | aB    | 818 | CLA  | 1       | 0            |
| 11  | cA    | 829 | CLA  | 5       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 11  | bA    | 803 | CLA  | 1       | 0            |
| 15  | cA    | 847 | BCR  | 2       | 0            |
| 11  | bB    | 827 | CLA  | 3       | 0            |
| 11  | bA    | 838 | CLA  | 2       | 0            |
| 11  | aB    | 839 | CLA  | 1       | 0            |
| 15  | bB    | 842 | BCR  | 1       | 0            |
| 11  | bB    | 825 | CLA  | 1       | 0            |
| 15  | aA    | 849 | BCR  | 2       | 0            |
| 11  | cA    | 831 | CLA  | 1       | 0            |
| 11  | cK    | 103 | CLA  | 1       | 0            |
| 13  | cB    | 841 | PQN  | 1       | 0            |
| 11  | bA    | 809 | CLA  | 2       | 0            |
| 11  | bA    | 831 | CLA  | 1       | 0            |
| 11  | aA    | 828 | CLA  | 2       | 0            |
| 15  | cB    | 846 | BCR  | 2       | 0            |
| 11  | aA    | 814 | CLA  | 3       | 0            |
| 15  | cA    | 850 | BCR  | 1       | 0            |
| 11  | cB    | 836 | CLA  | 2       | 0            |
| 11  | aA    | 836 | CLA  | 2       | 0            |
| 11  | bA    | 812 | CLA  | 1       | 0            |
| 11  | cA    | 812 | CLA  | 1       | 0            |
| 11  | bL    | 204 | CLA  | 2       | 0            |
| 11  | bB    | 833 | CLA  | 1       | 0            |
| 11  | cB    | 837 | CLA  | 3       | 0            |
| 11  | aB    | 802 | CLA  | 4       | 0            |
| 15  | cB    | 842 | BCR  | 1       | 0            |
| 11  | aB    | 816 | CLA  | 4       | 0            |
| 11  | aA    | 821 | CLA  | 2       | 0            |
| 11  | bB    | 801 | CLA  | 2       | 0            |
| 11  | aA    | 803 | CLA  | 3       | 0            |
| 11  | bB    | 817 | CLA  | 1       | 0            |
| 11  | cB    | 808 | CLA  | 3       | 0            |
| 11  | bB    | 810 | CLA  | 1       | 0            |
| 11  | cA    | 828 | CLA  | 1       | 0            |
| 11  | cB    | 815 | CLA  | 2       | 0            |
| 15  | bM    | 101 | BCR  | 2       | 0            |
| 11  | cB    | 839 | CLA  | 1       | 0            |
| 11  | cB    | 817 | CLA  | 1       | 0            |
| 11  | cA    | 825 | CLA  | 2       | 0            |
| 11  | cA    | 836 | CLA  | 2       | 0            |
| 15  | bK    | 102 | BCR  | 2       | 0            |
| 15  | bA    | 849 | BCR  | 3       | 0            |

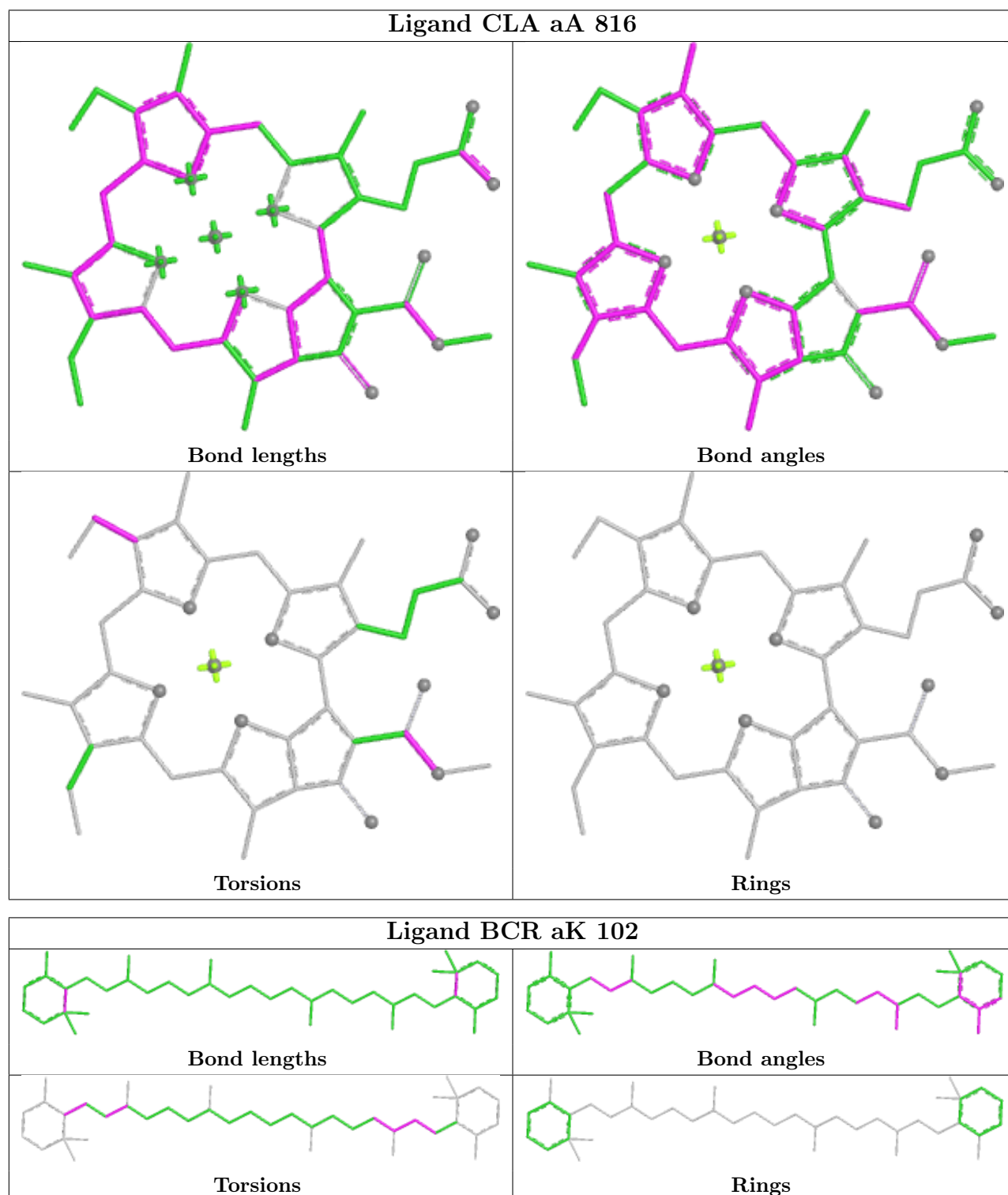
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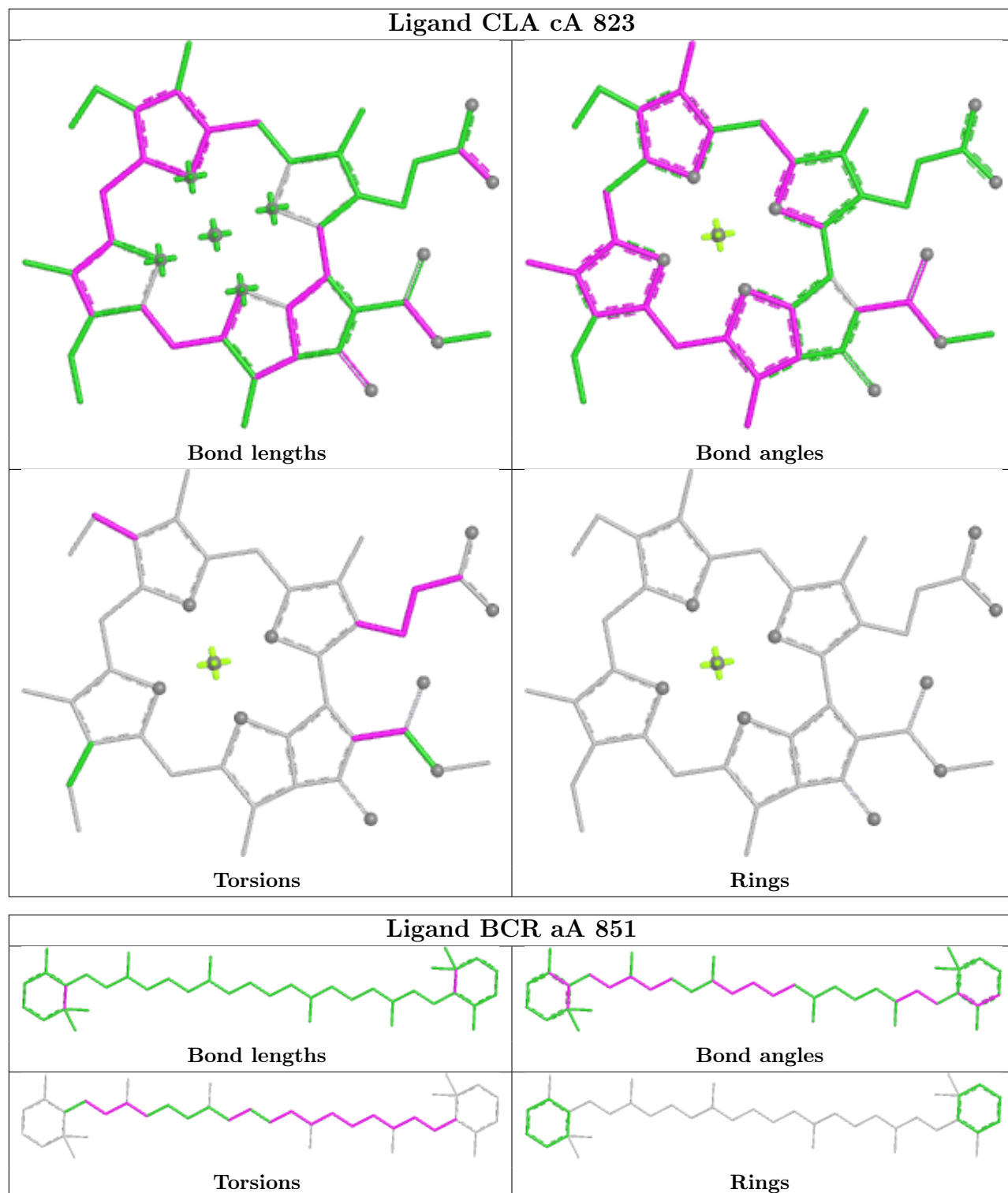
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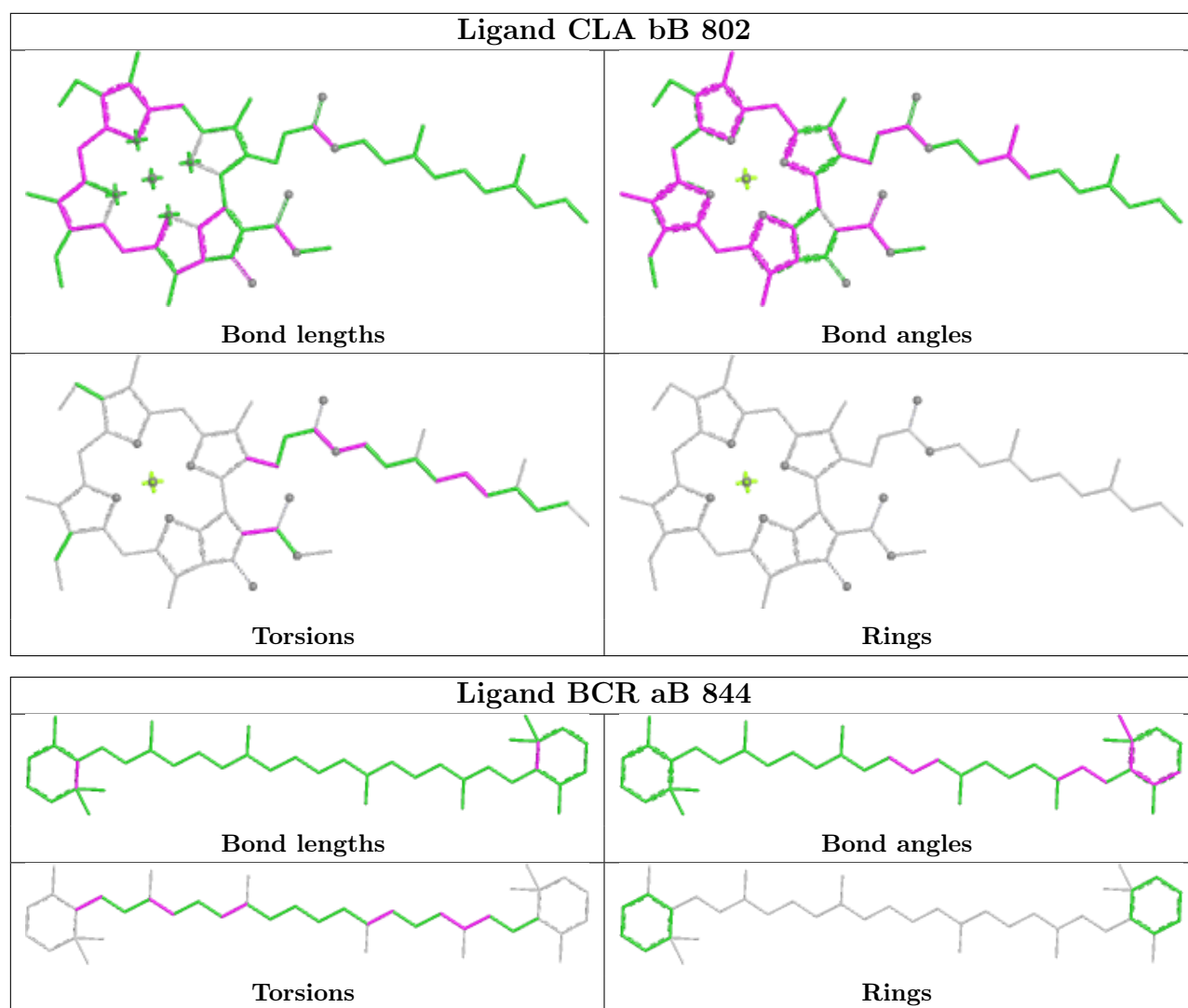
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 15  | bL    | 208 | BCR  | 2       | 0            |
| 15  | cA    | 848 | BCR  | 3       | 0            |
| 11  | bB    | 807 | CLA  | 1       | 0            |
| 16  | aA    | 852 | LHG  | 1       | 0            |
| 11  | aA    | 823 | CLA  | 1       | 0            |
| 11  | cA    | 843 | CLA  | 2       | 0            |
| 11  | bA    | 813 | CLA  | 1       | 0            |
| 11  | bA    | 843 | CLA  | 2       | 0            |
| 11  | bA    | 829 | CLA  | 4       | 0            |
| 11  | aB    | 803 | CLA  | 1       | 0            |
| 11  | bL    | 206 | CLA  | 3       | 0            |
| 11  | bB    | 804 | CLA  | 3       | 0            |
| 15  | cL    | 208 | BCR  | 5       | 0            |
| 11  | bB    | 837 | CLA  | 2       | 0            |
| 15  | bB    | 848 | BCR  | 2       | 0            |
| 11  | cB    | 806 | CLA  | 3       | 0            |
| 11  | bB    | 838 | CLA  | 1       | 0            |
| 11  | aB    | 833 | CLA  | 1       | 0            |
| 11  | cB    | 823 | CLA  | 5       | 0            |
| 11  | aA    | 831 | CLA  | 1       | 0            |
| 11  | aB    | 808 | CLA  | 4       | 0            |
| 11  | bB    | 818 | CLA  | 1       | 0            |
| 15  | cL    | 203 | BCR  | 2       | 0            |
| 11  | aL    | 204 | CLA  | 1       | 0            |
| 11  | bA    | 824 | CLA  | 2       | 0            |
| 11  | cB    | 816 | CLA  | 3       | 0            |
| 11  | aA    | 839 | CLA  | 3       | 0            |
| 11  | bB    | 839 | CLA  | 1       | 0            |
| 17  | bA    | 853 | LMT  | 2       | 0            |
| 11  | bA    | 833 | CLA  | 3       | 0            |
| 11  | bB    | 816 | CLA  | 4       | 0            |
| 11  | cA    | 806 | CLA  | 5       | 0            |
| 15  | bA    | 847 | BCR  | 4       | 0            |
| 11  | aL    | 205 | CLA  | 3       | 0            |
| 11  | cA    | 824 | CLA  | 2       | 0            |
| 15  | cB    | 844 | BCR  | 2       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

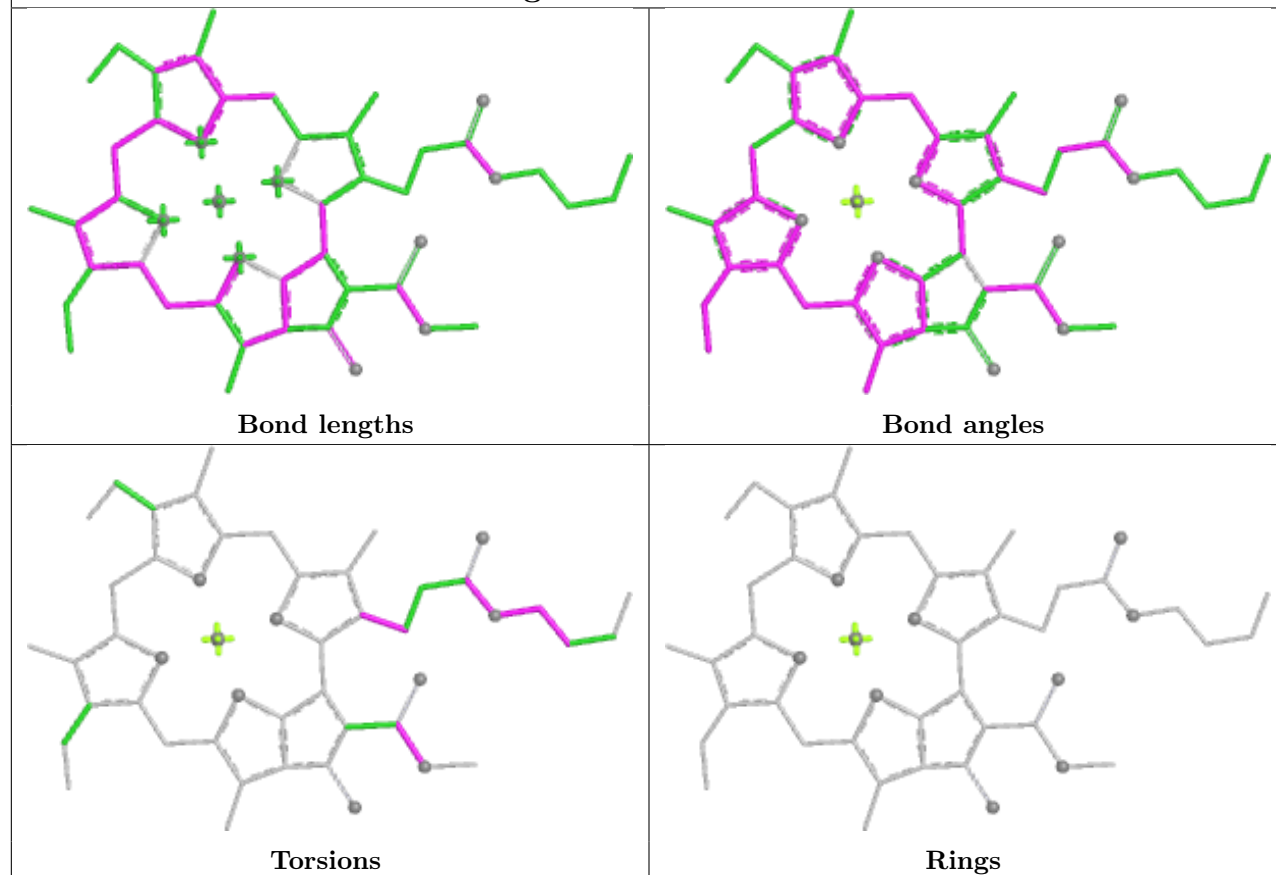
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



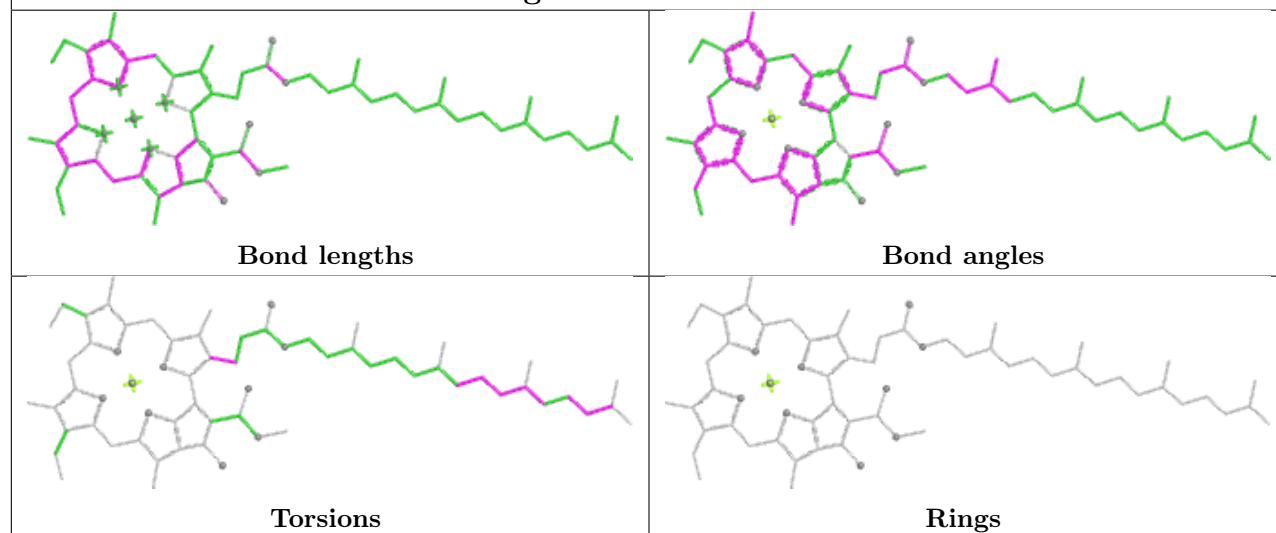




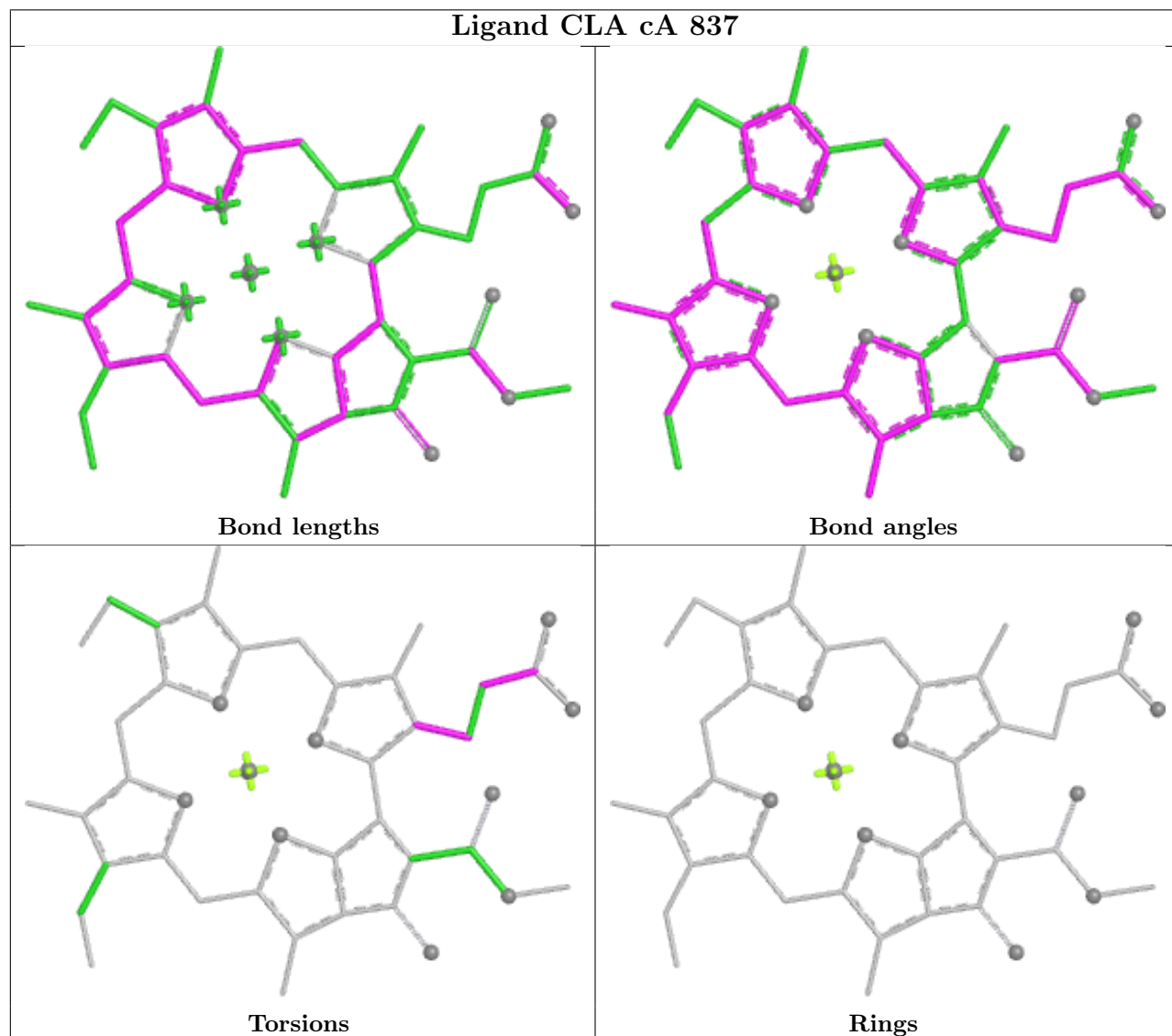
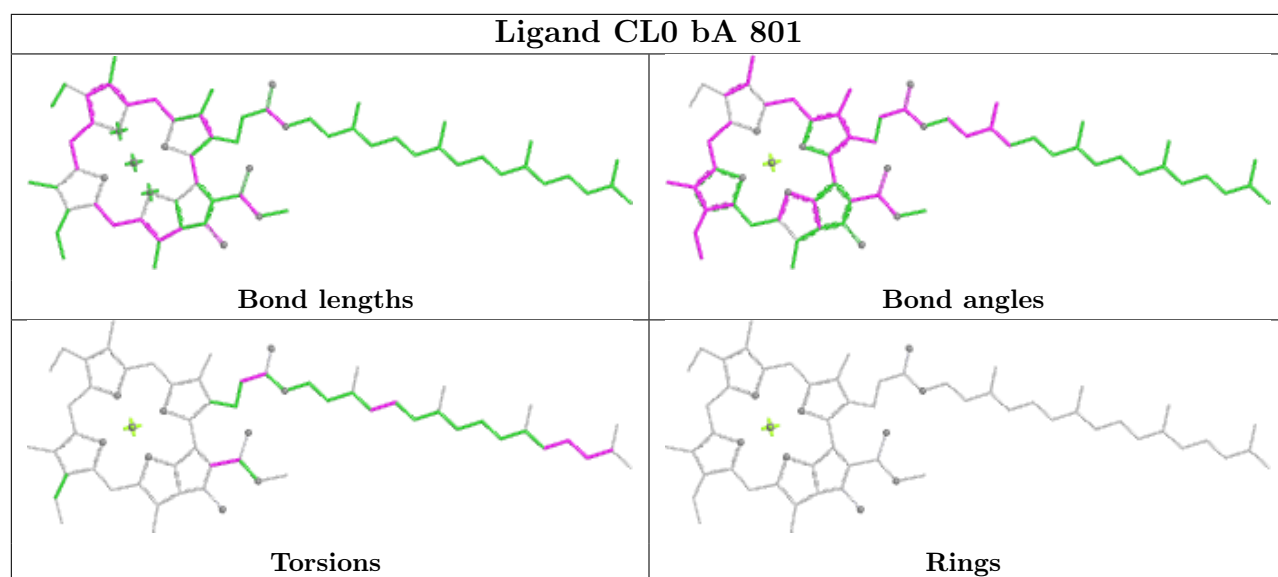
## Ligand CLA cA 817

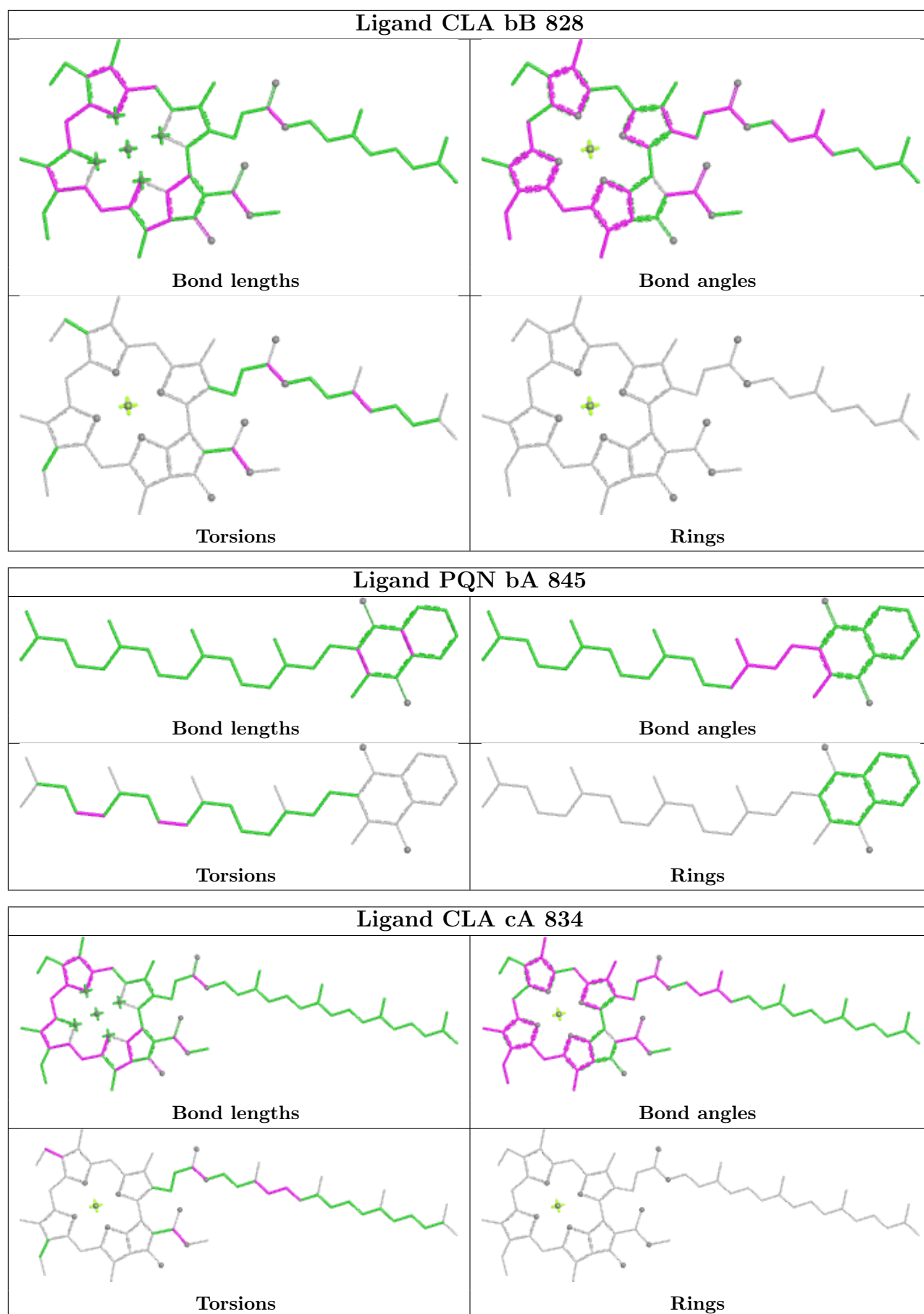


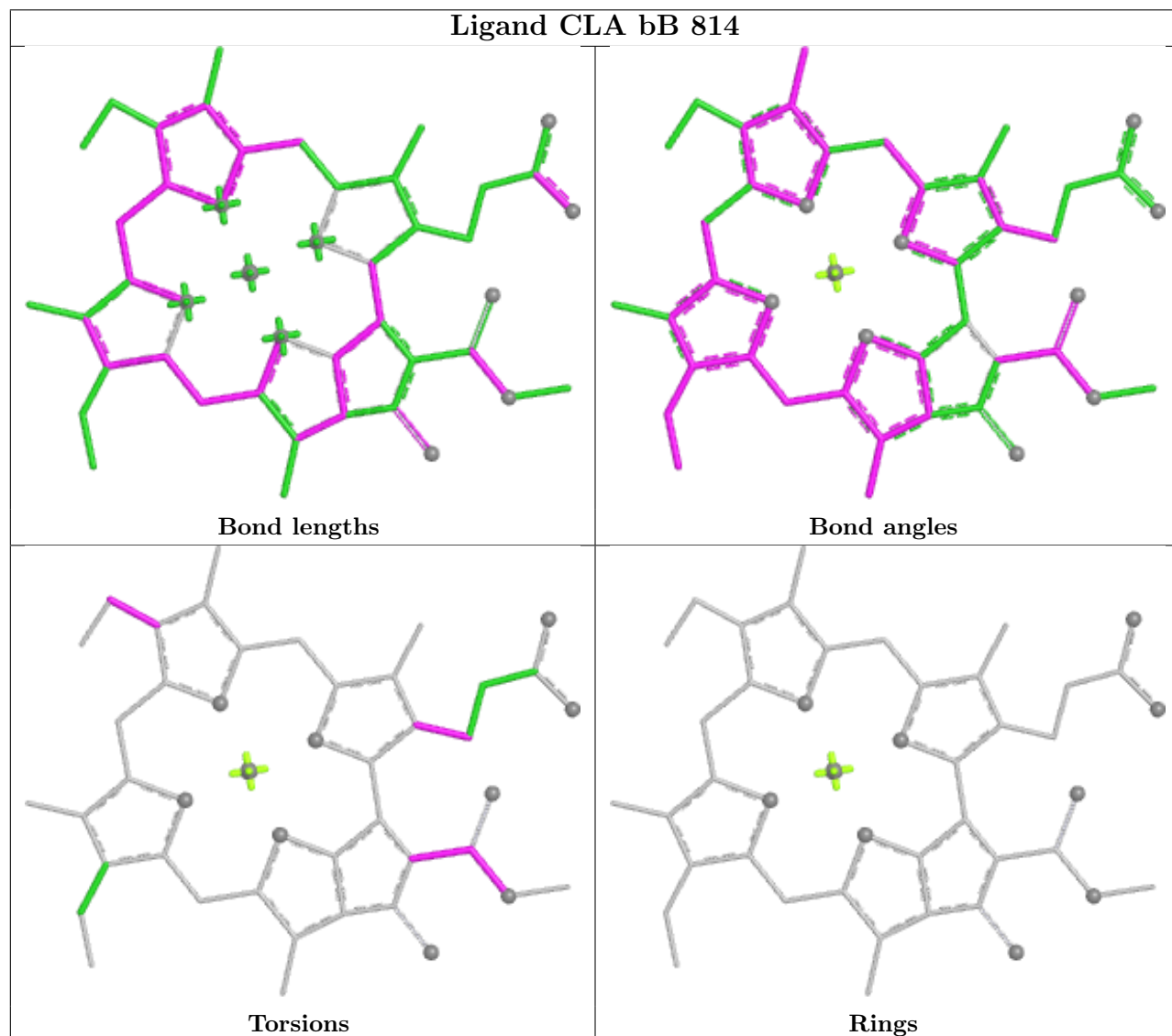
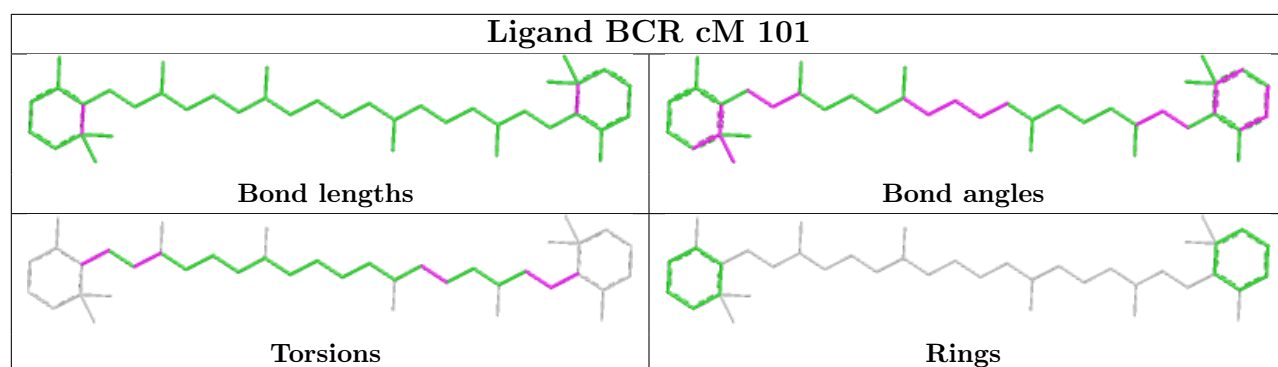
## Ligand CLA aB 825



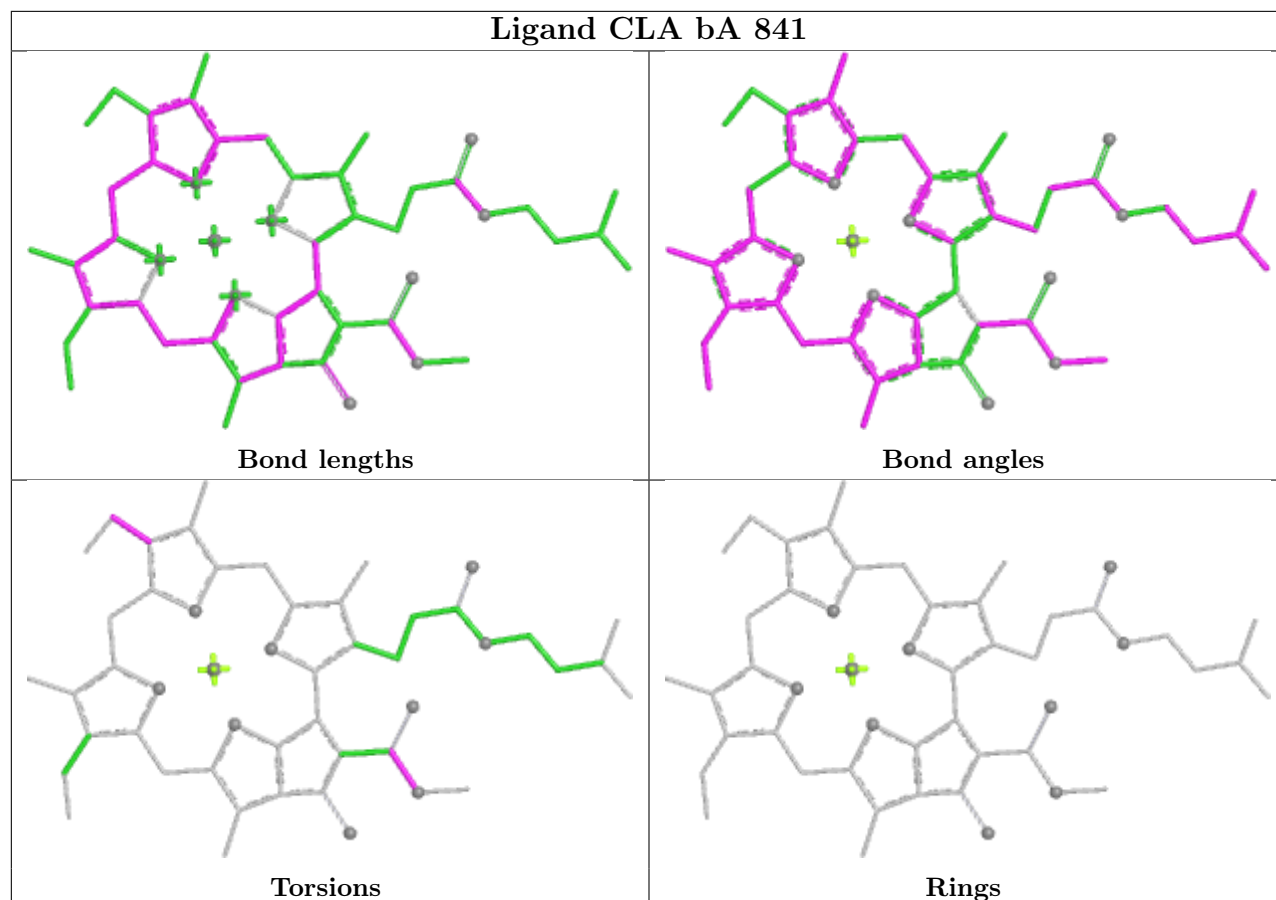




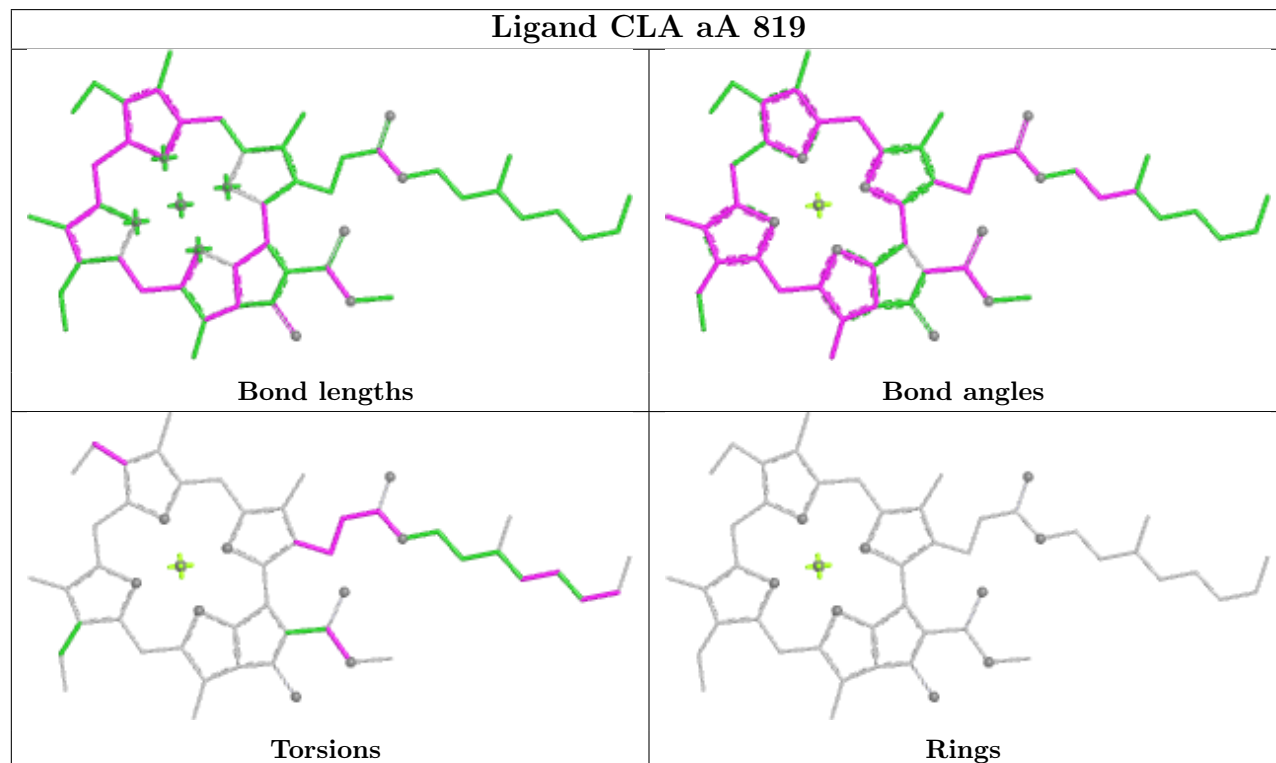


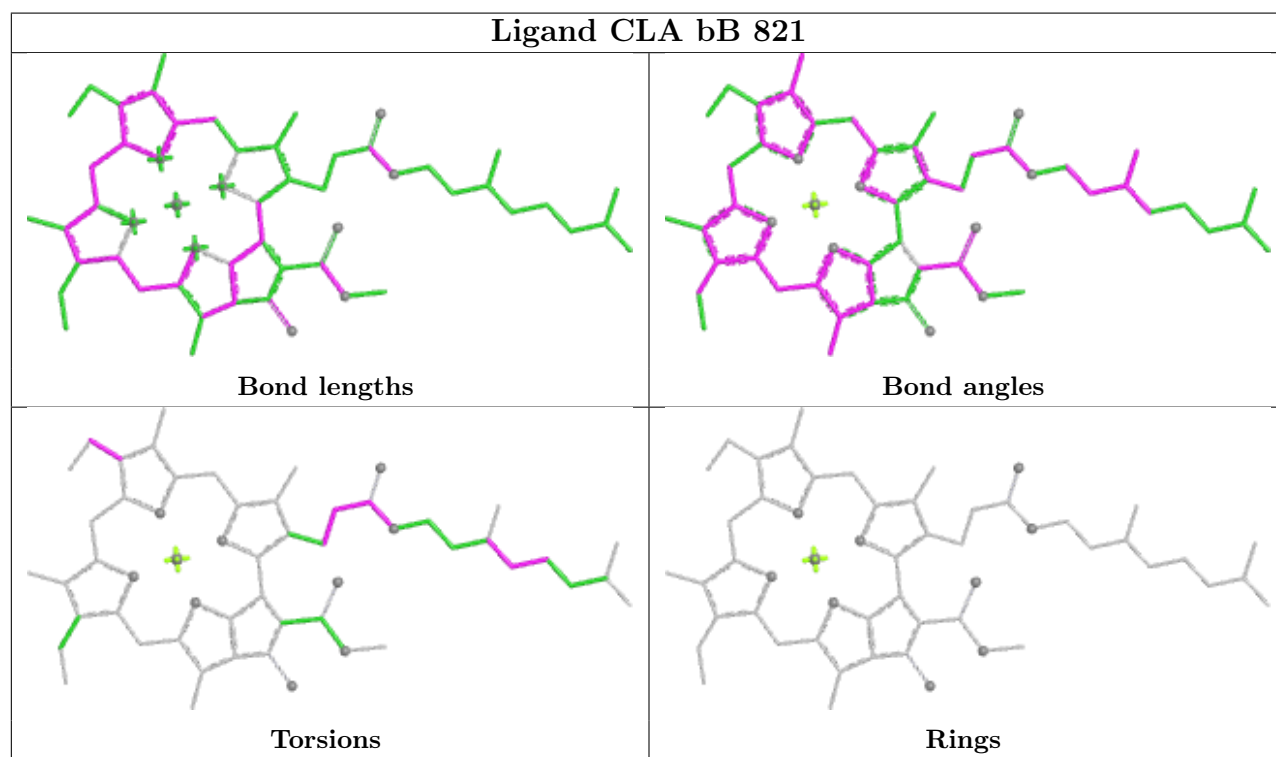
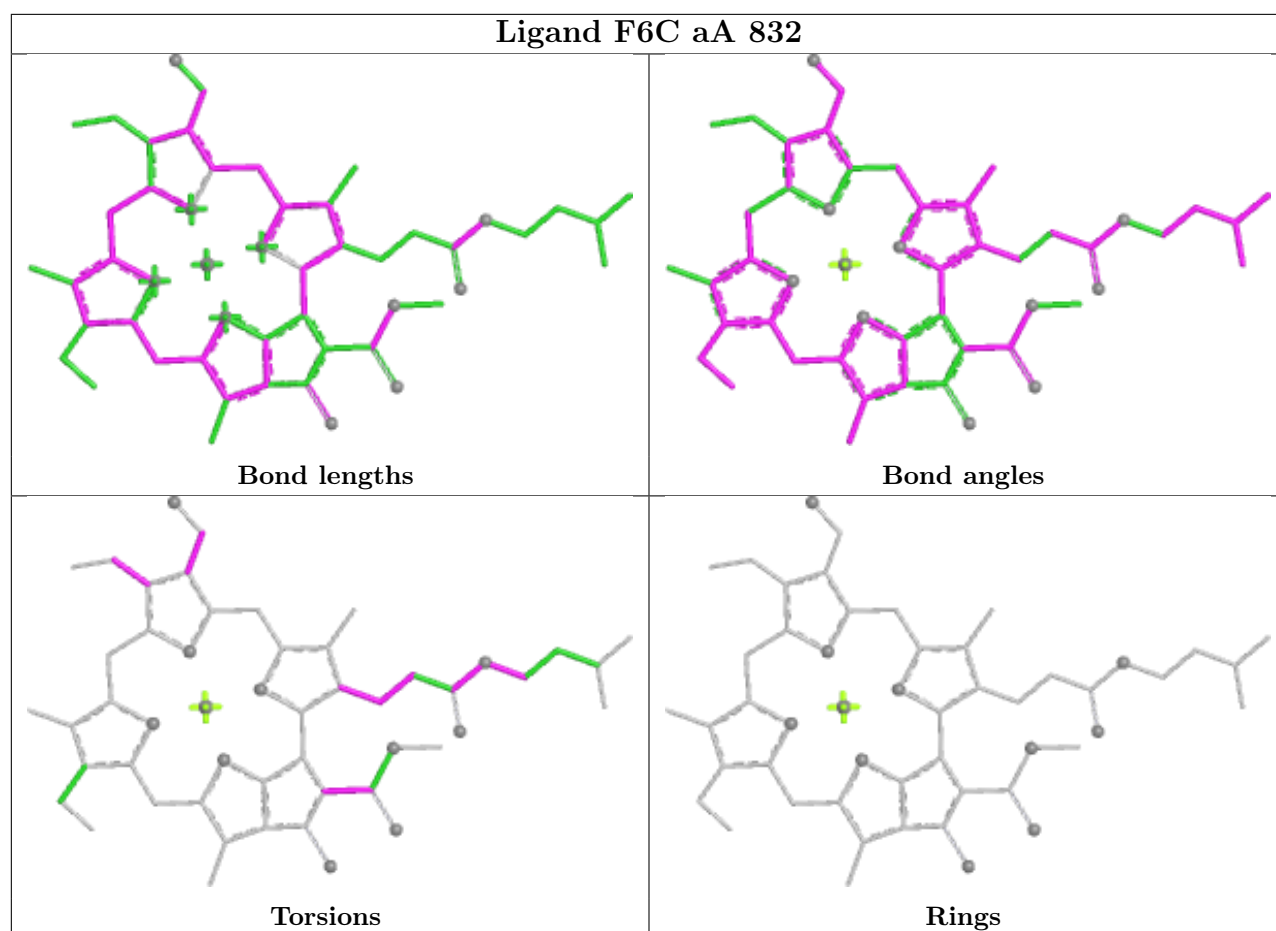


## Ligand CLA bA 841

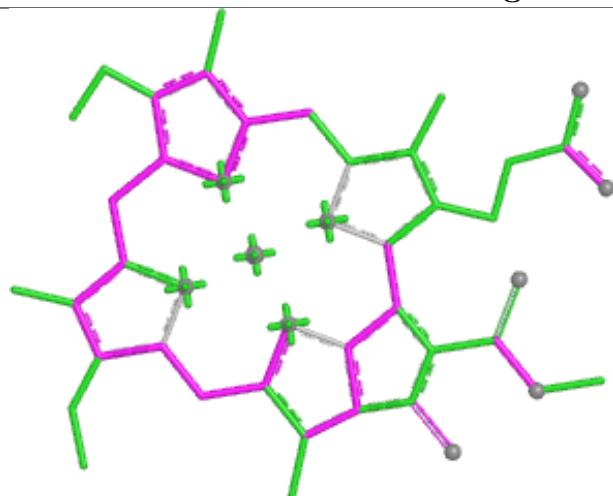


## Ligand CLA aA 819

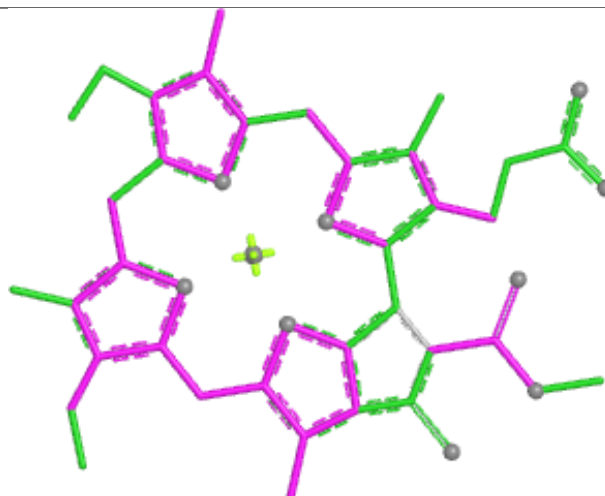




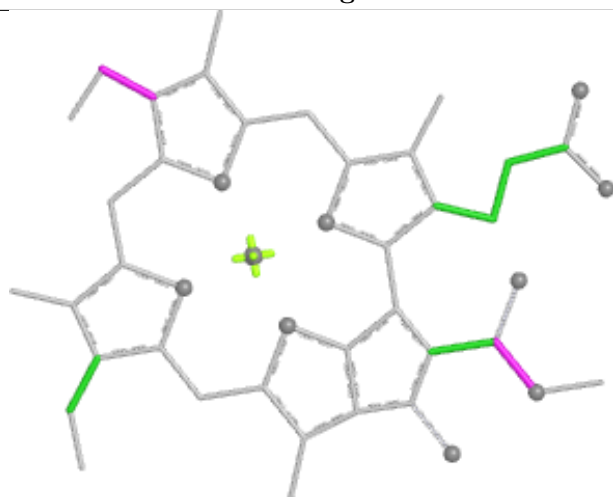
## Ligand CLA bA 816



Bond lengths



Bond angles

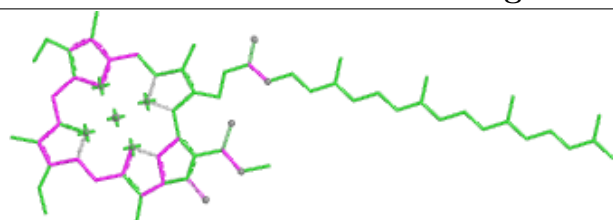


Torsions

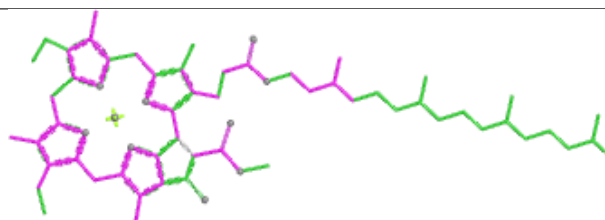


Rings

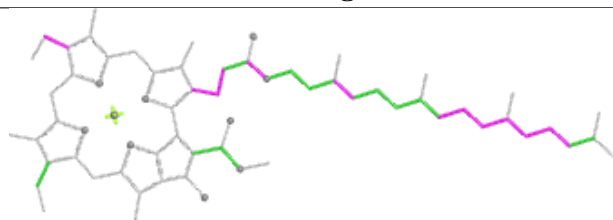
## Ligand CLA bB 812



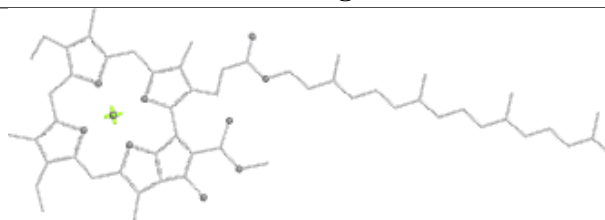
Bond lengths



Bond angles

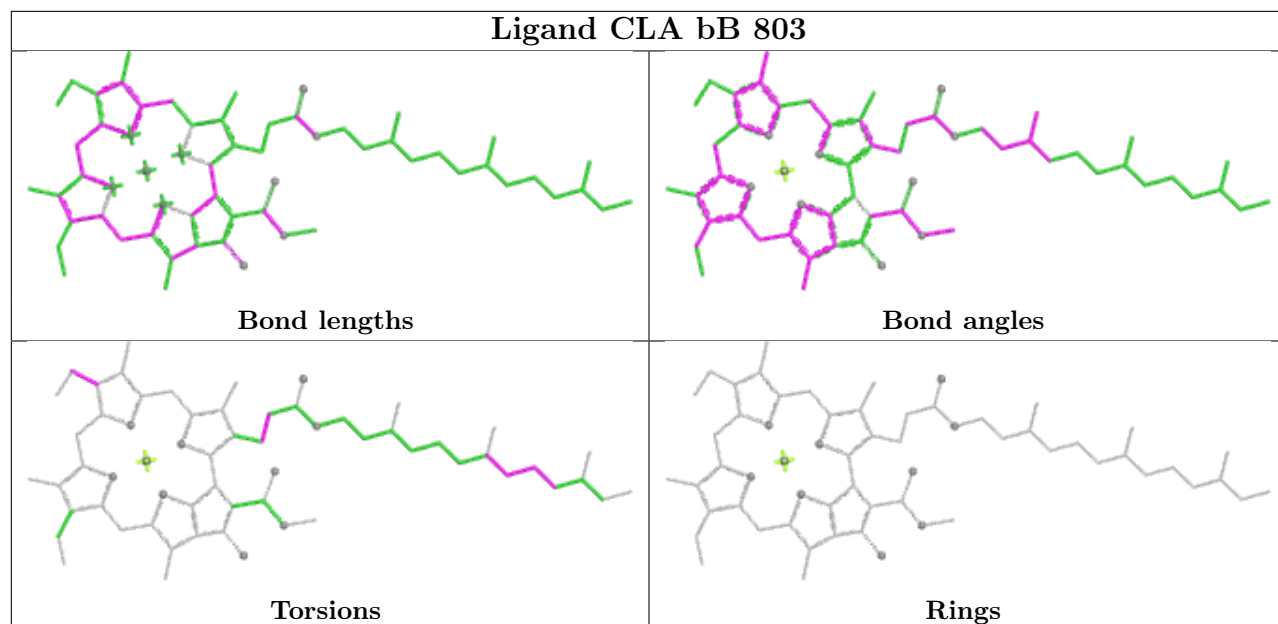


Torsions

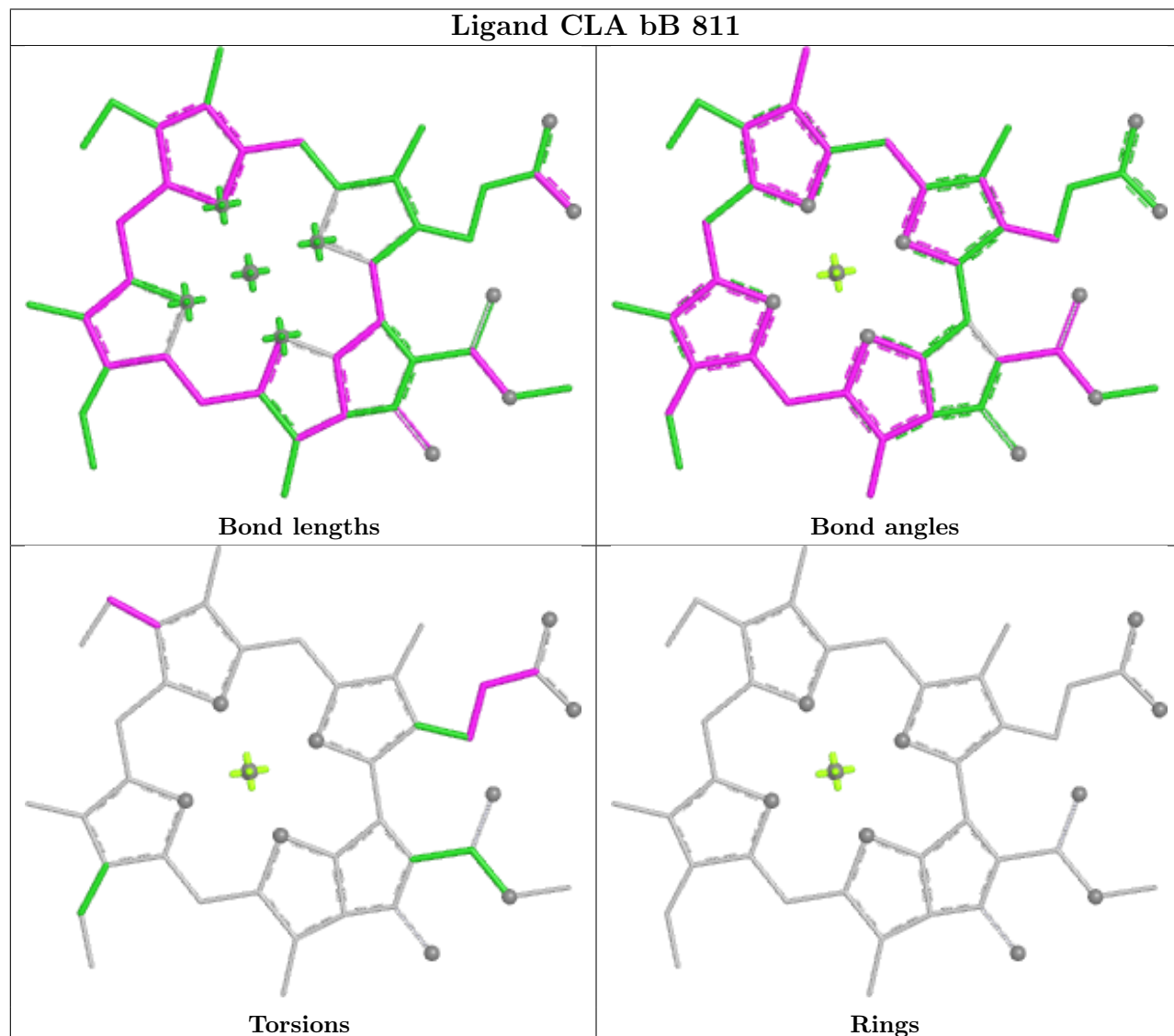


Rings

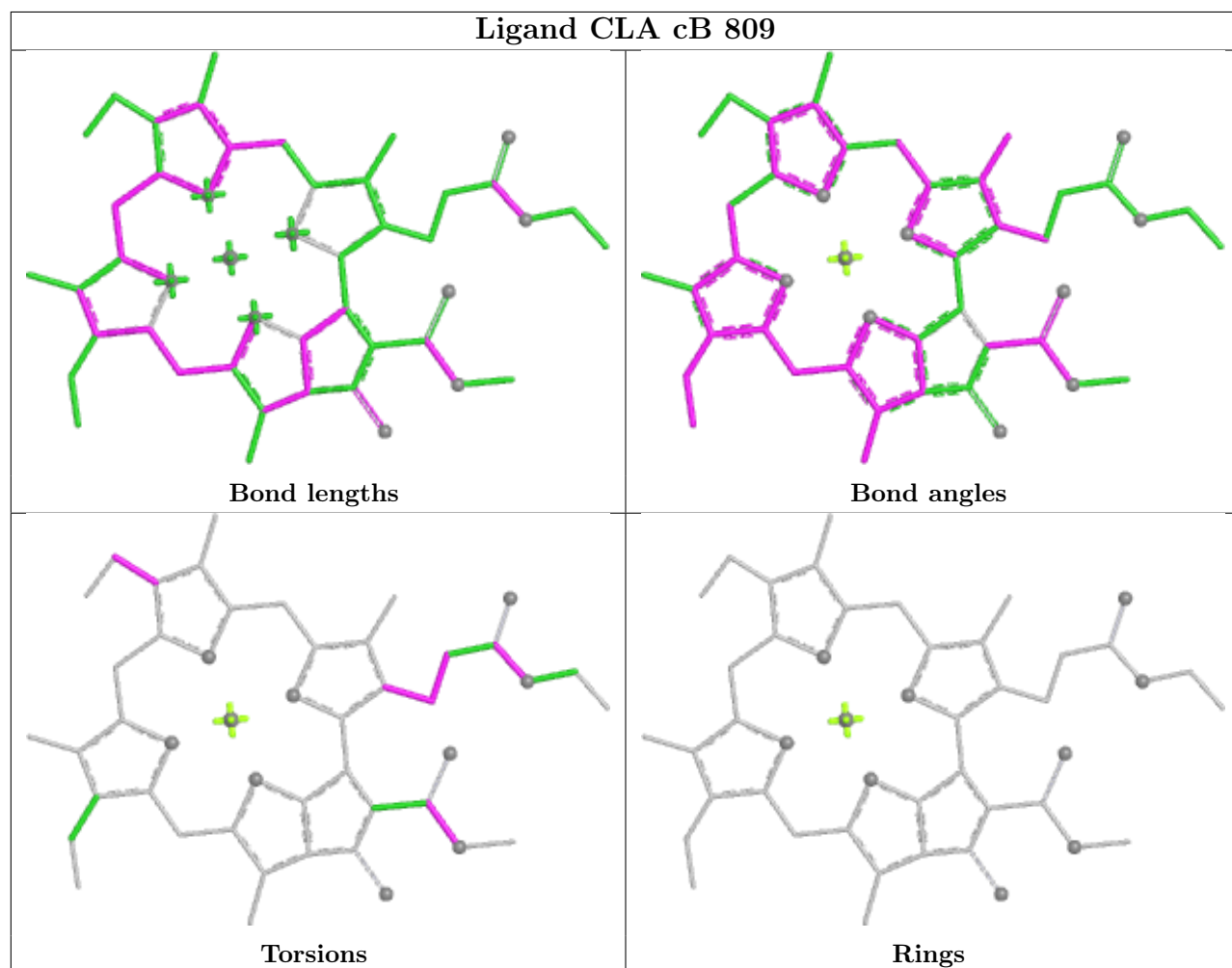
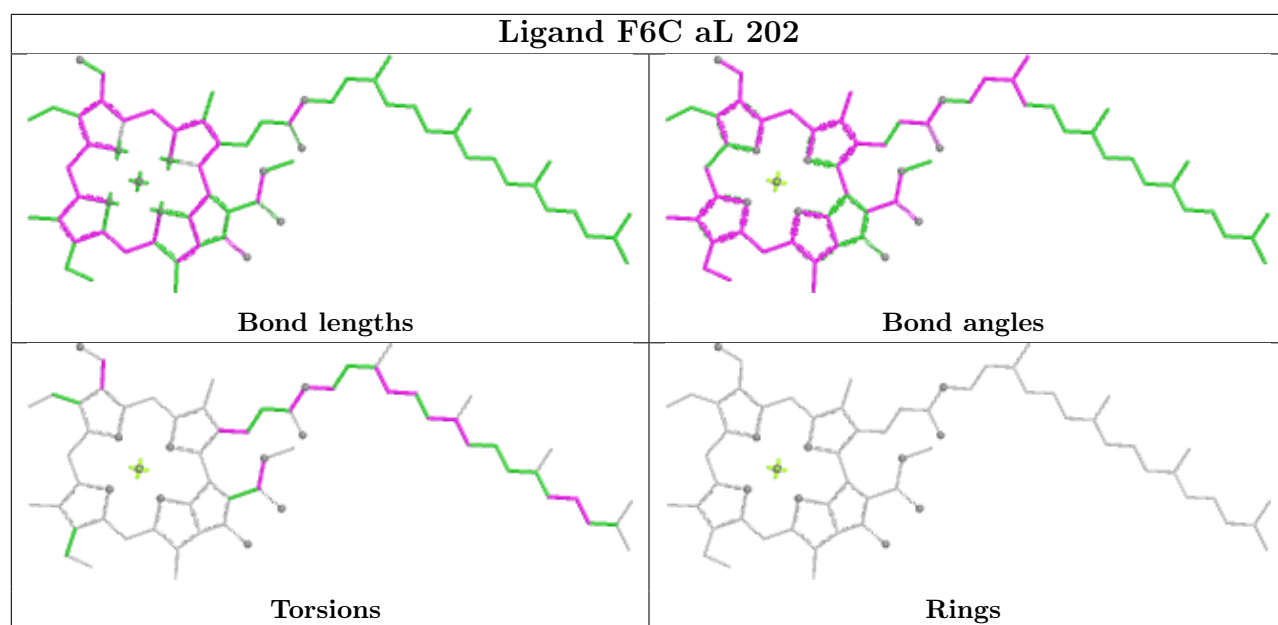
## Ligand CLA bB 803

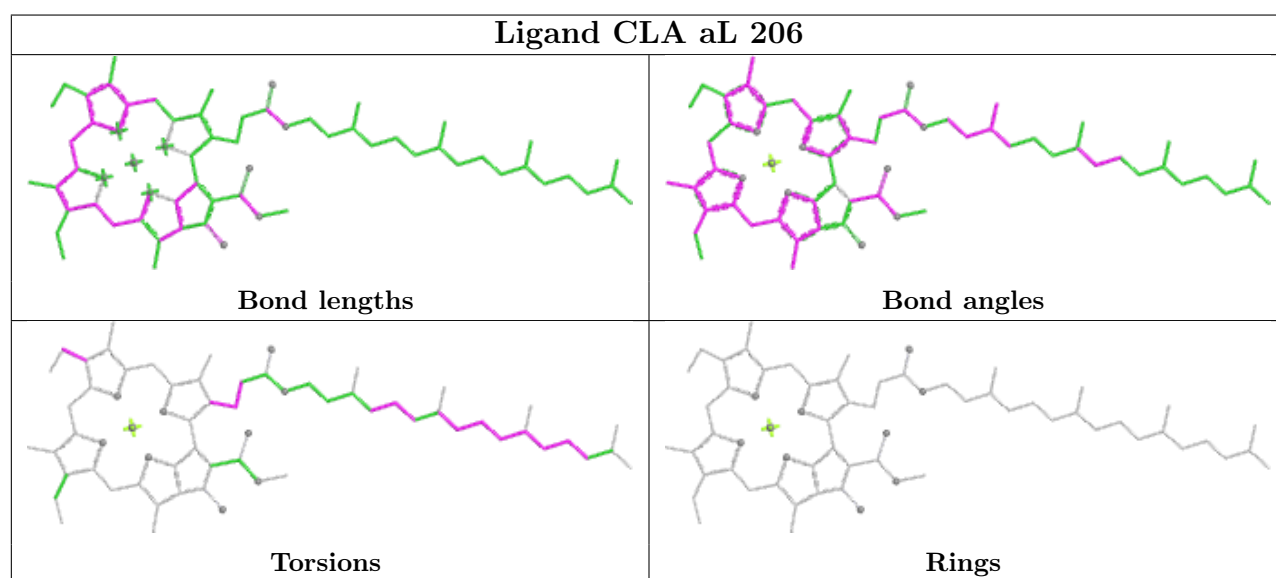
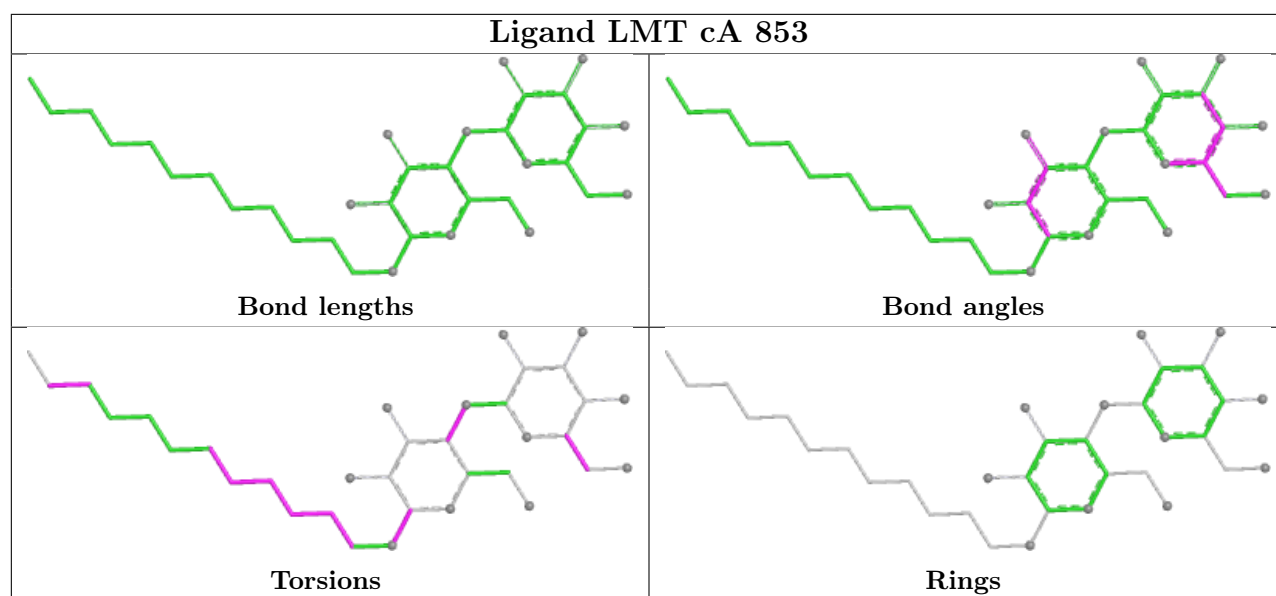


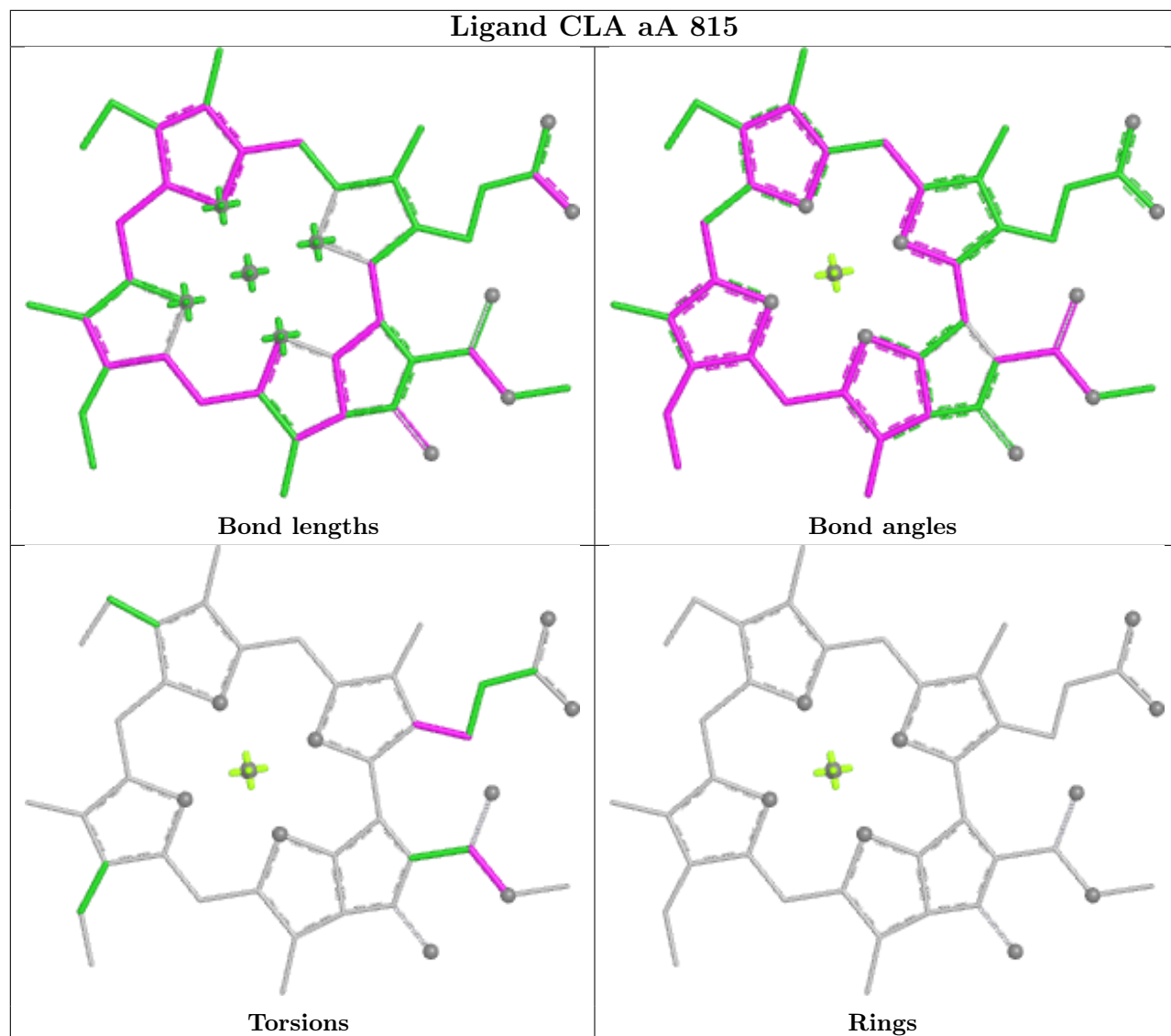
## Ligand CLA bB 811



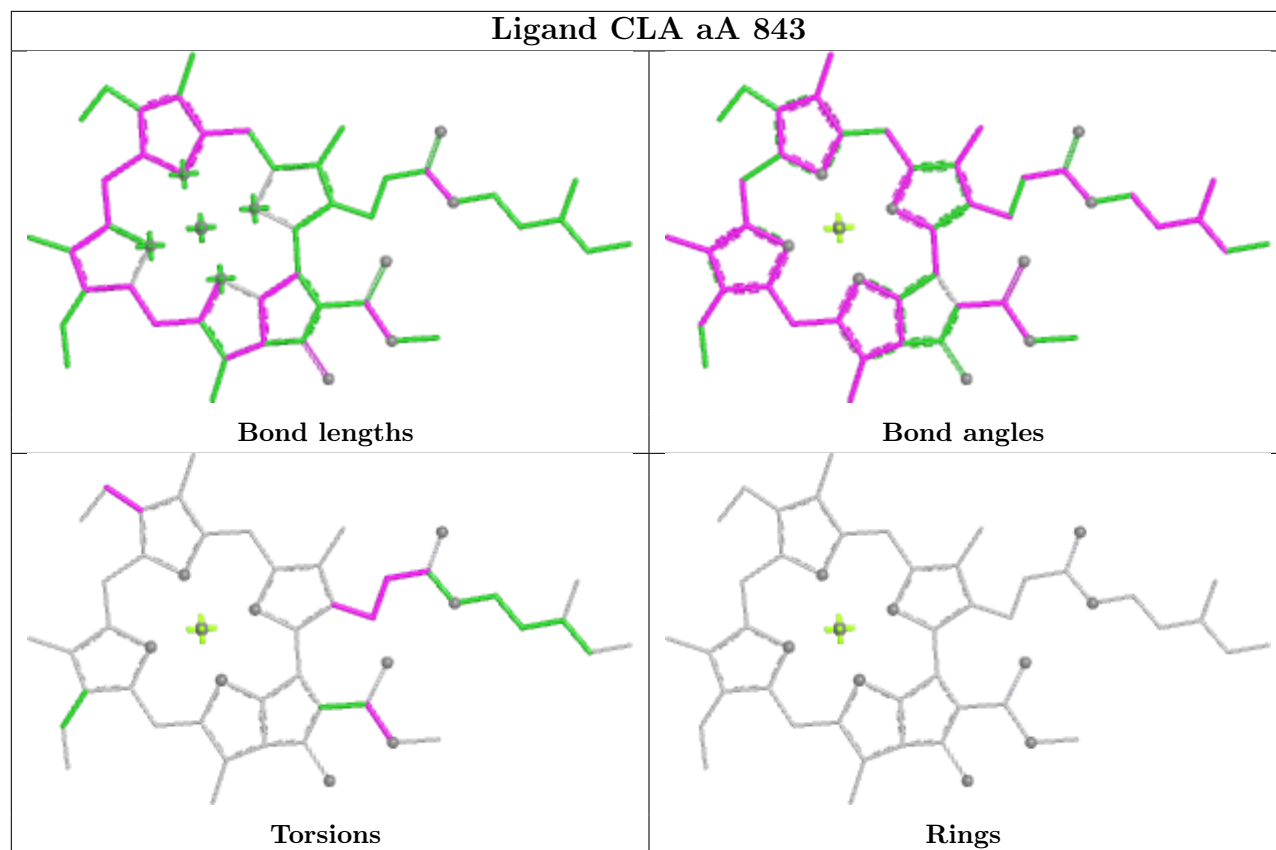




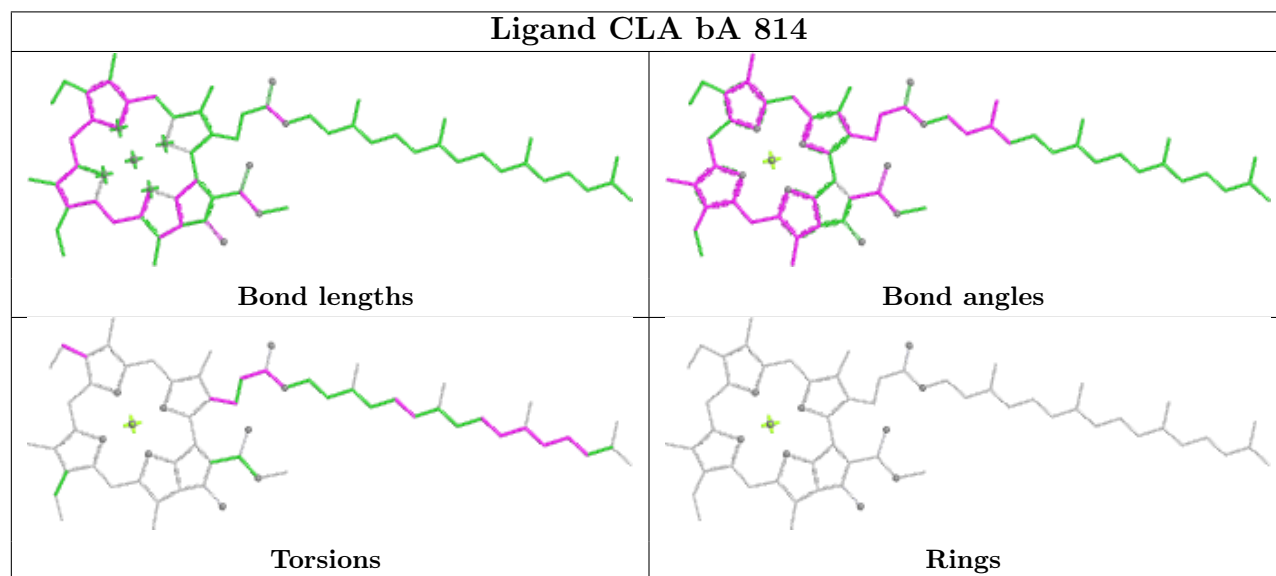


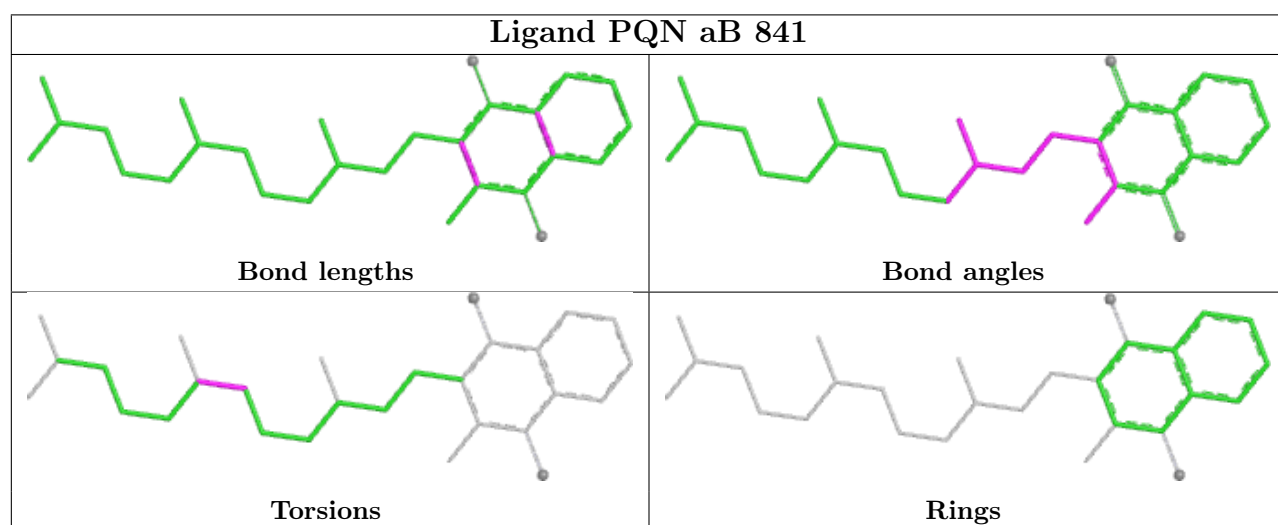
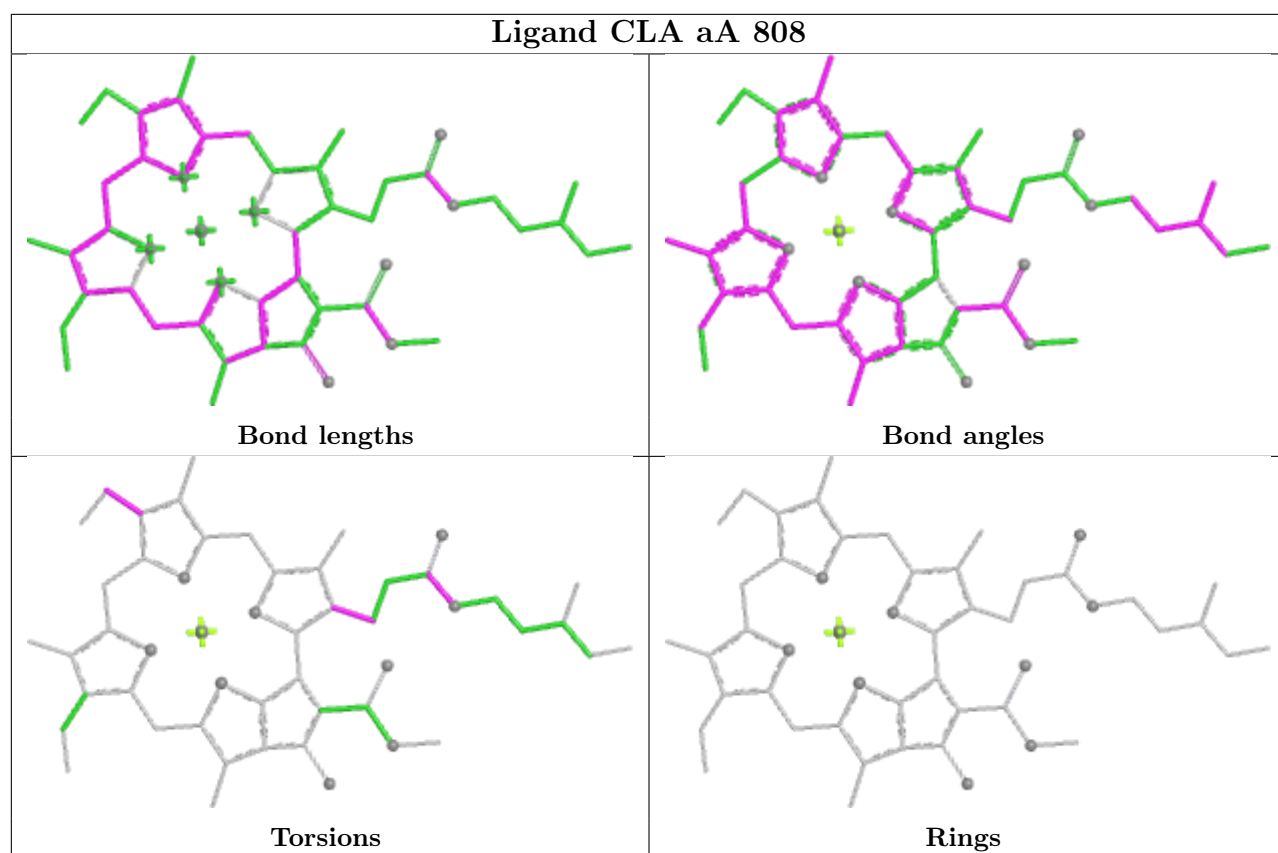


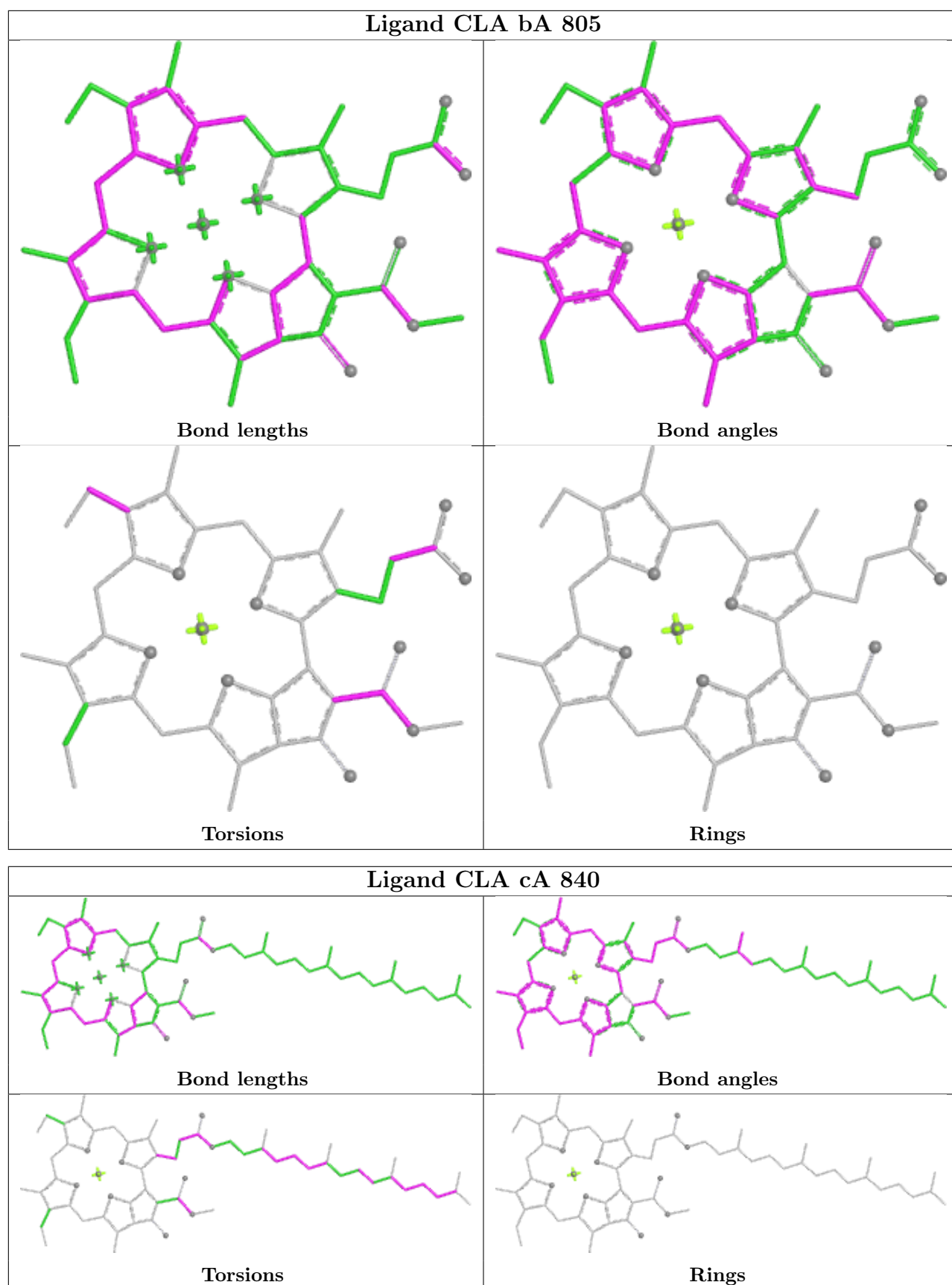
## Ligand CLA aA 843



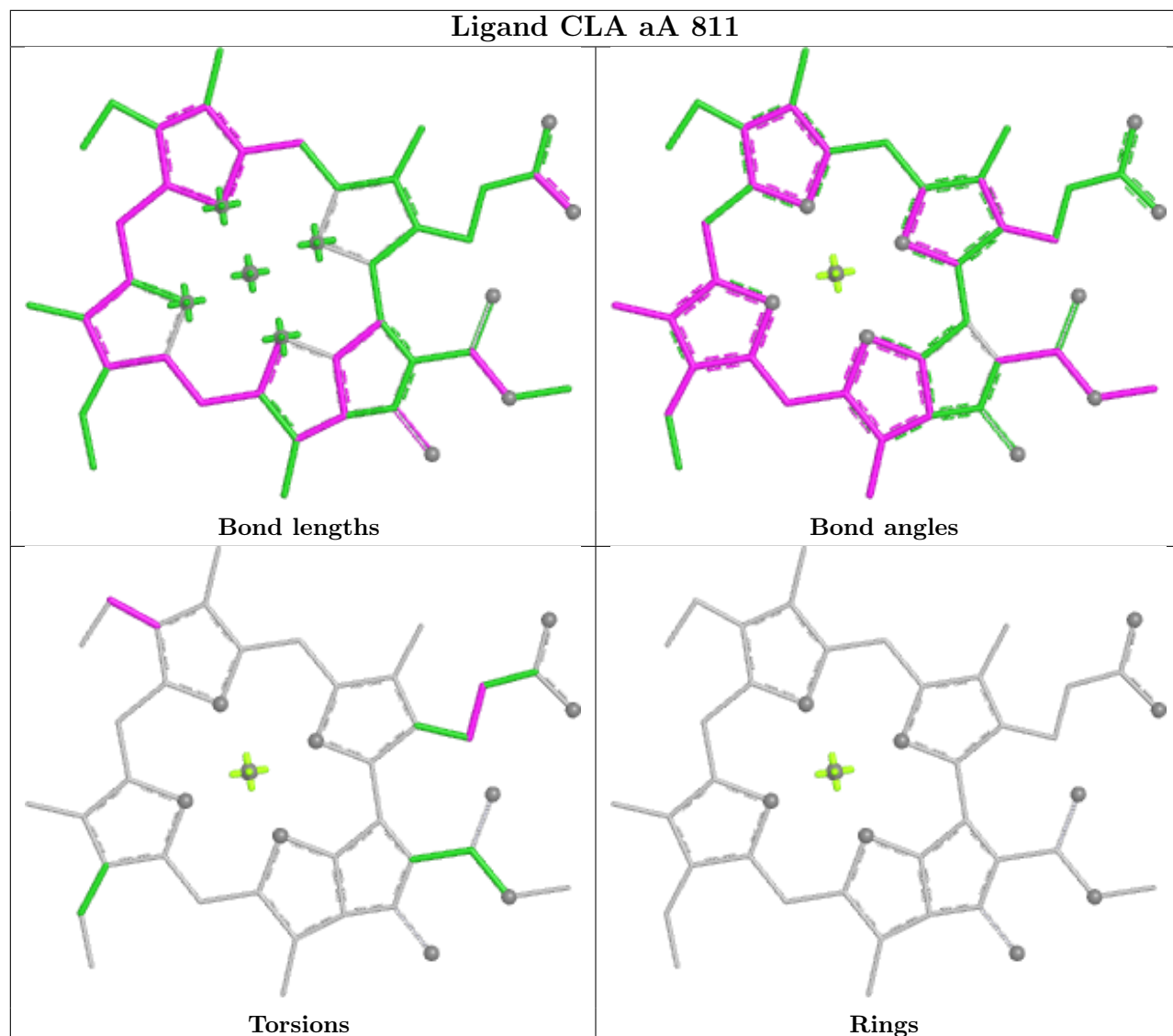
## Ligand CLA bA 814



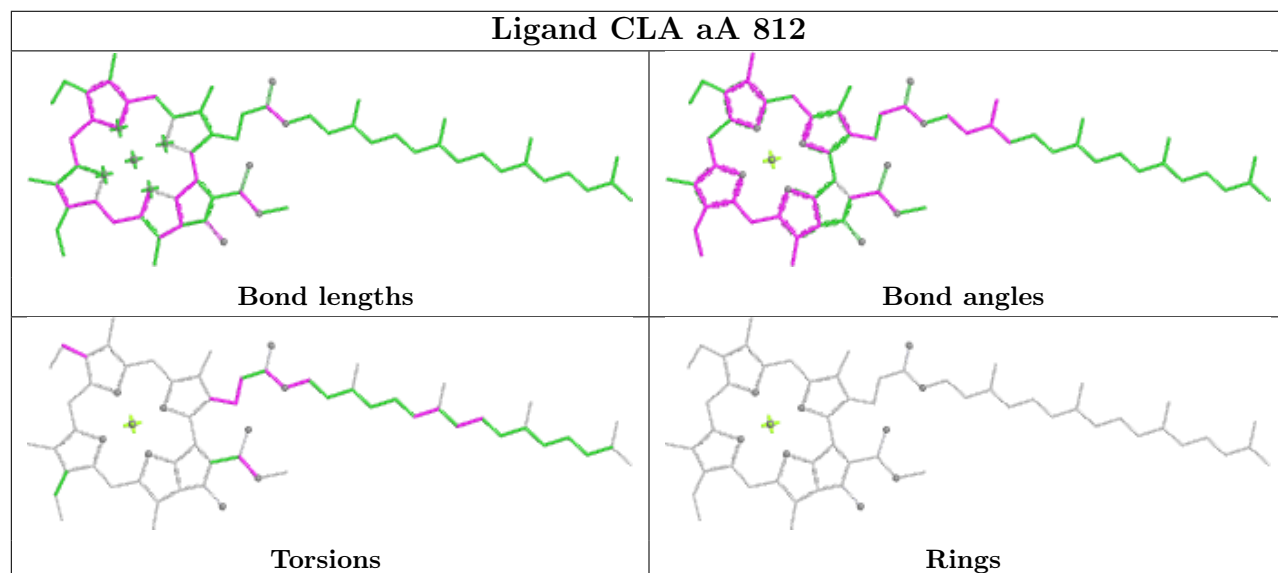




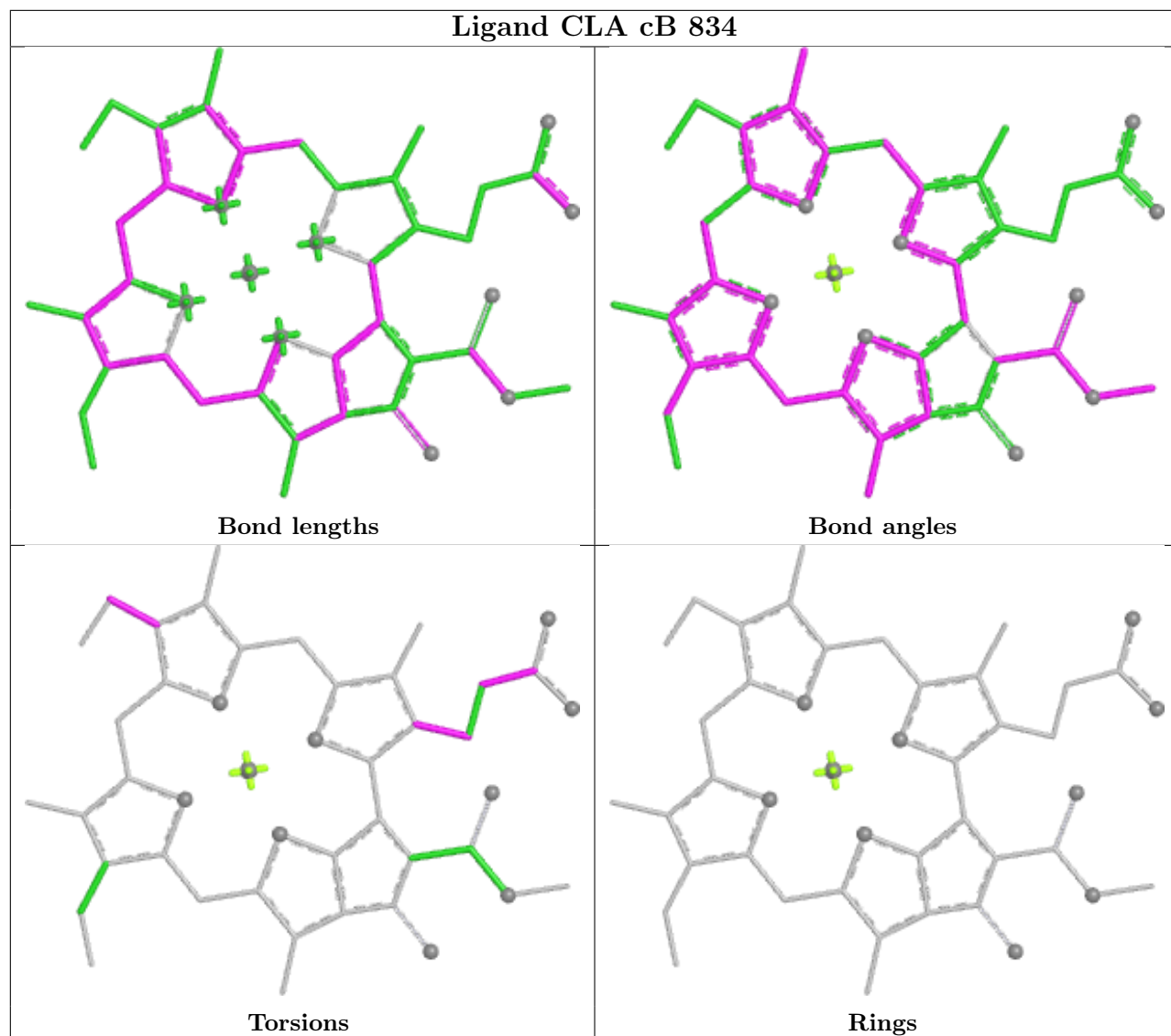
## Ligand CLA aA 811

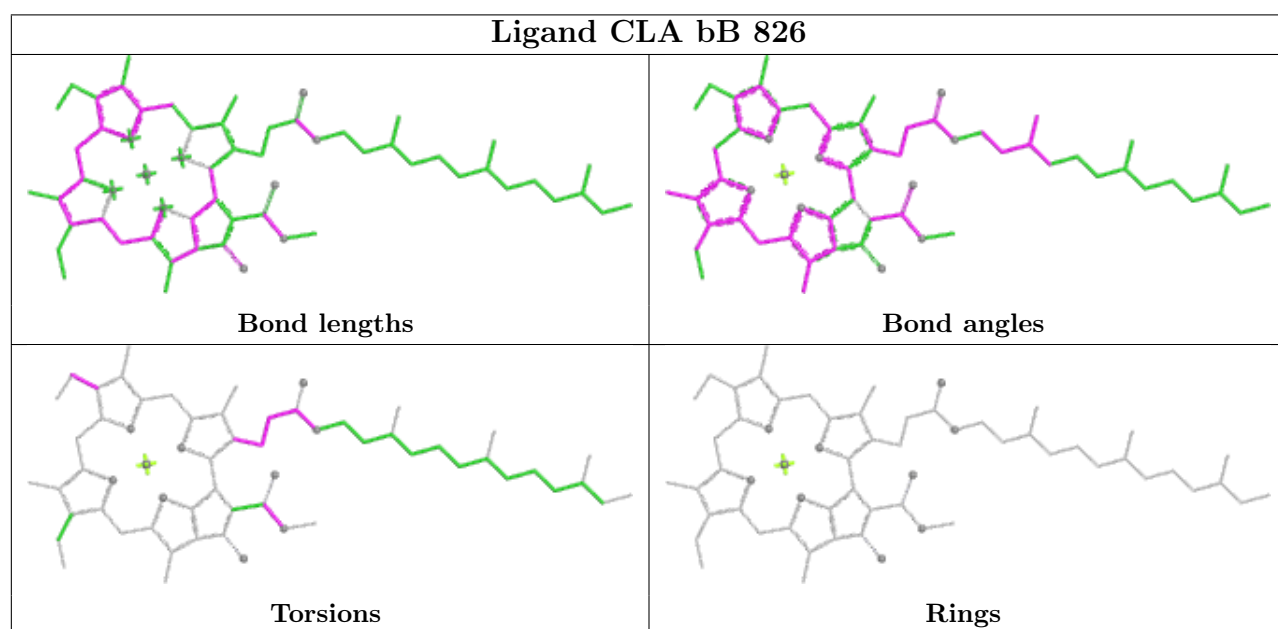
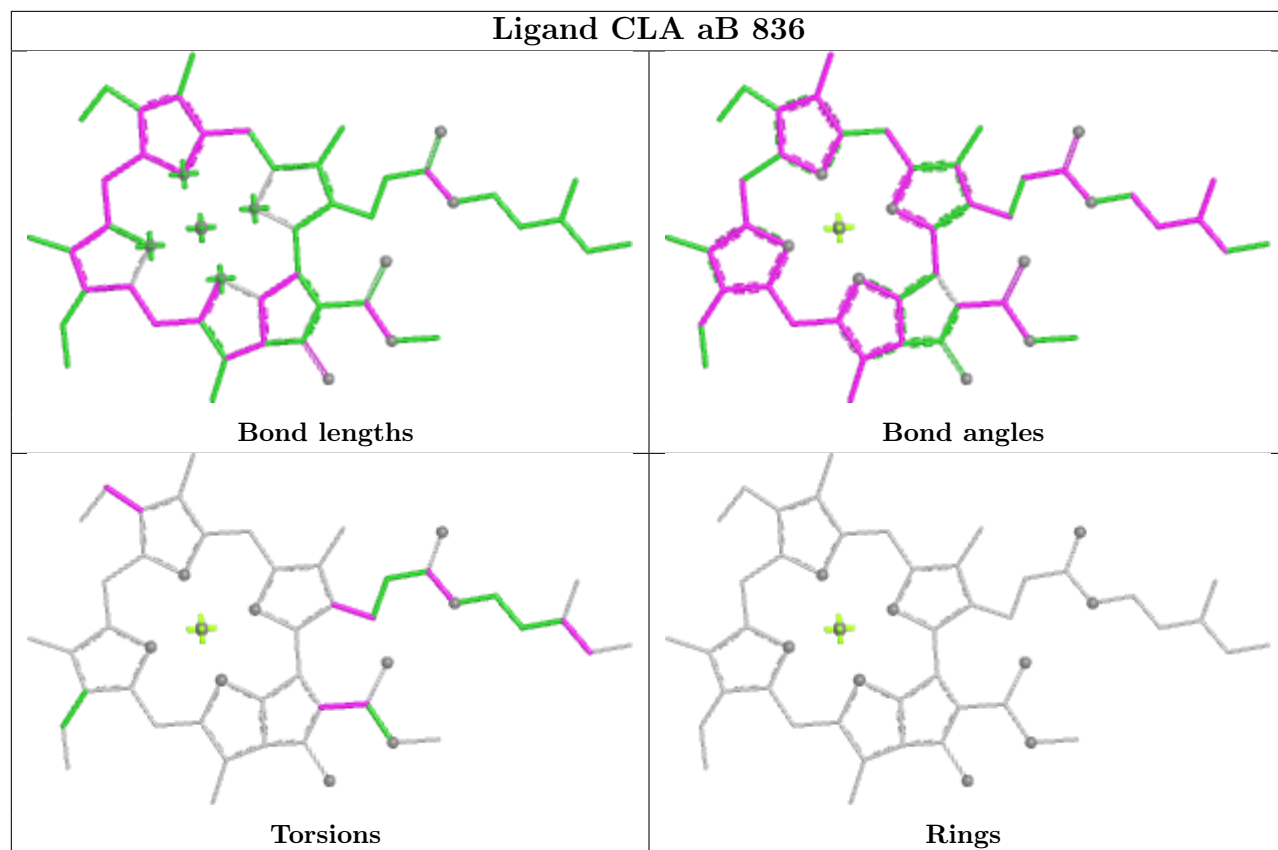


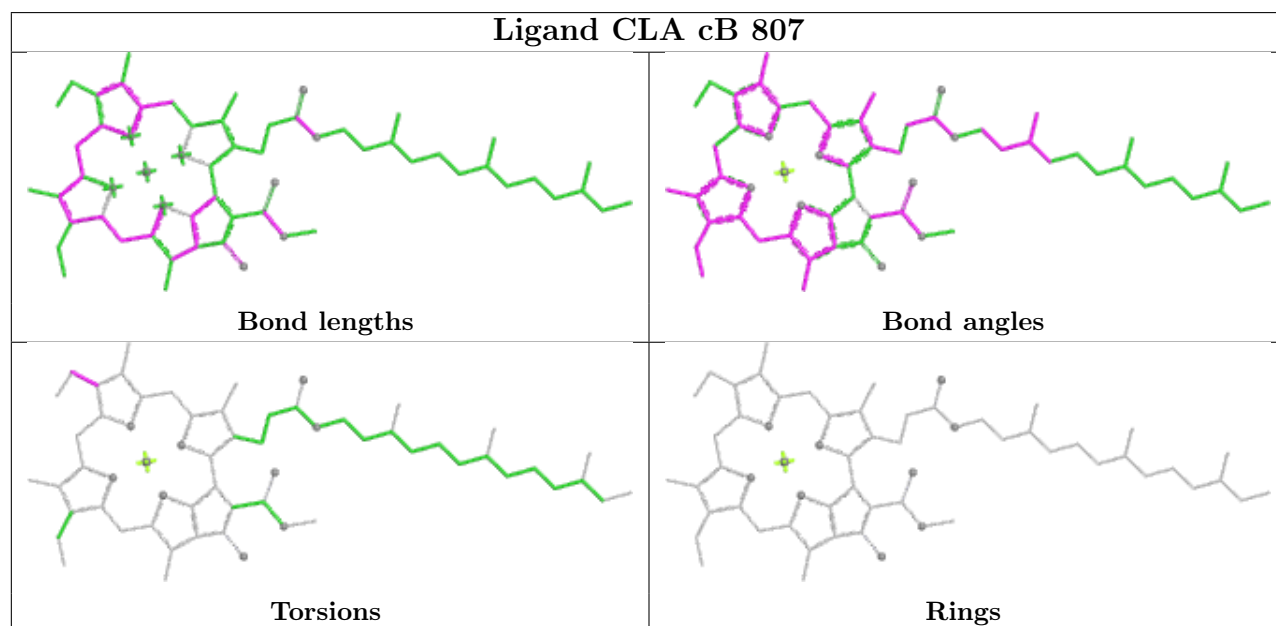
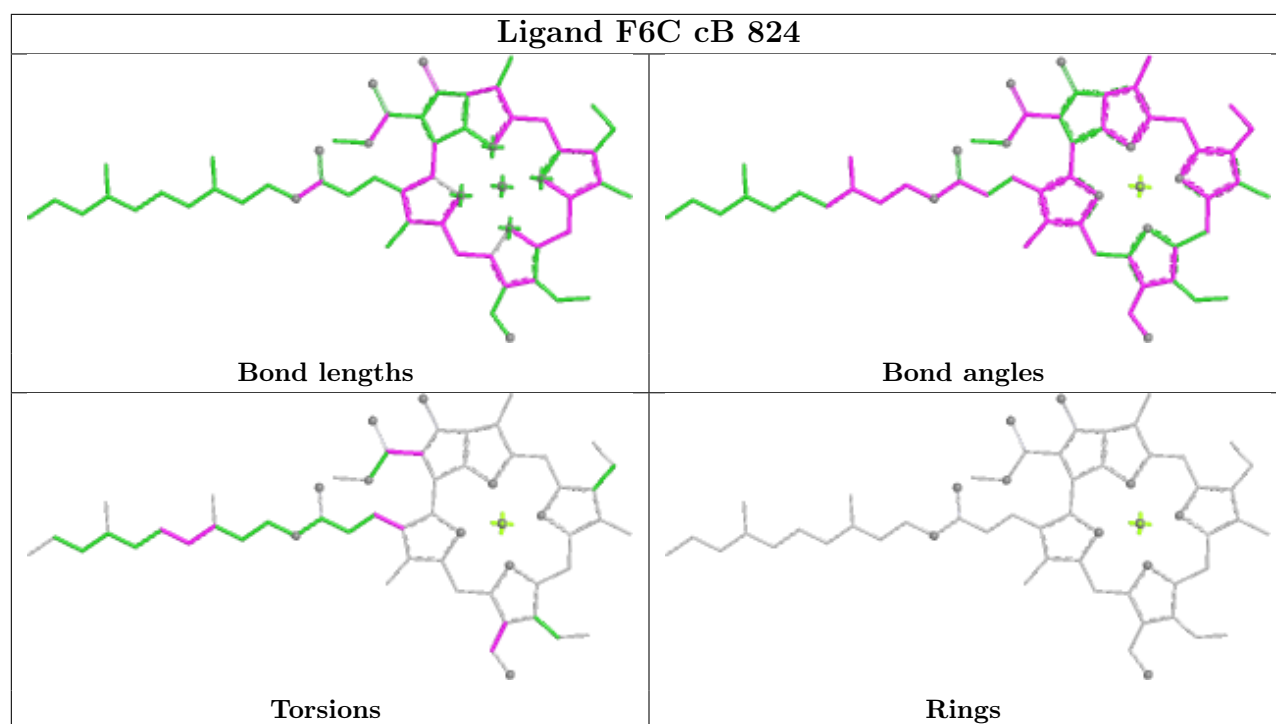
## Ligand CLA aA 812

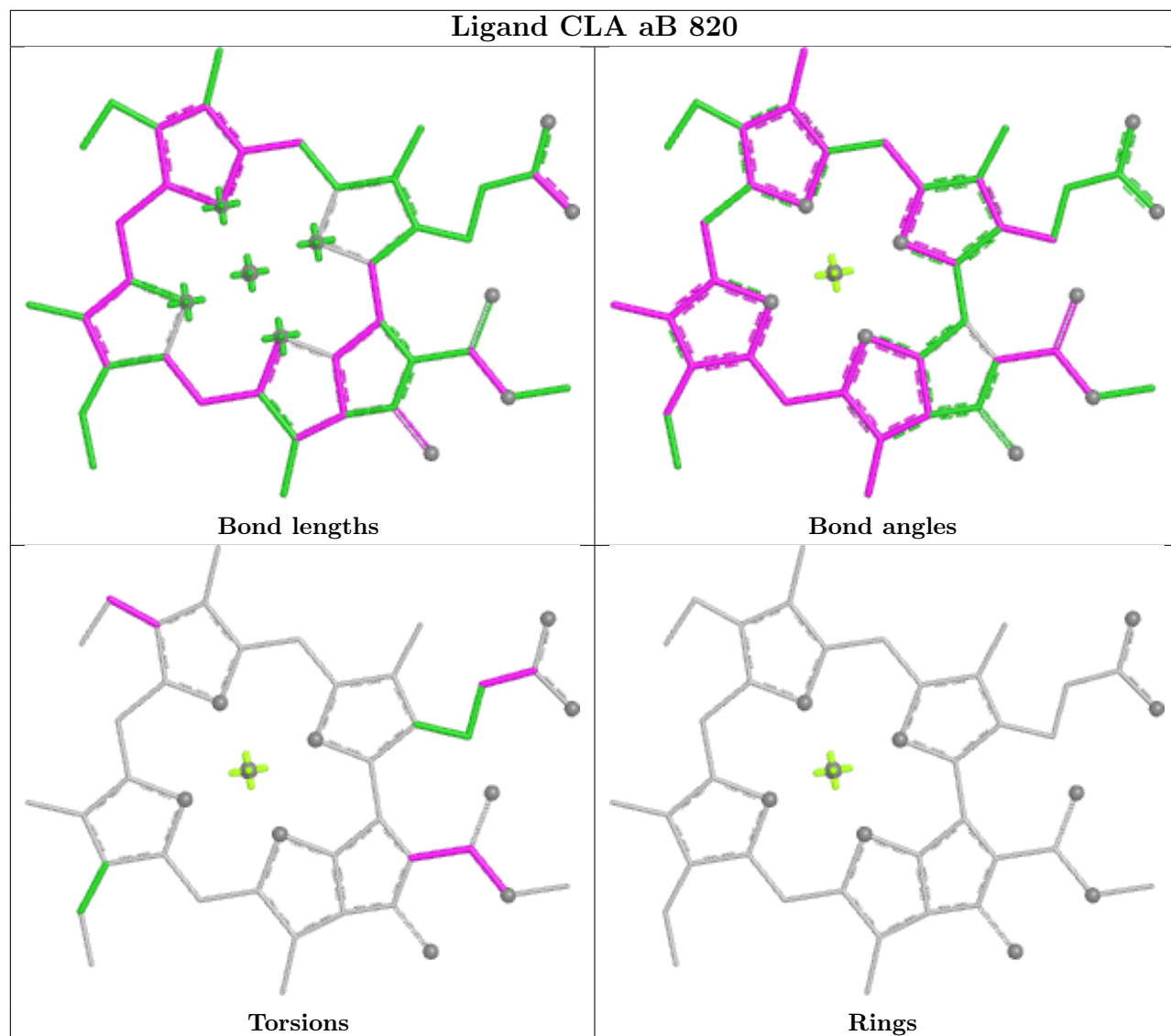


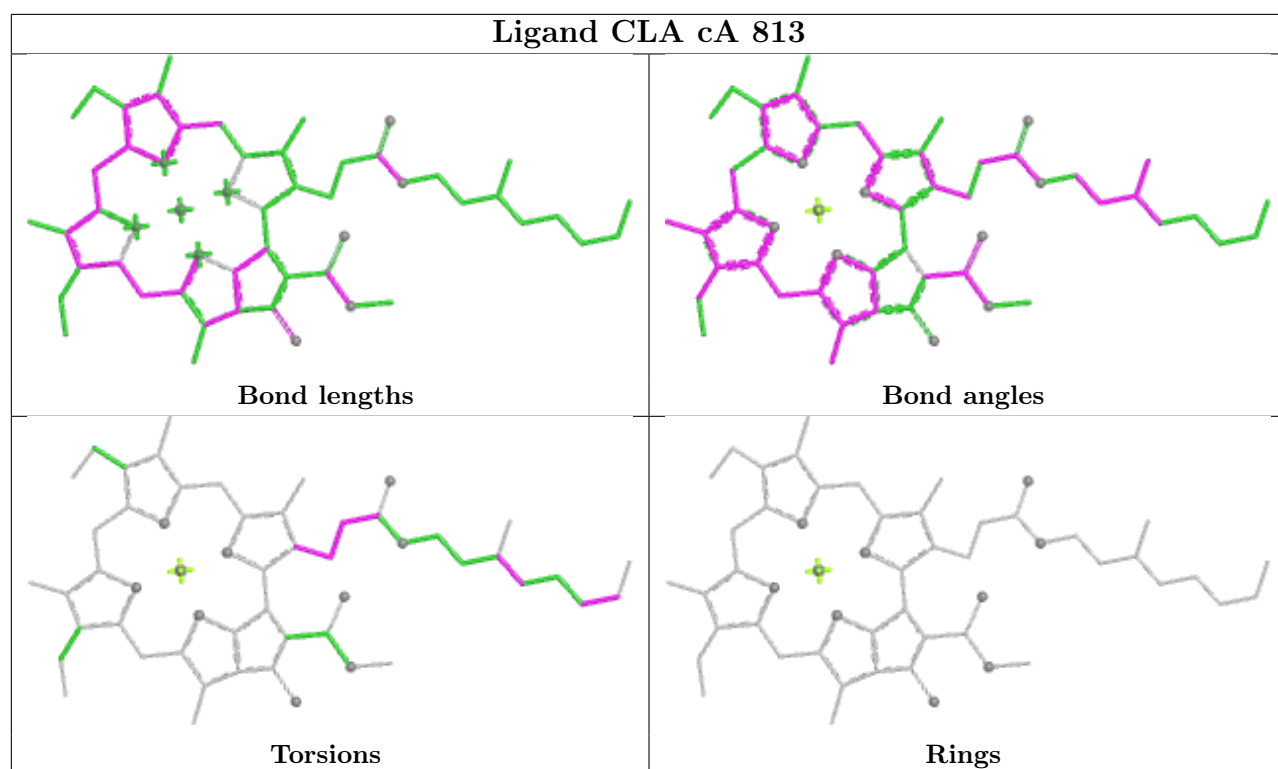




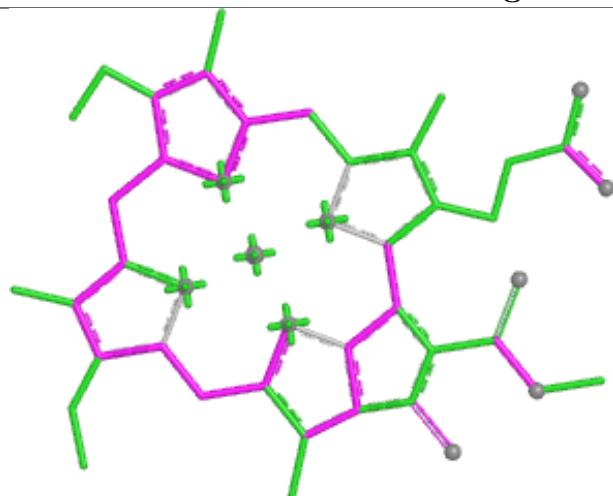




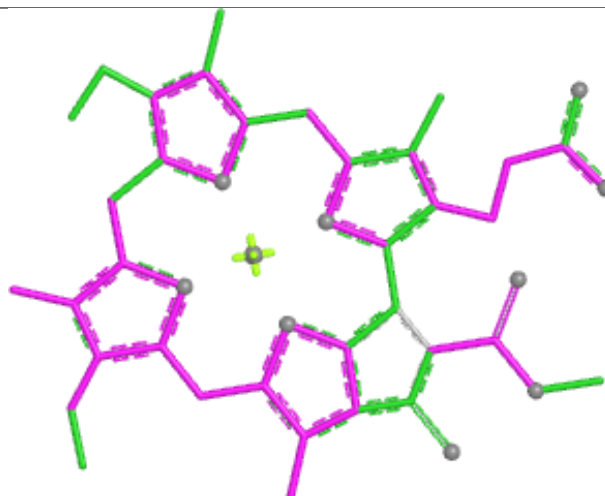




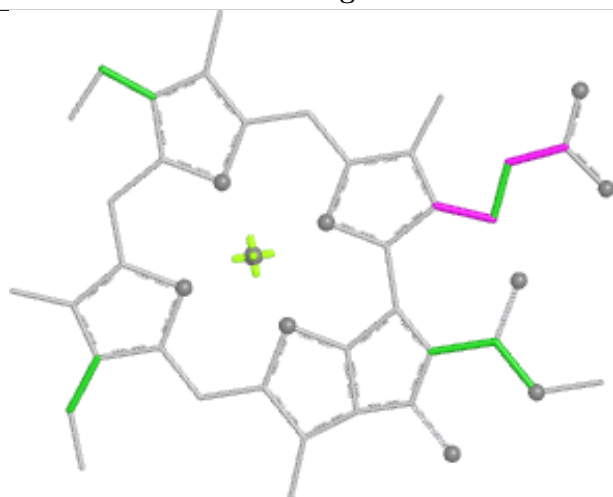
## Ligand CLA bA 837



Bond lengths



Bond angles

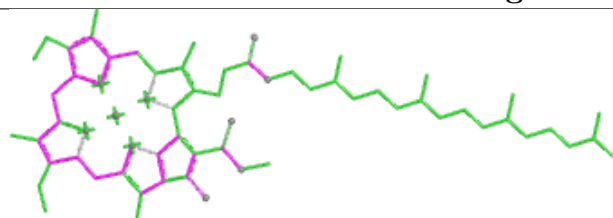


Torsions

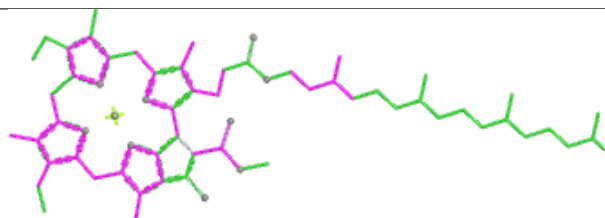


Rings

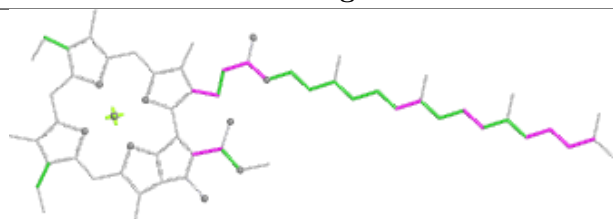
## Ligand CLA aB 805



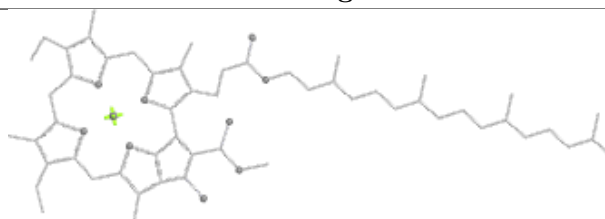
Bond lengths



Bond angles

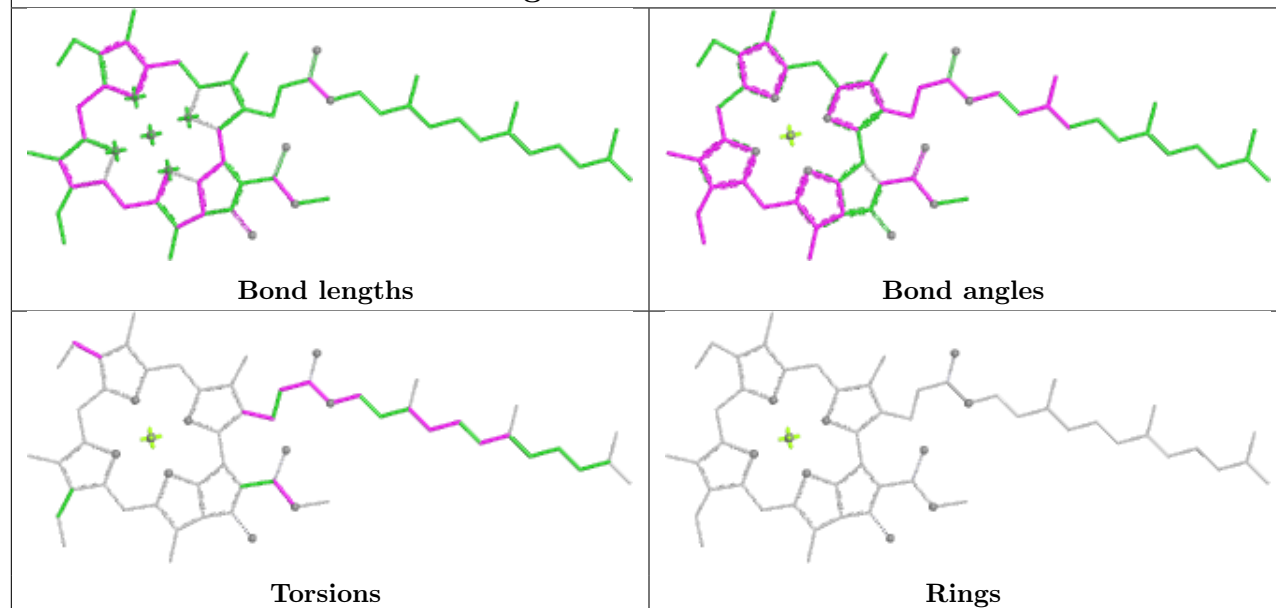


Torsions

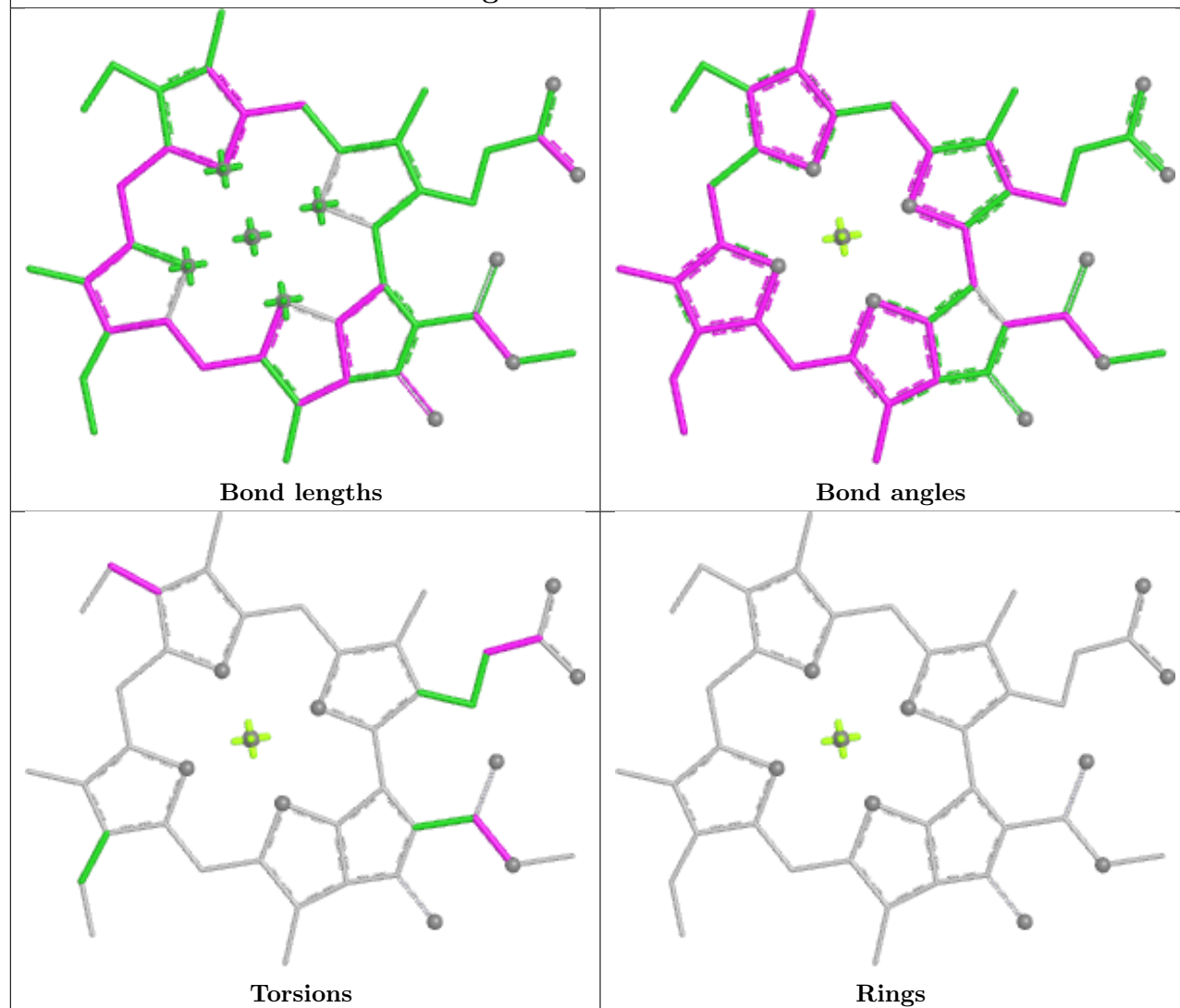


Rings

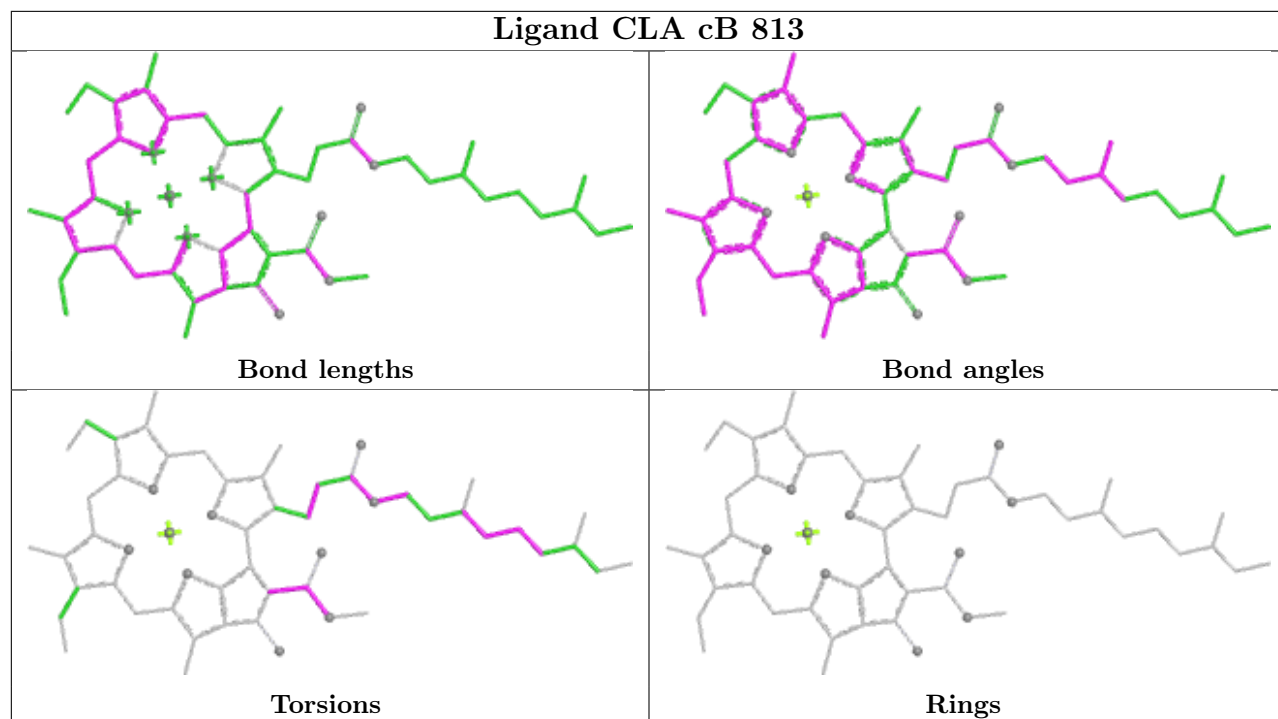
## Ligand CLA aB 817



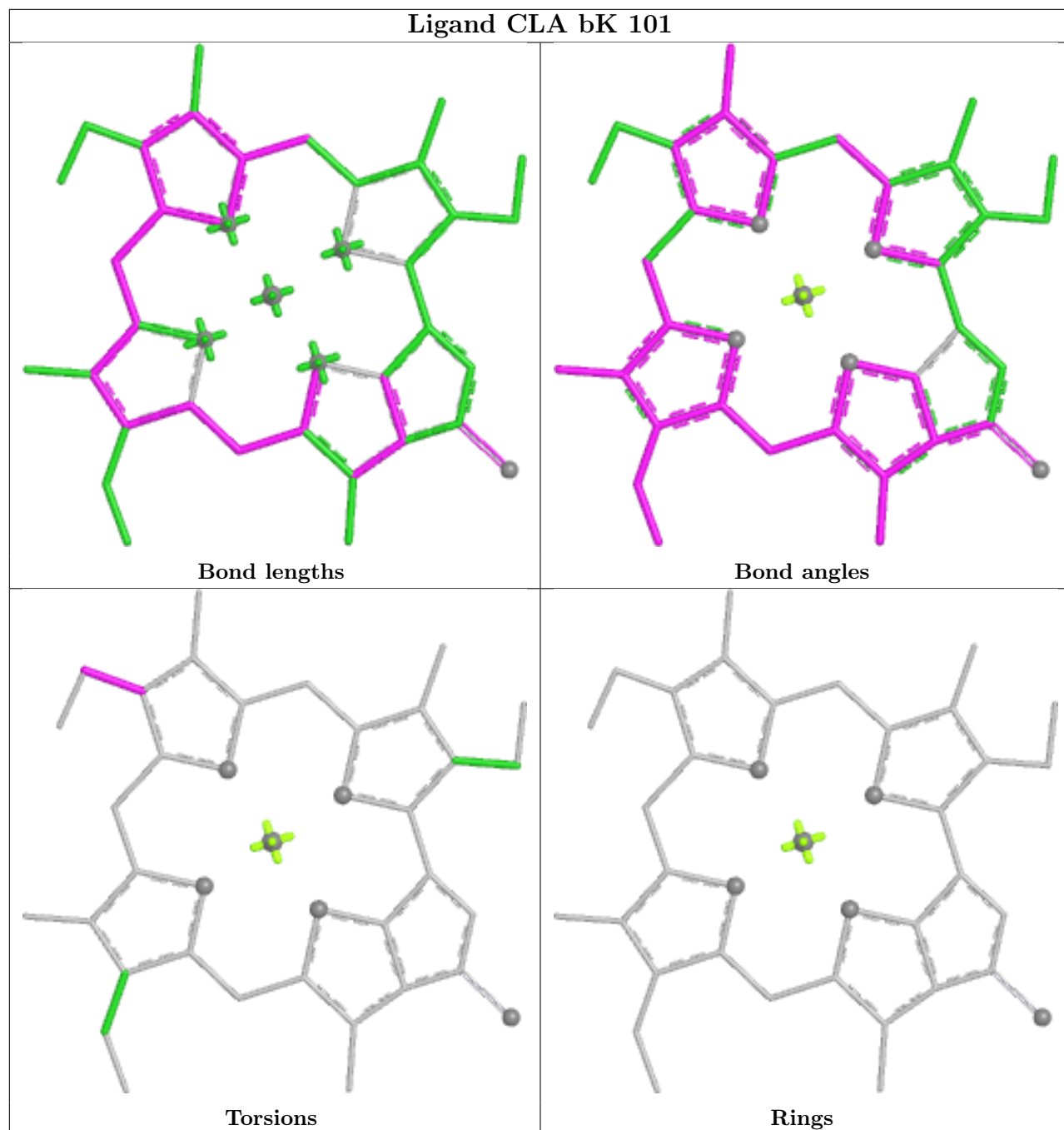
## Ligand CLA bA 836

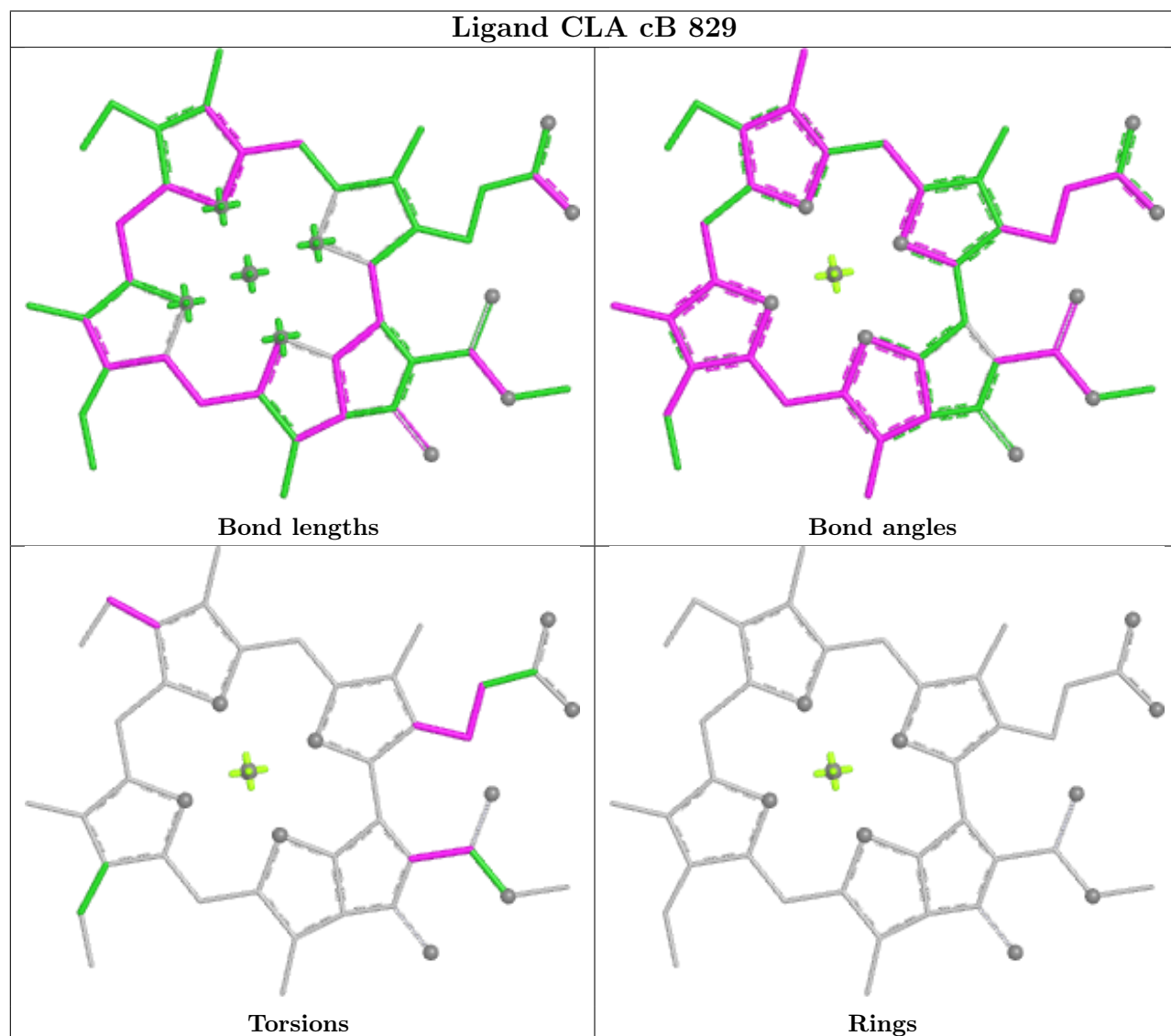
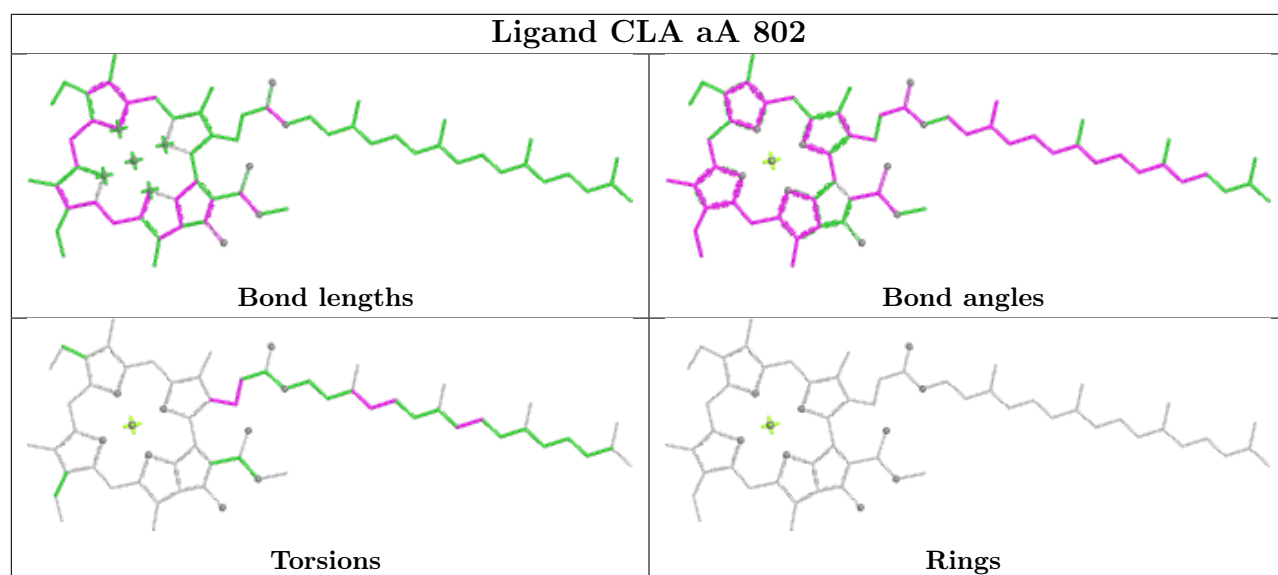


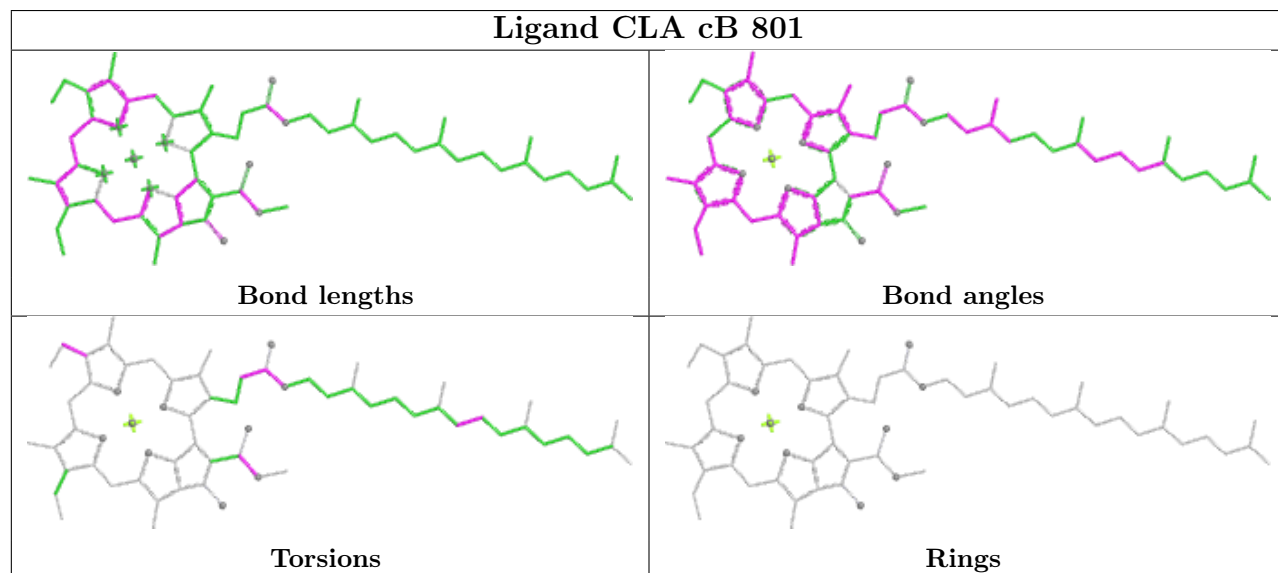
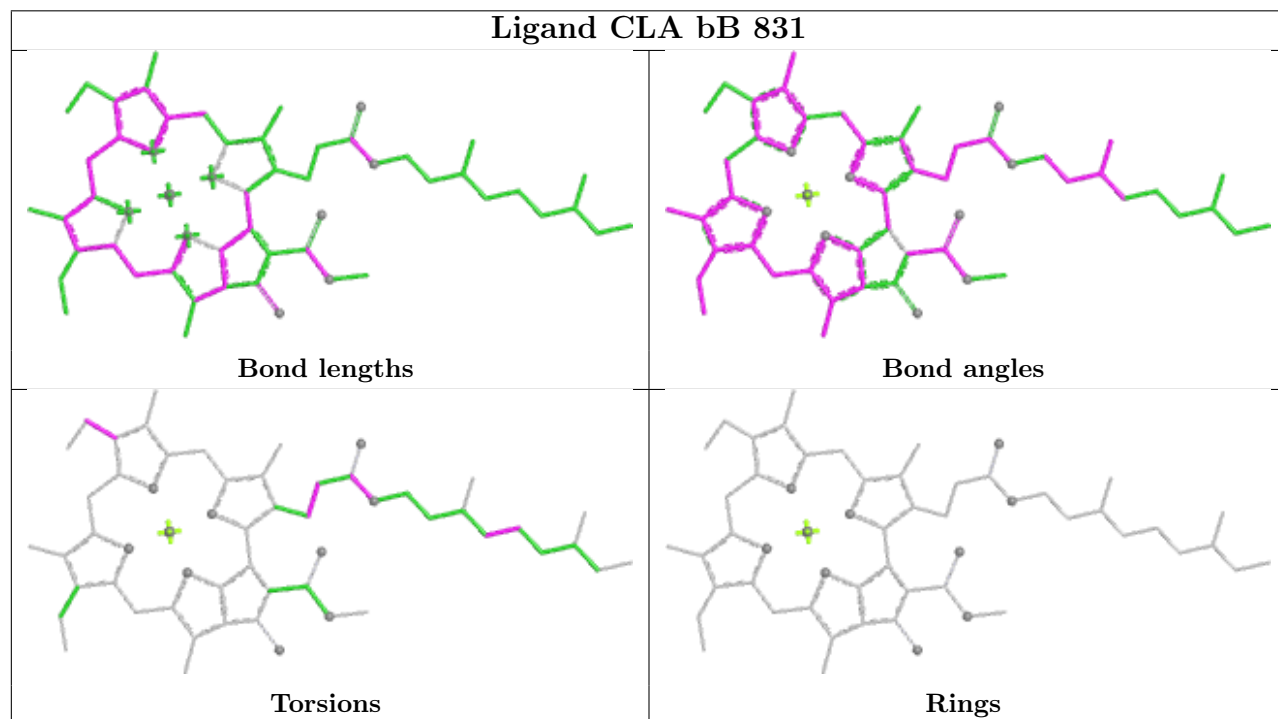
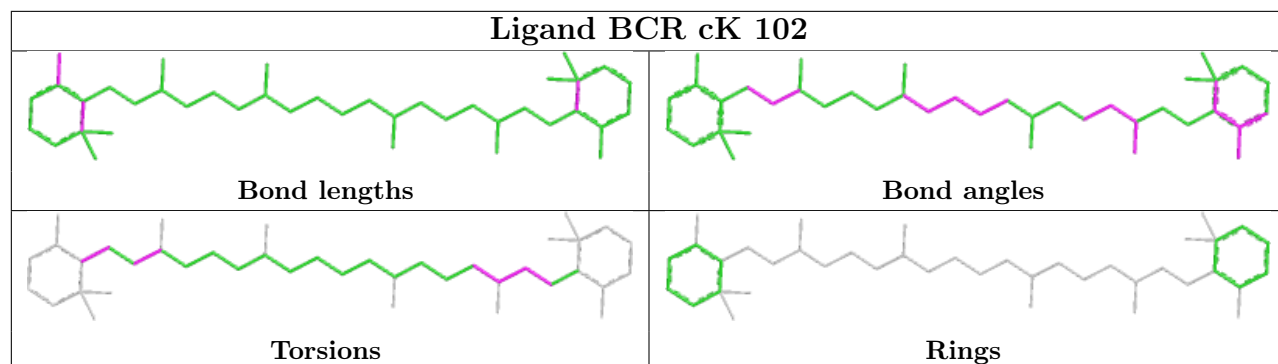


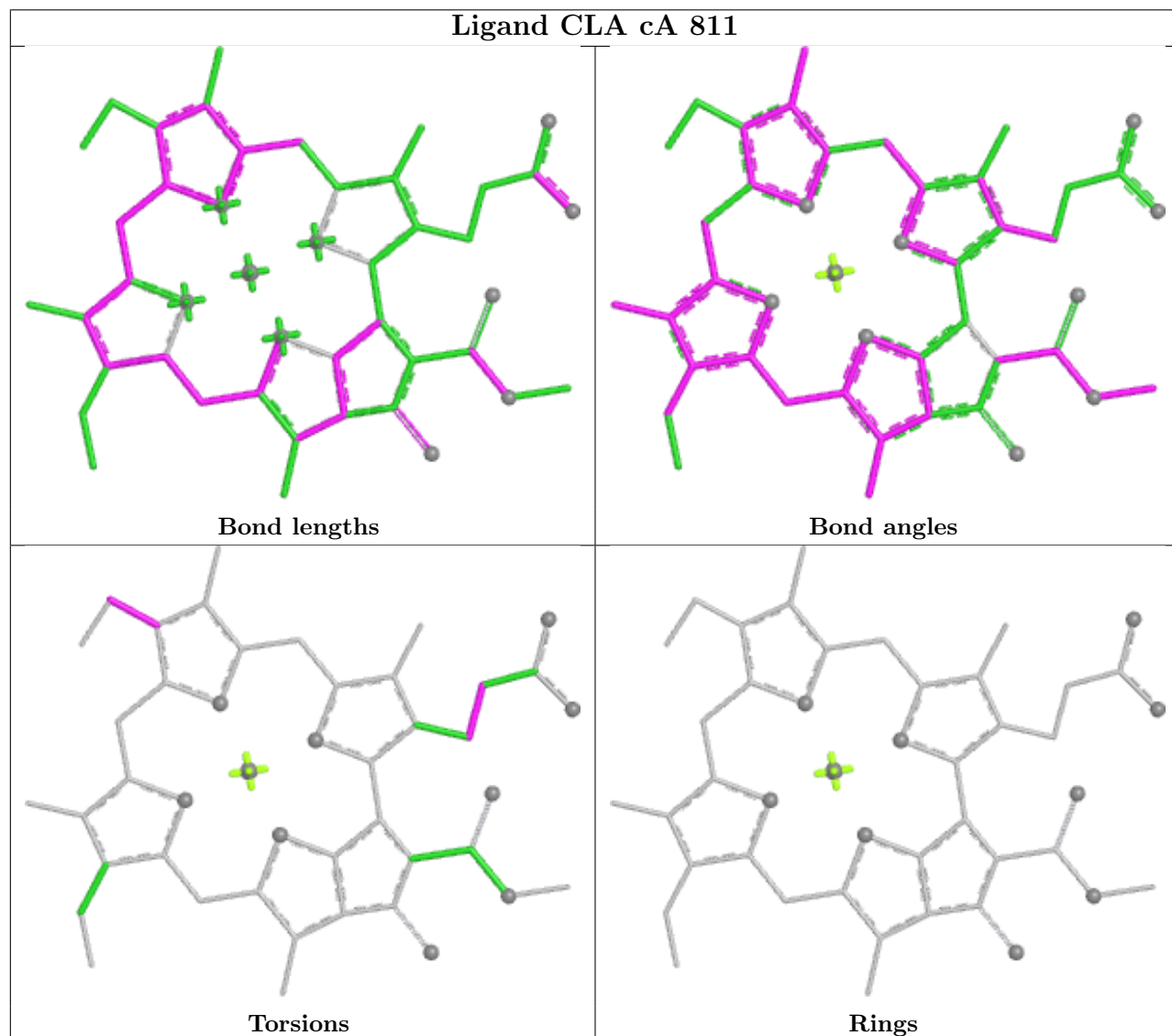
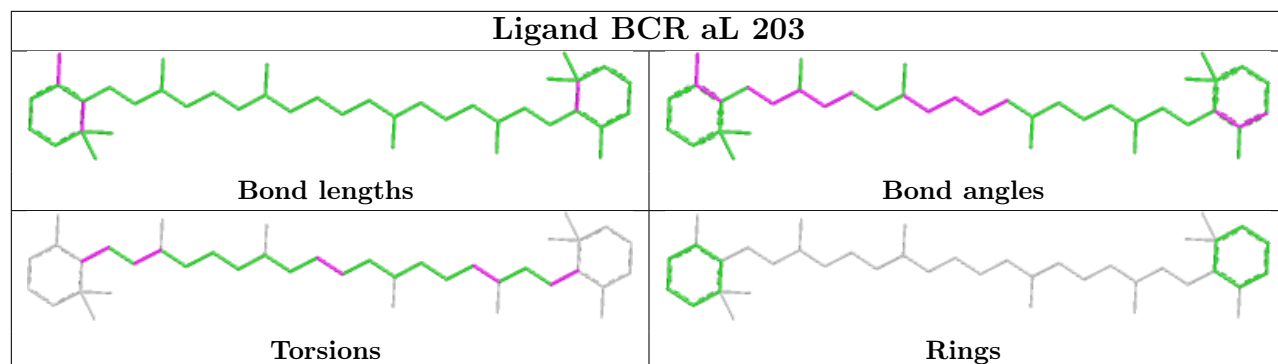


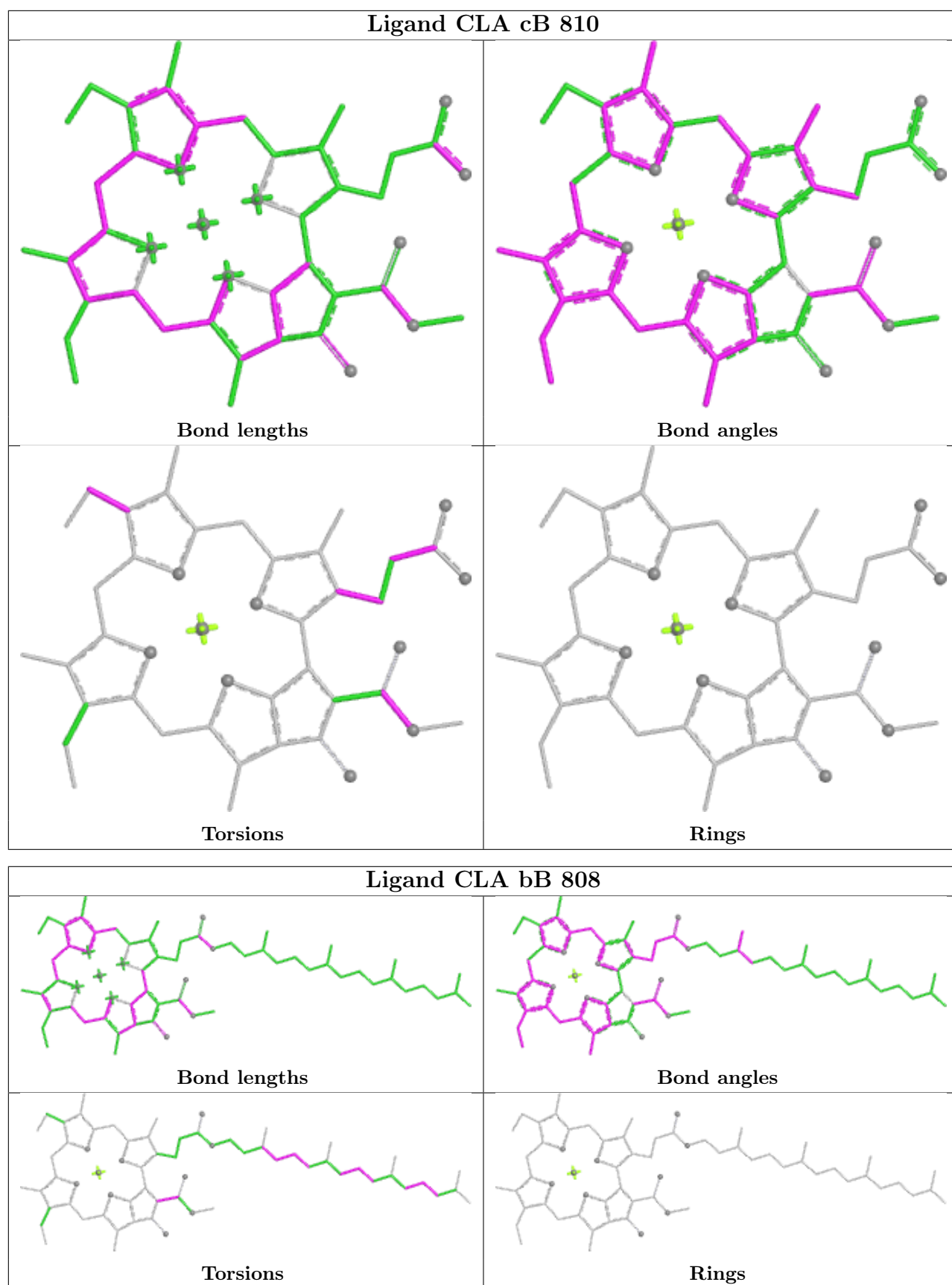
## Ligand CLA bK 101

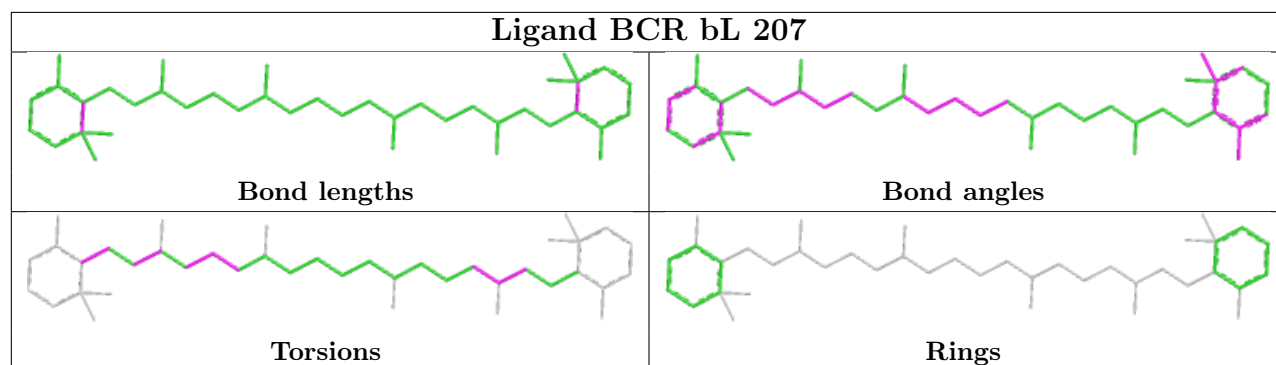
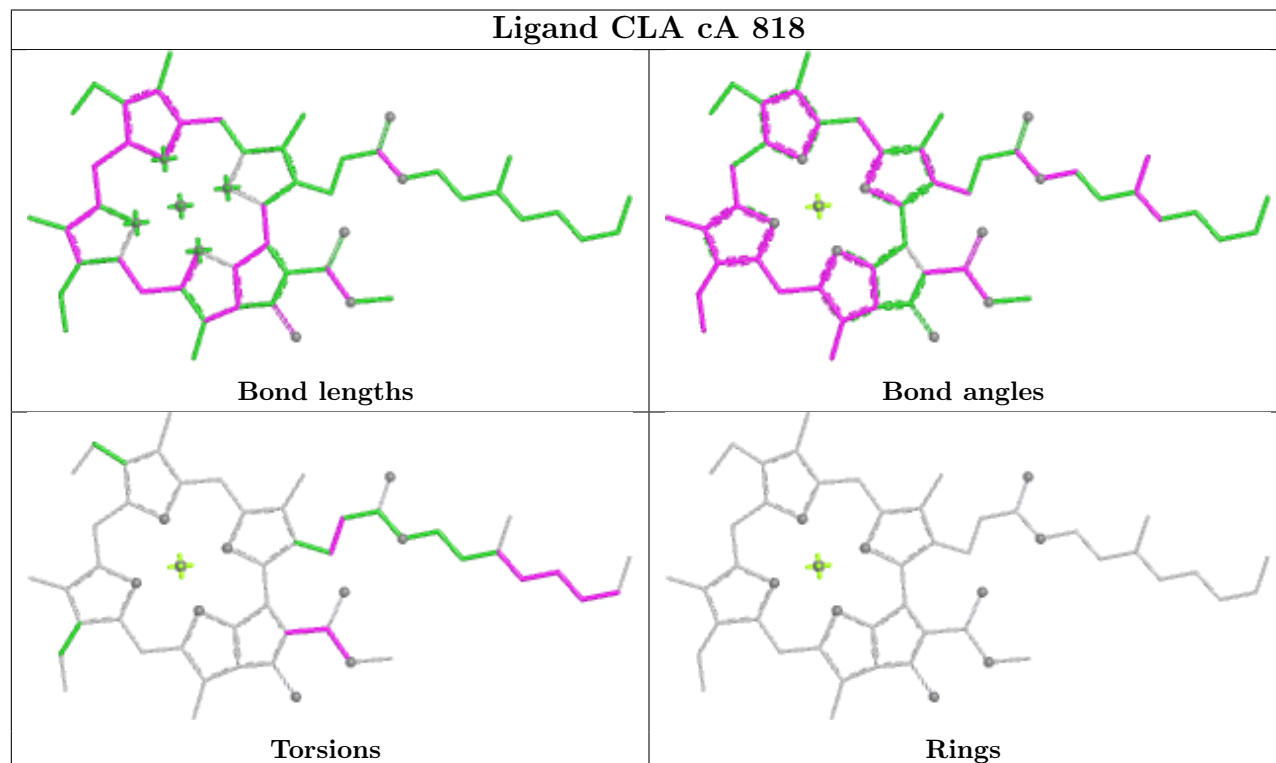
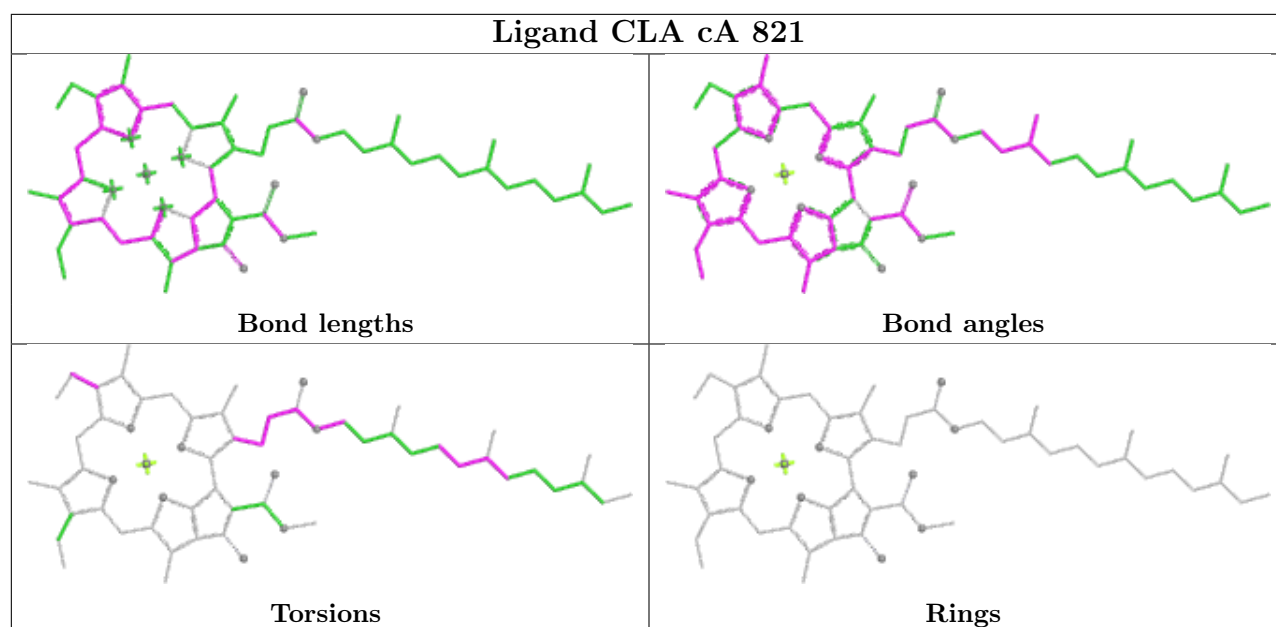




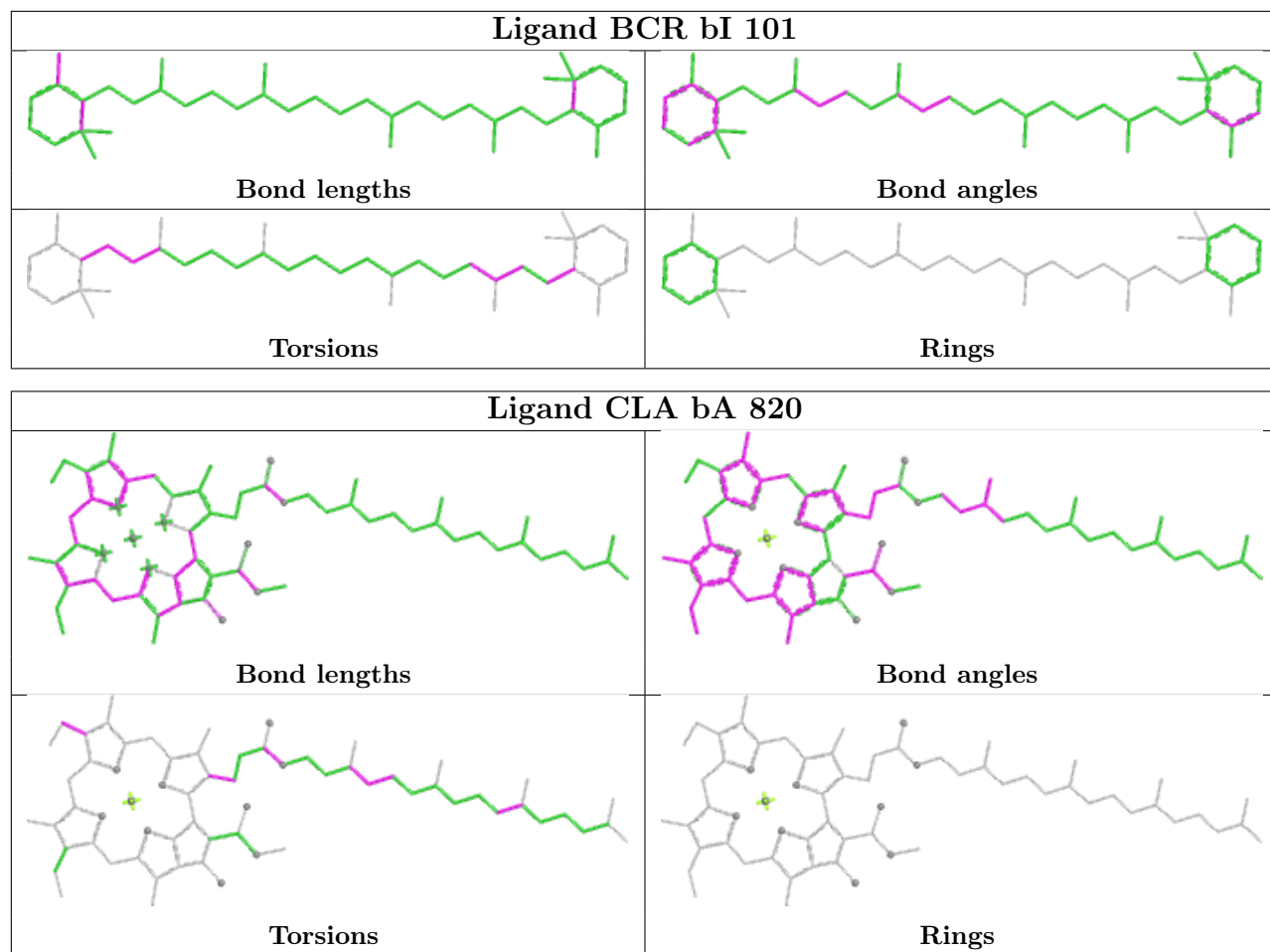


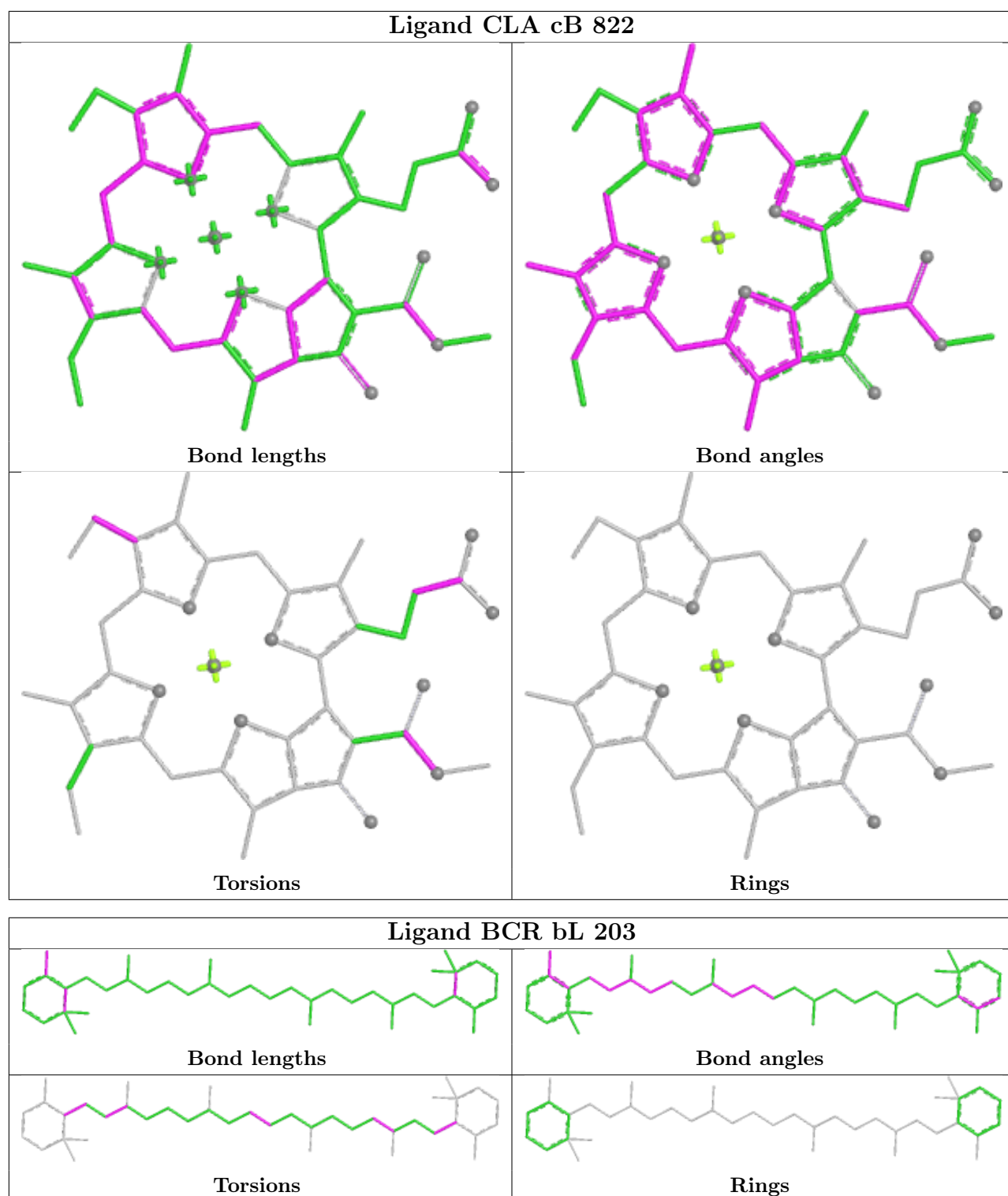


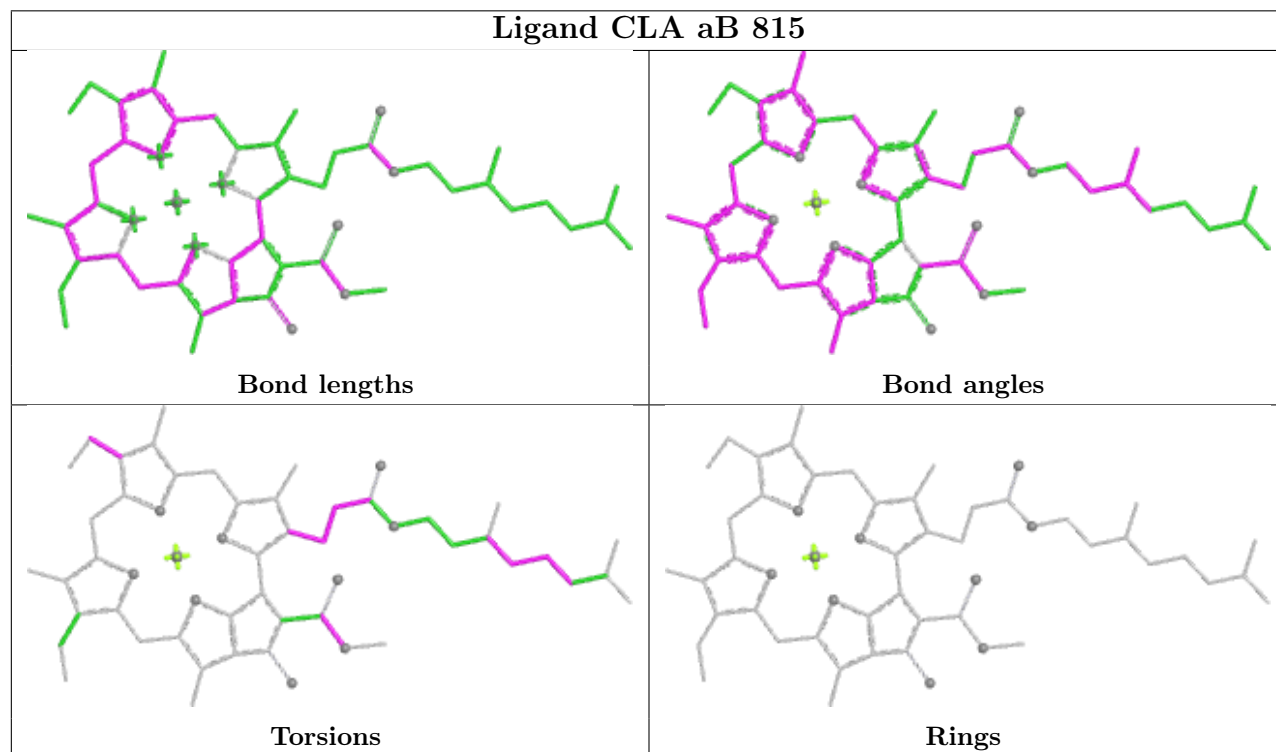
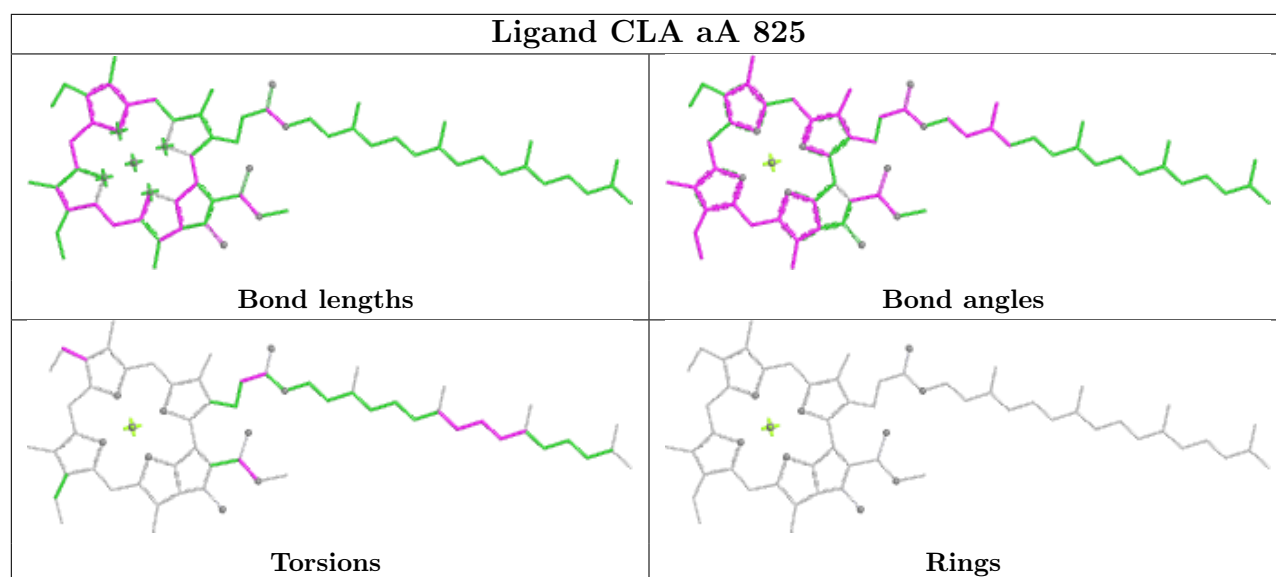


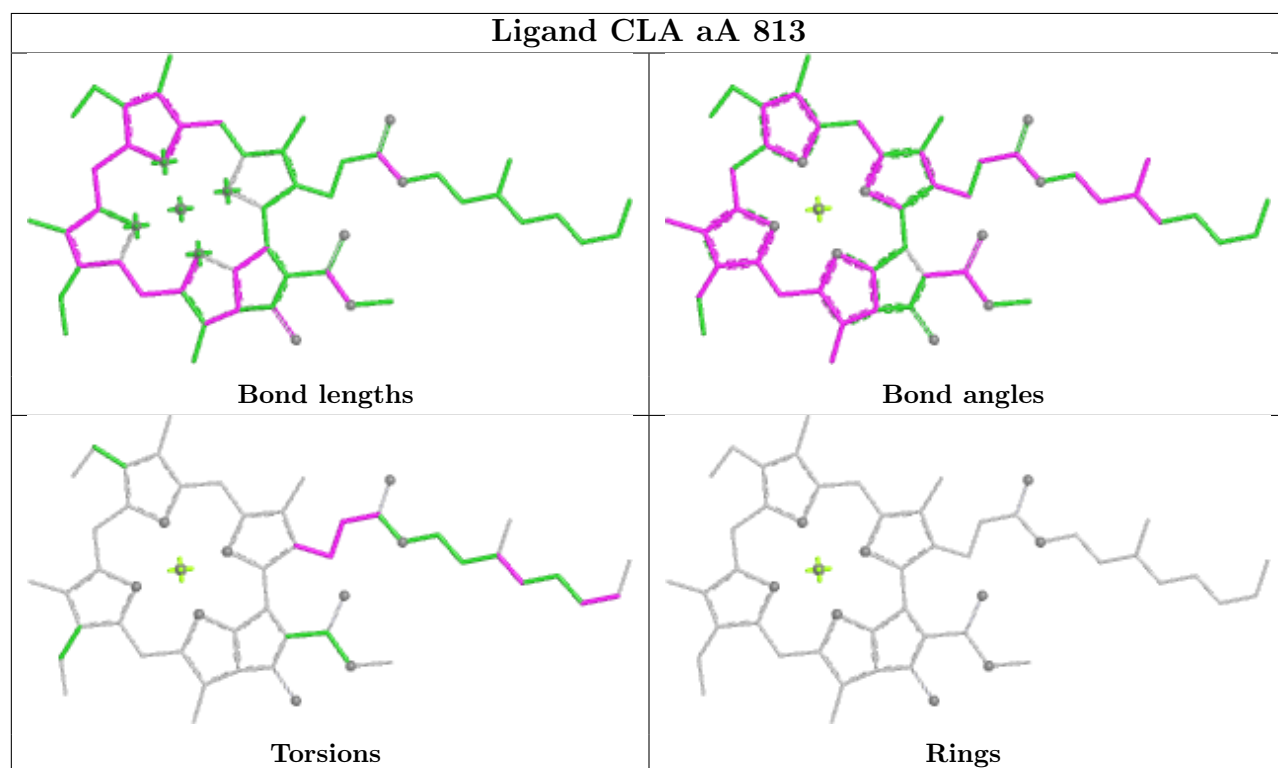
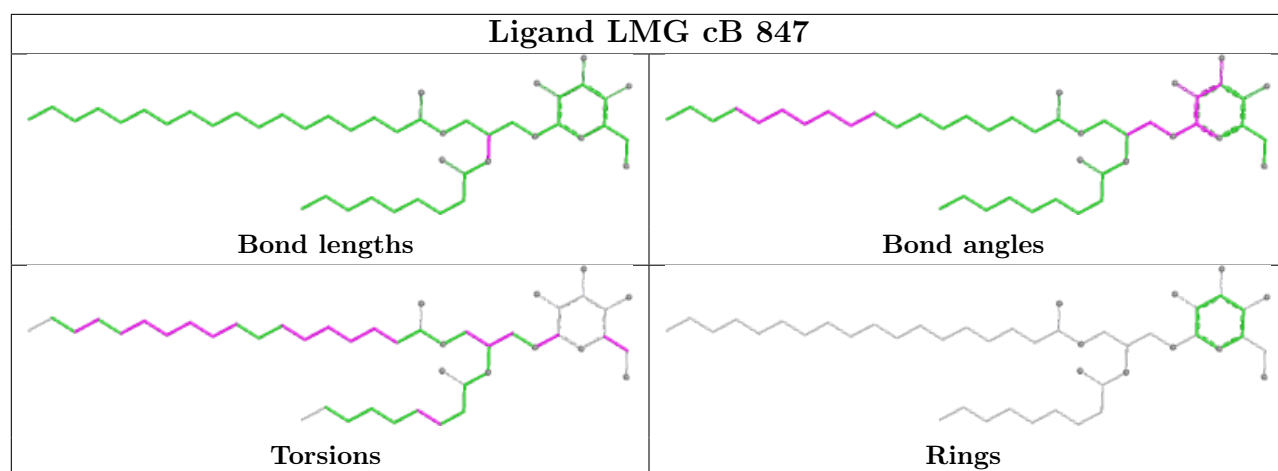


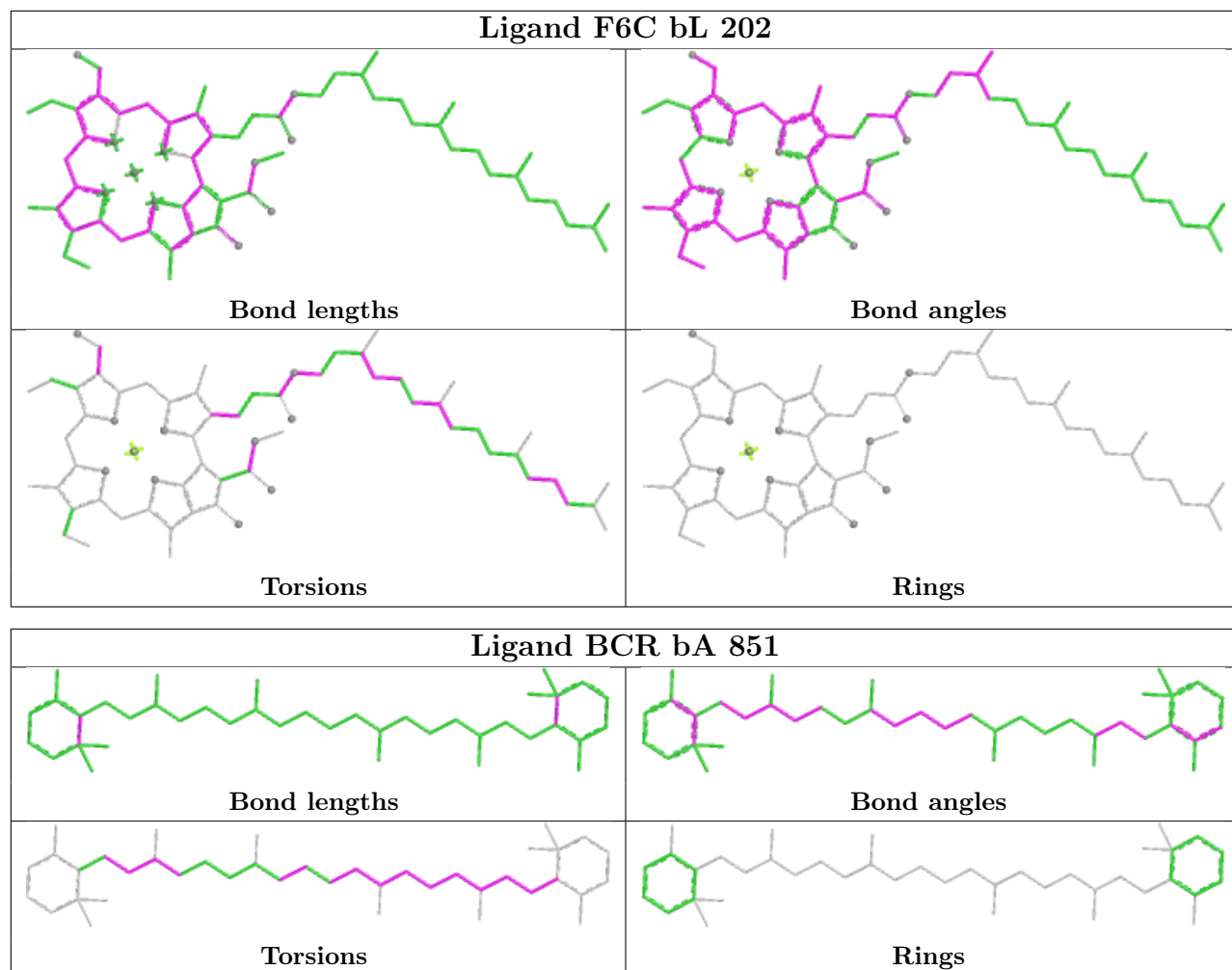




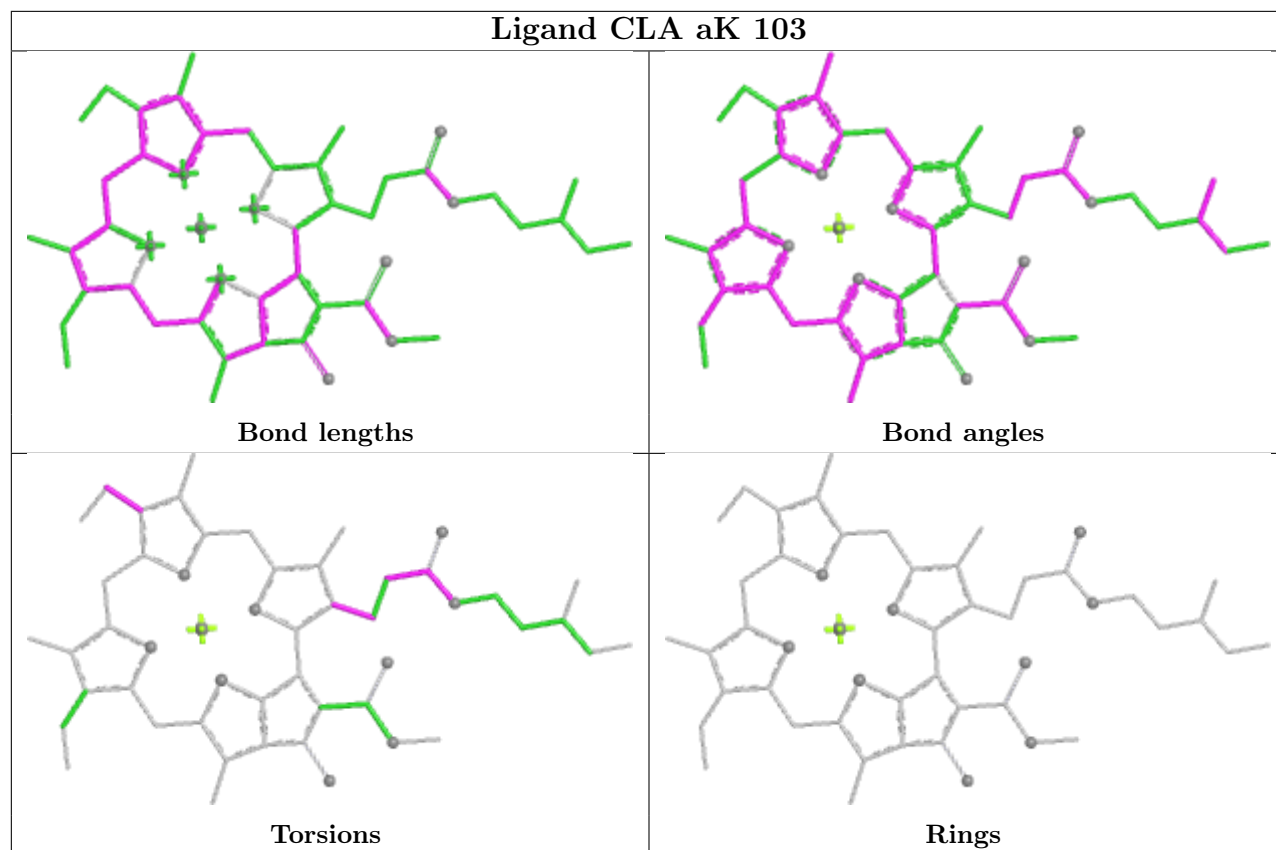




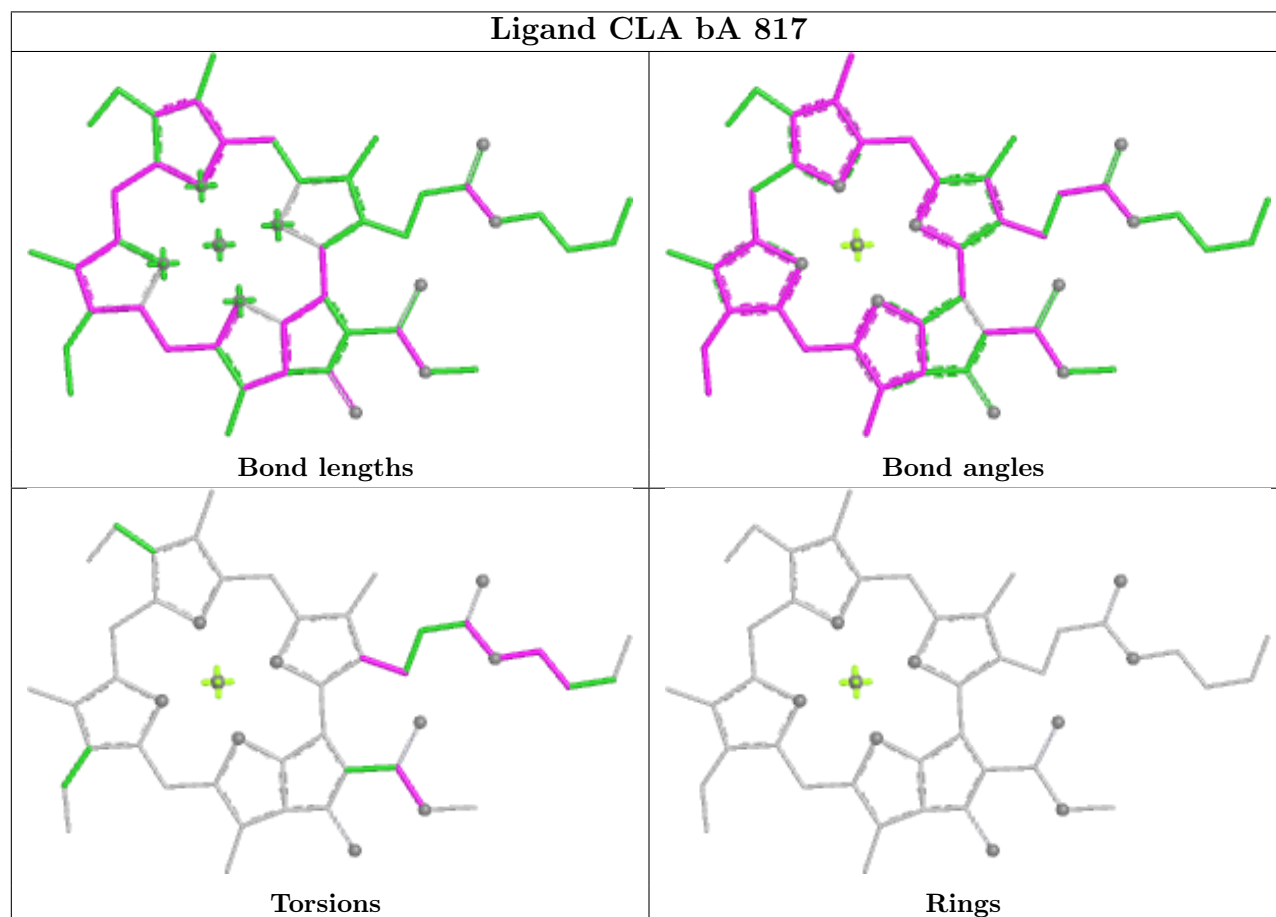




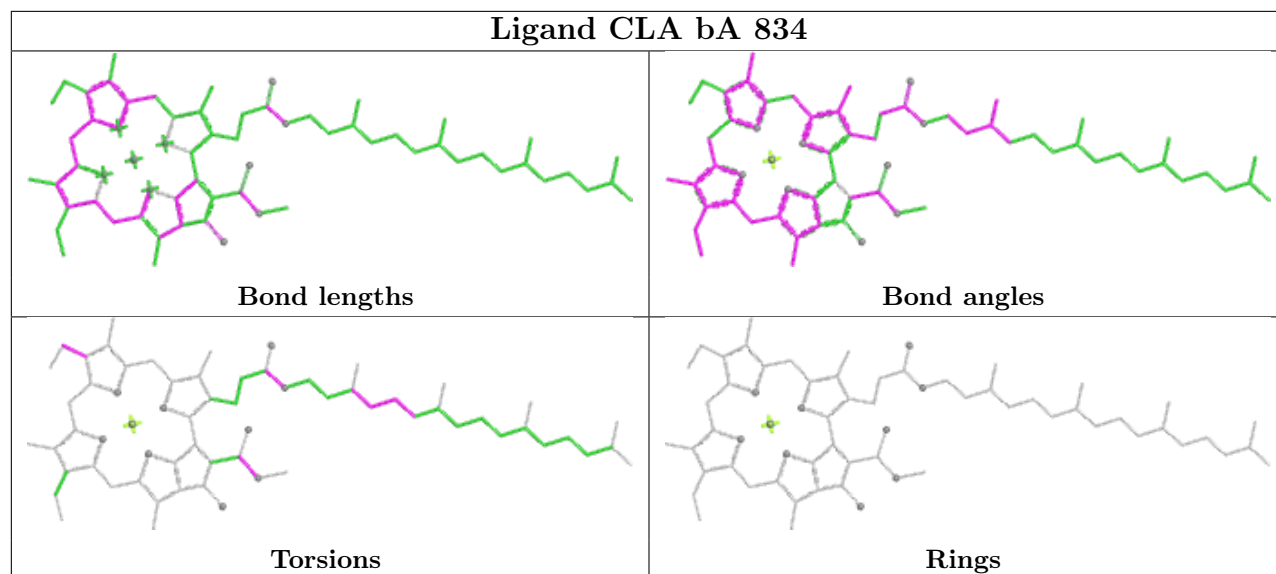
## Ligand CLA aK 103



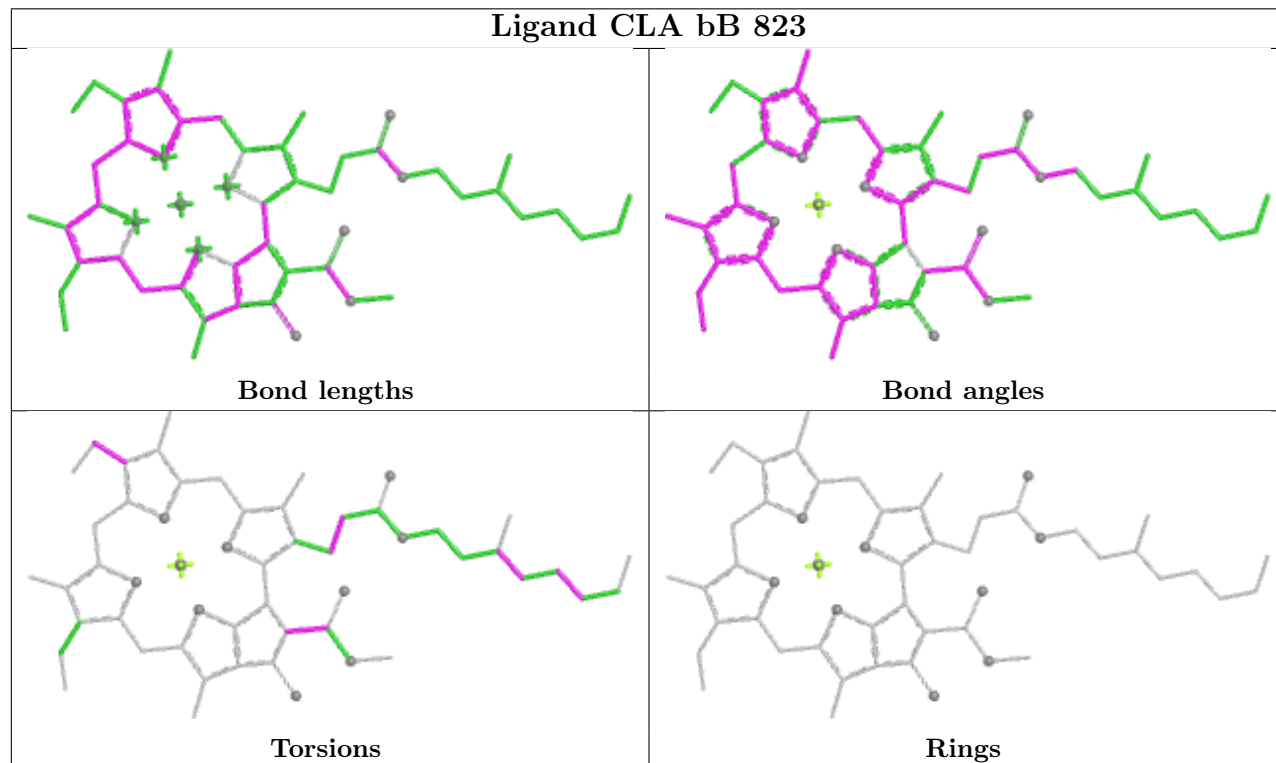
## Ligand CLA bA 817



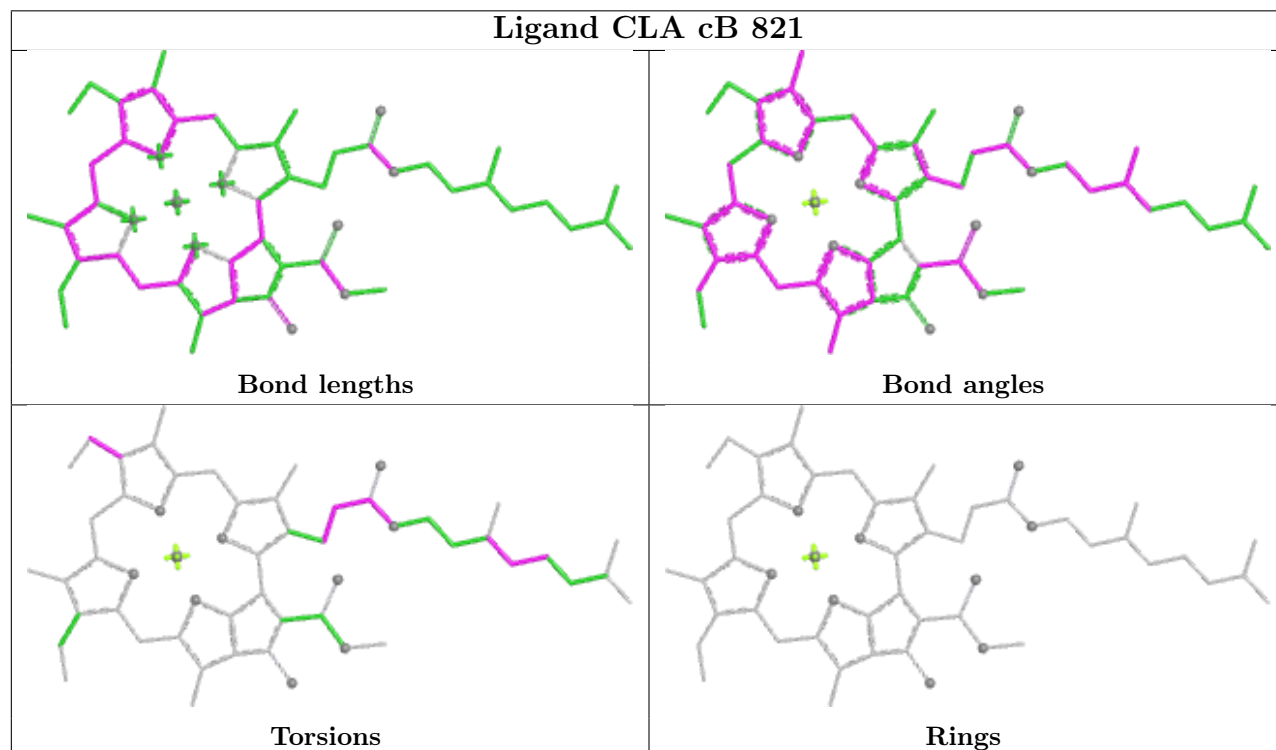
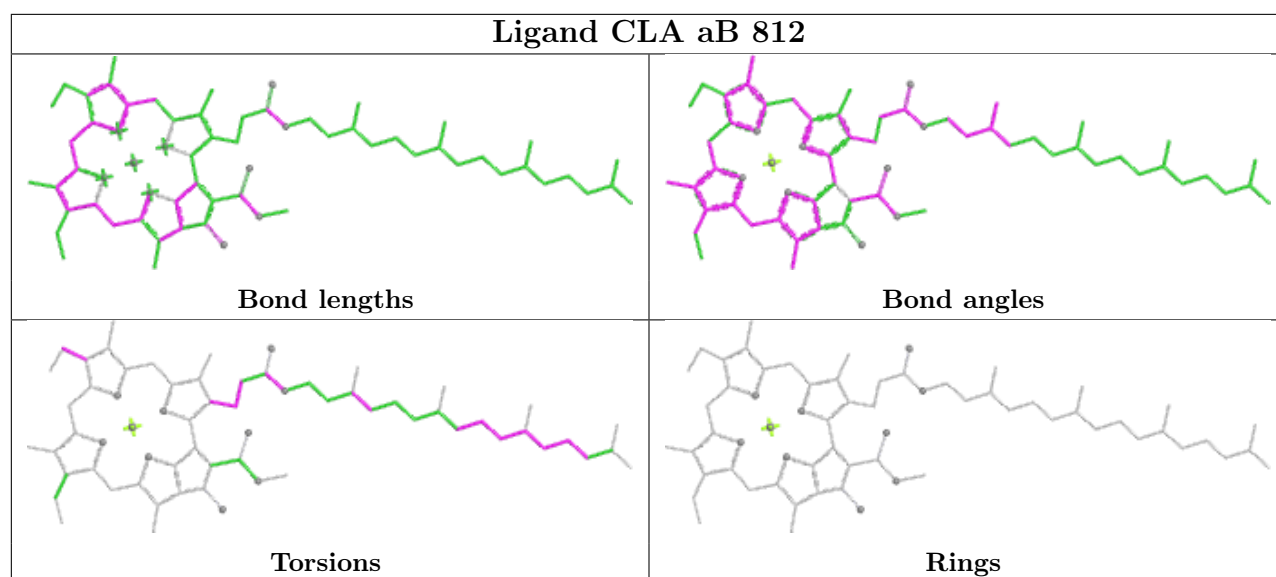
## Ligand CLA bA 834

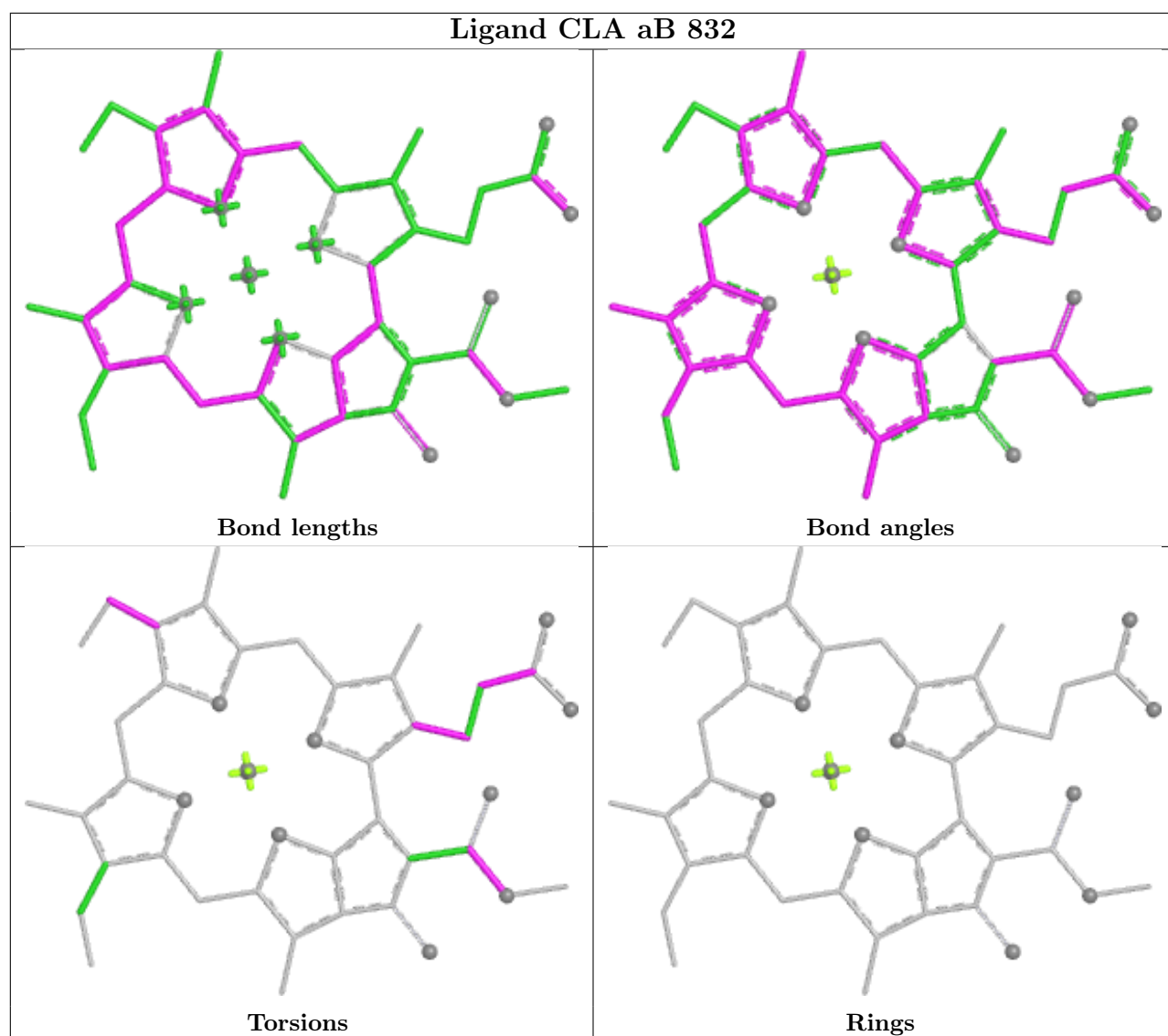


## Ligand CLA bB 823

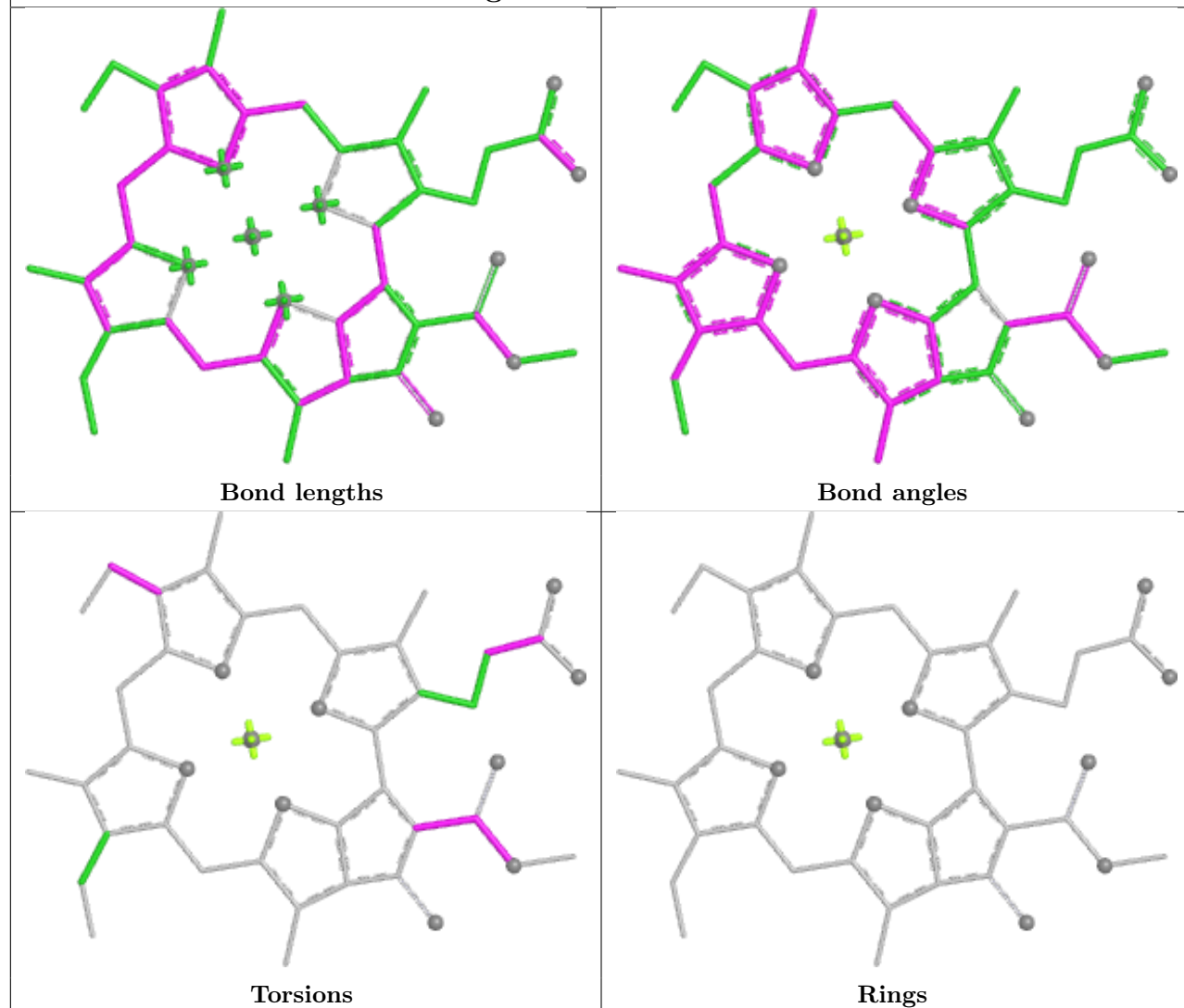




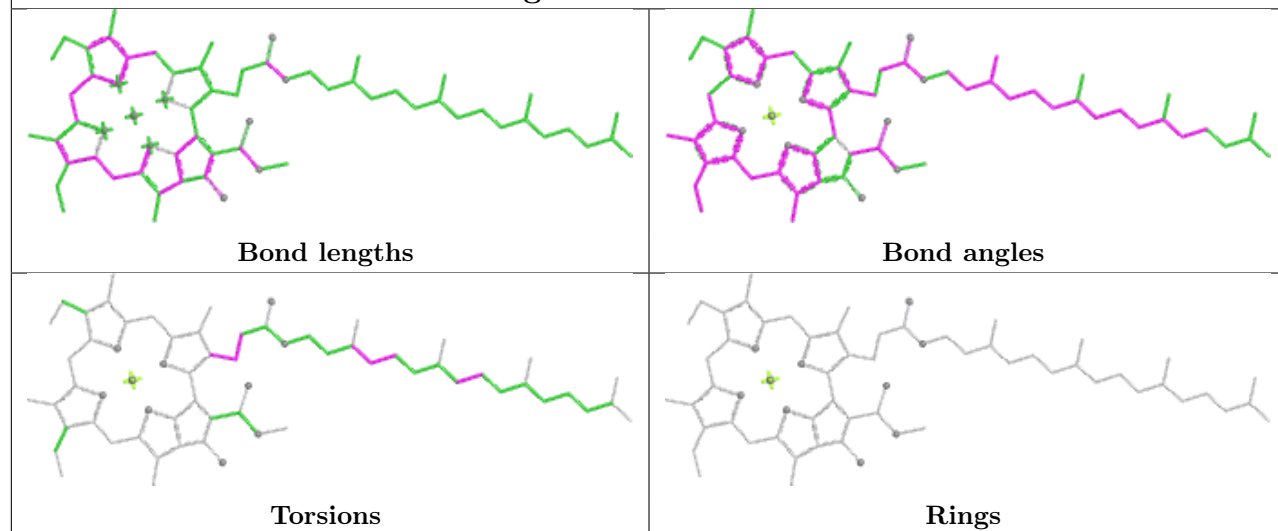




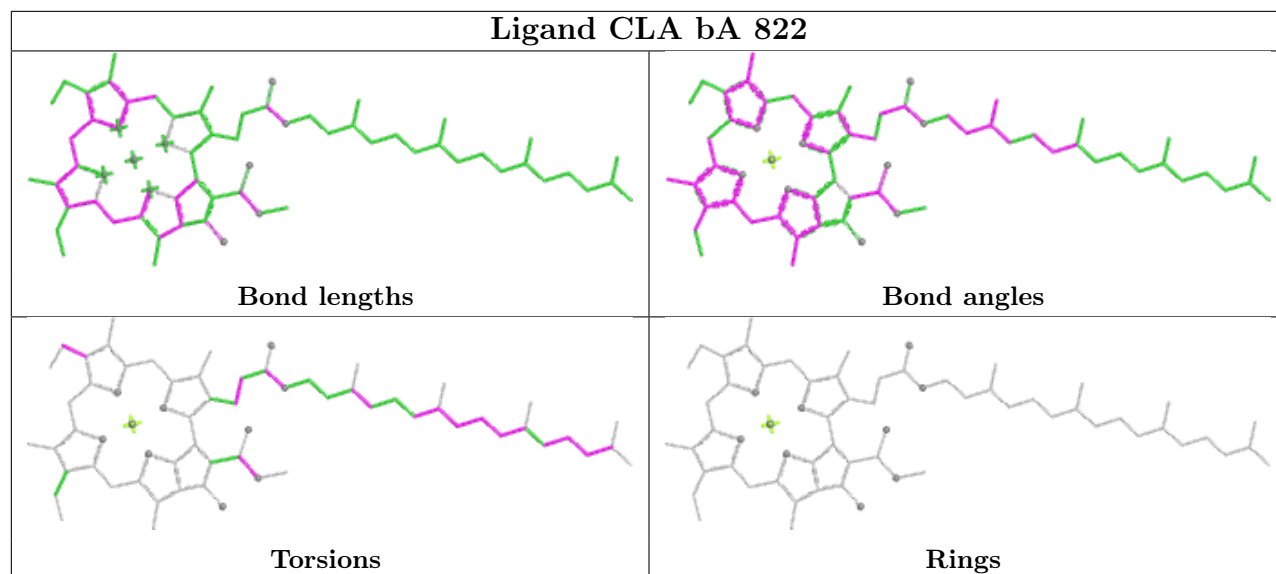
## Ligand CLA cB 820



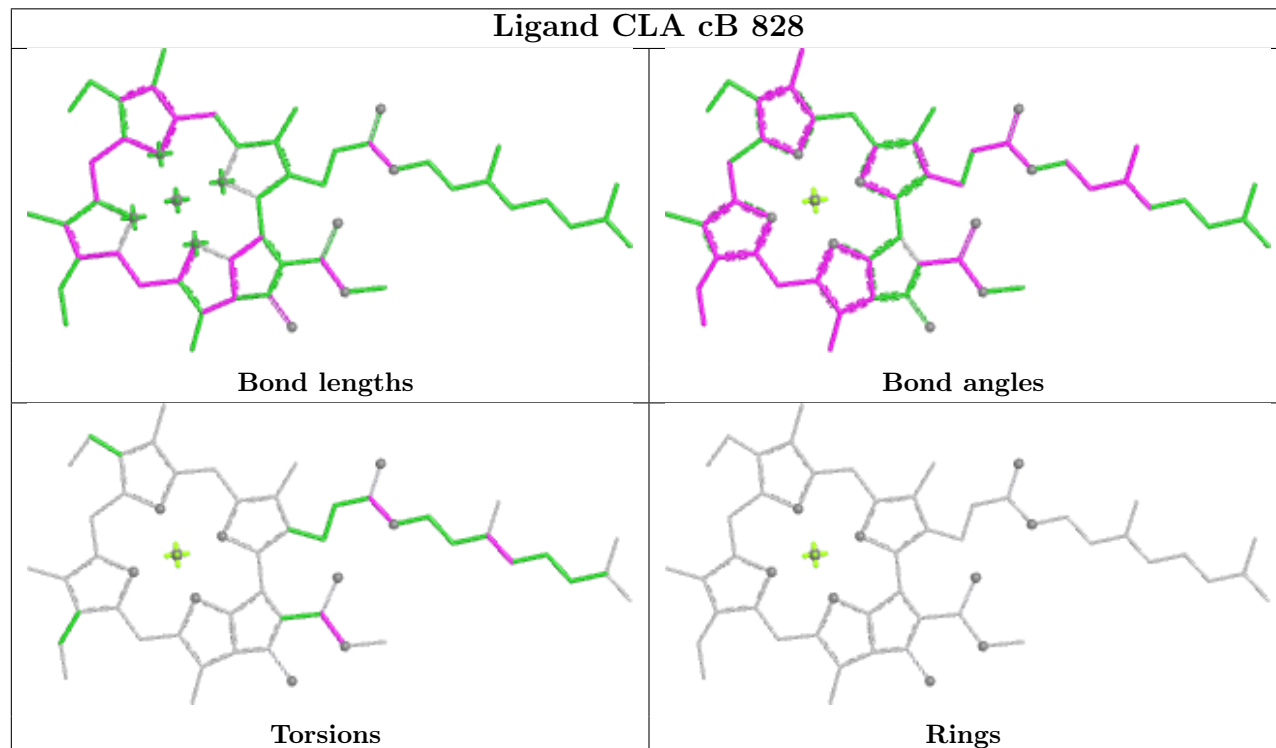
## Ligand CLA cA 802

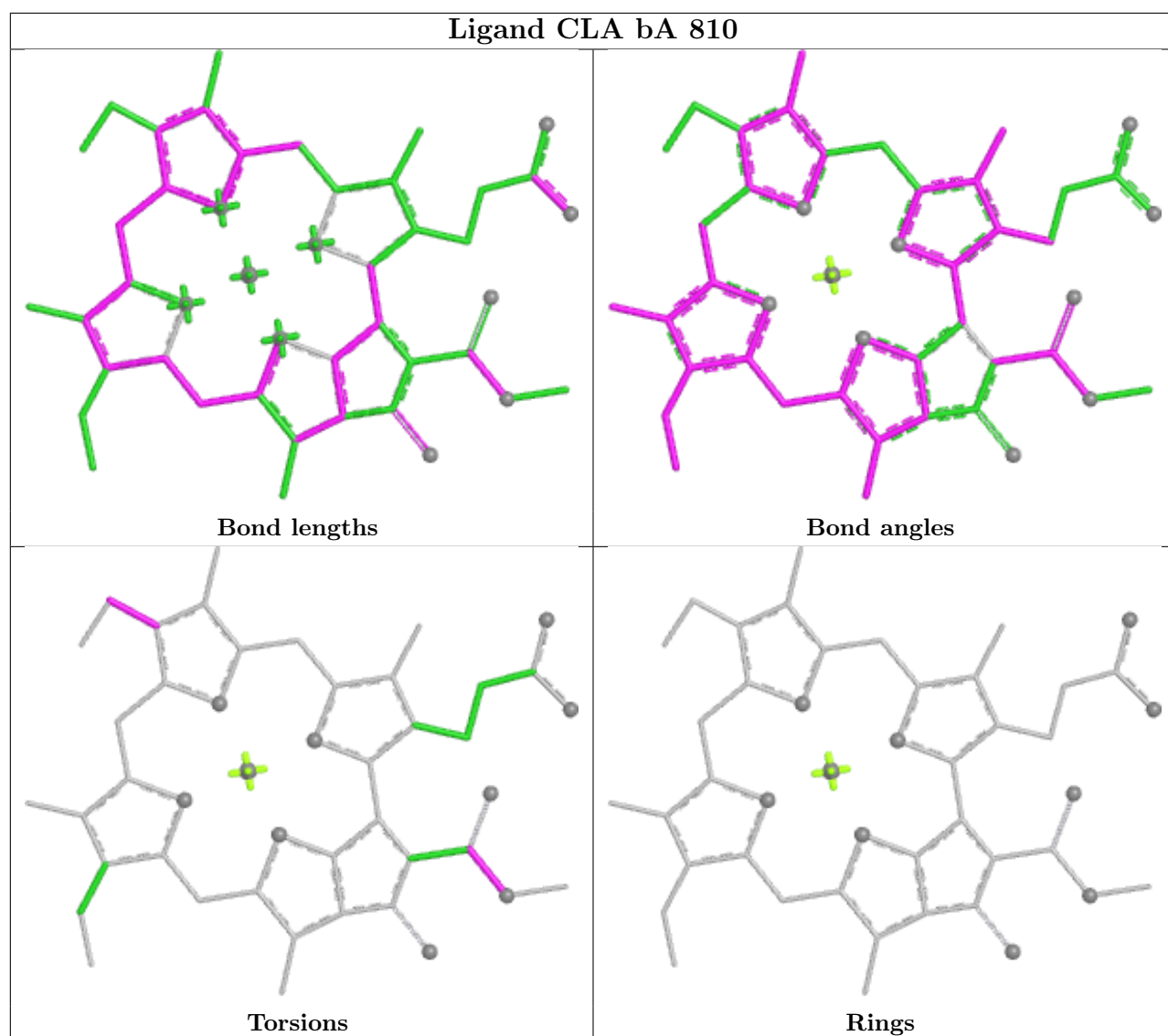


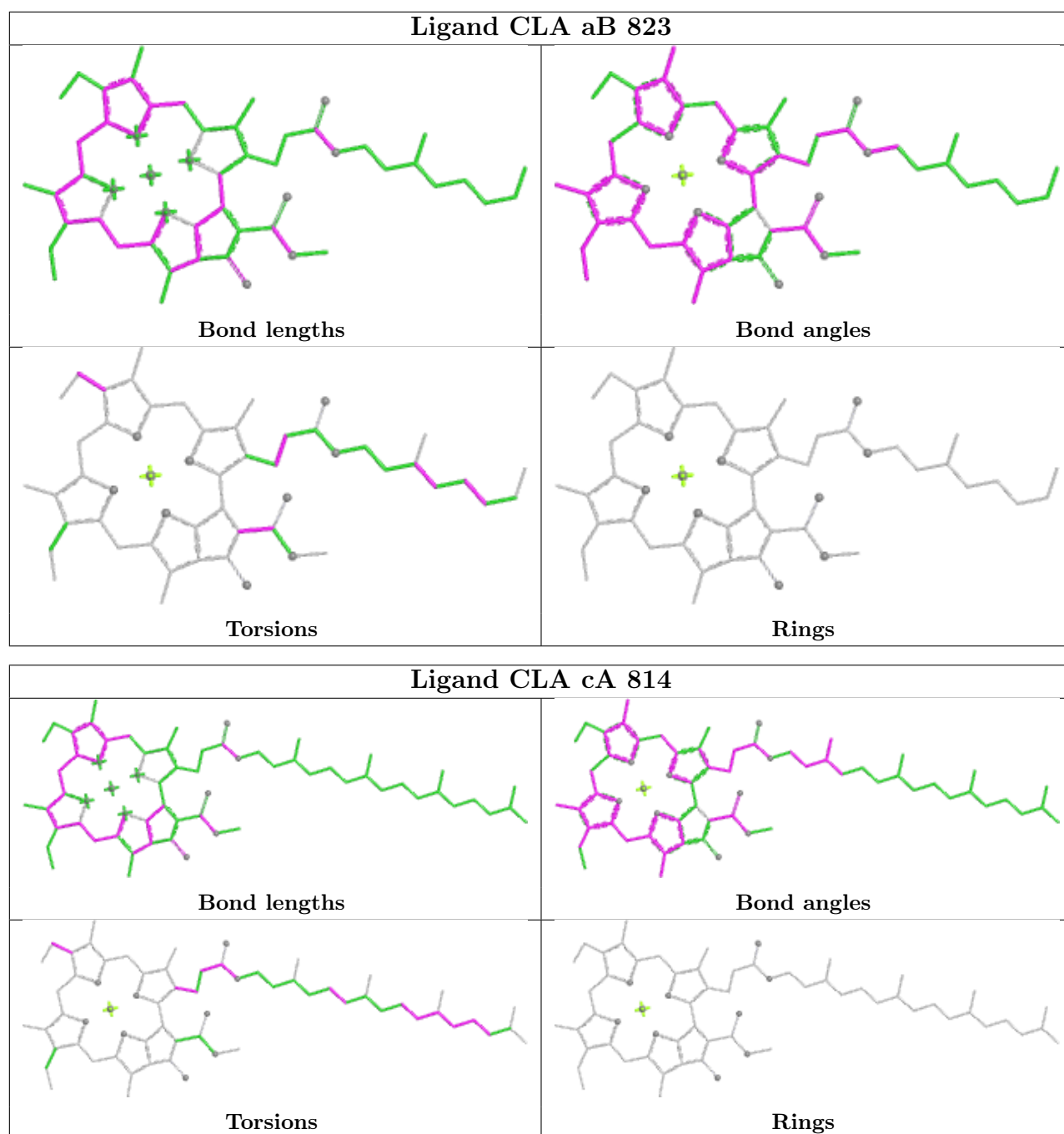
## Ligand CLA bA 822



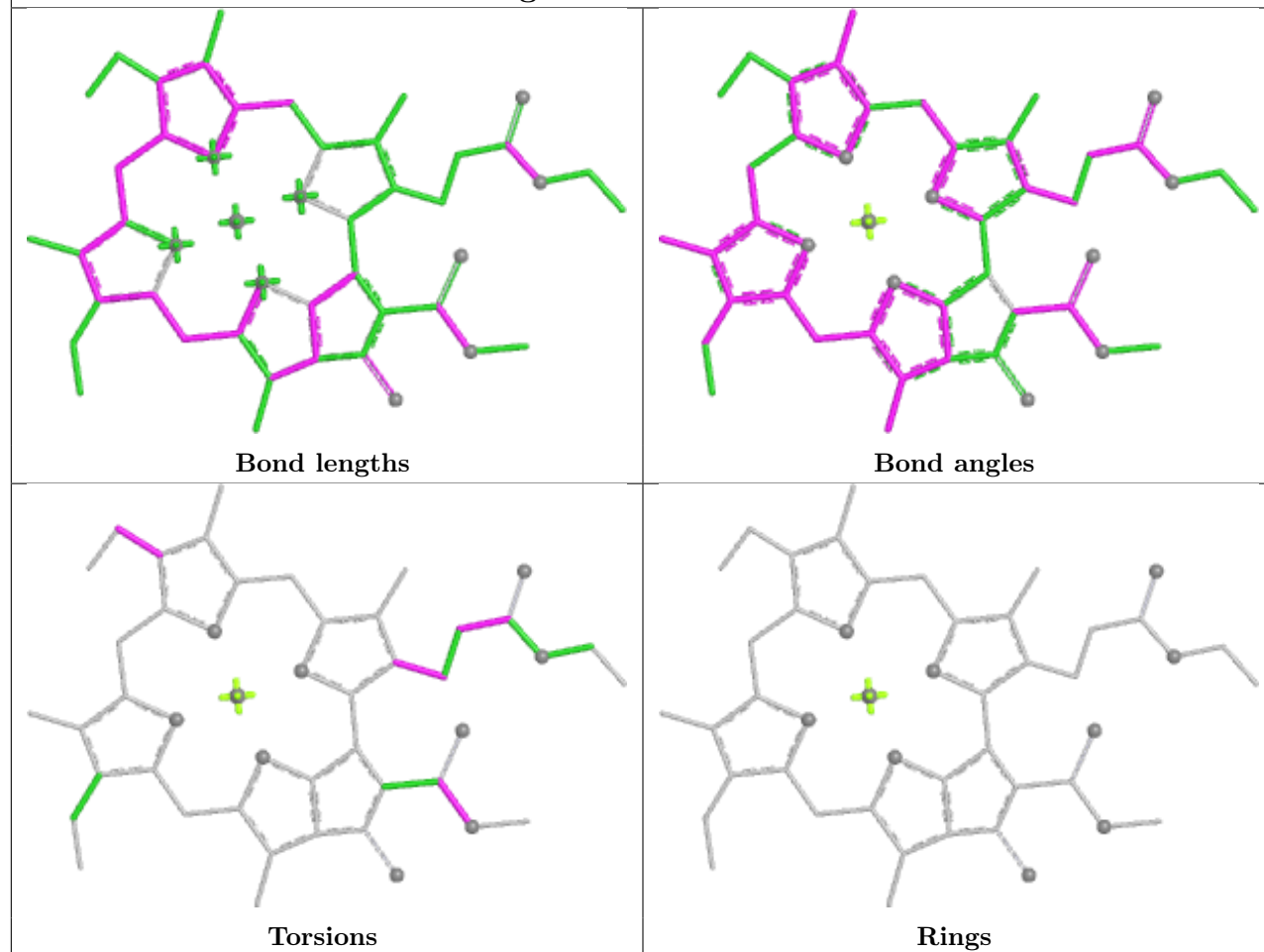
## Ligand CLA cB 828



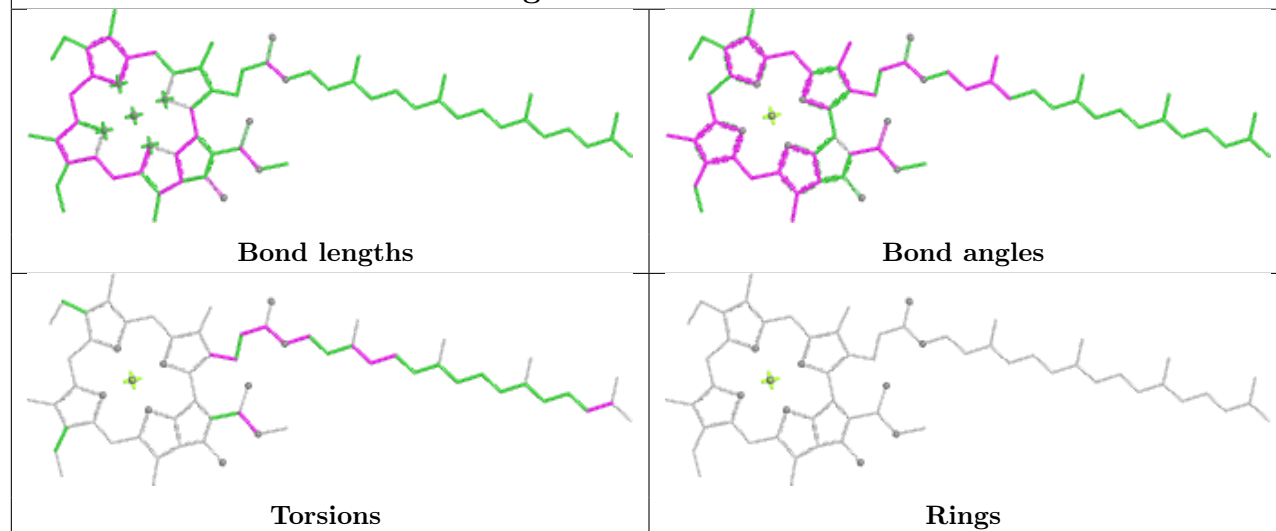




## Ligand CLA cB 838

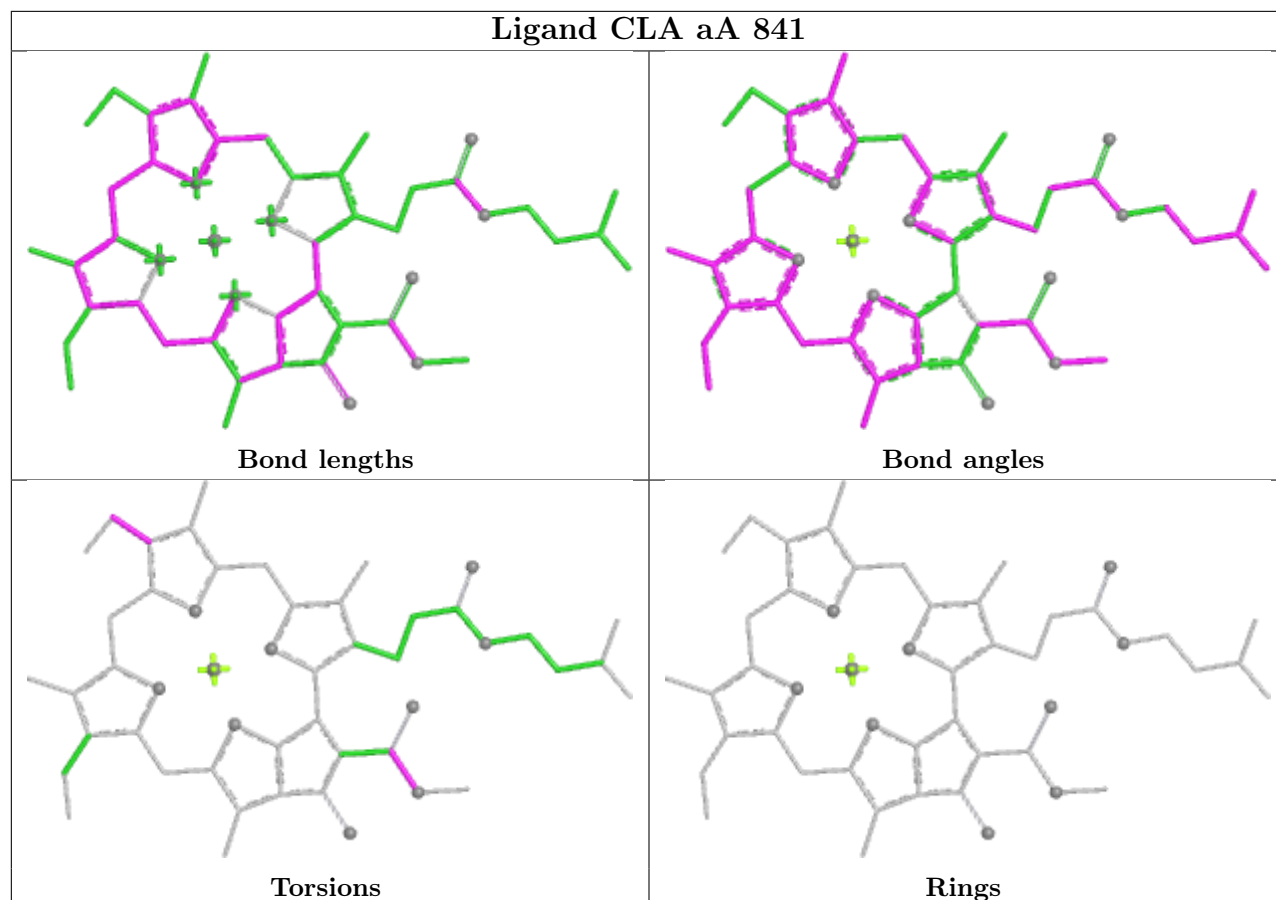


## Ligand CLA aA 829

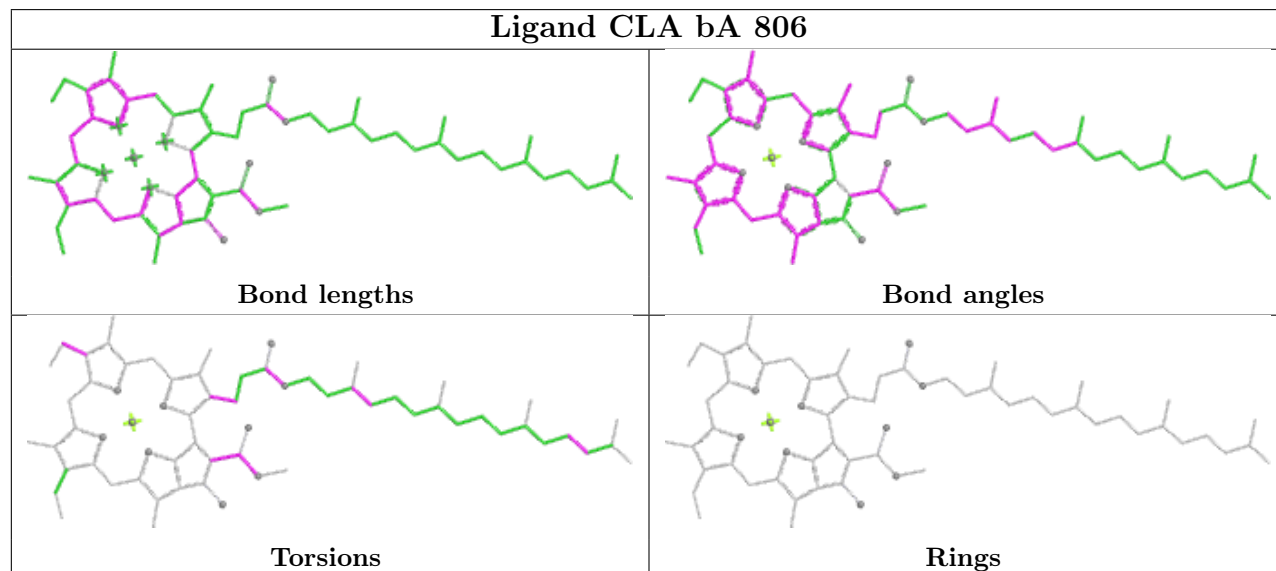


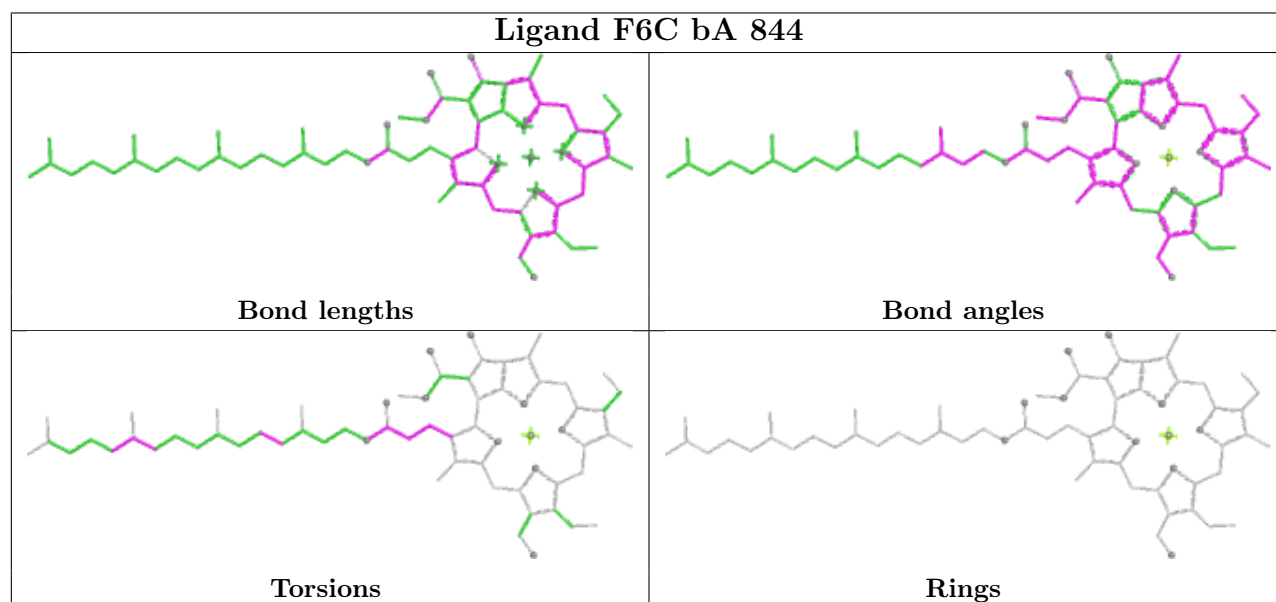
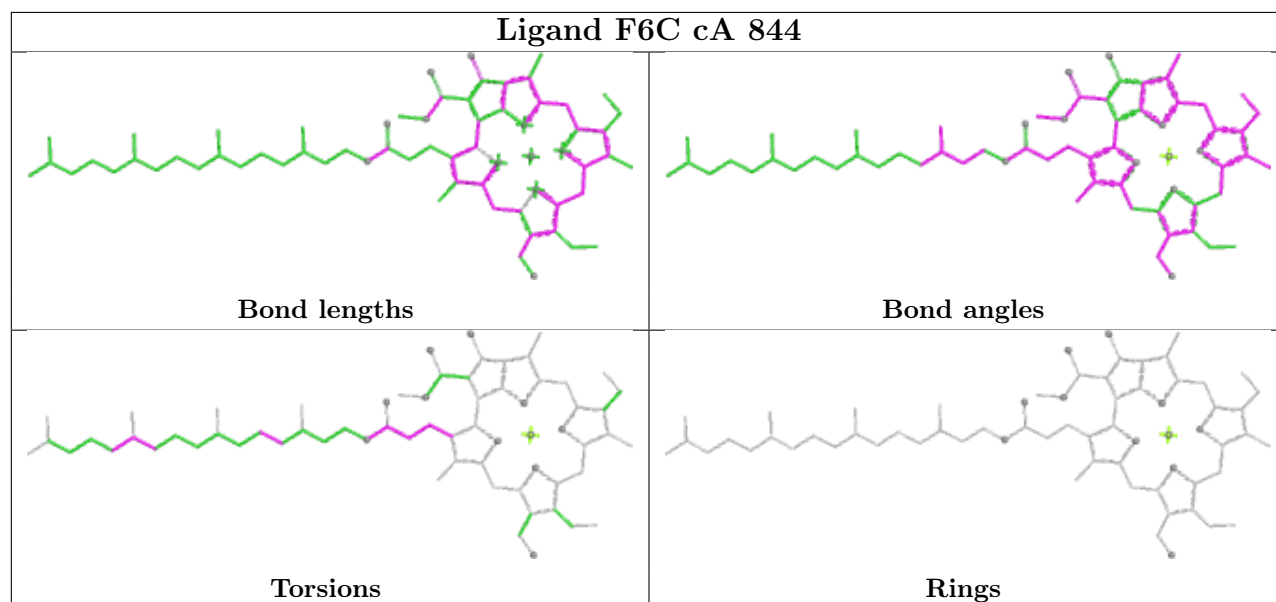
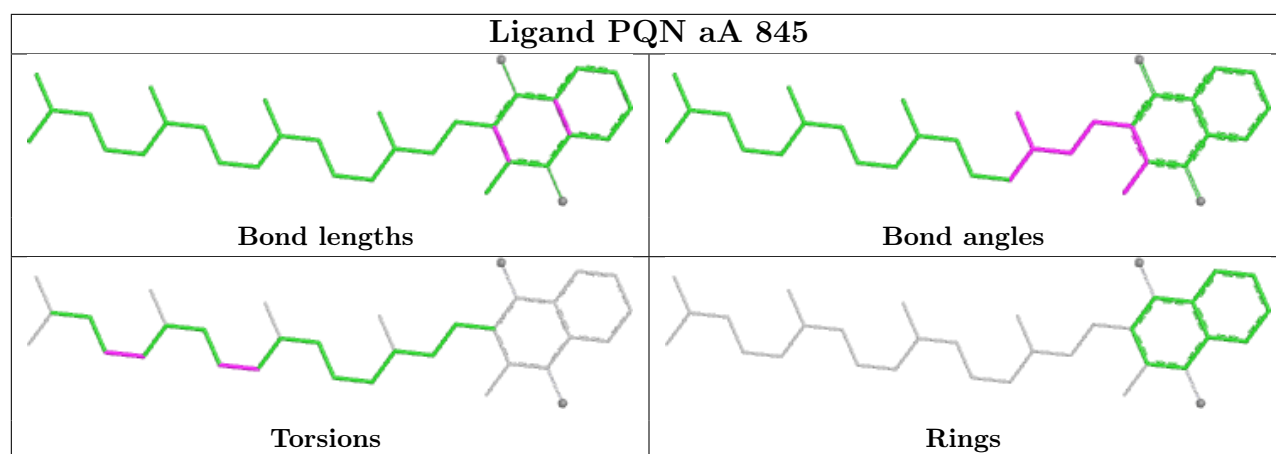


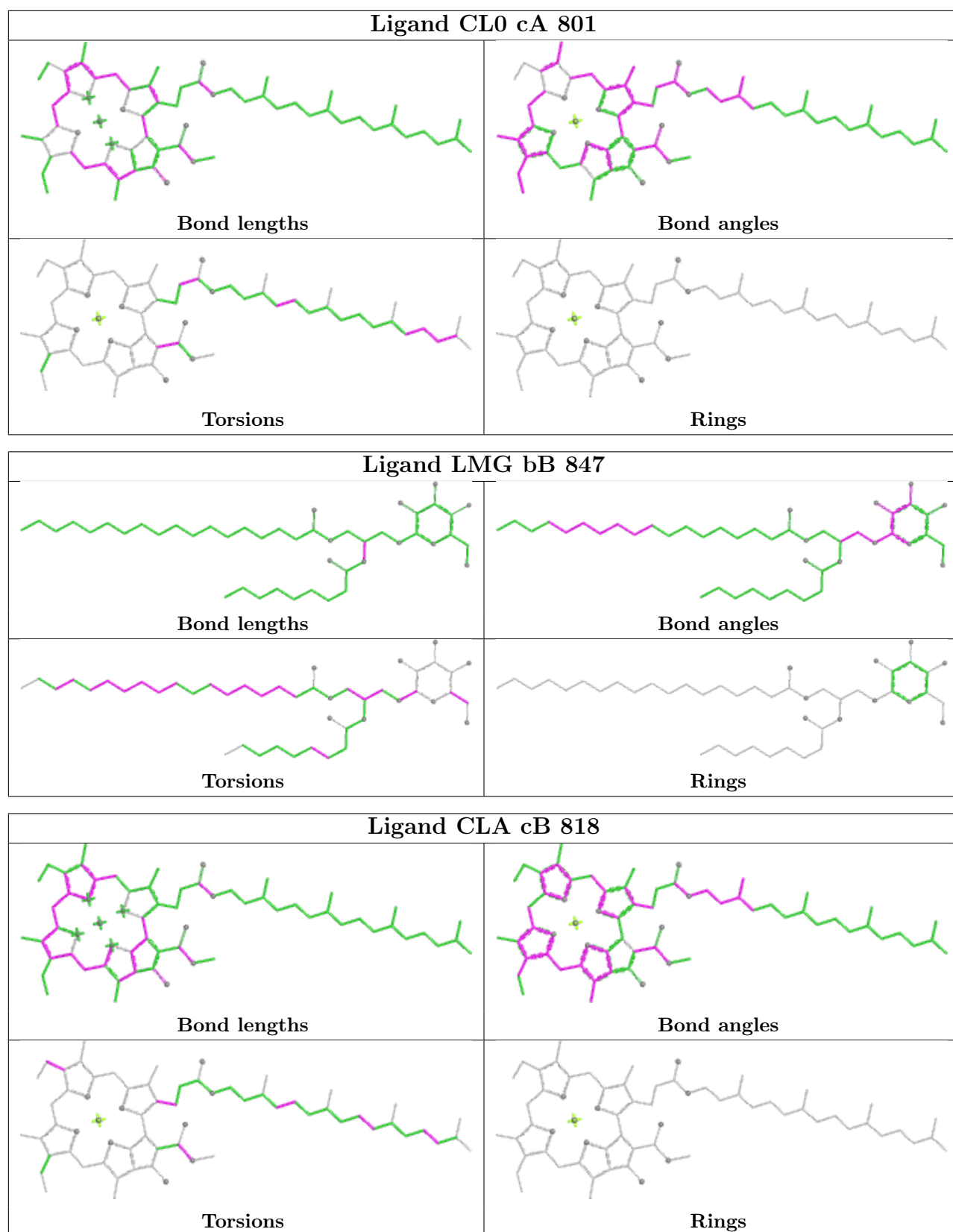
## Ligand CLA aA 841

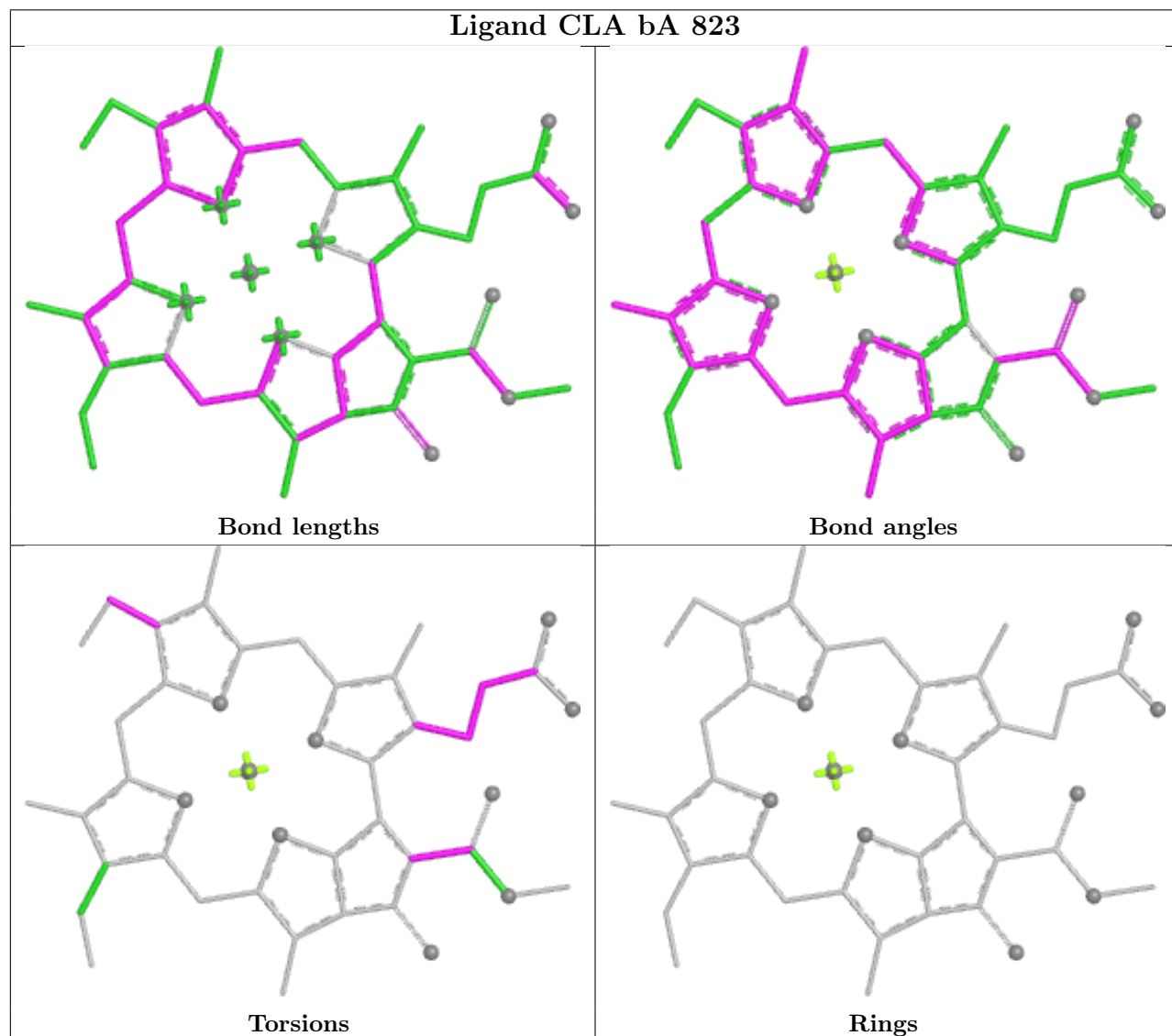
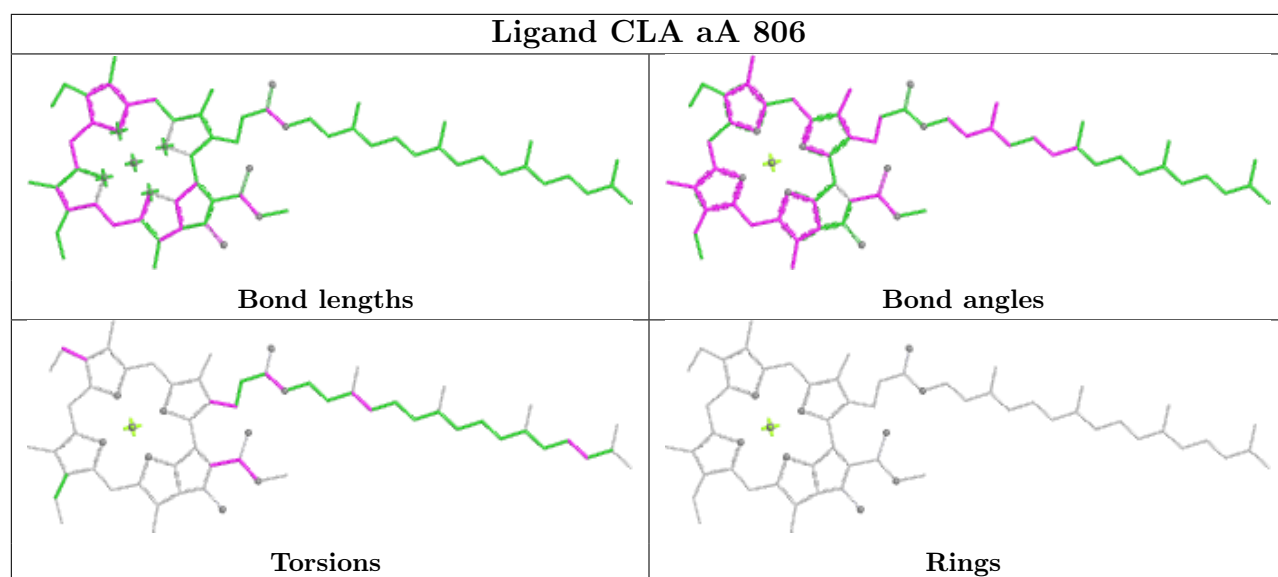


## Ligand CLA bA 806

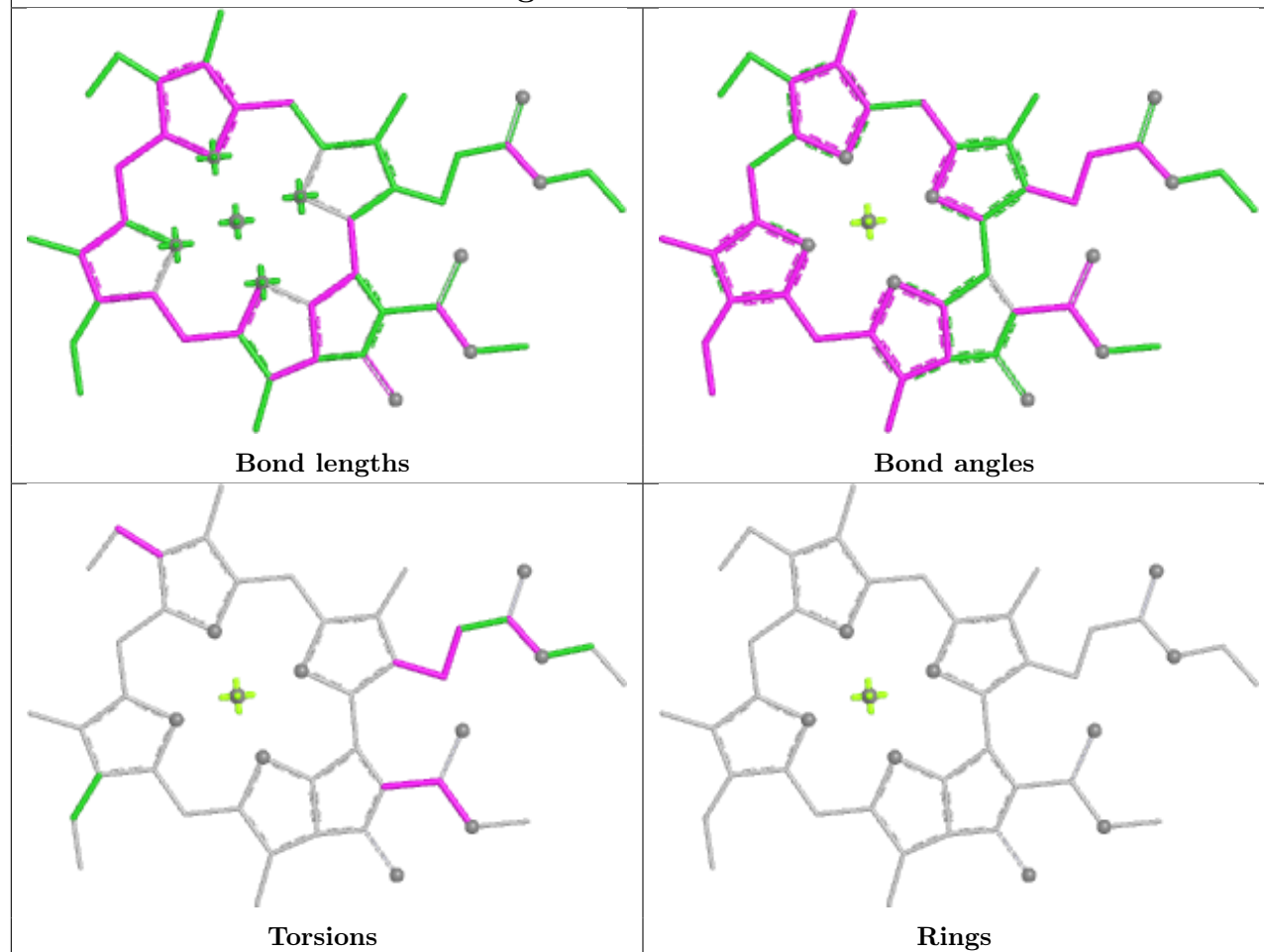




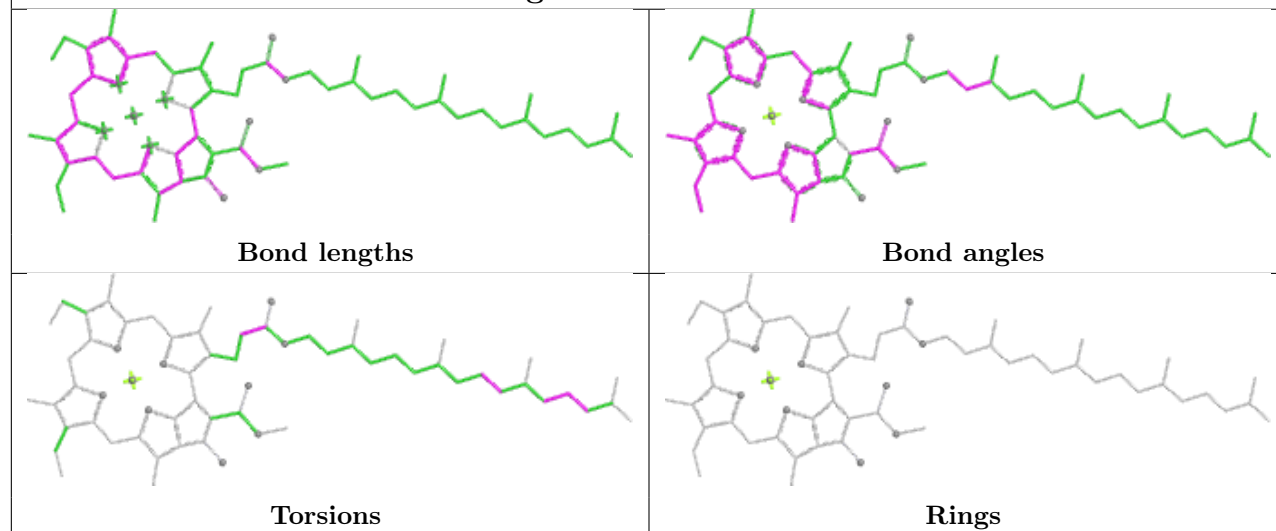


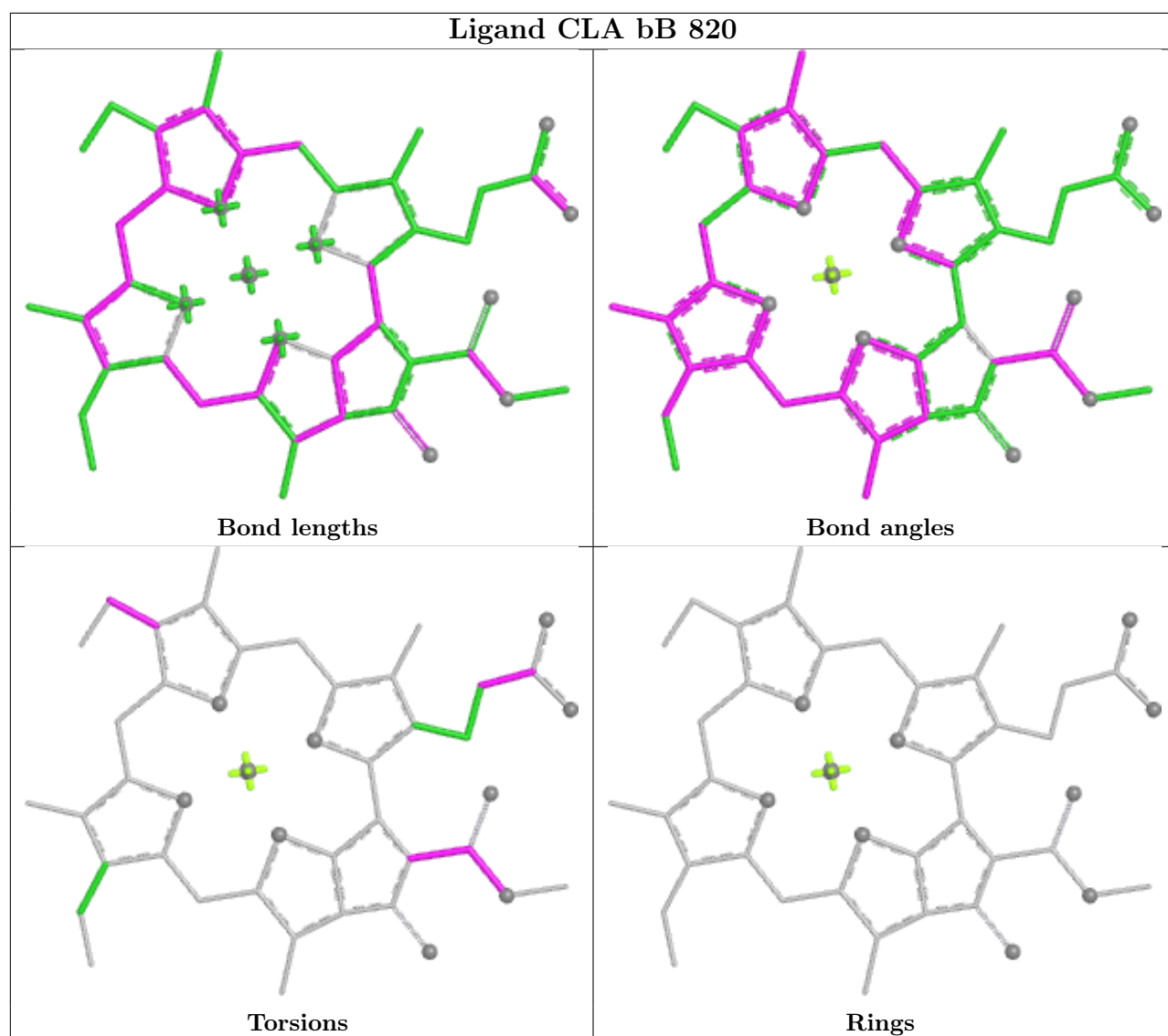


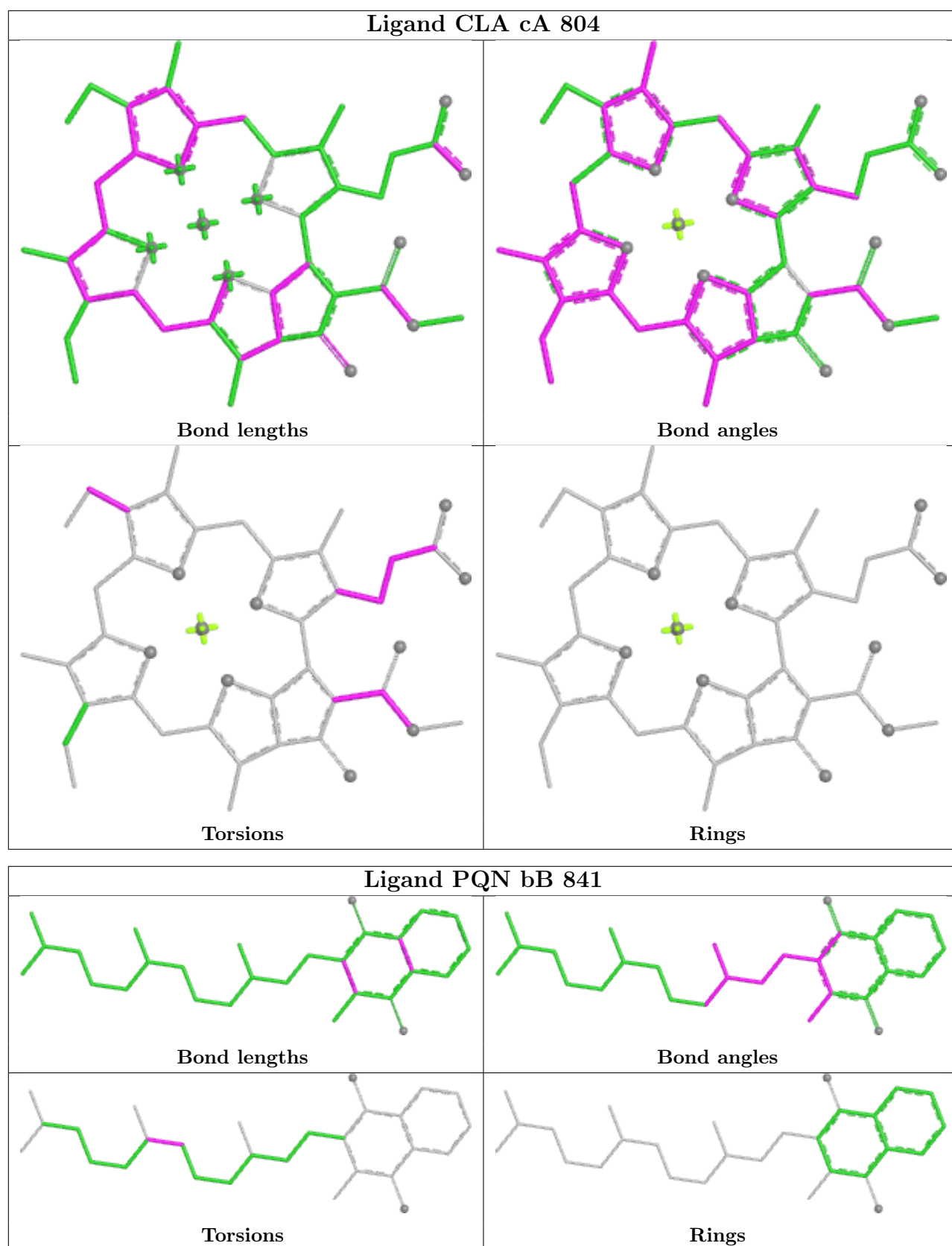
## Ligand CLA bB 819



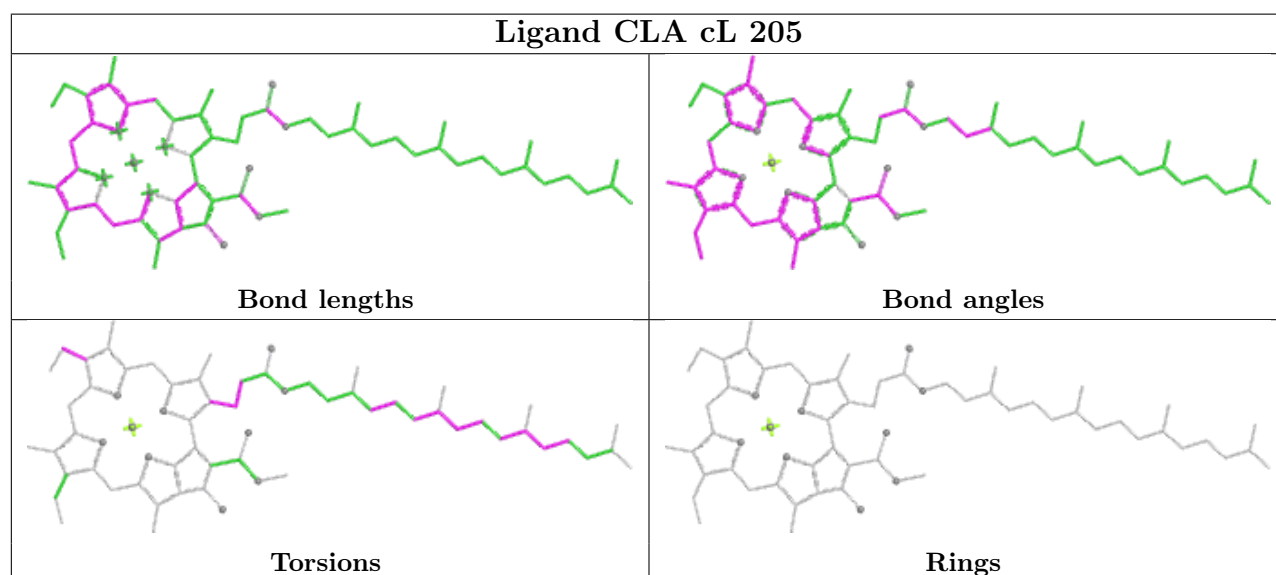
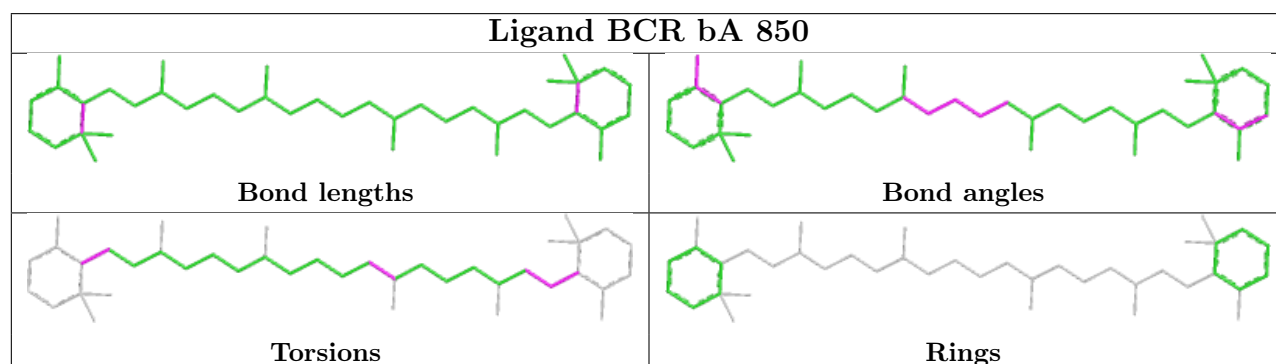
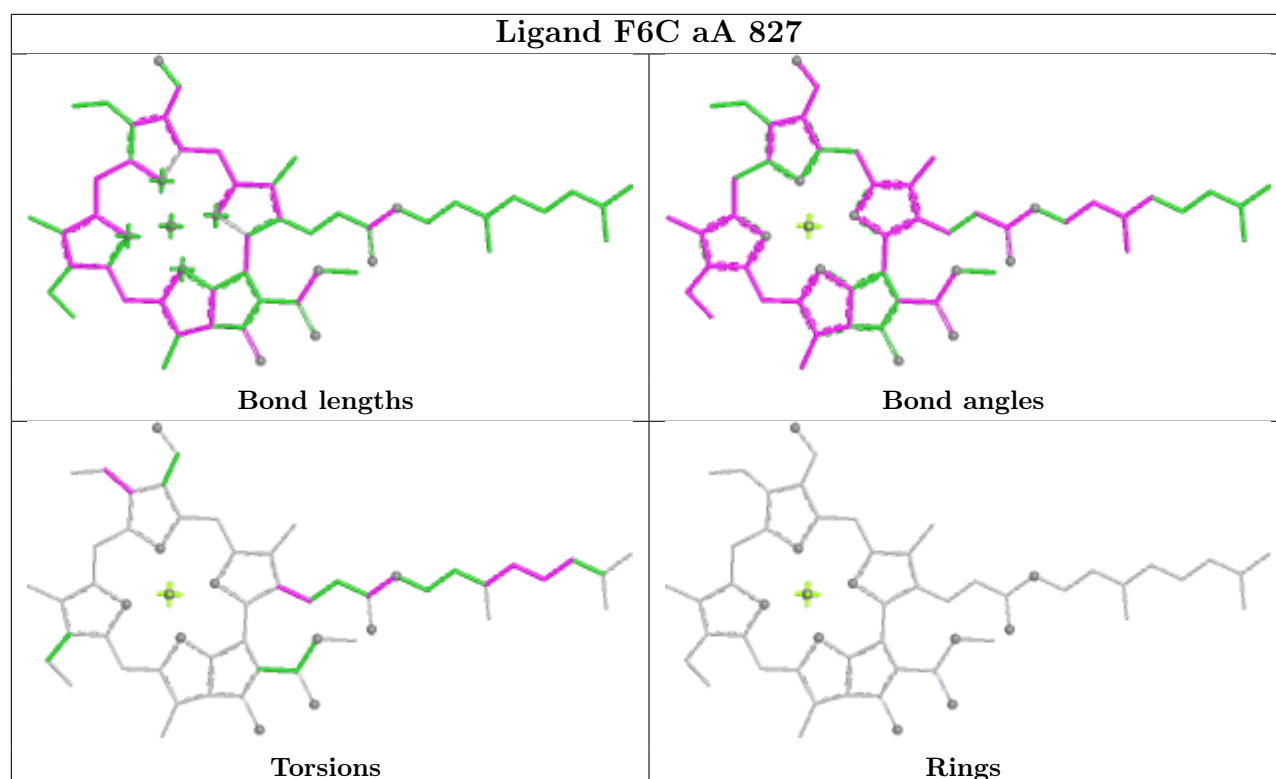
## Ligand CLA cL 204

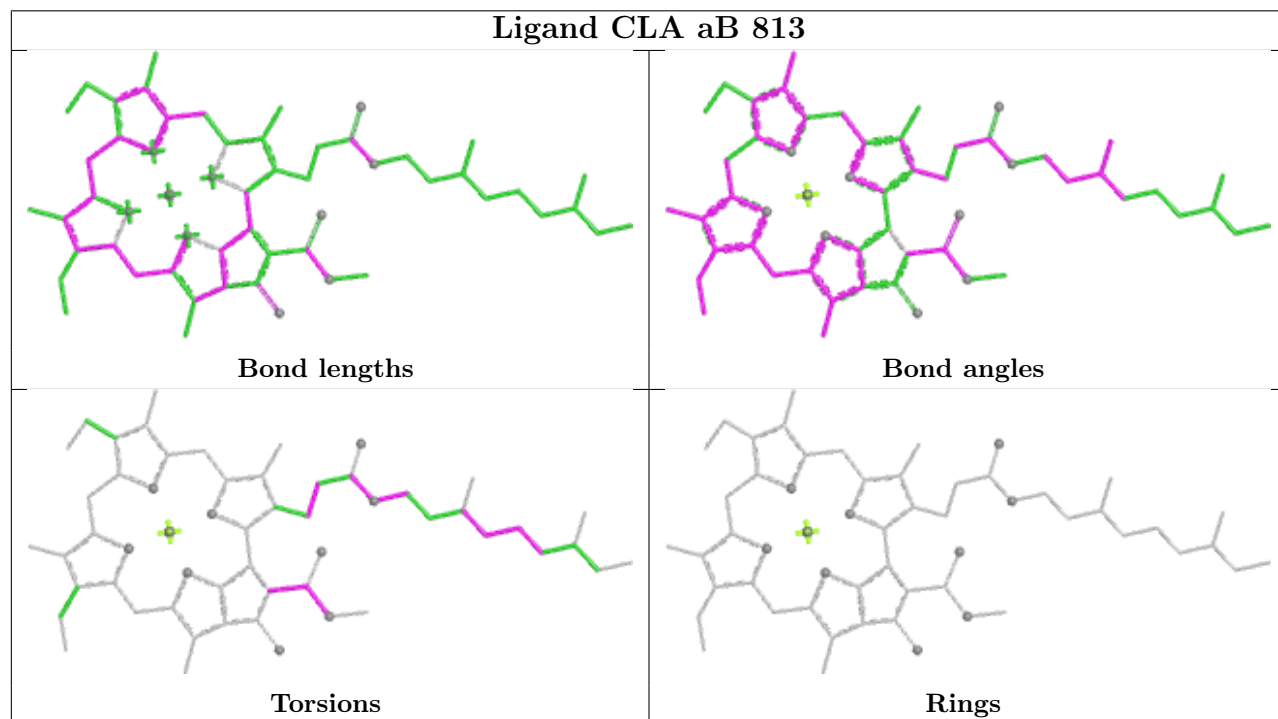
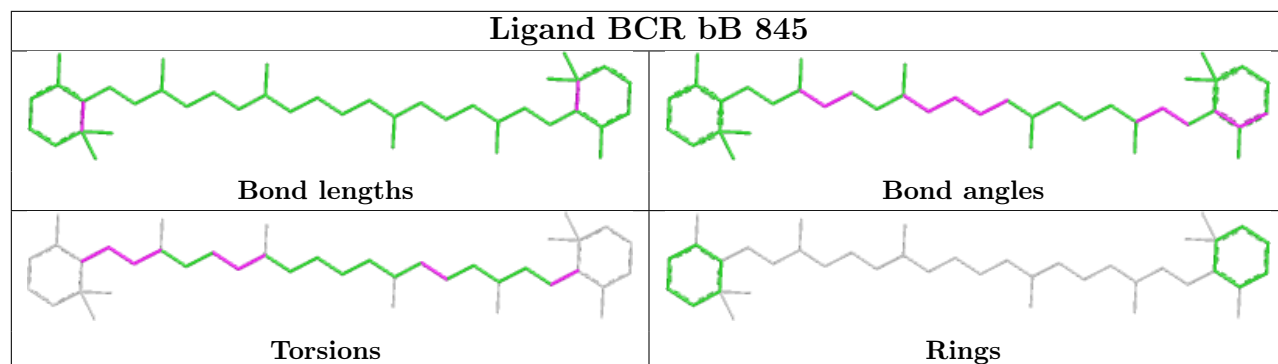




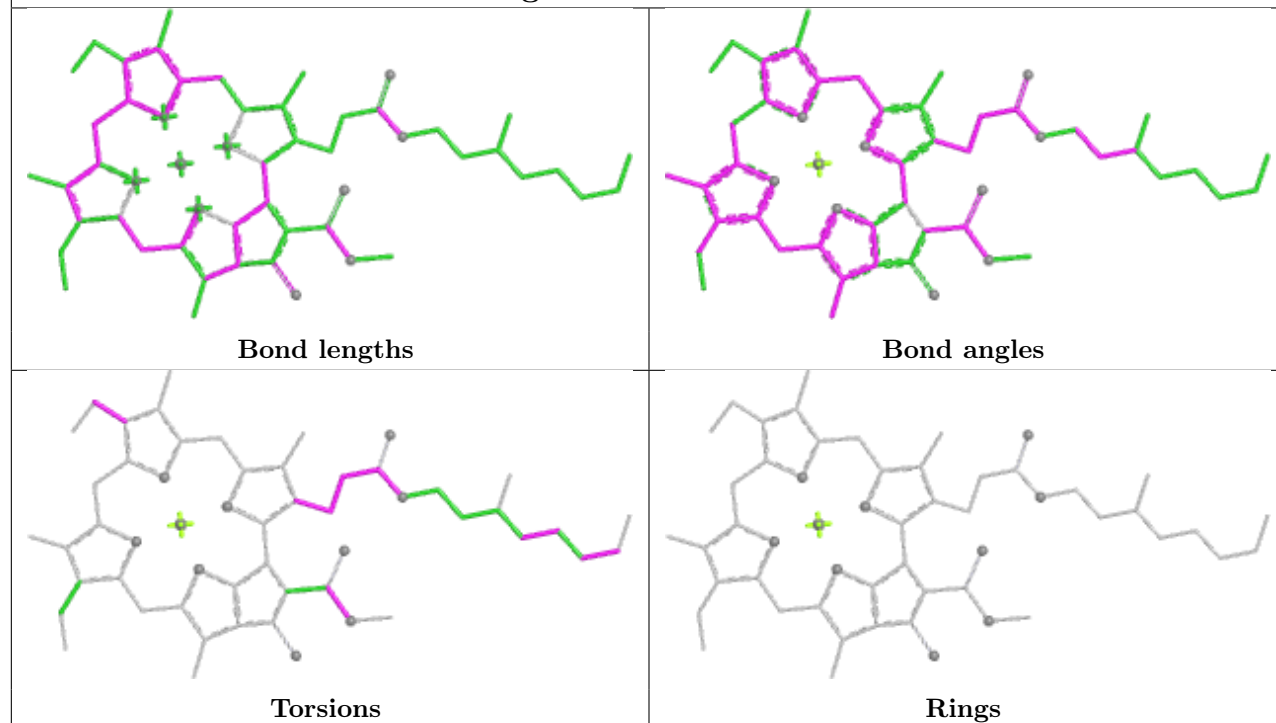




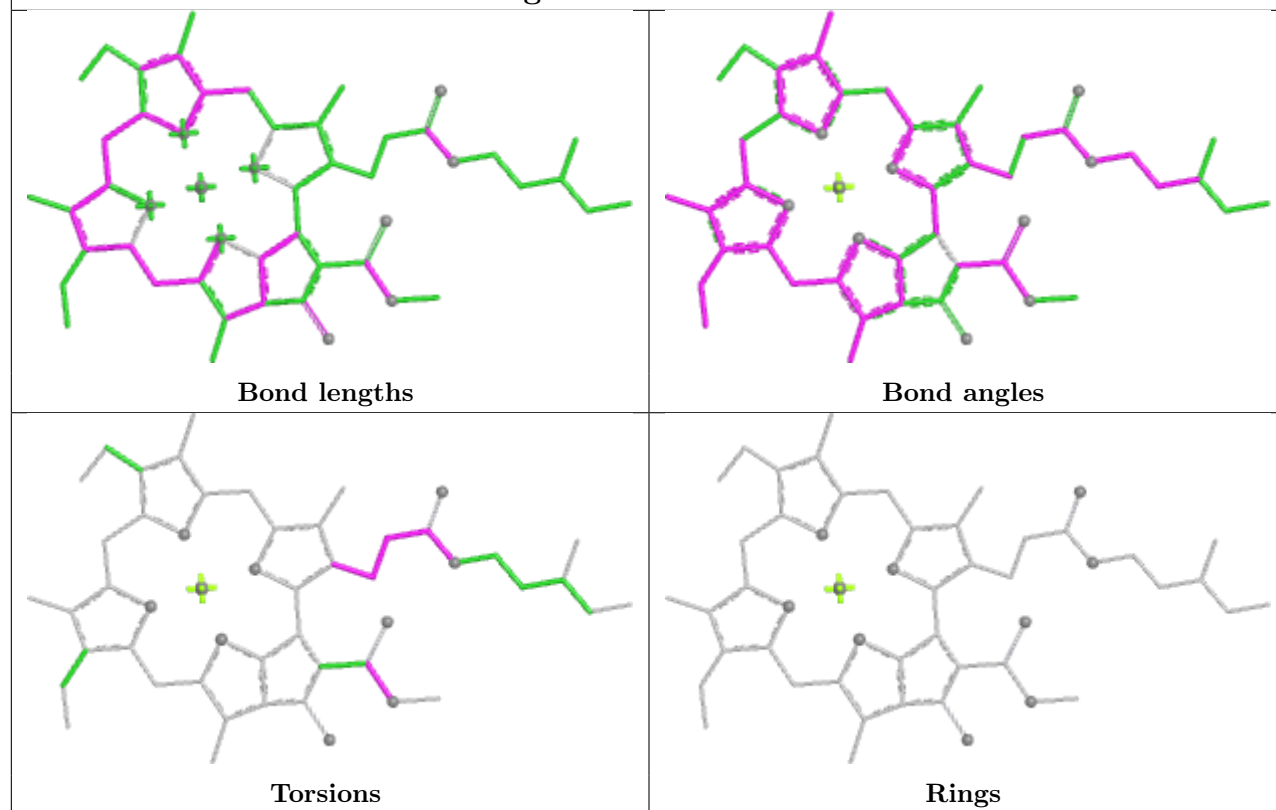




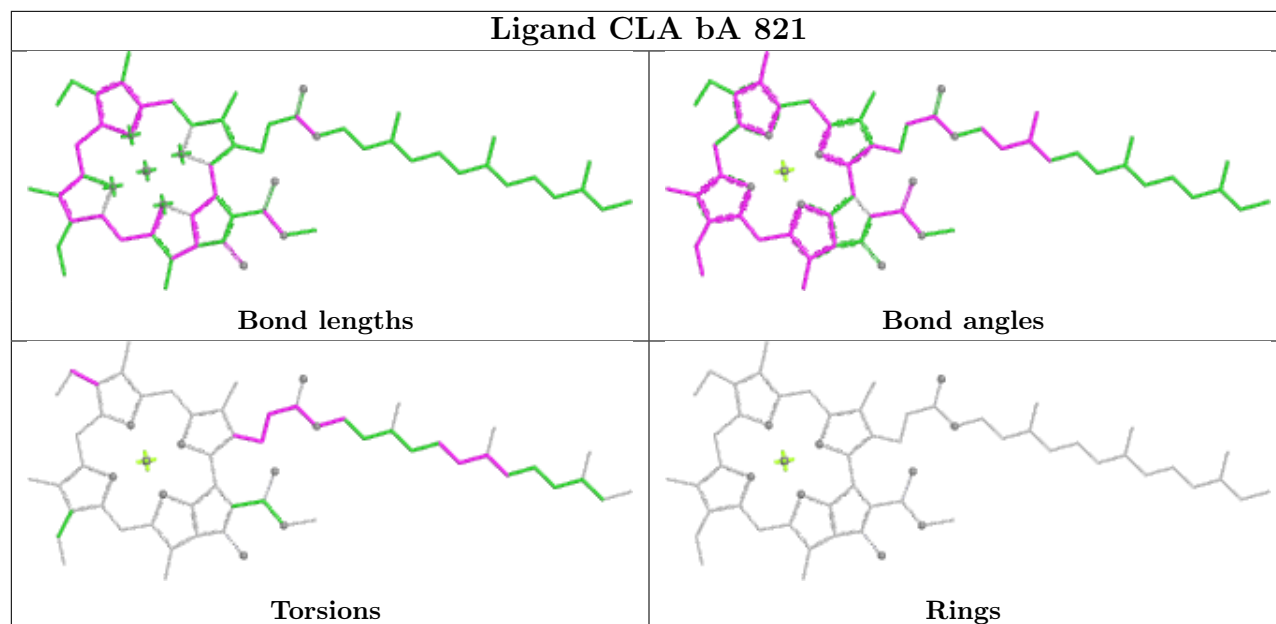
## Ligand CLA bA 819



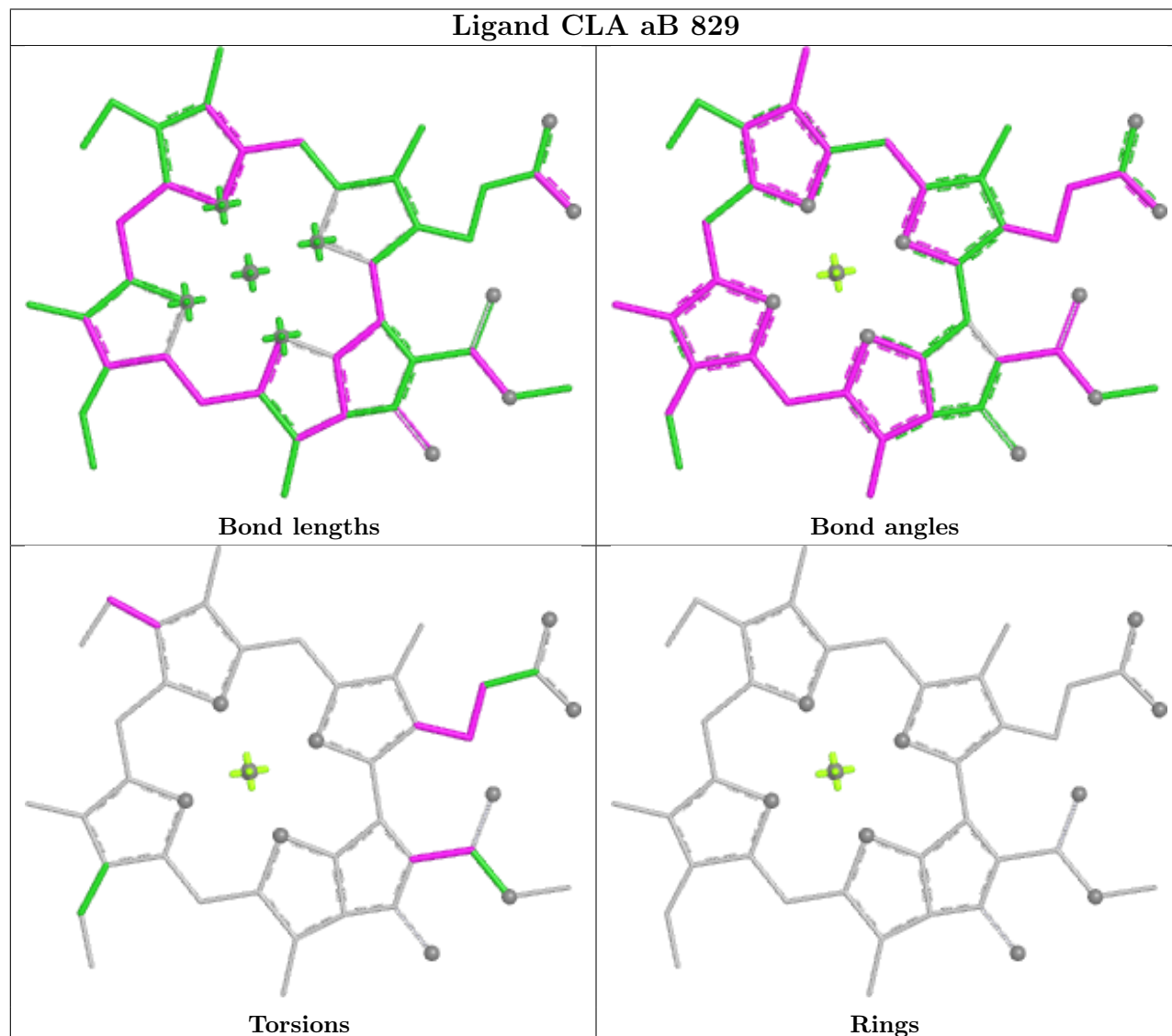
## Ligand CLA cA 838

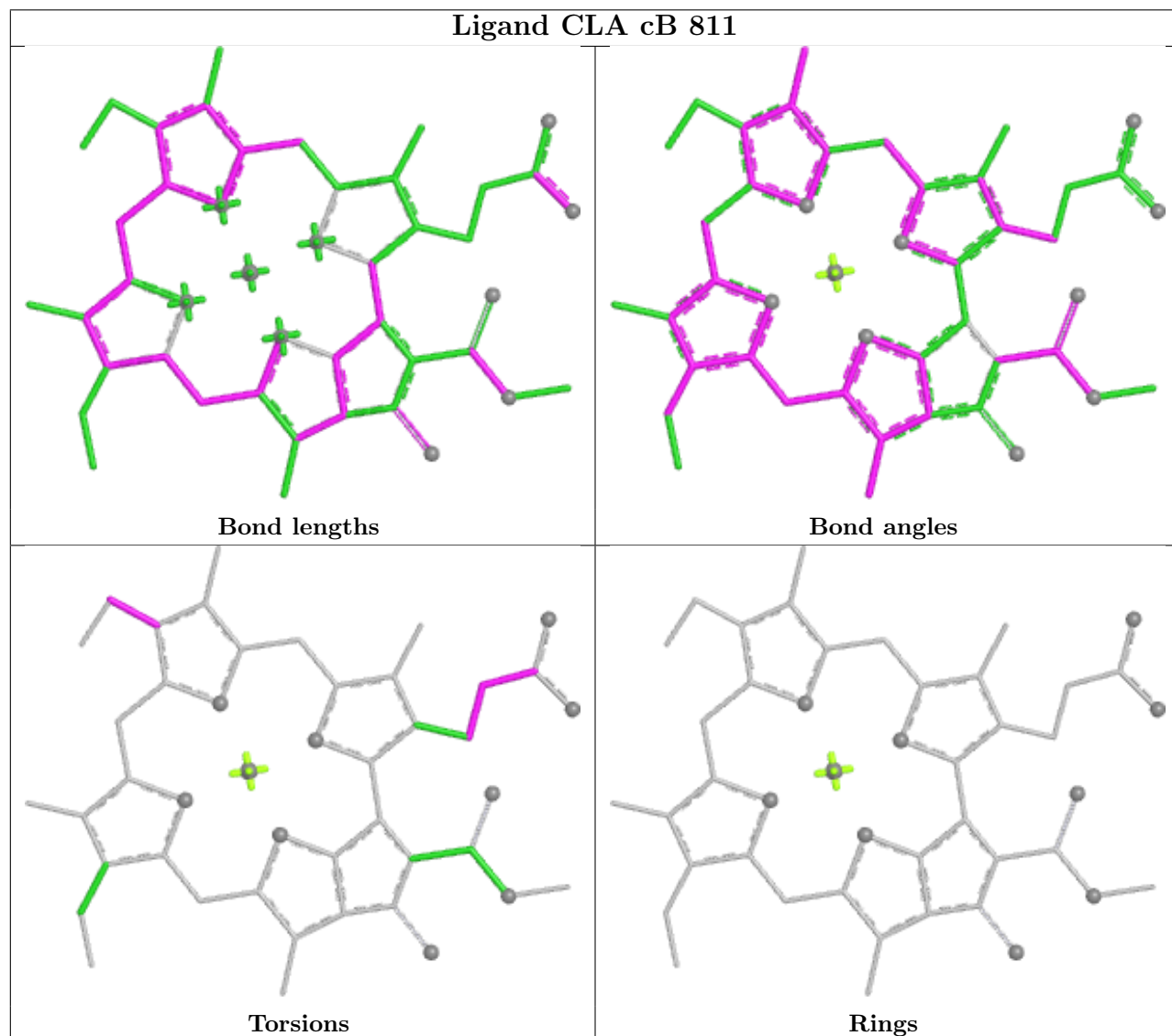
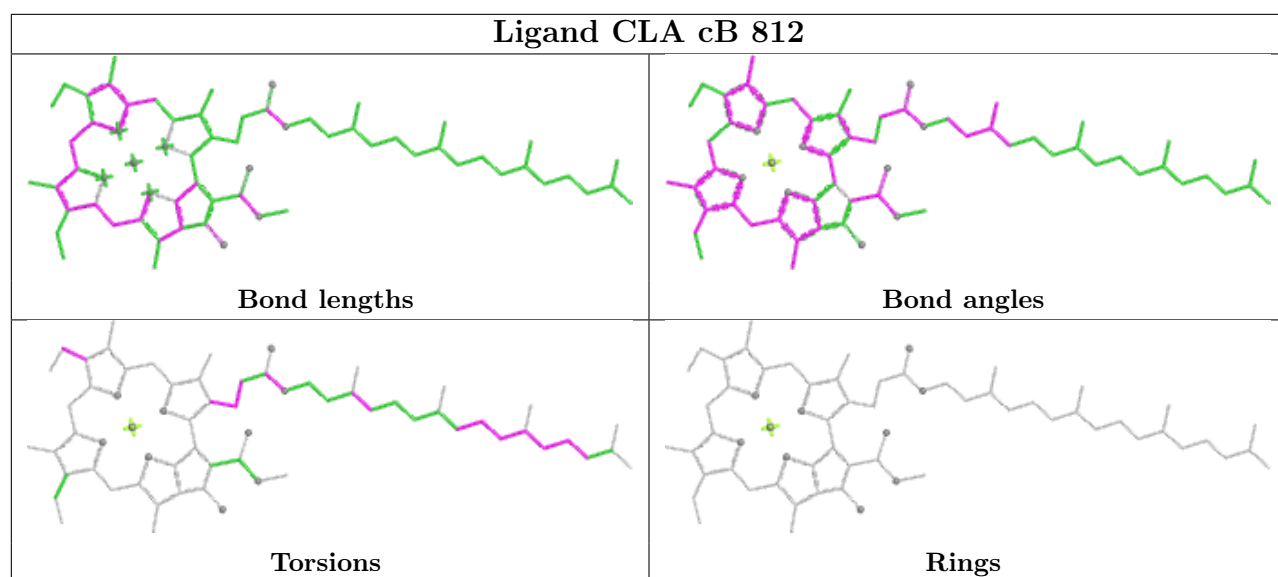


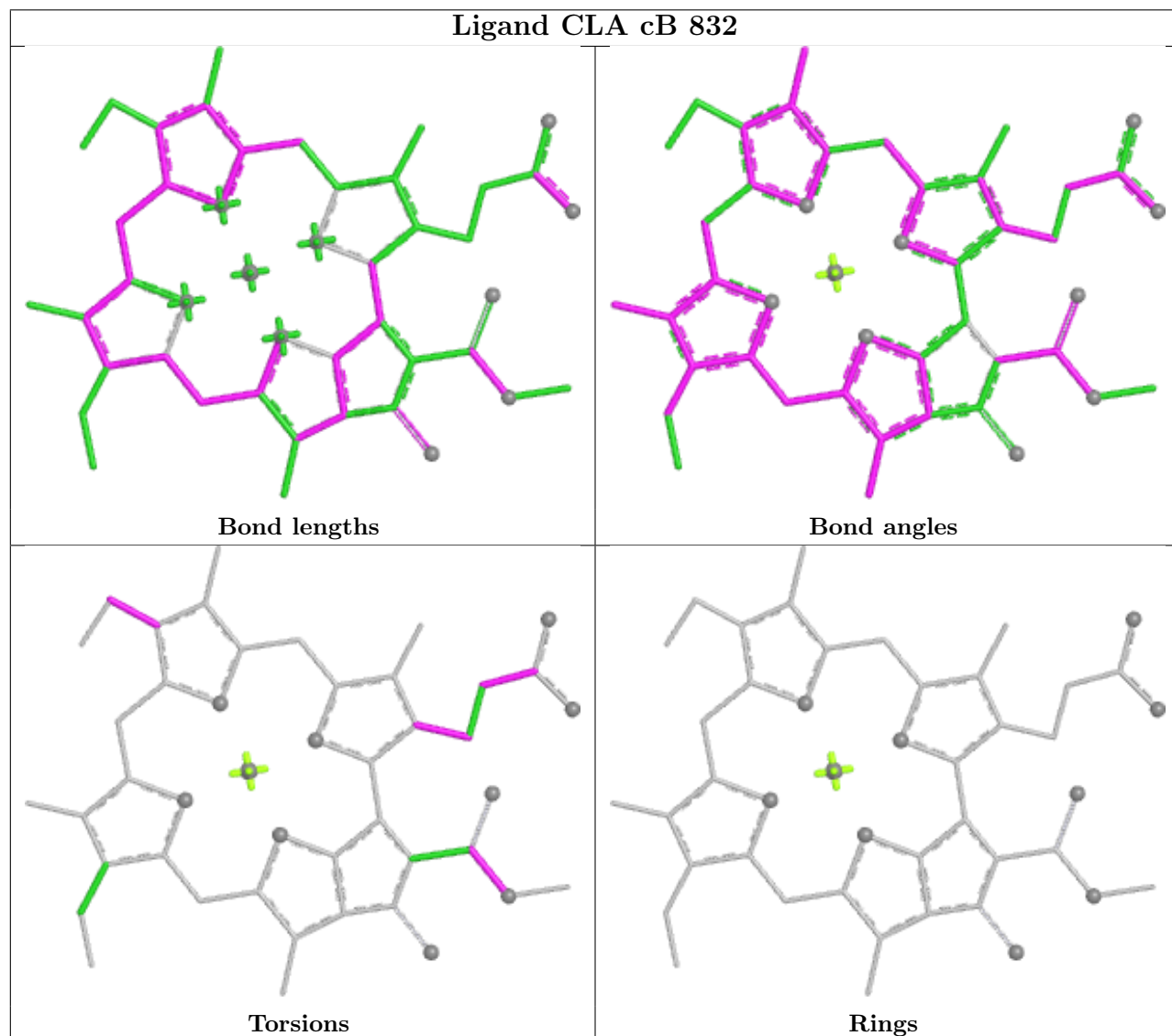
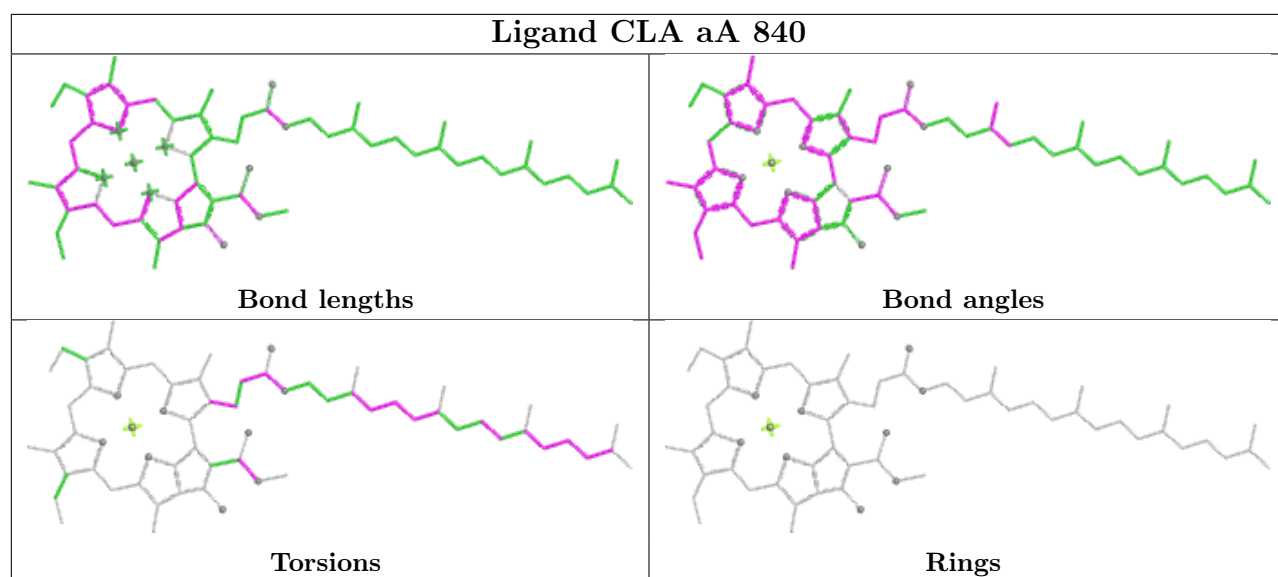
## Ligand CLA bA 821

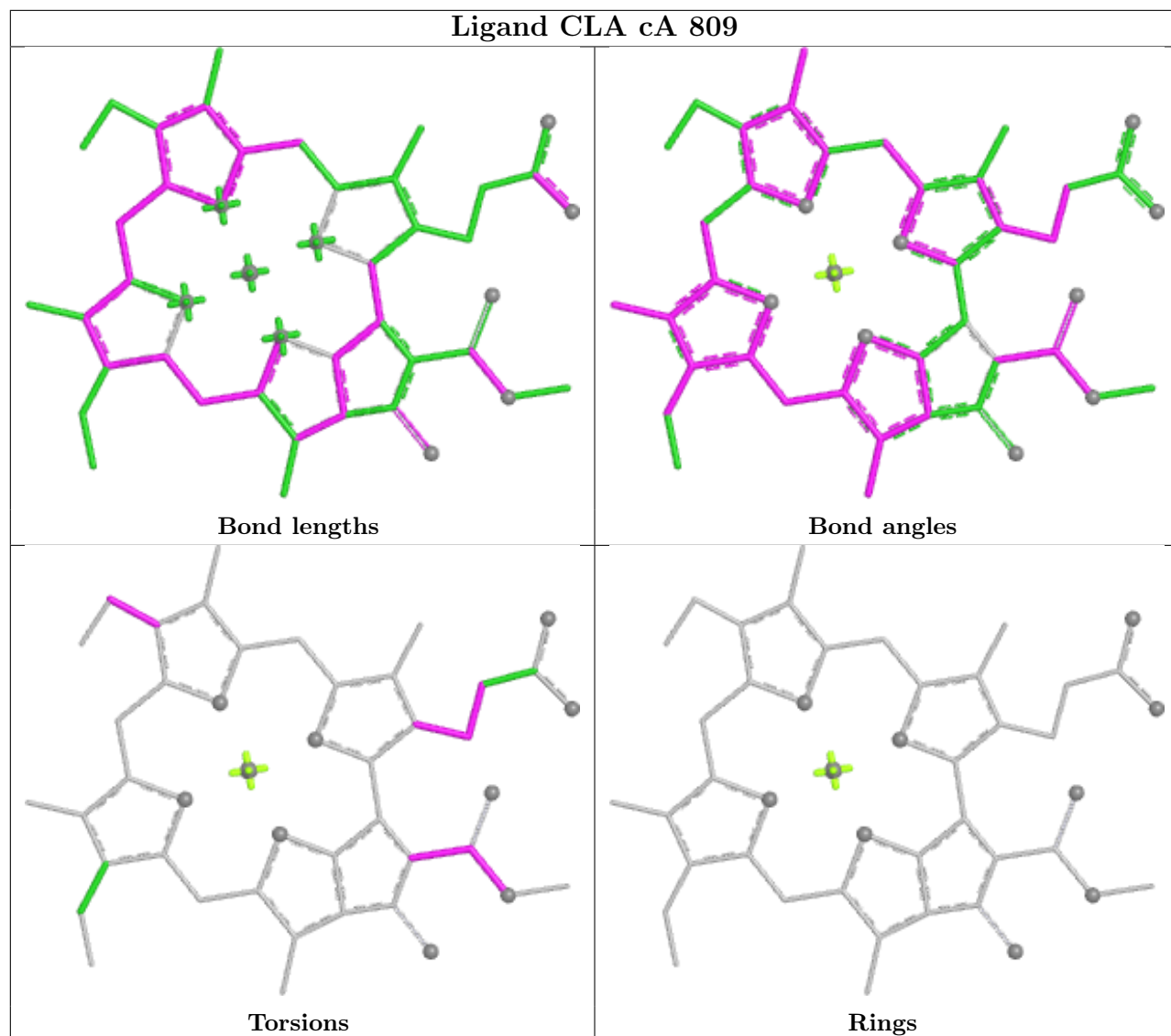


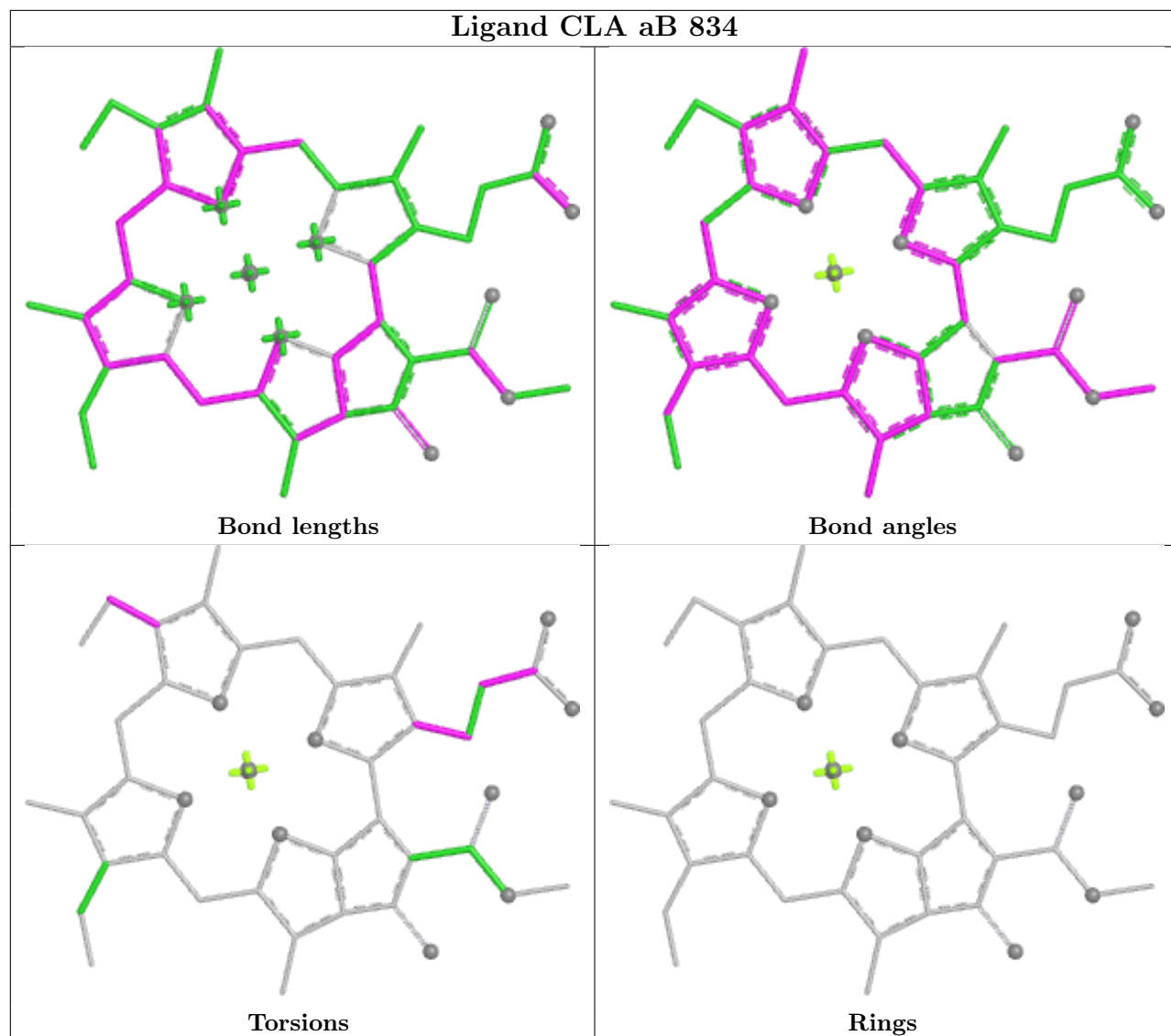
## Ligand CLA aB 829



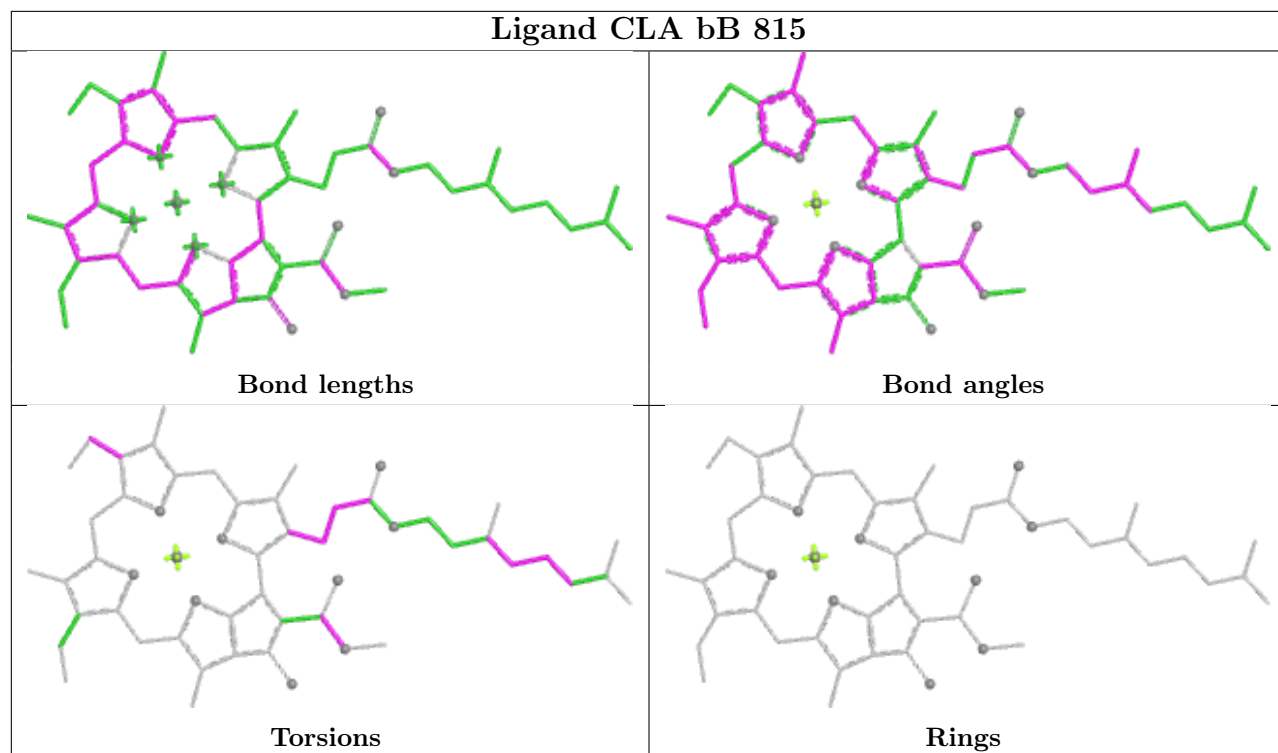


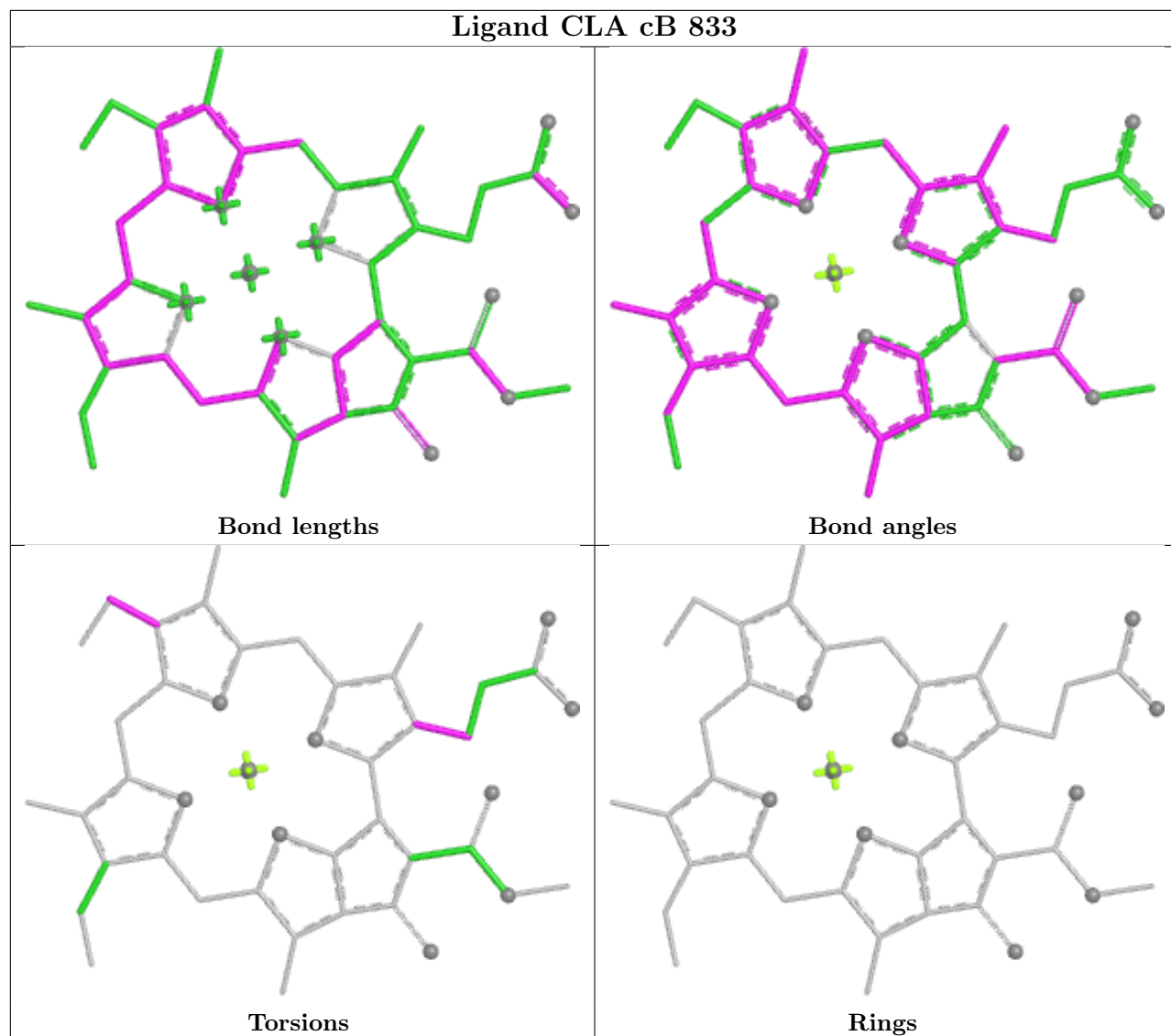


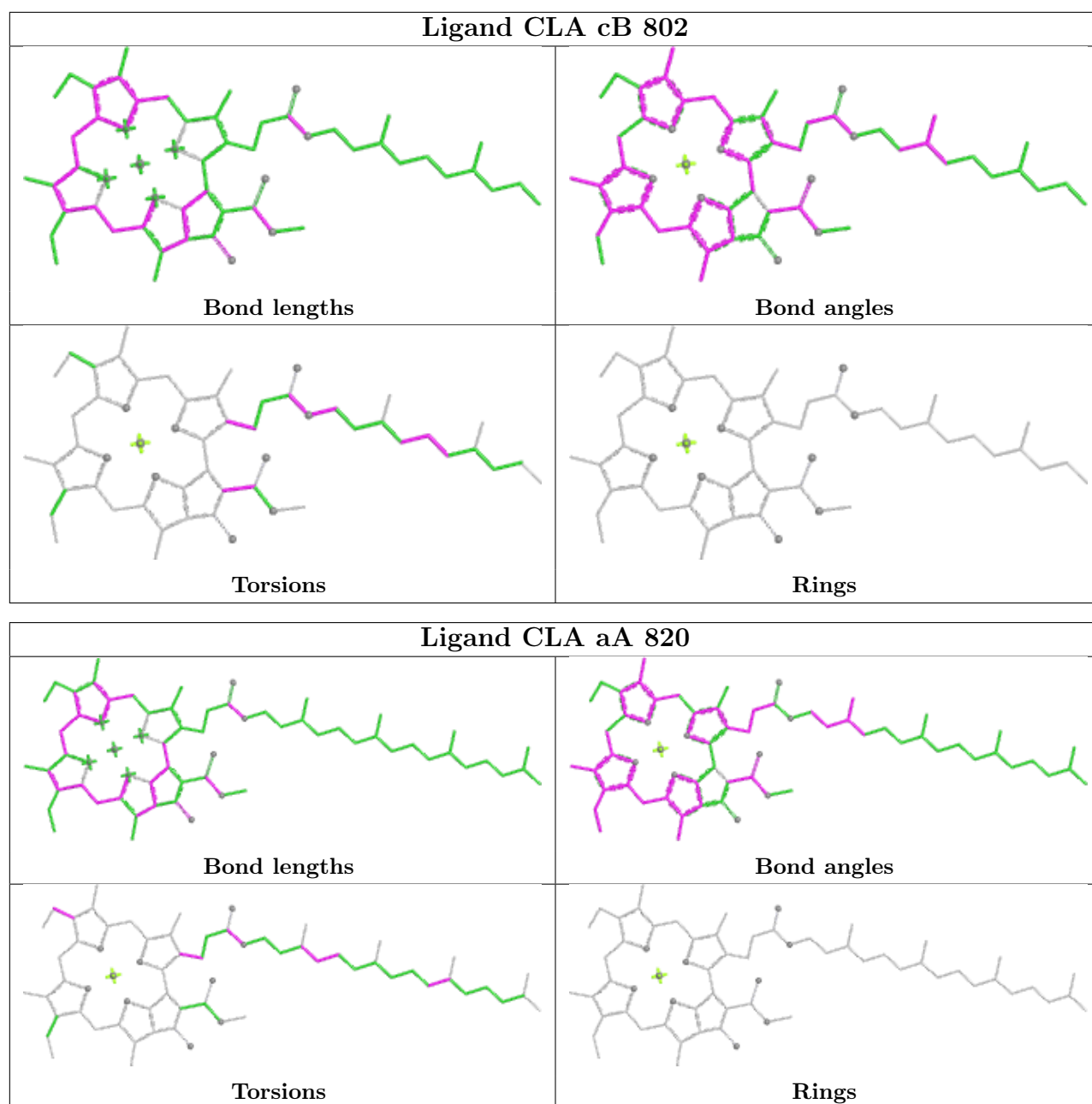


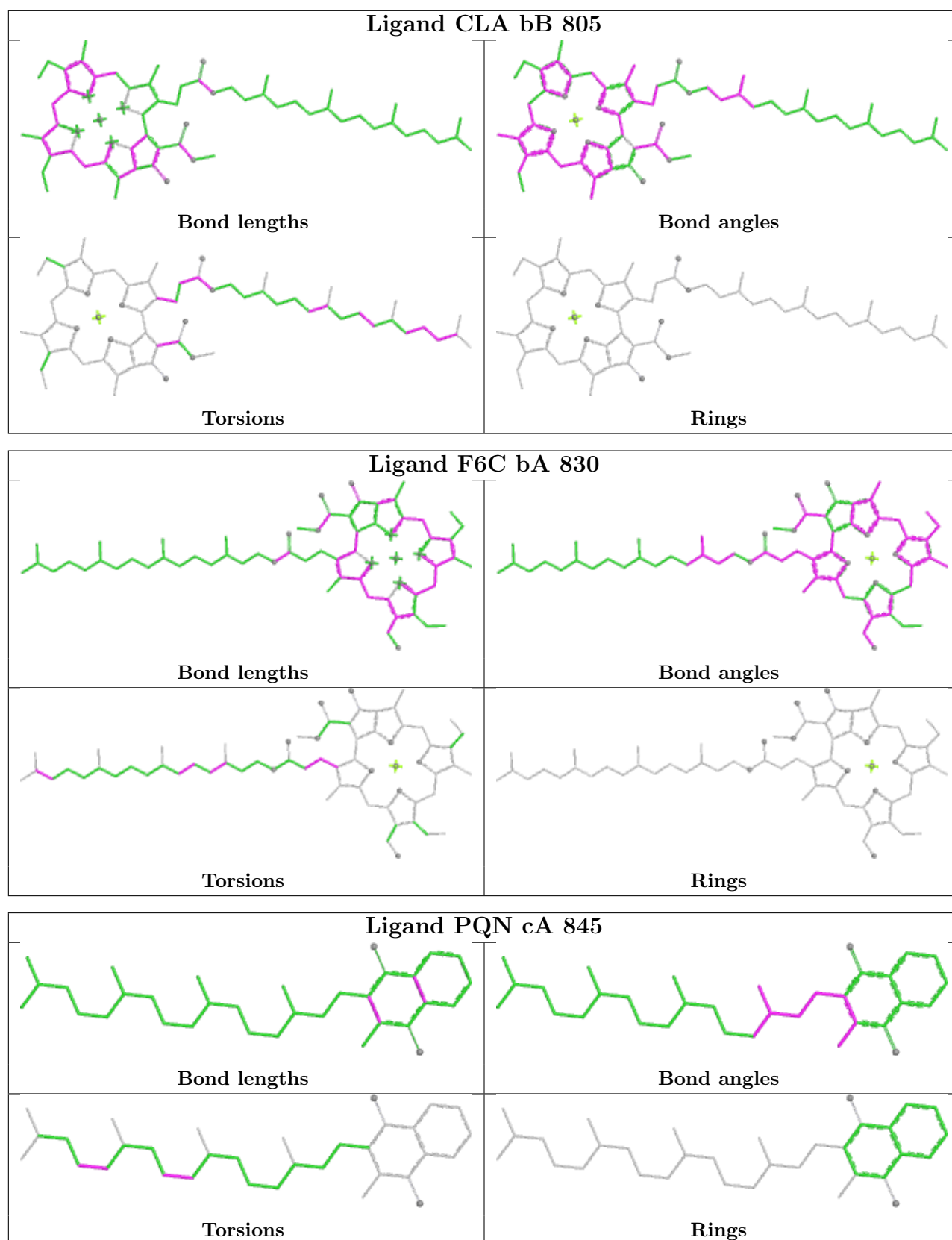


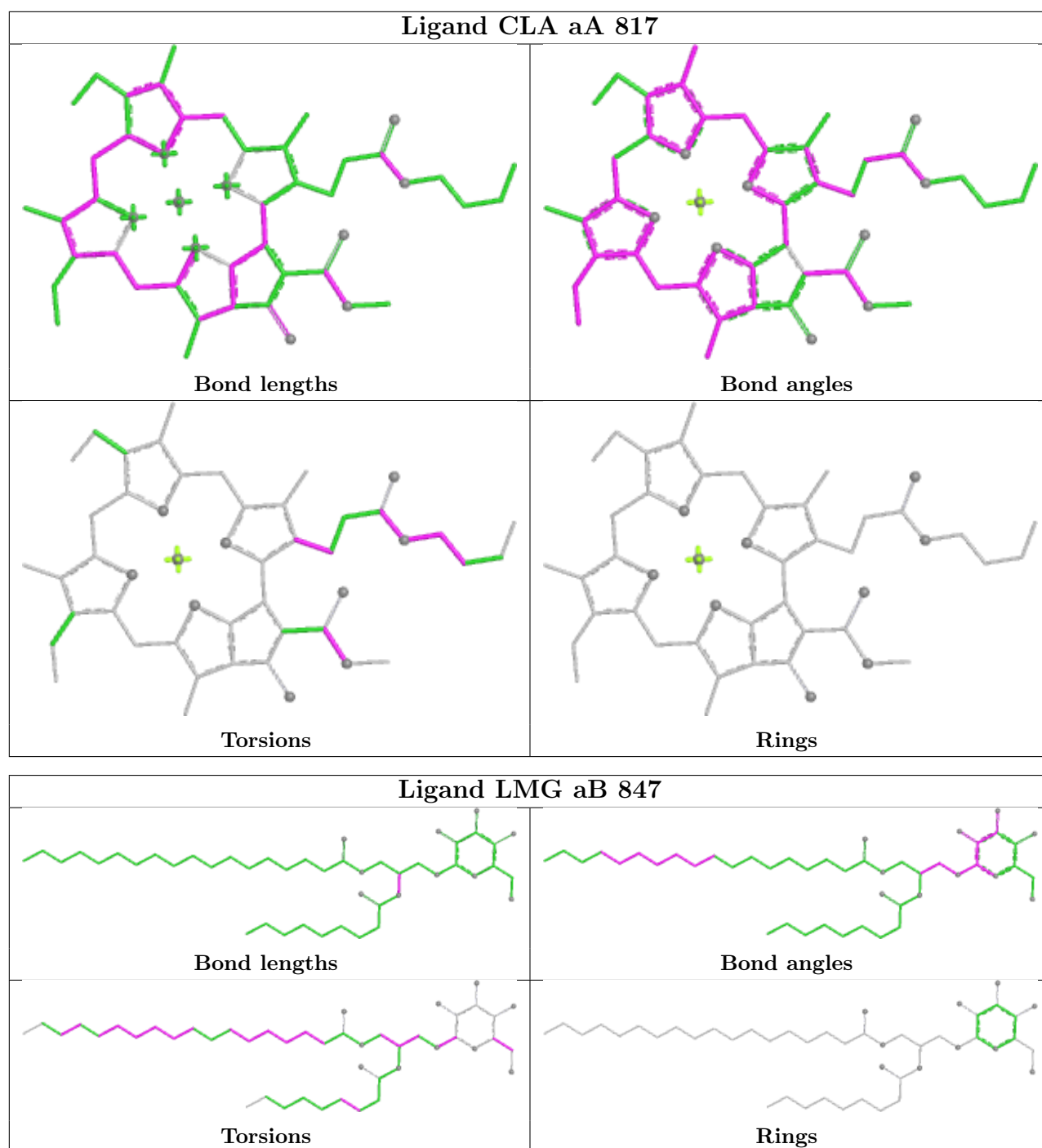


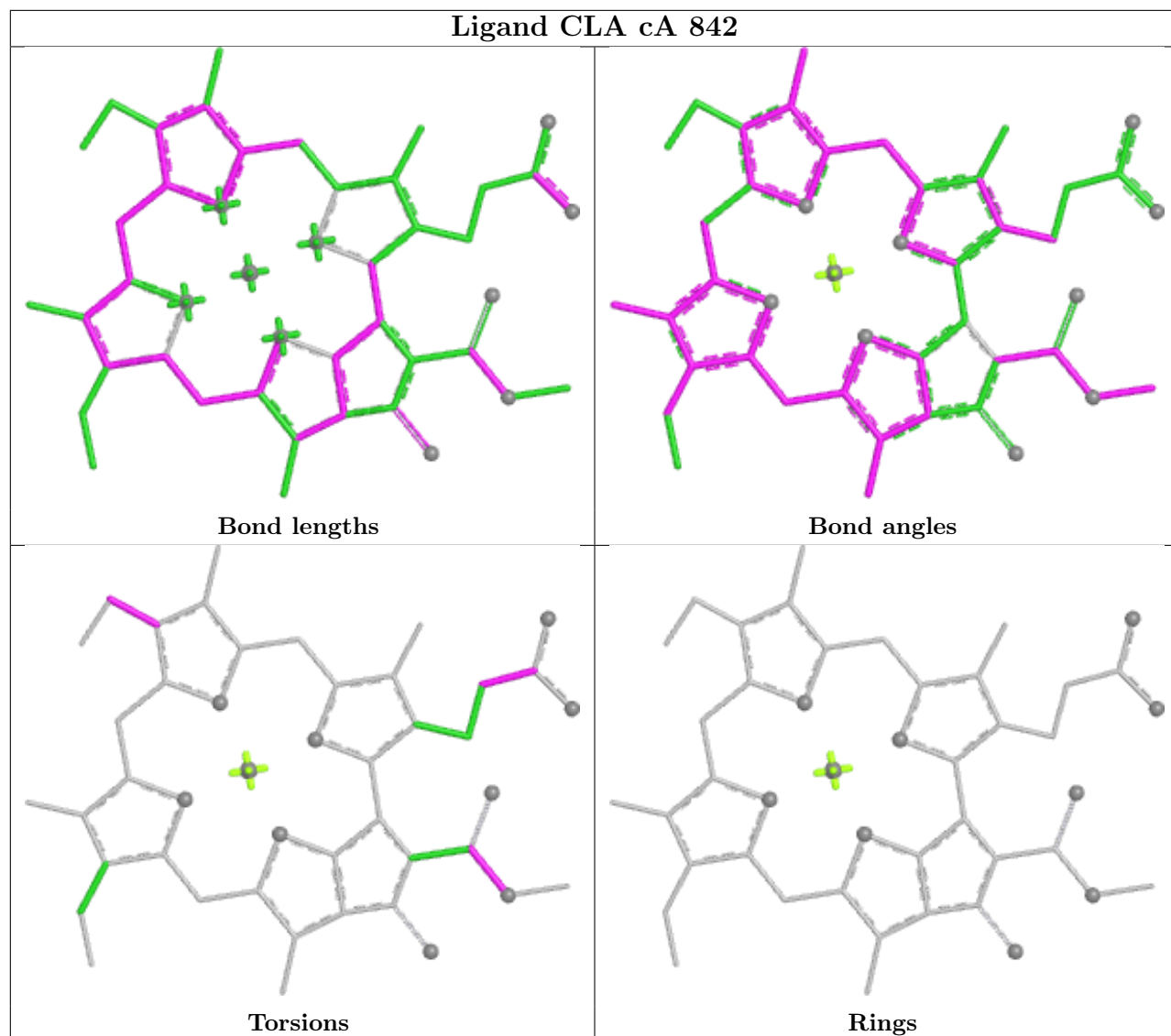


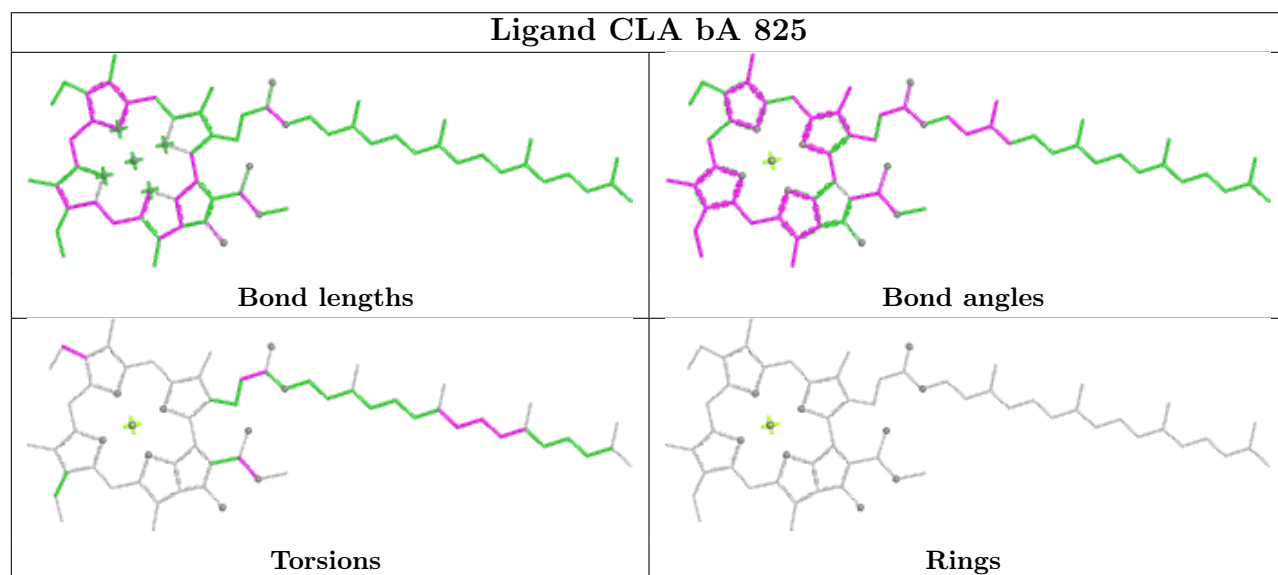
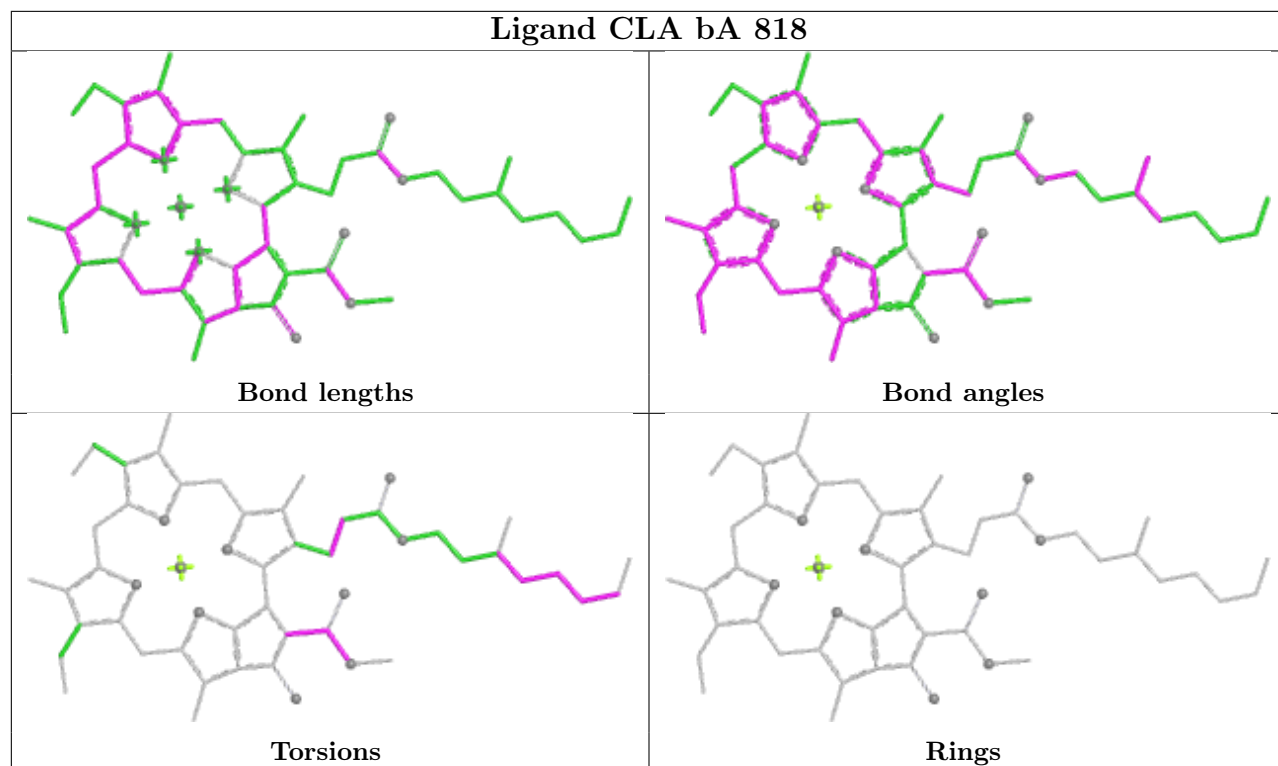


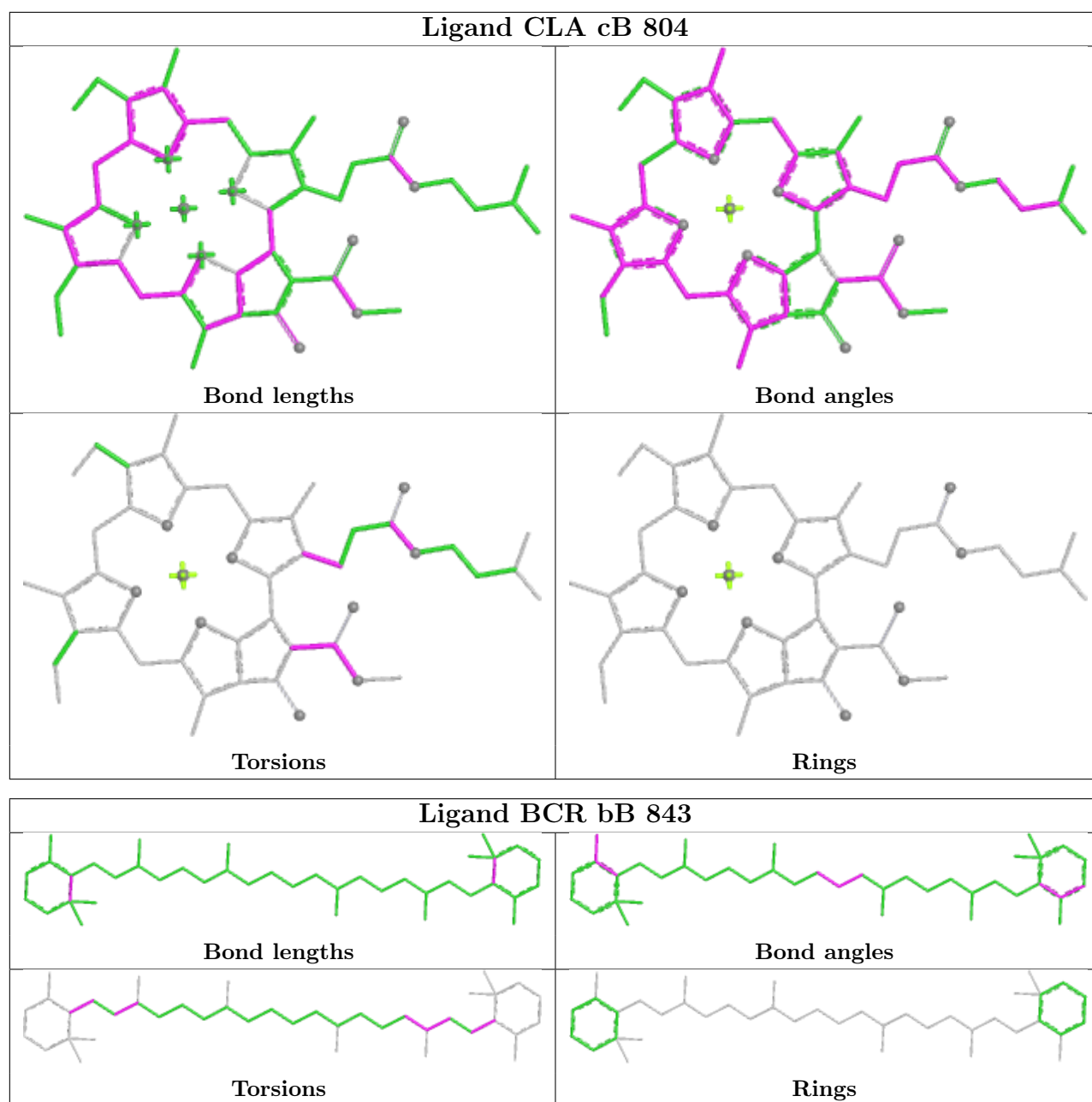




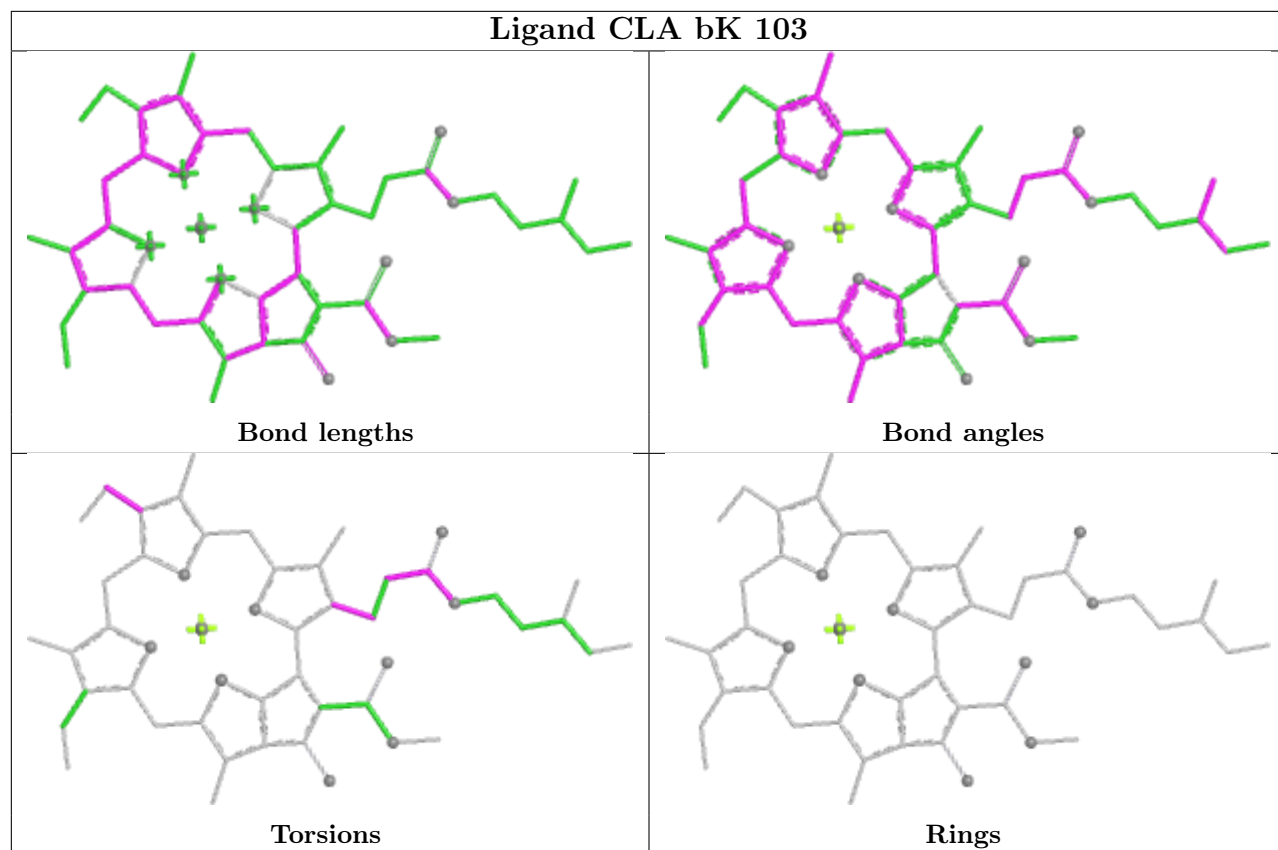


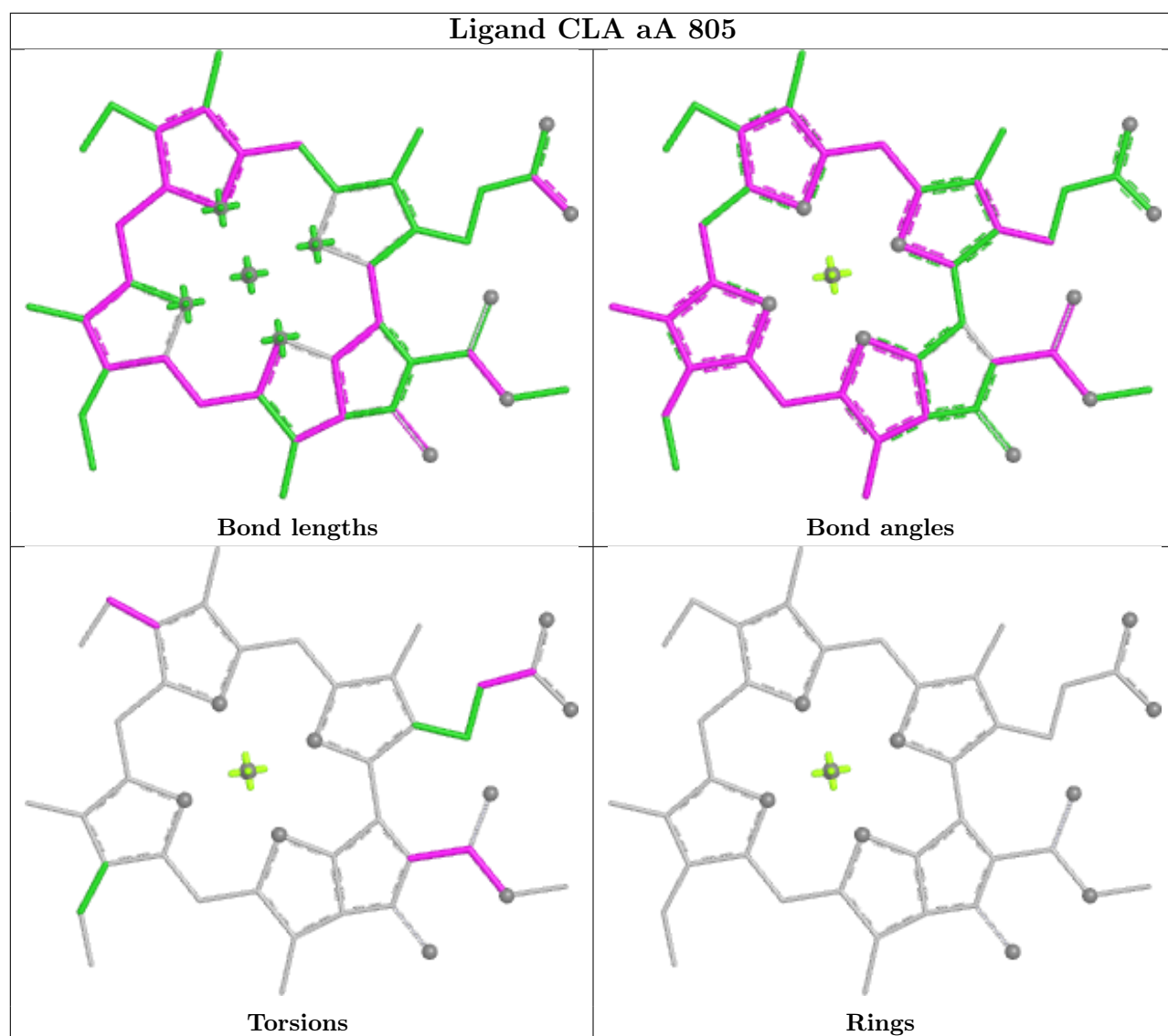




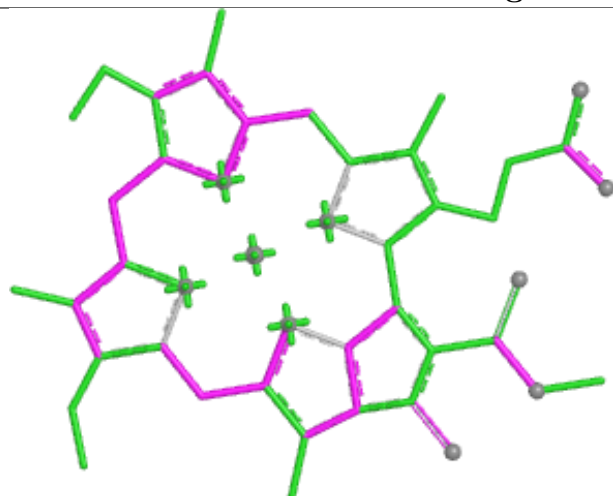




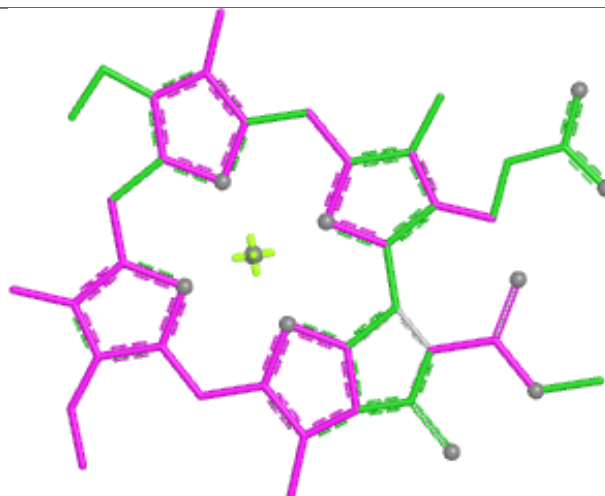




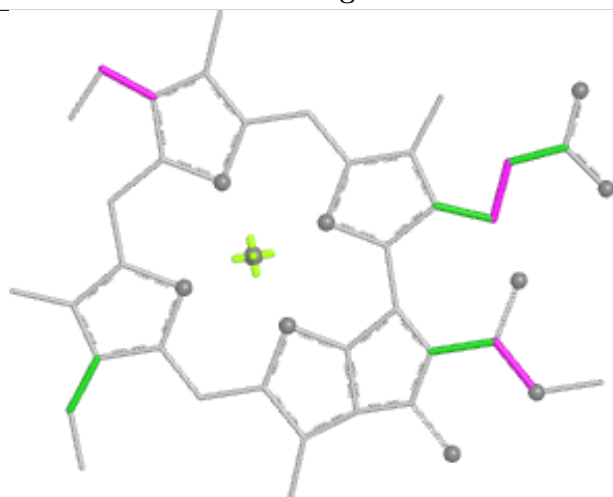
## Ligand CLA aB 840



Bond lengths



Bond angles

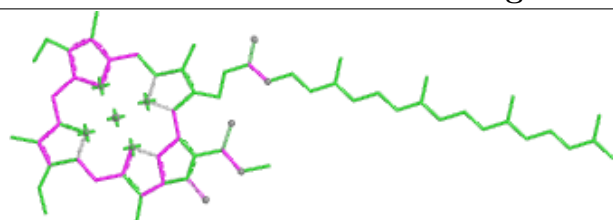


Torsions

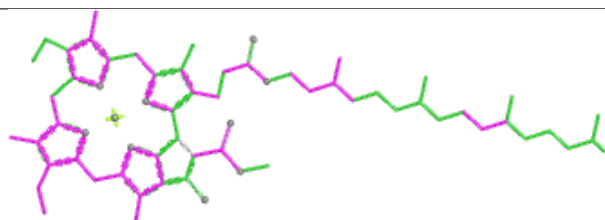


Rings

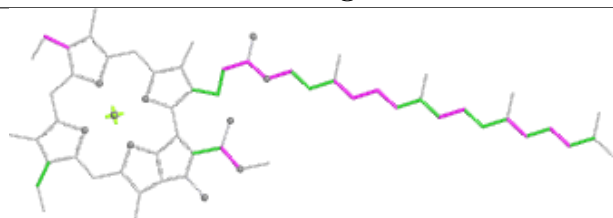
## Ligand CLA cA 807



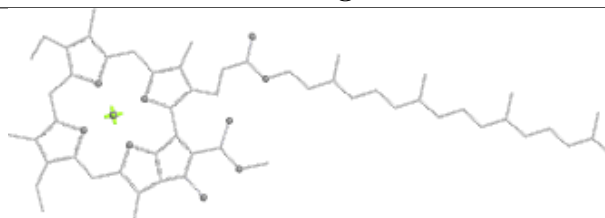
Bond lengths



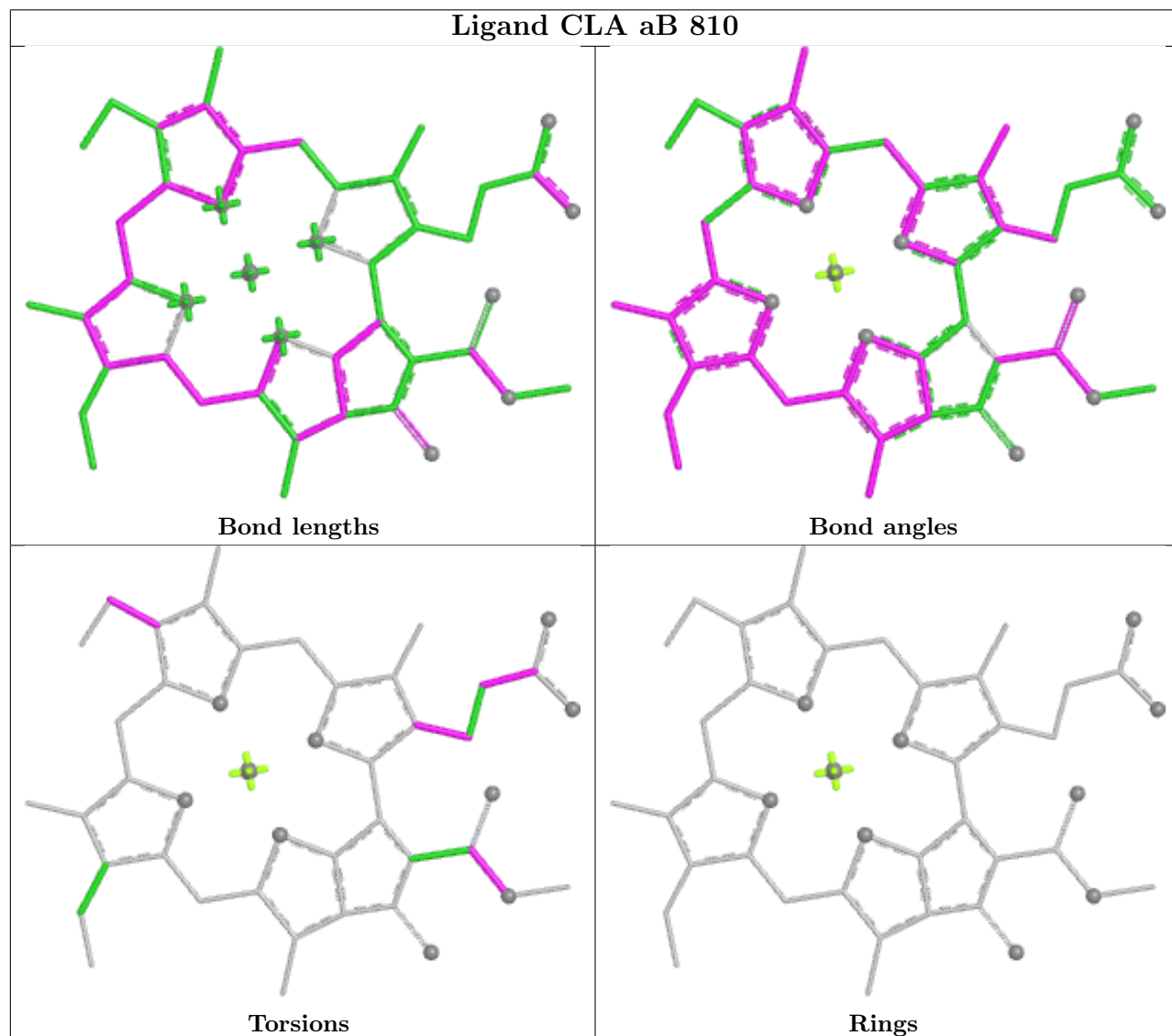
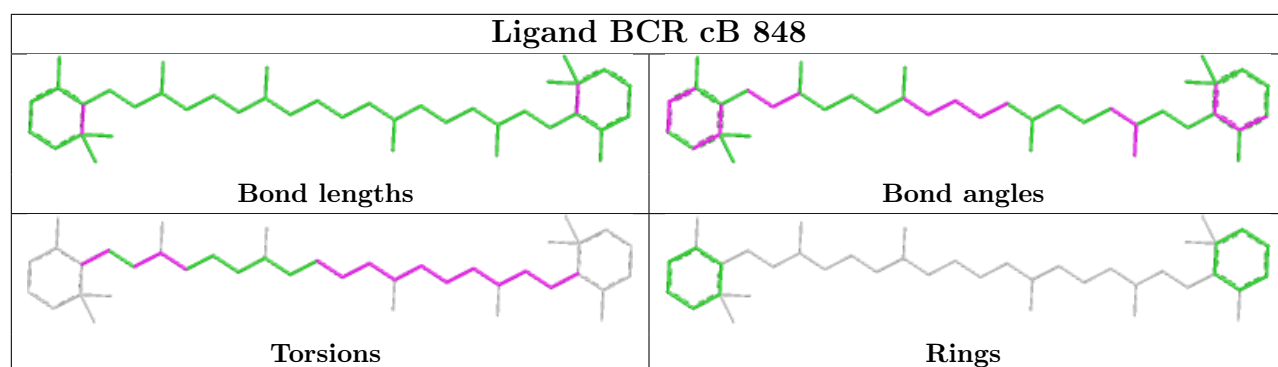
Bond angles

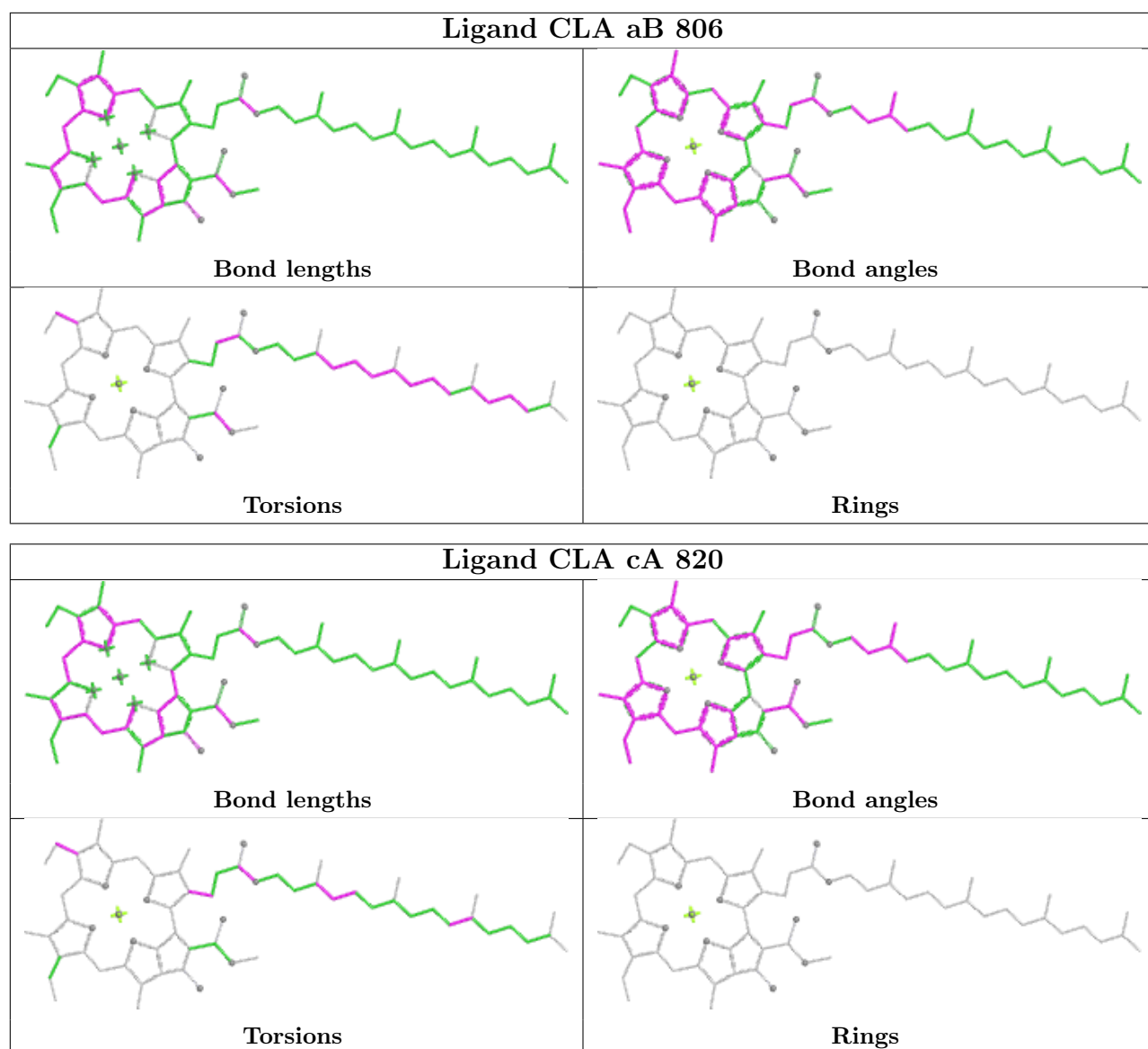


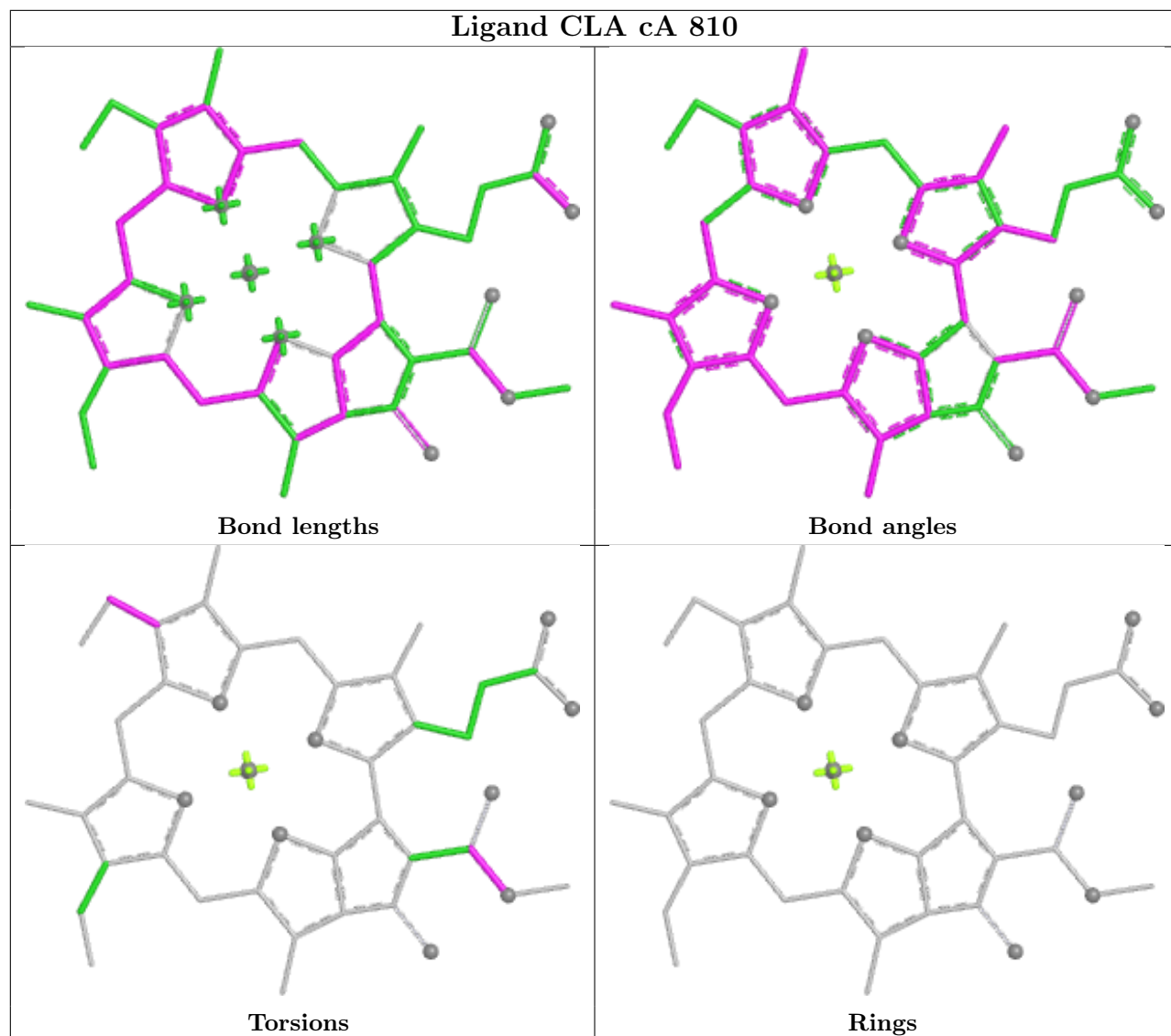
Torsions

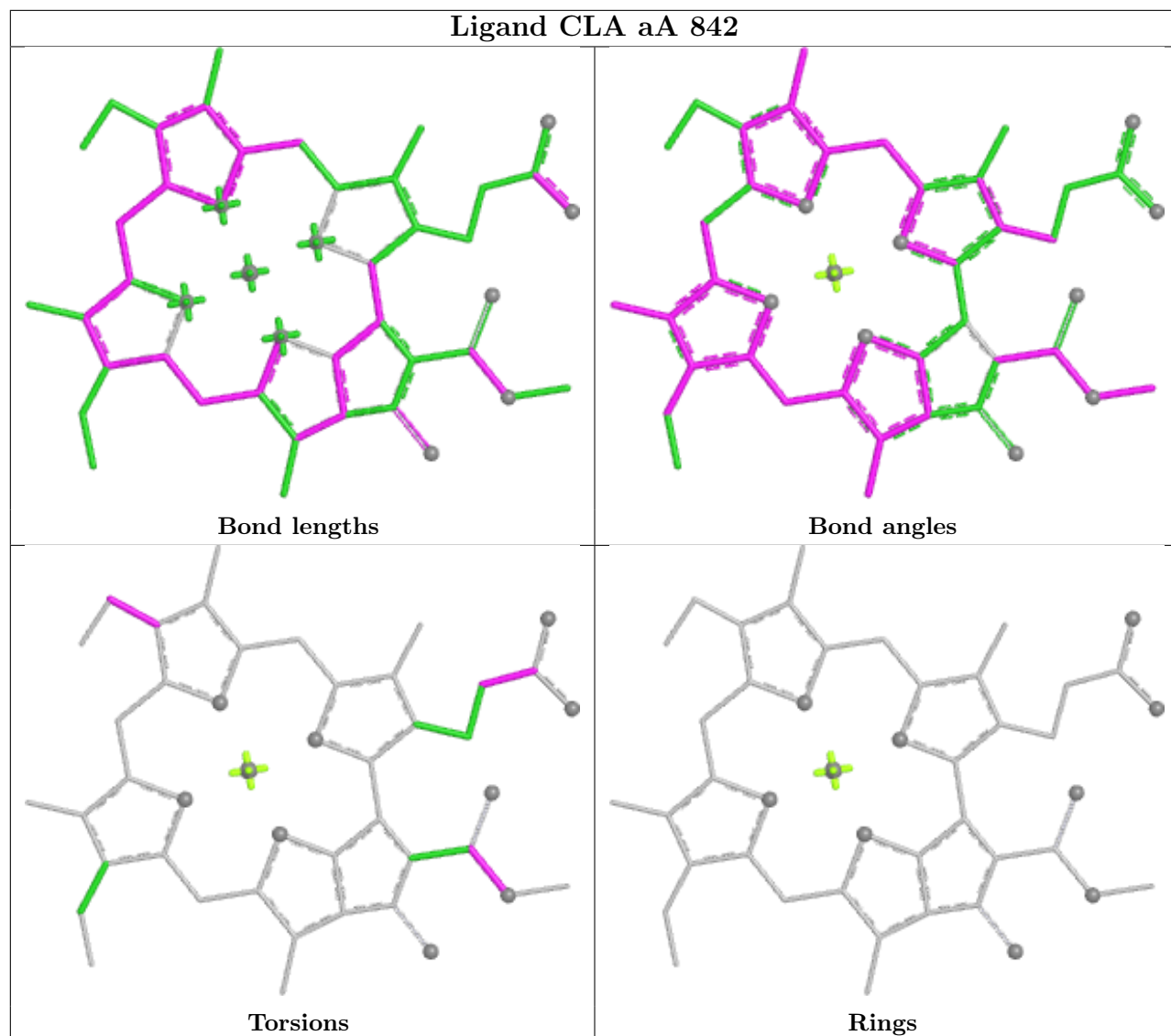


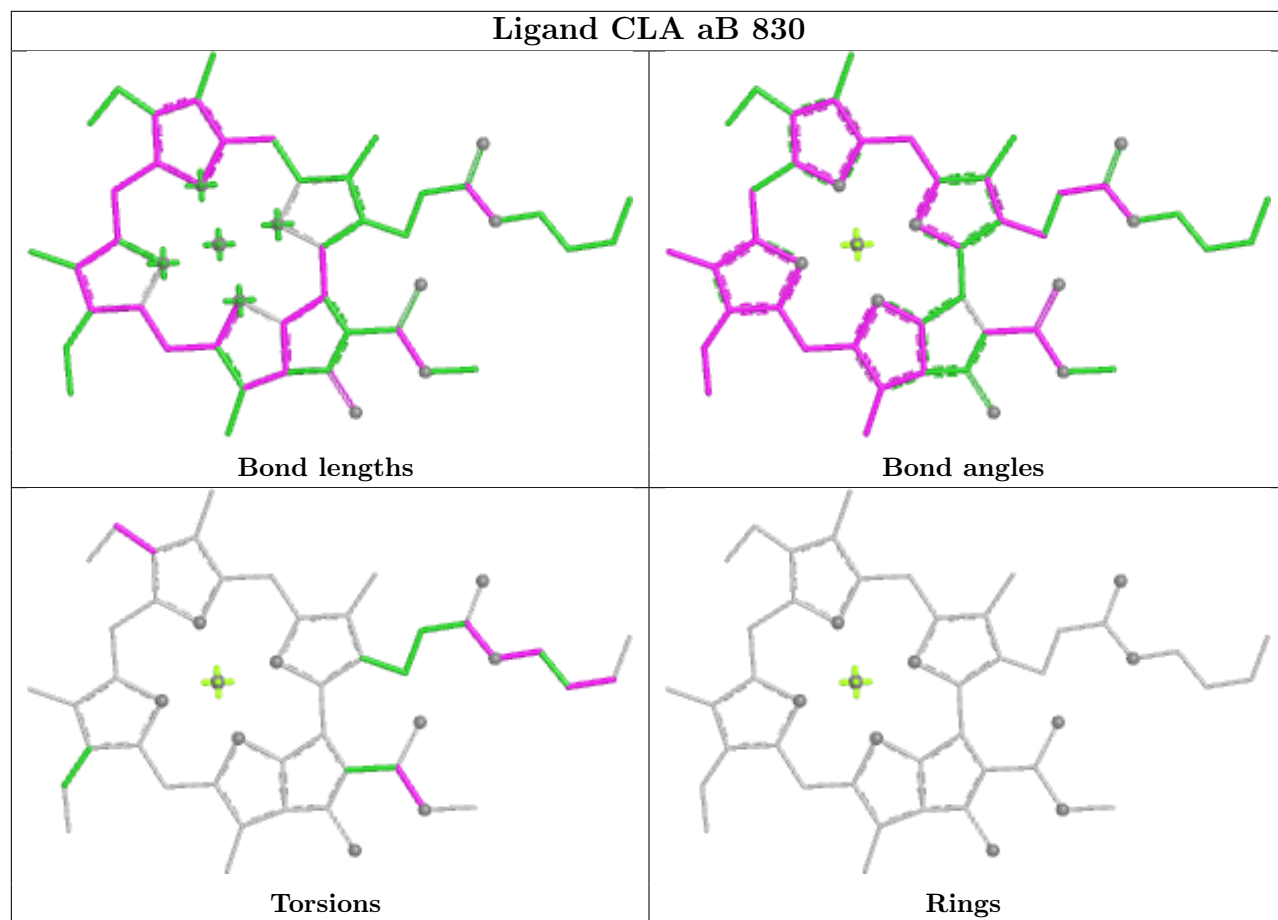
Rings



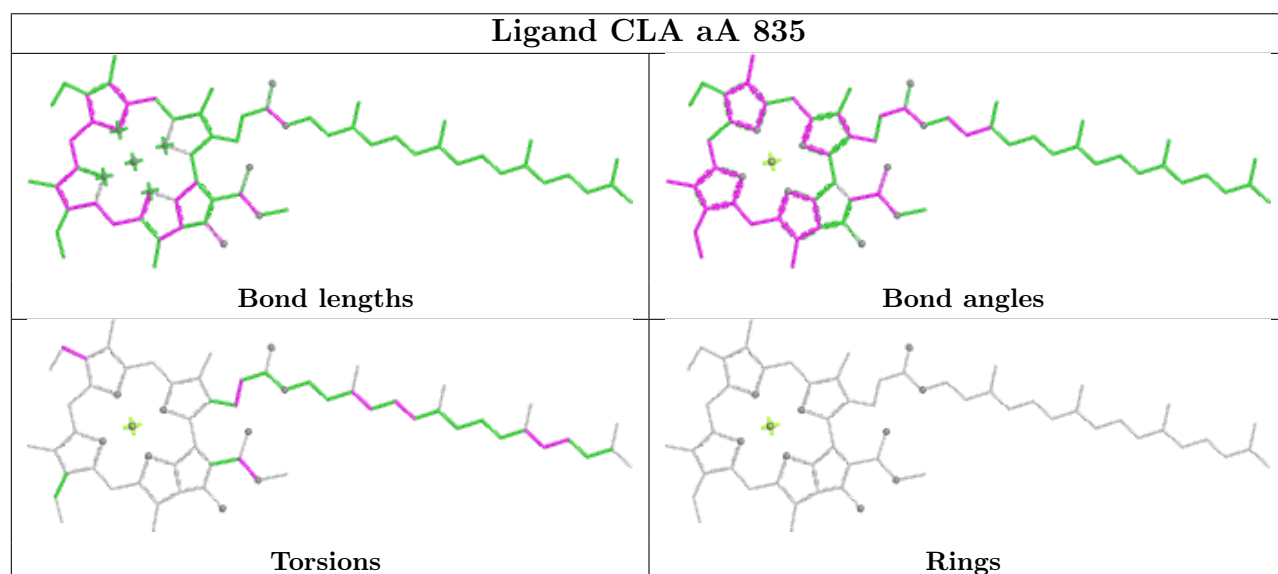
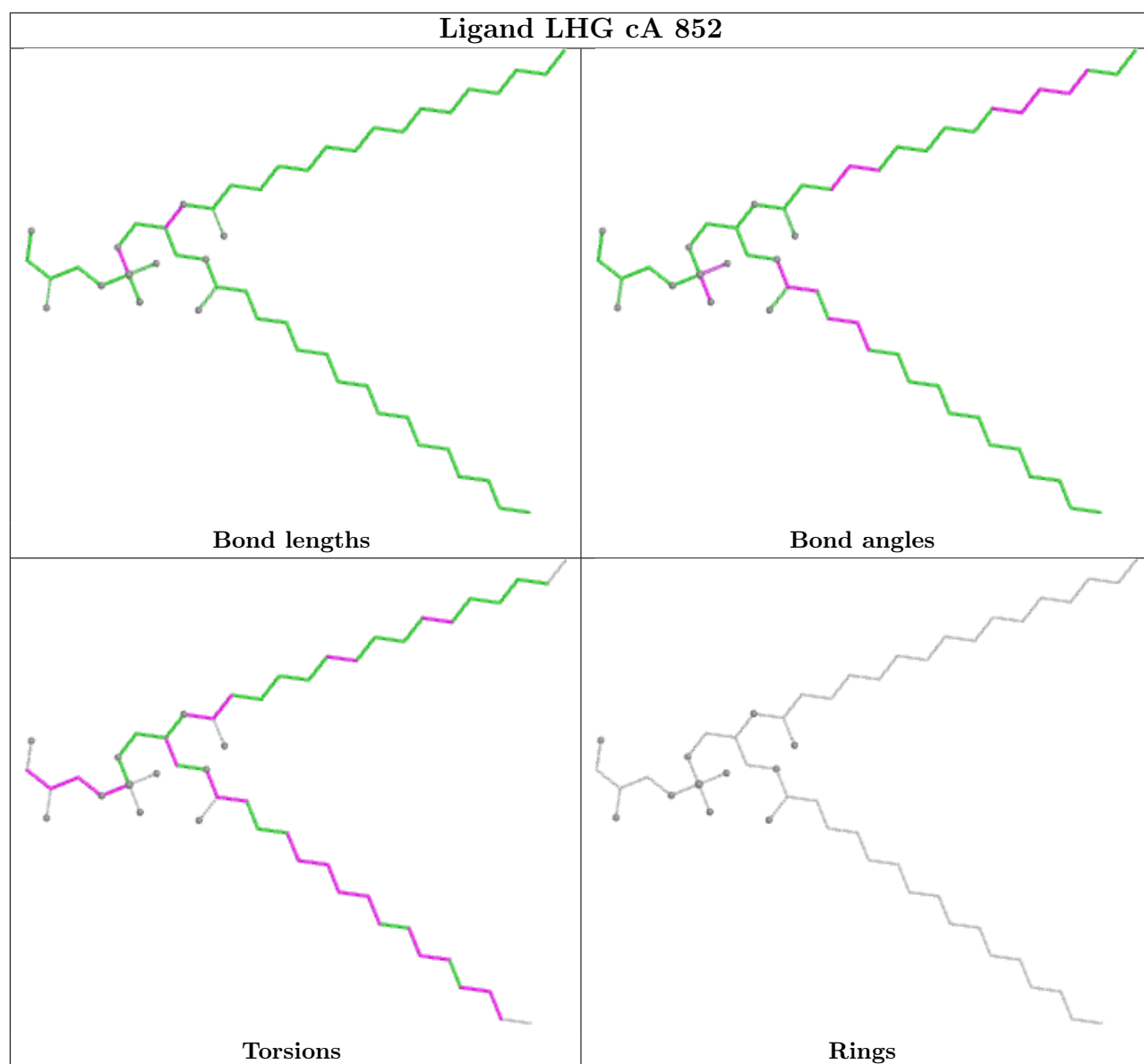


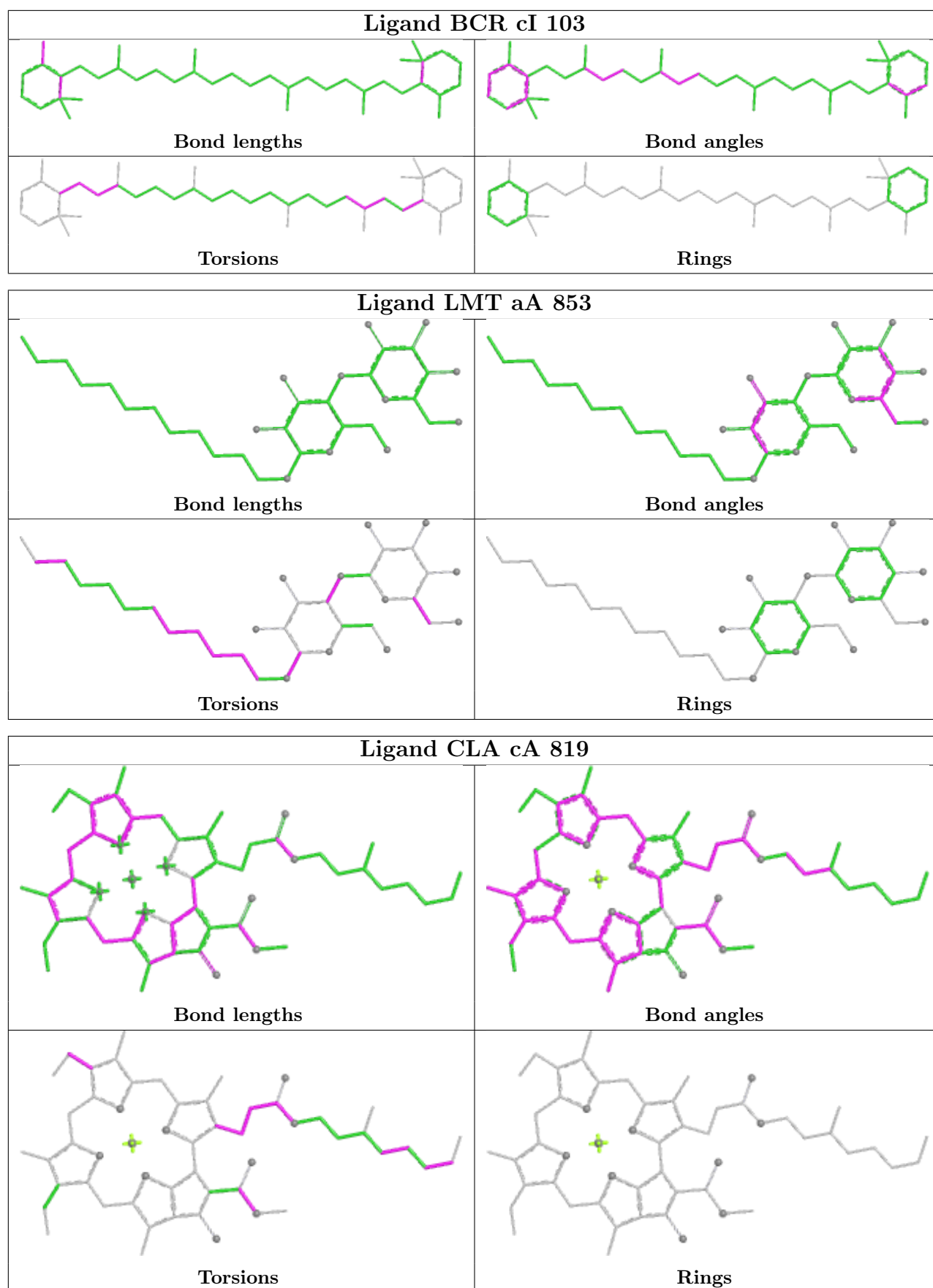


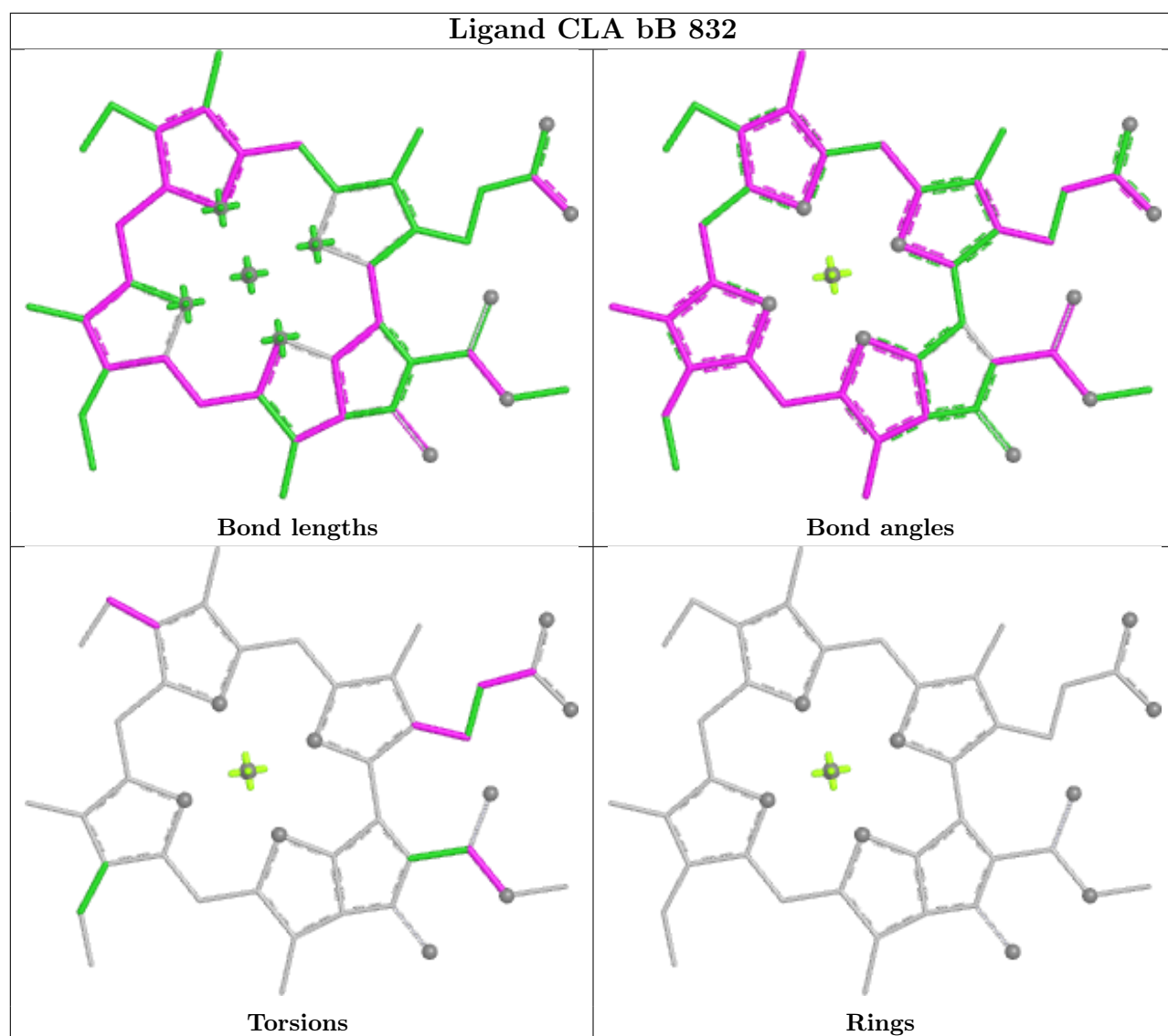


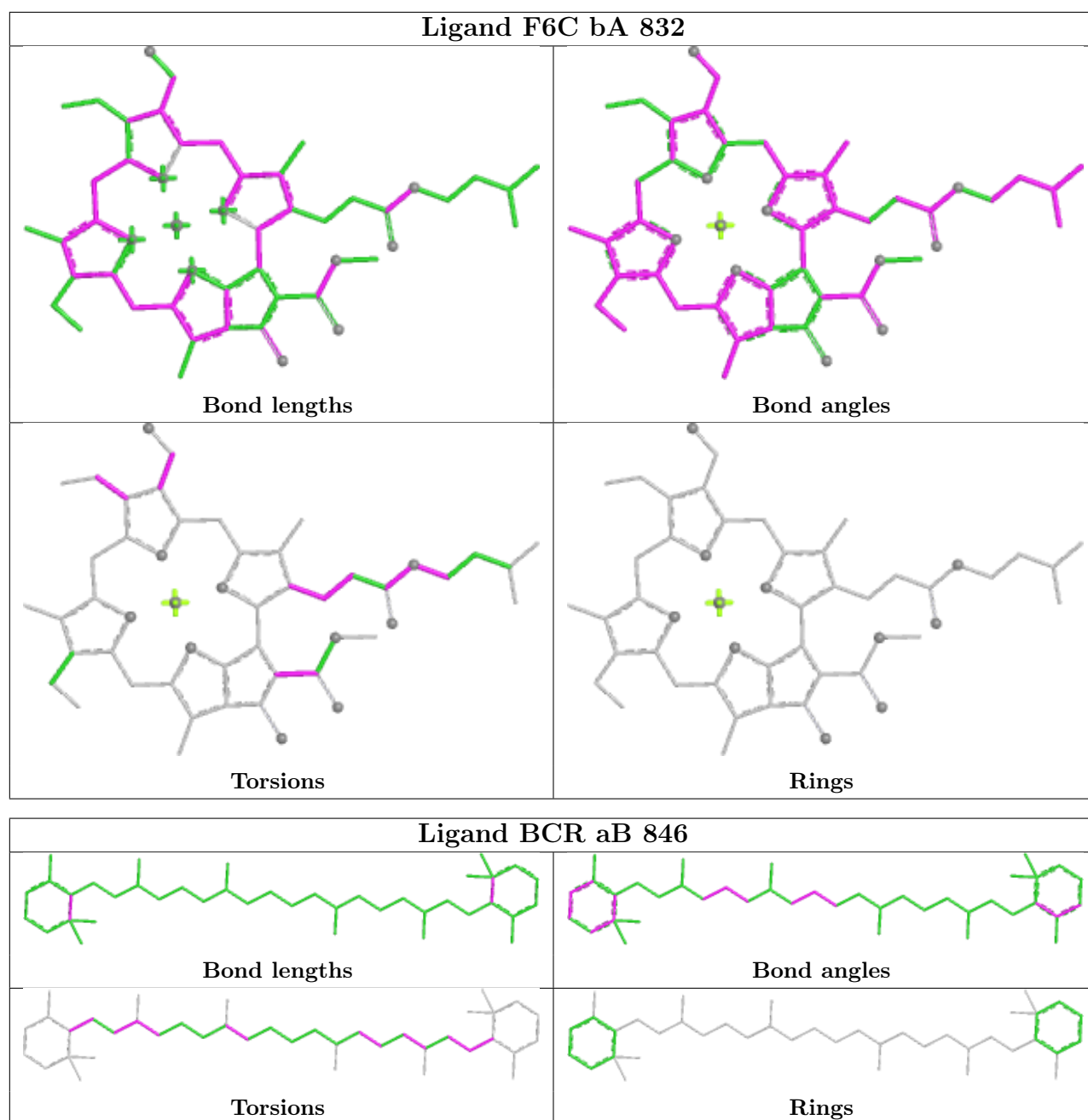


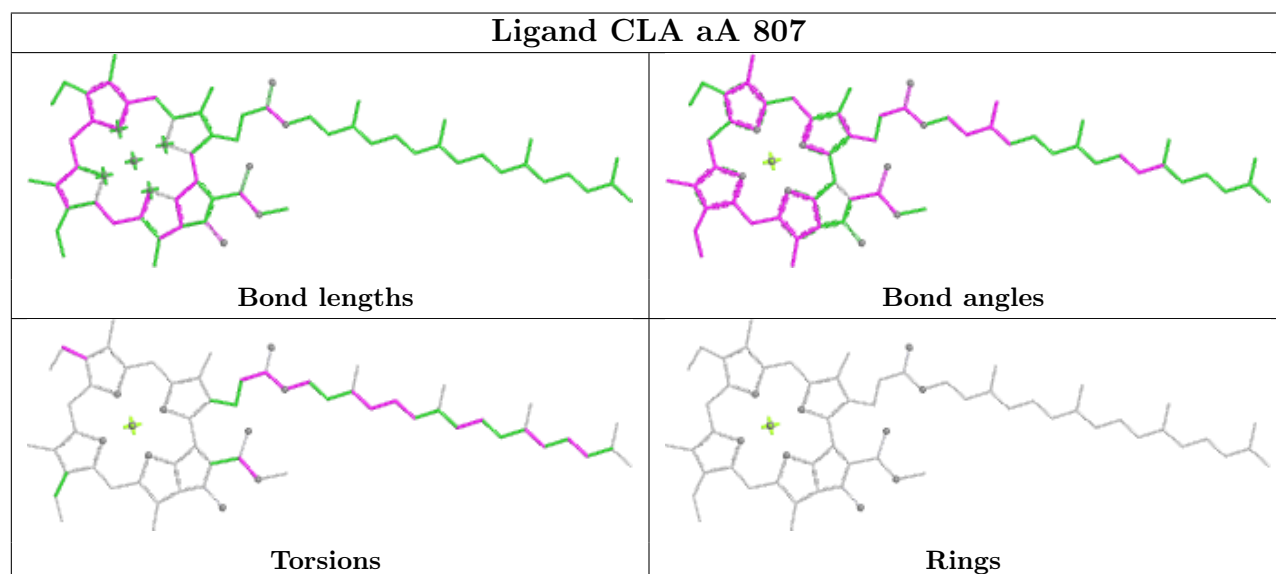
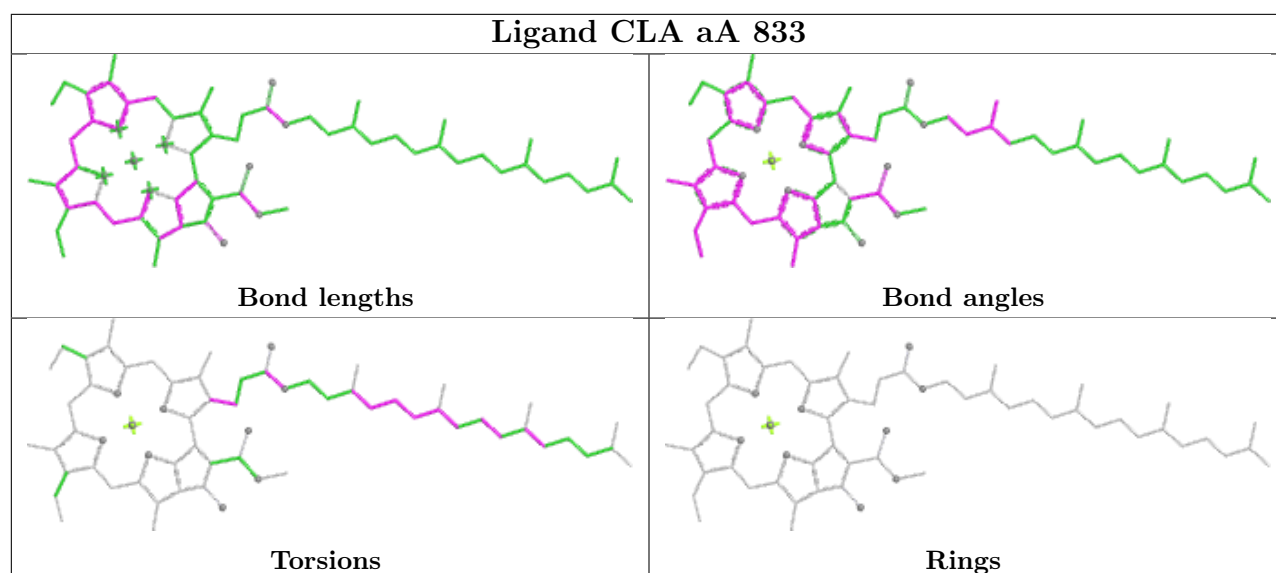
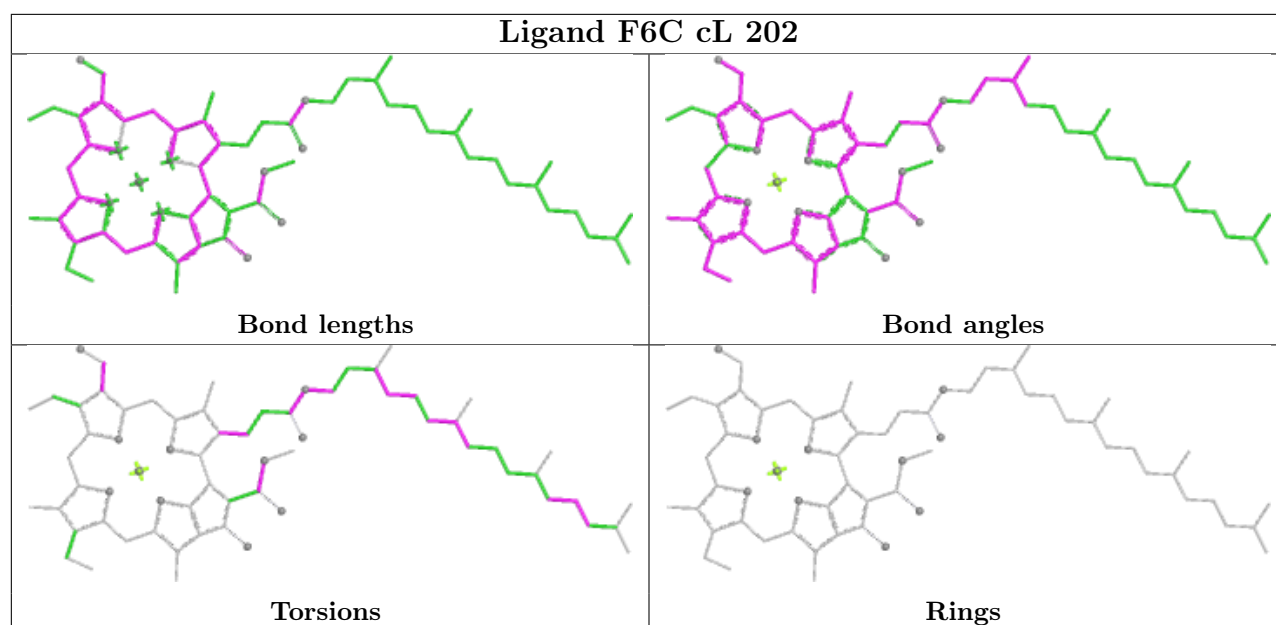


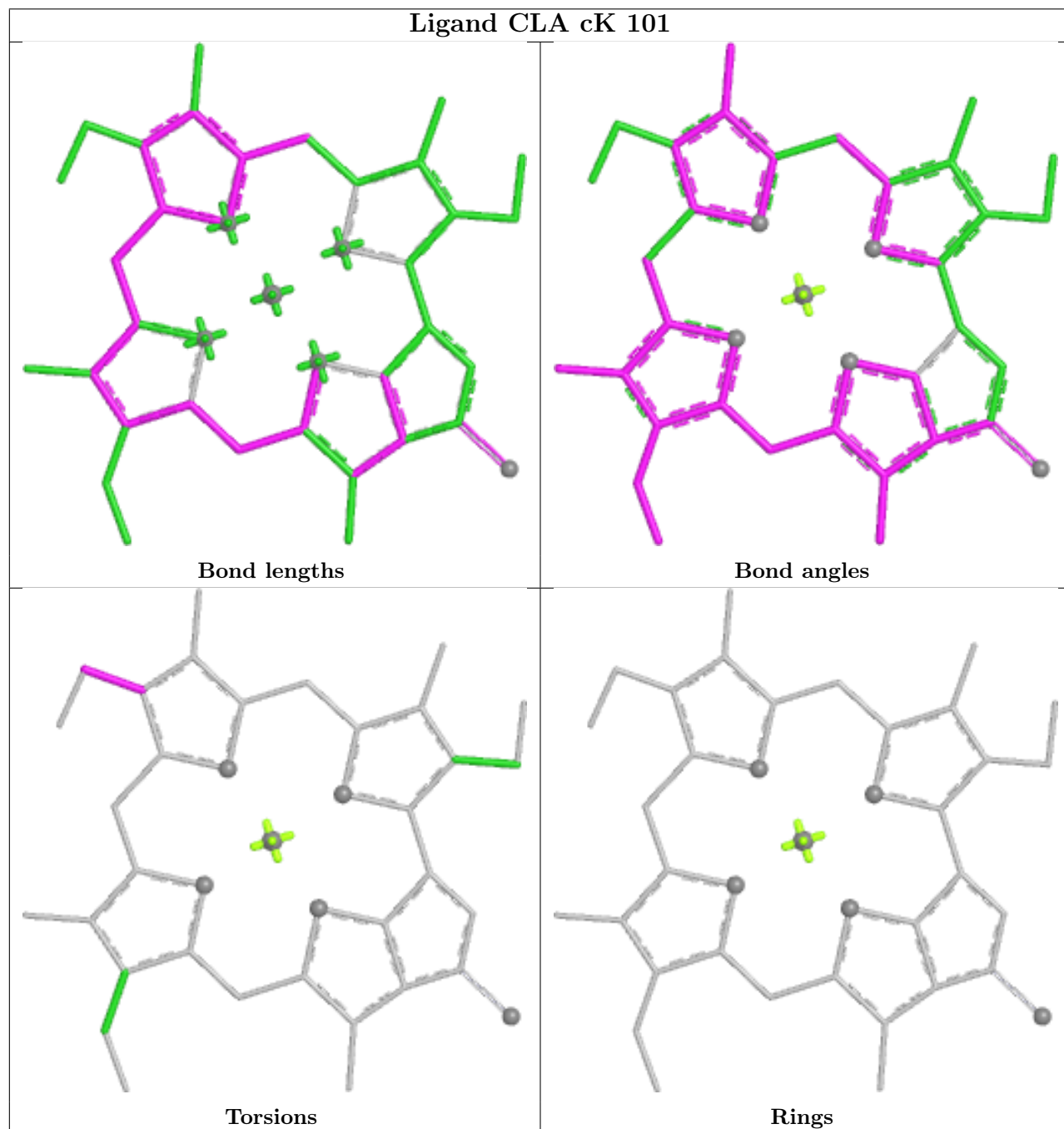
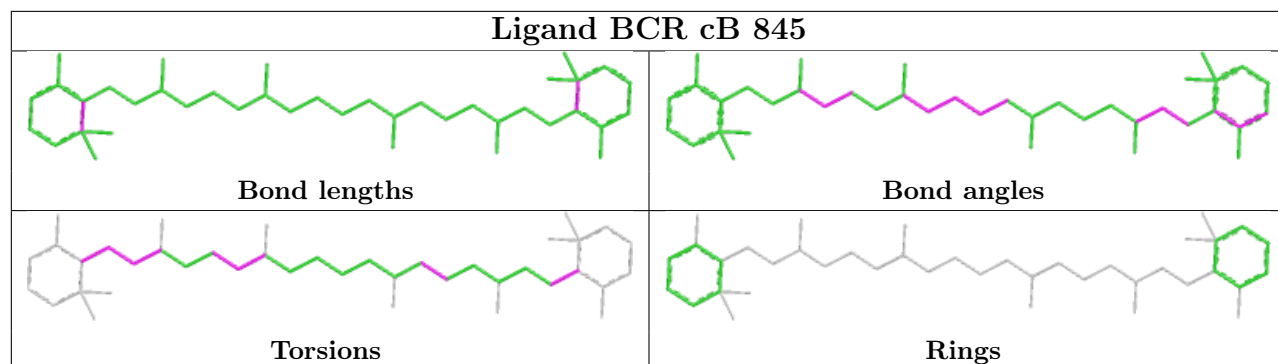


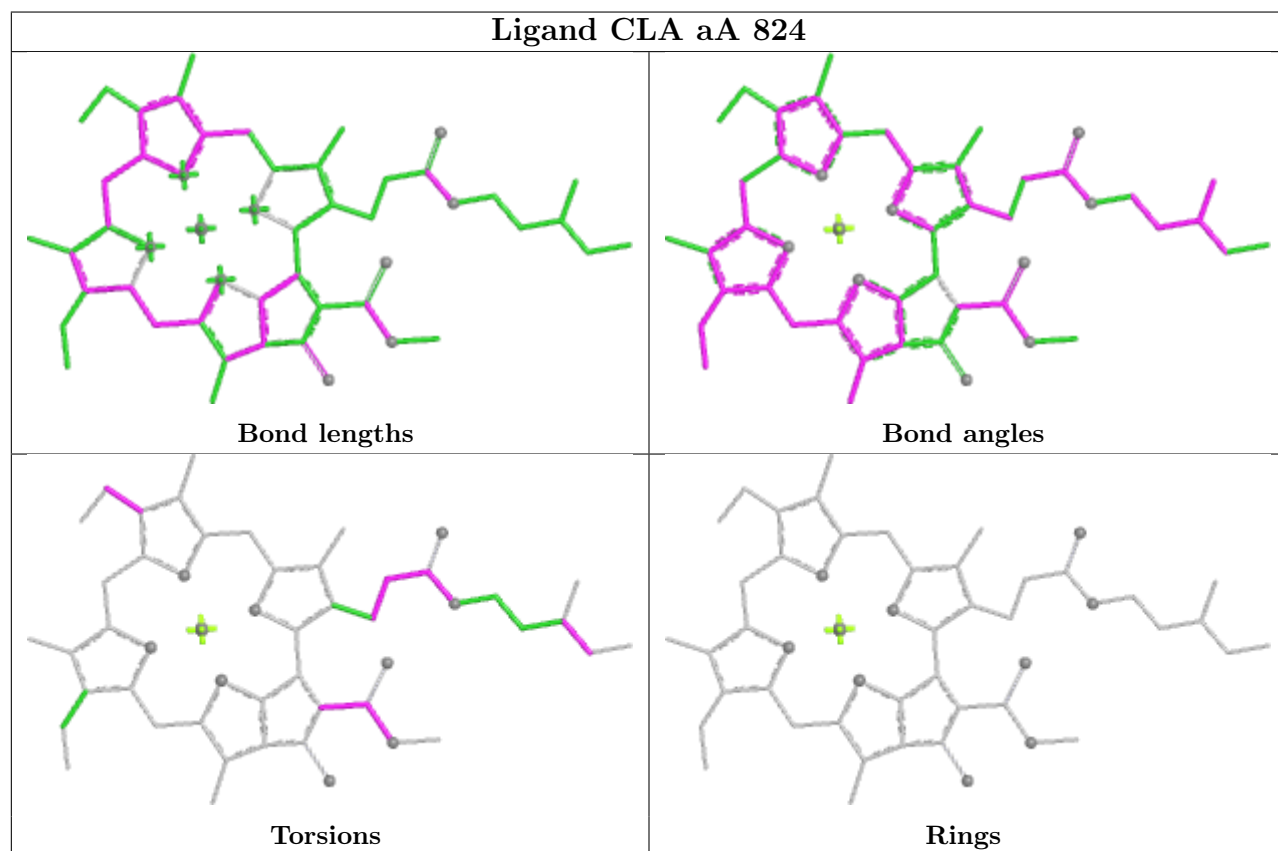
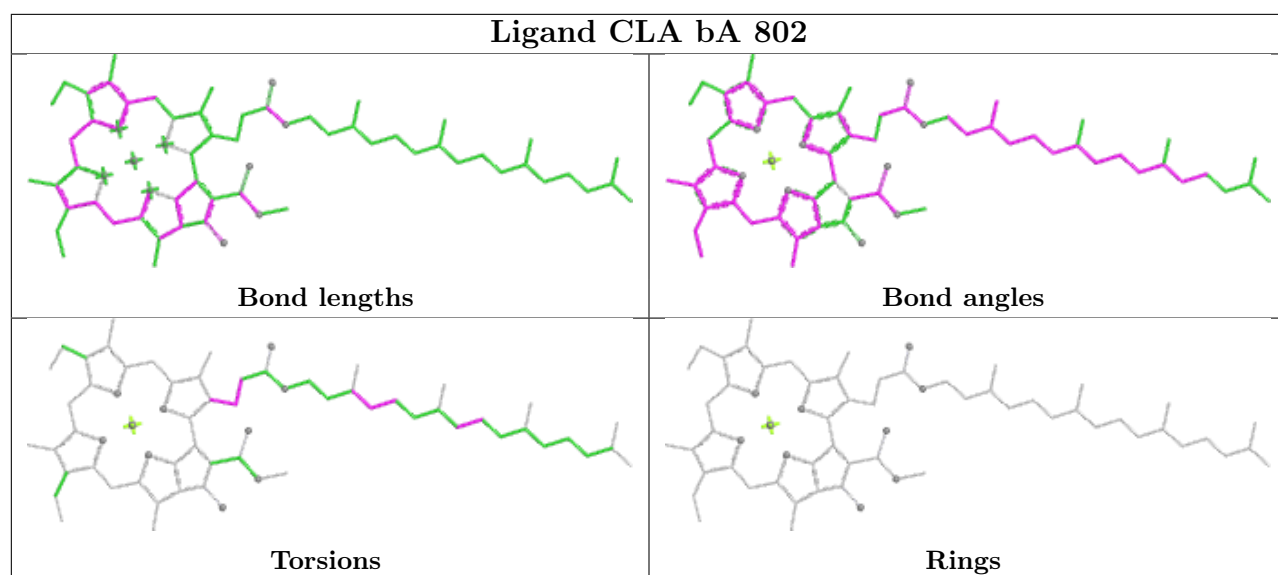




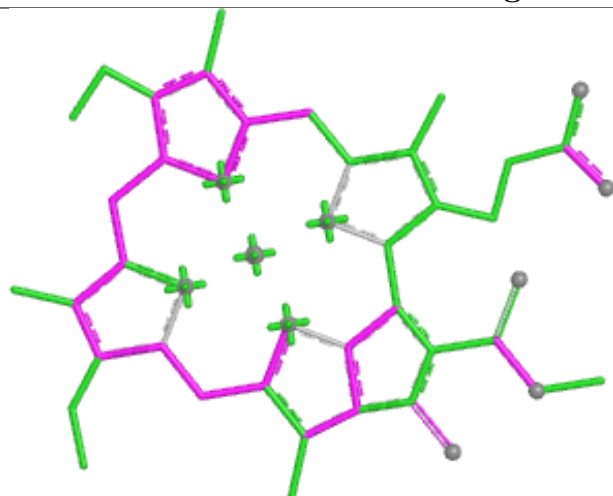




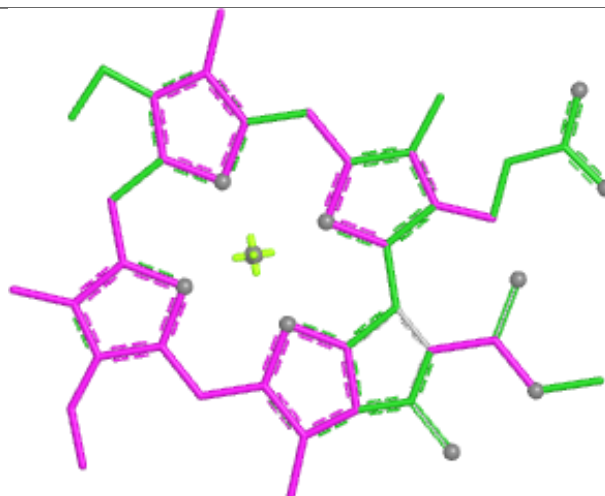




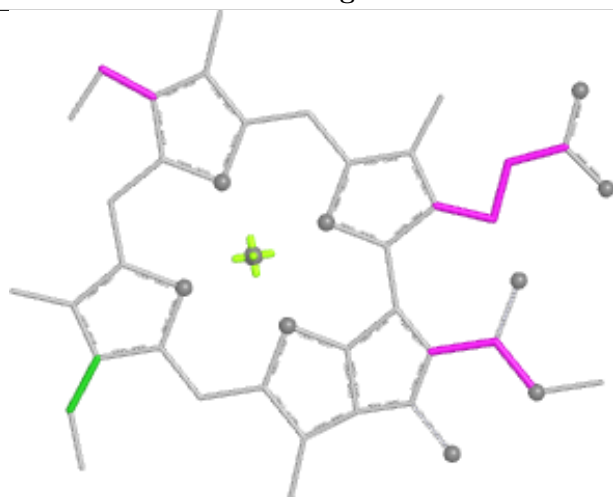
## Ligand CLA bA 804



Bond lengths



Bond angles

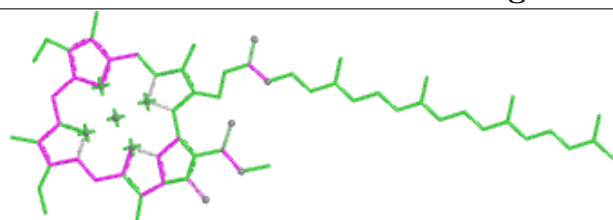


Torsions

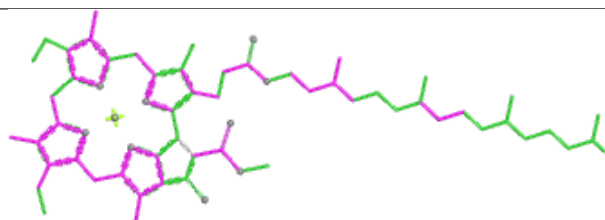


Rings

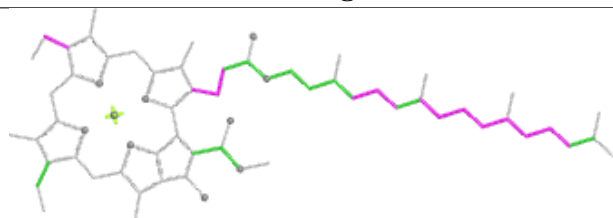
## Ligand CLA cL 206



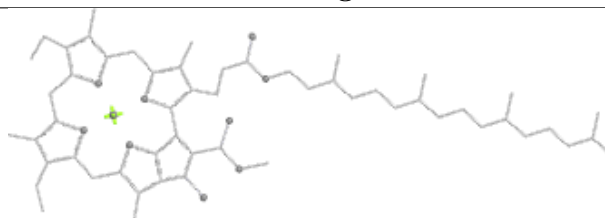
Bond lengths



Bond angles



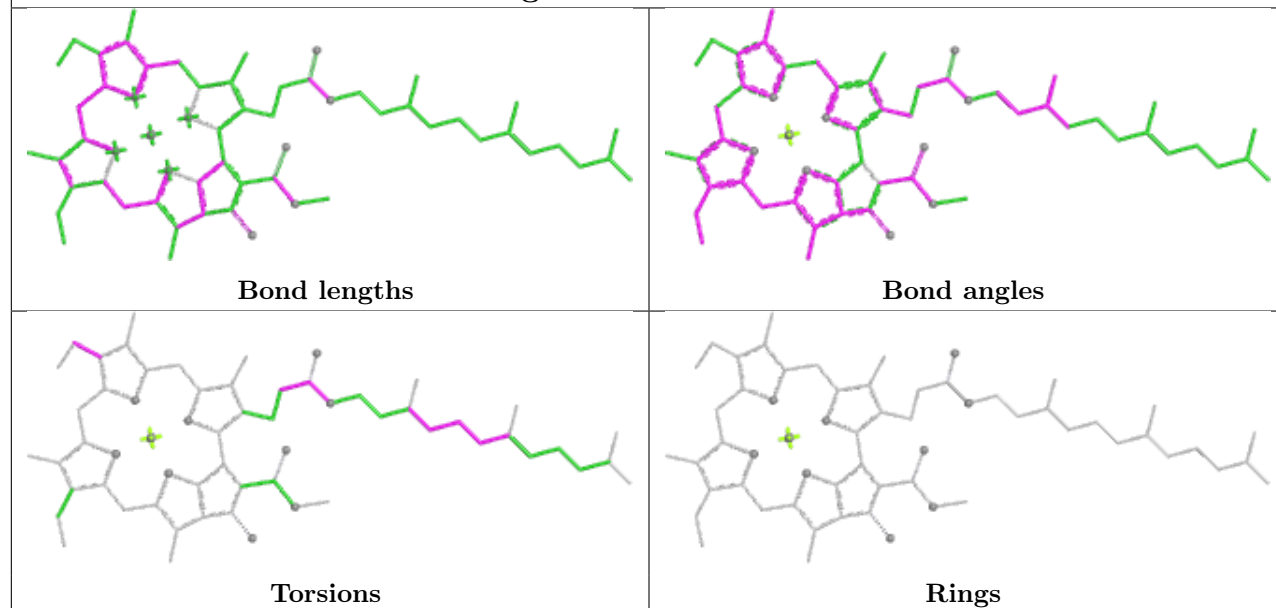
Torsions



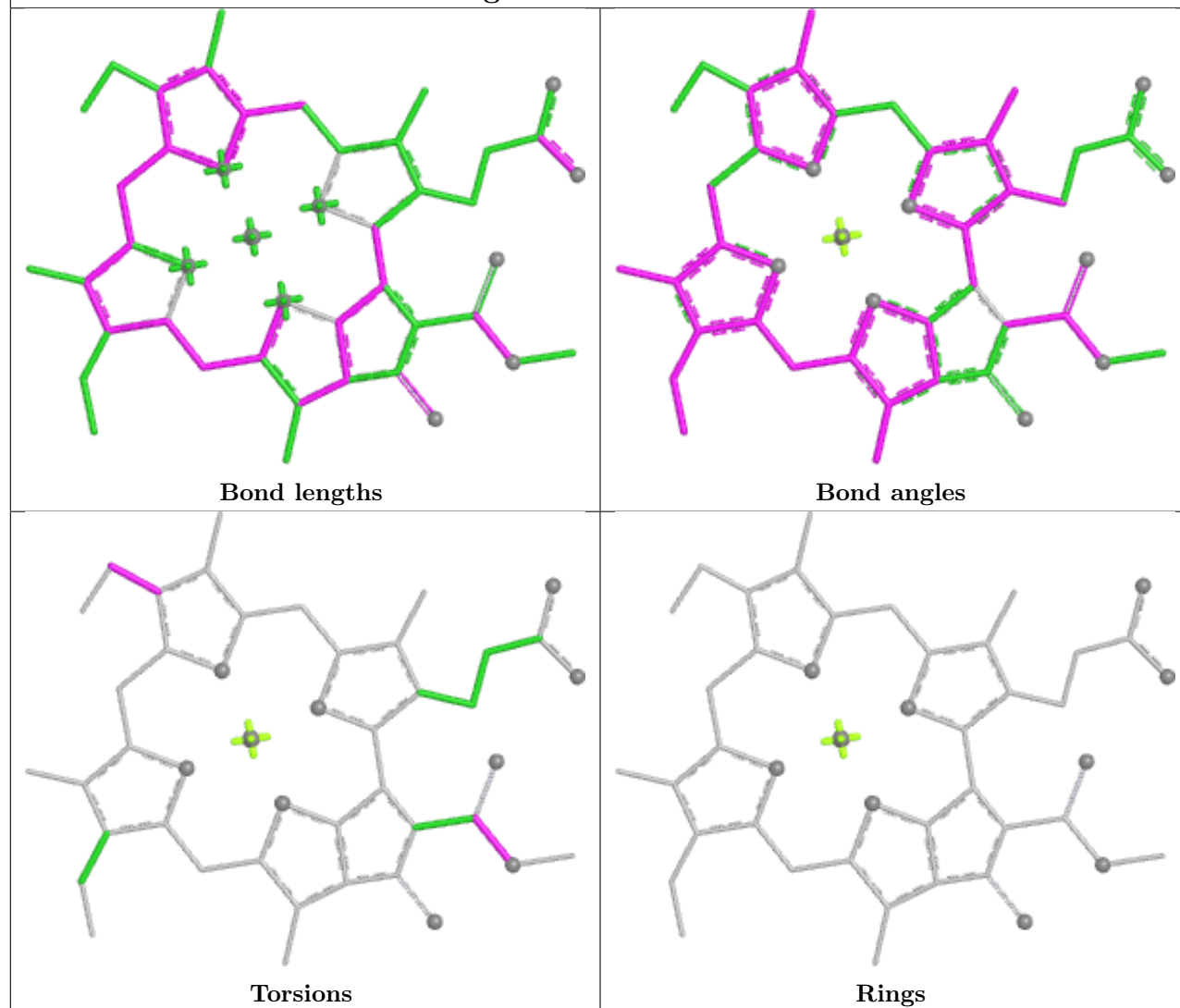
Rings

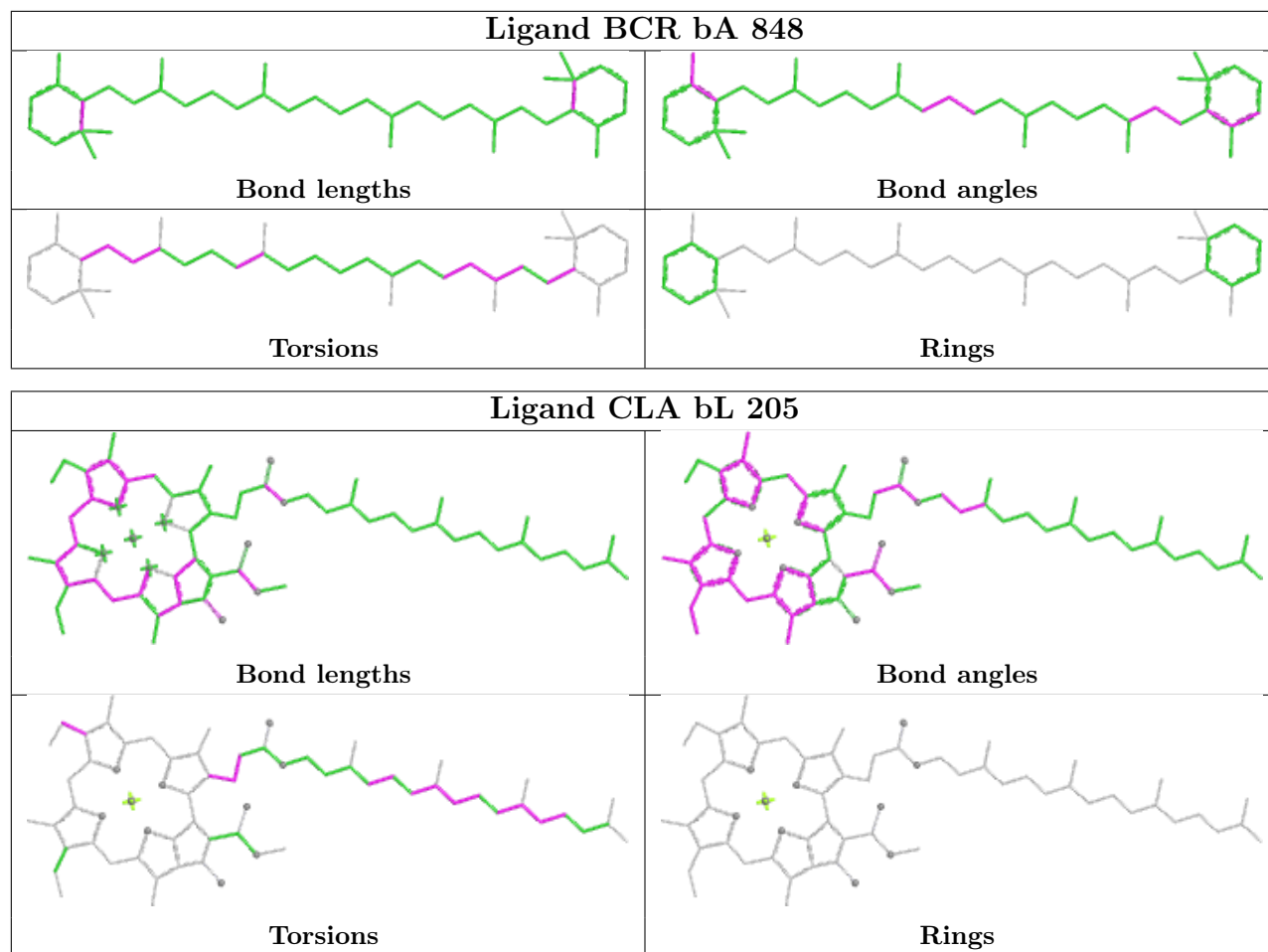


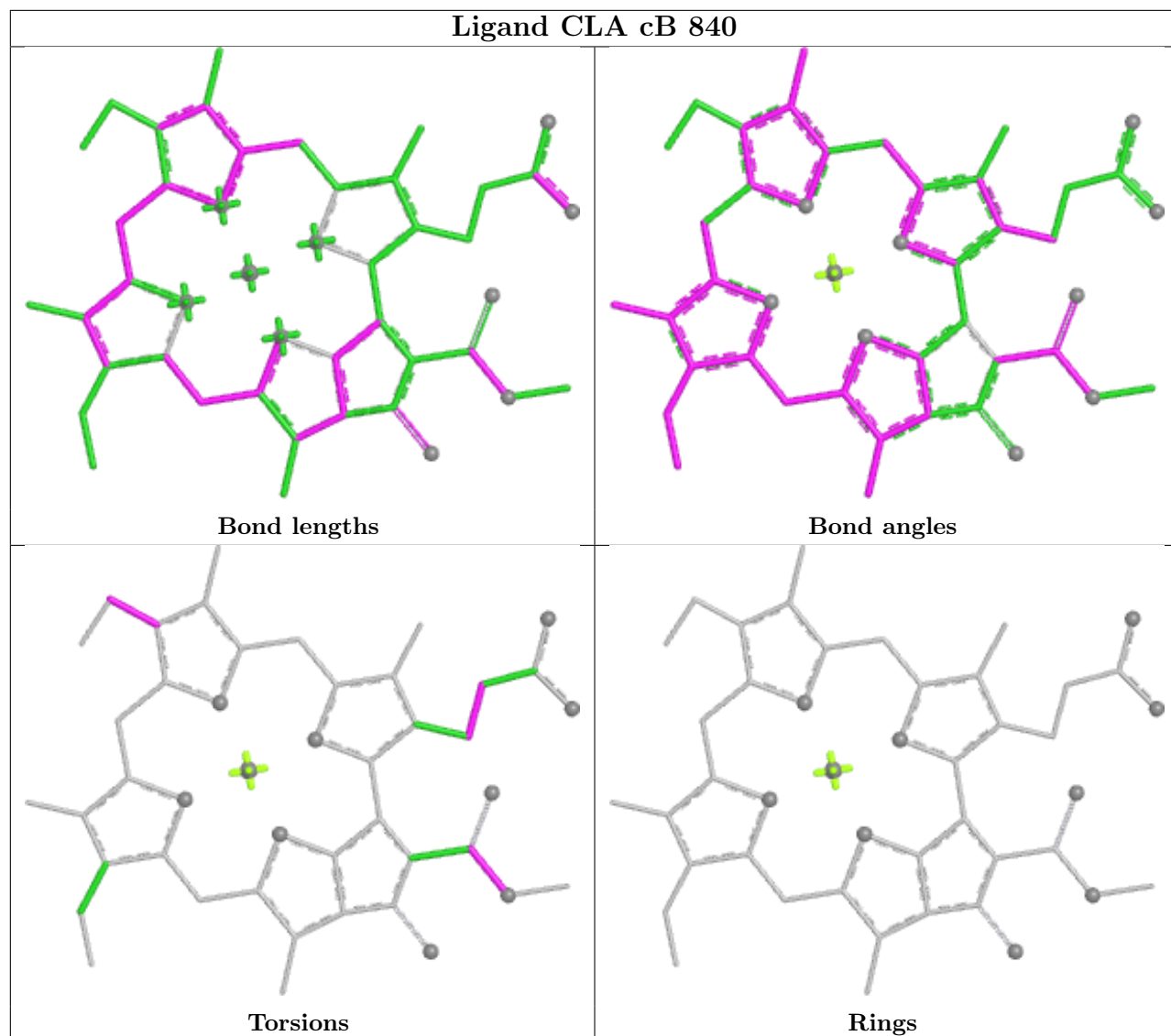
## Ligand CLA bA 828

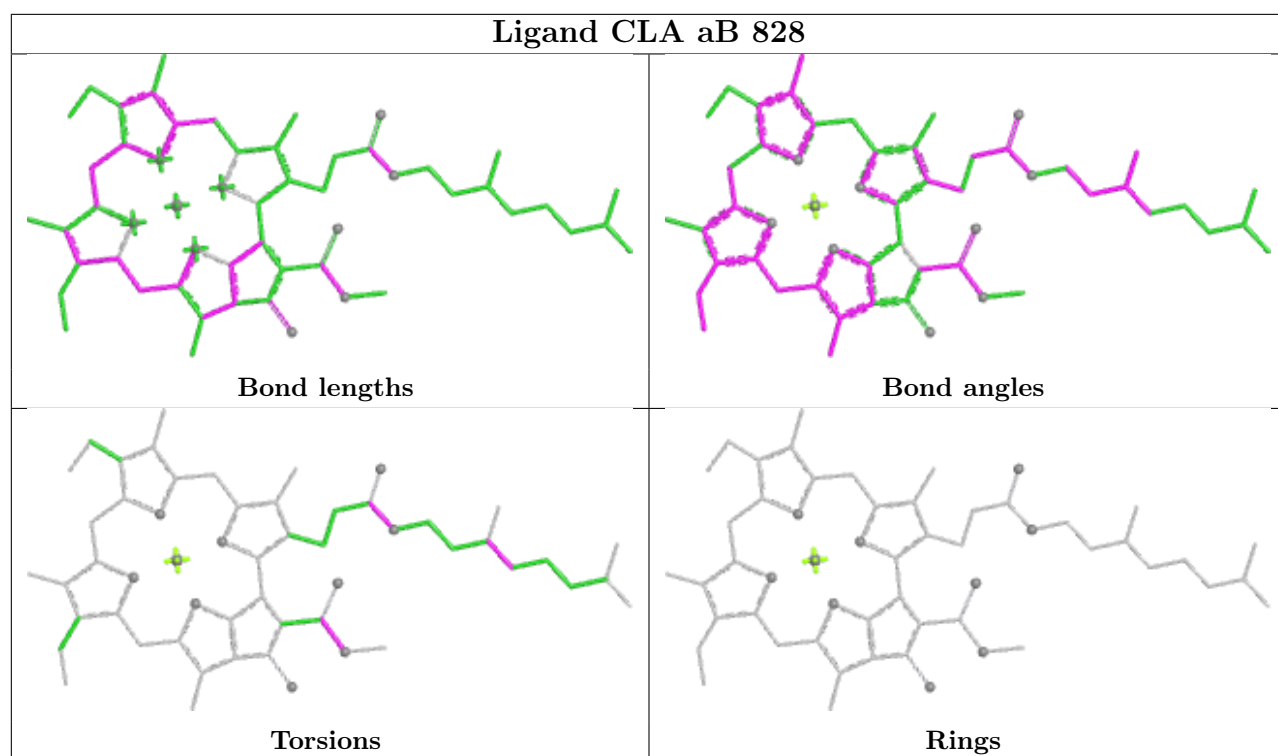


## Ligand CLA aA 810

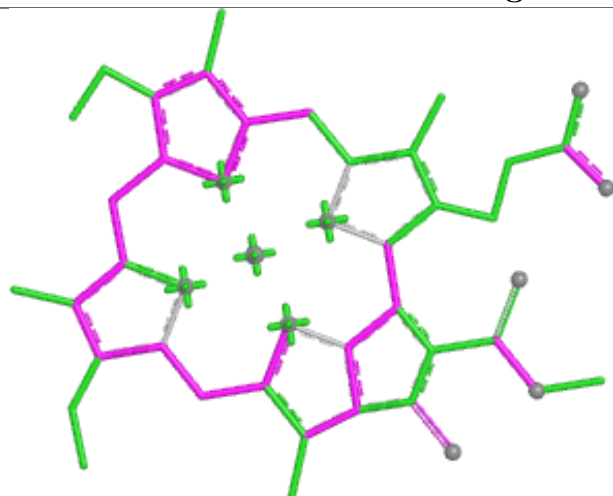




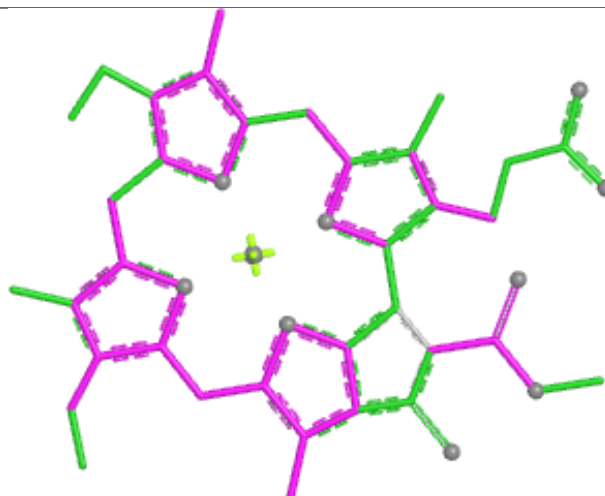




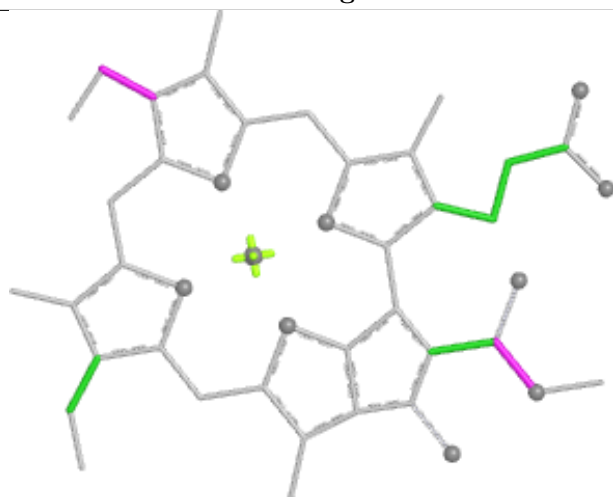
## Ligand CLA cA 816



Bond lengths



Bond angles

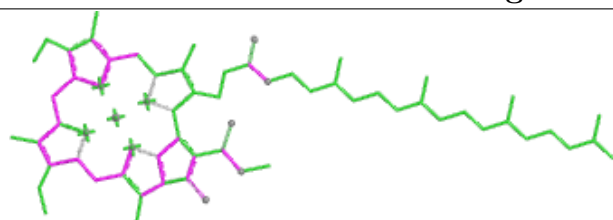


Torsions

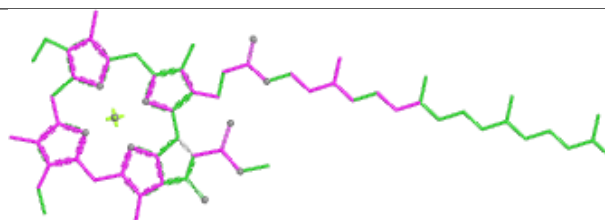


Rings

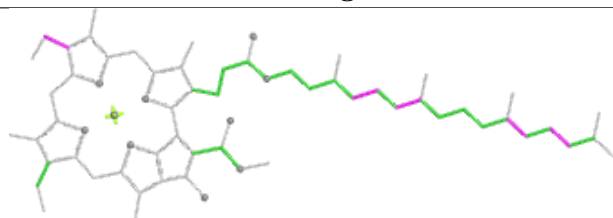
## Ligand CLA cA 839



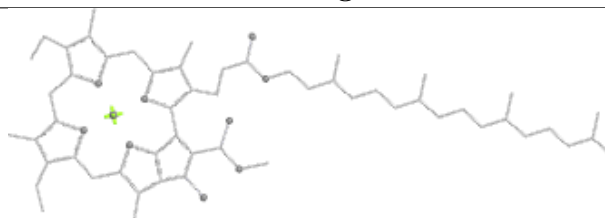
Bond lengths



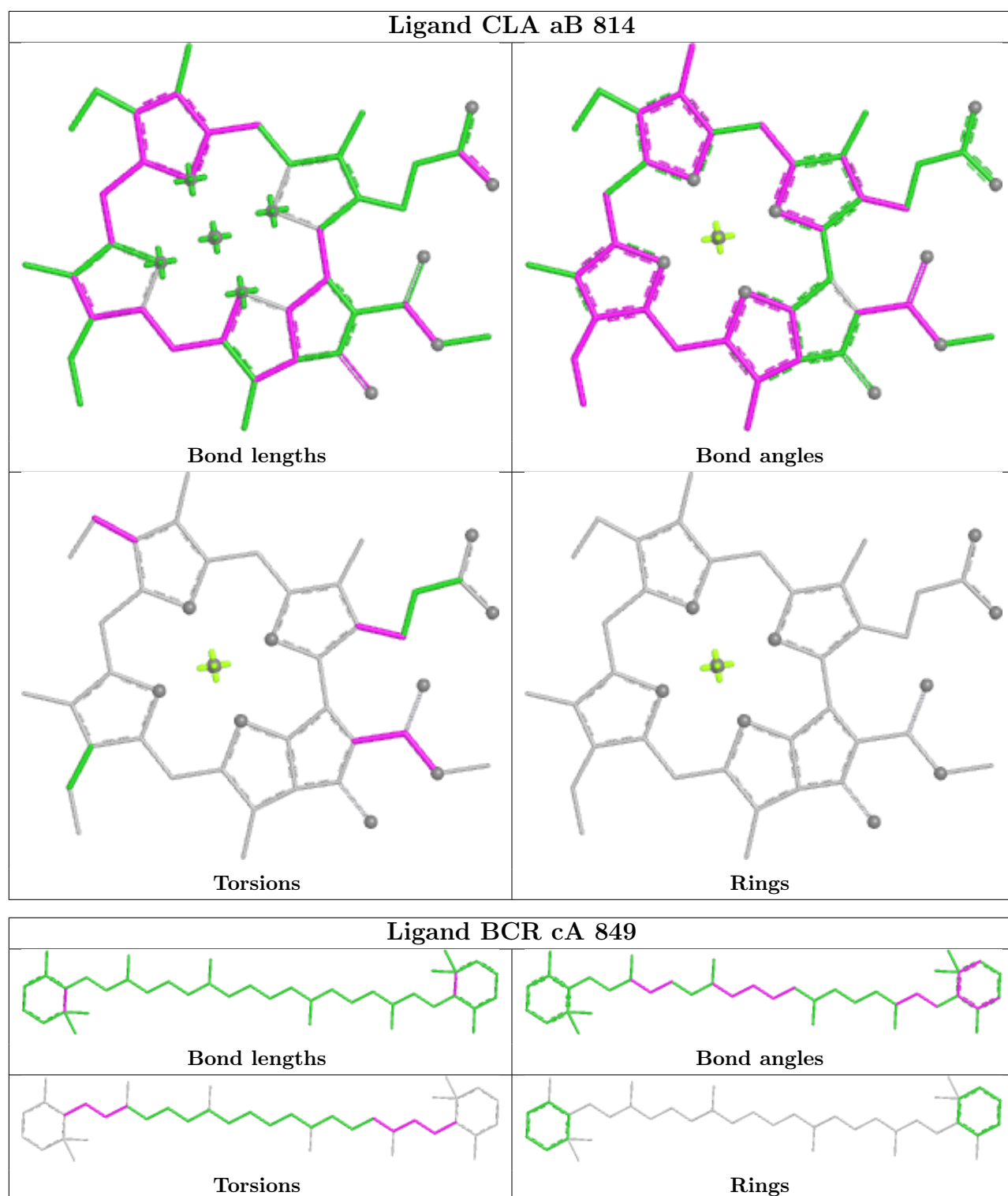
Bond angles



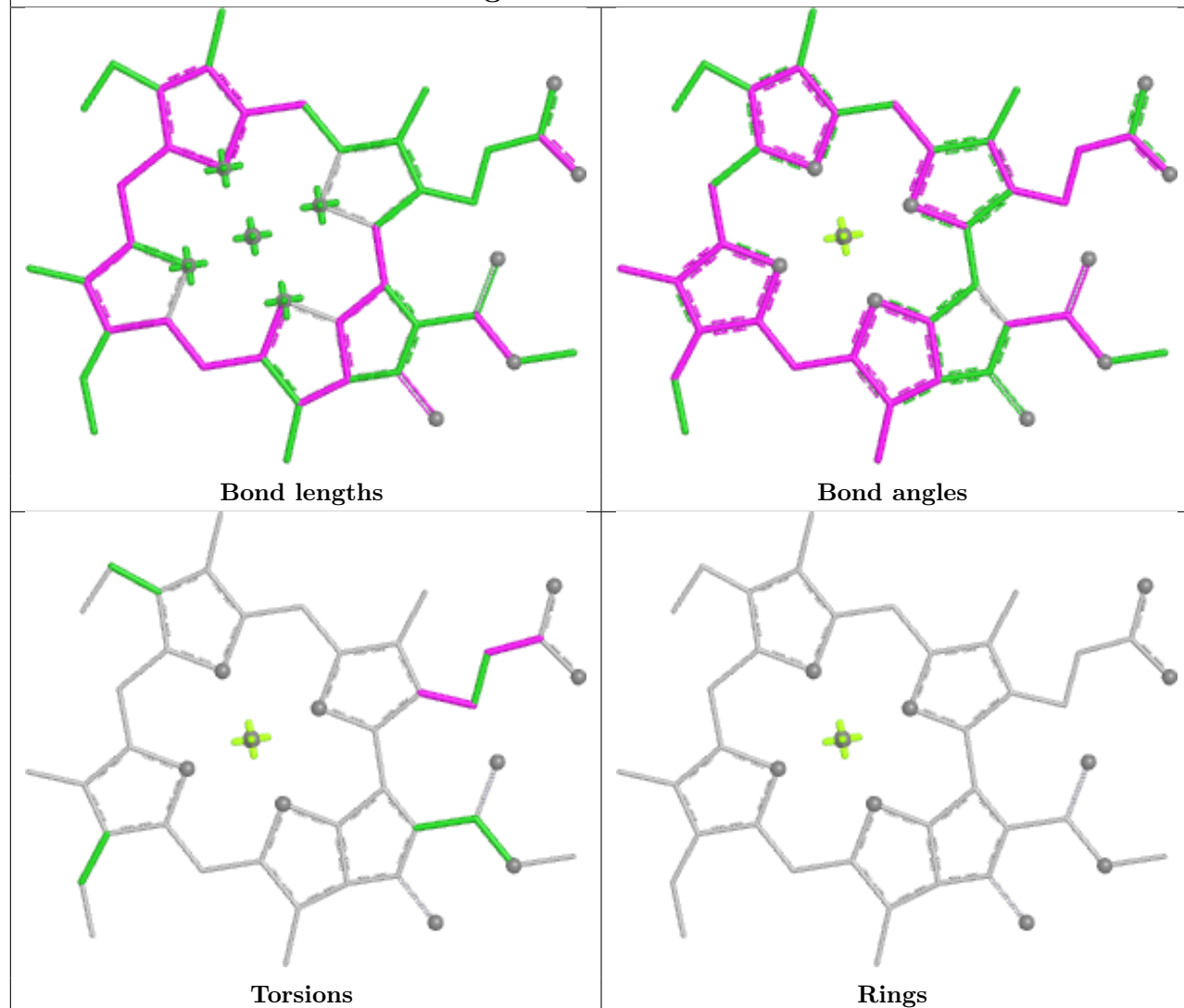
Torsions



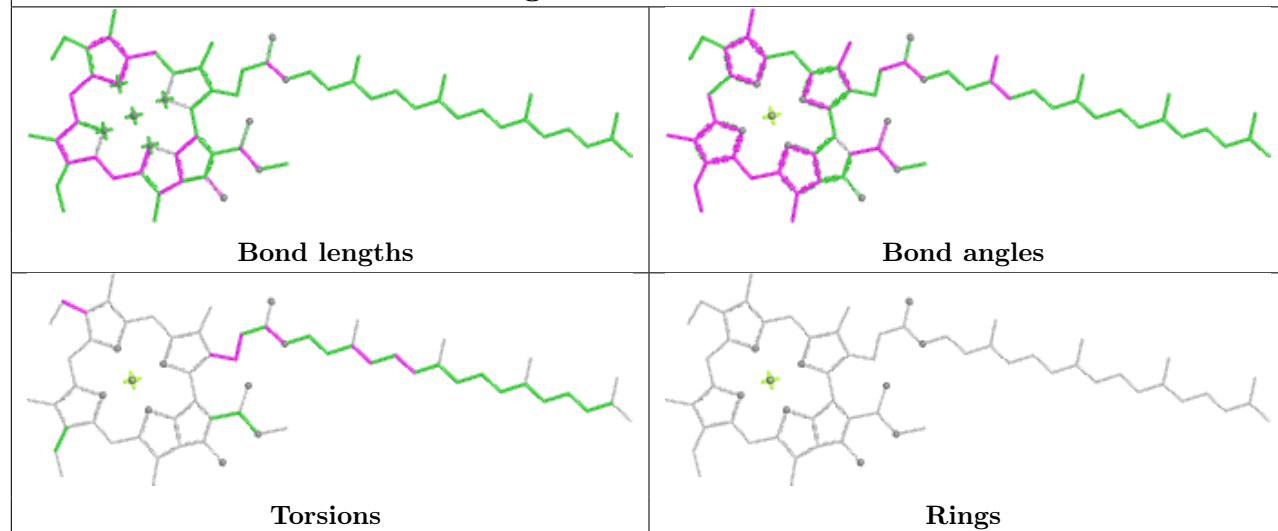
Rings

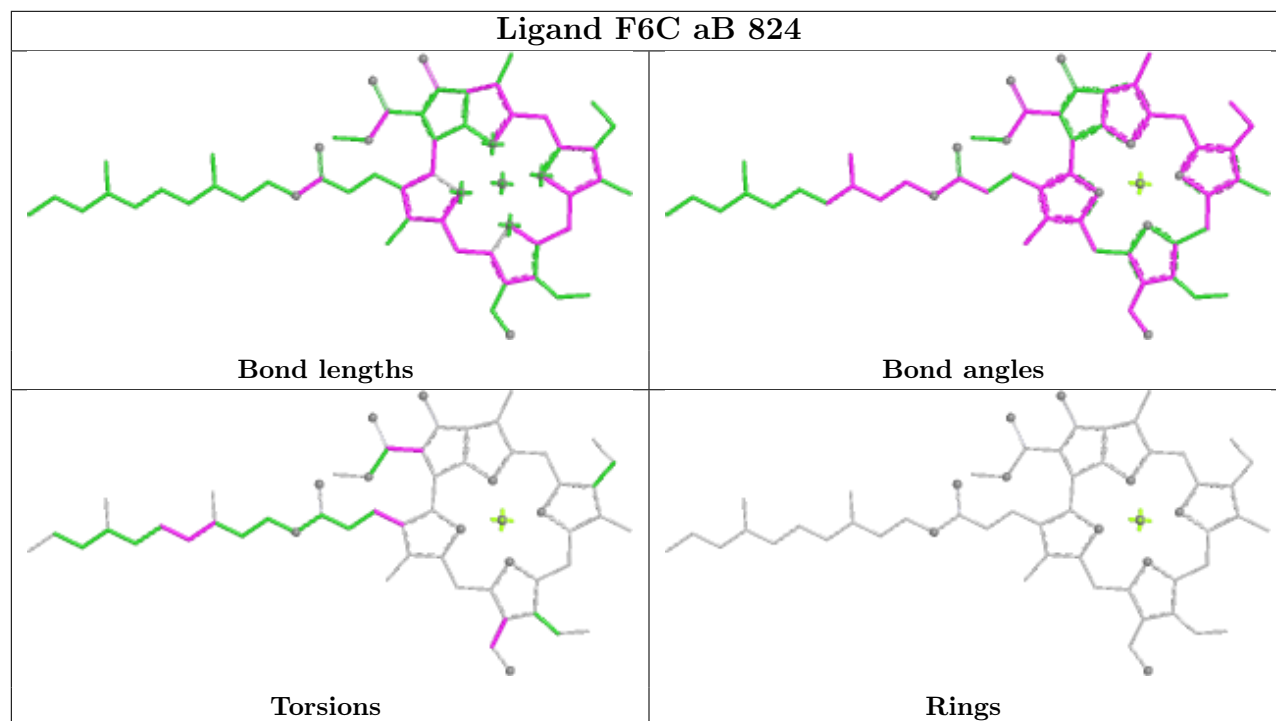
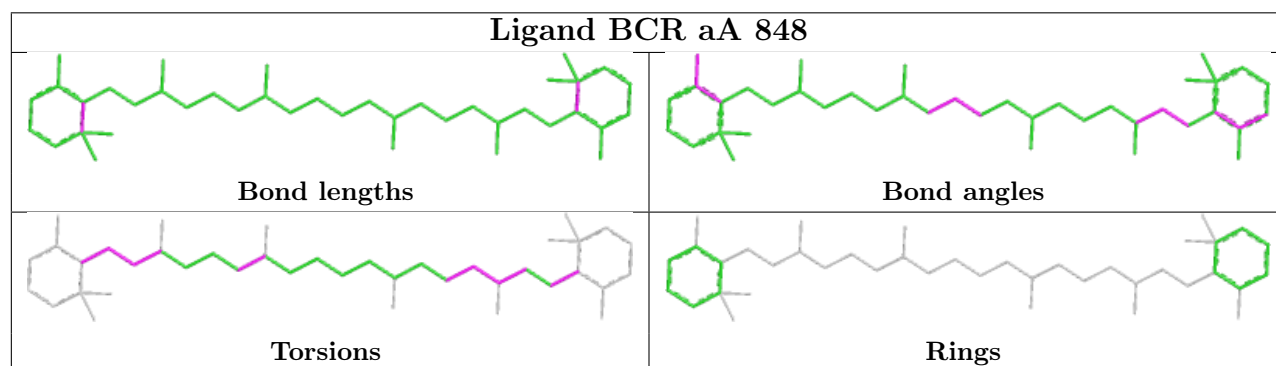
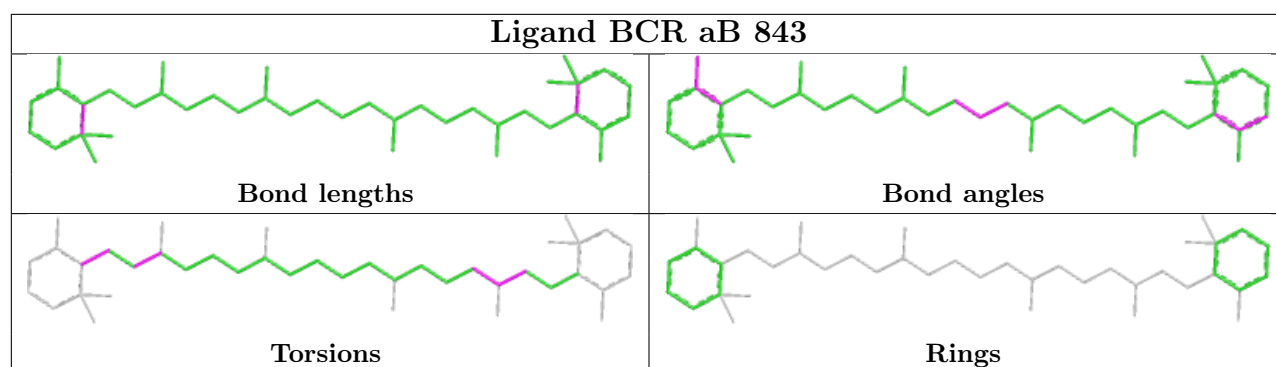


## Ligand CLA aA 837

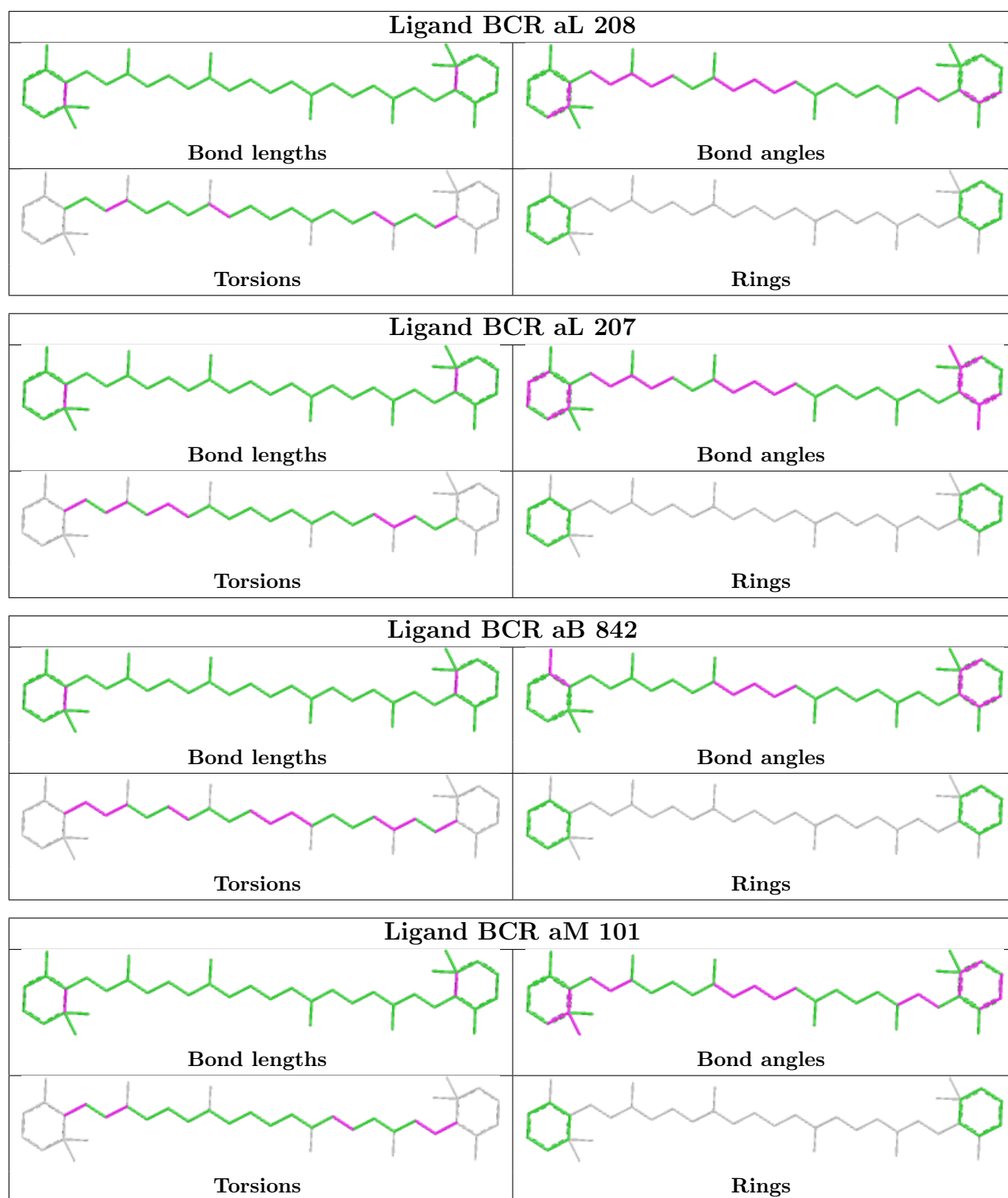


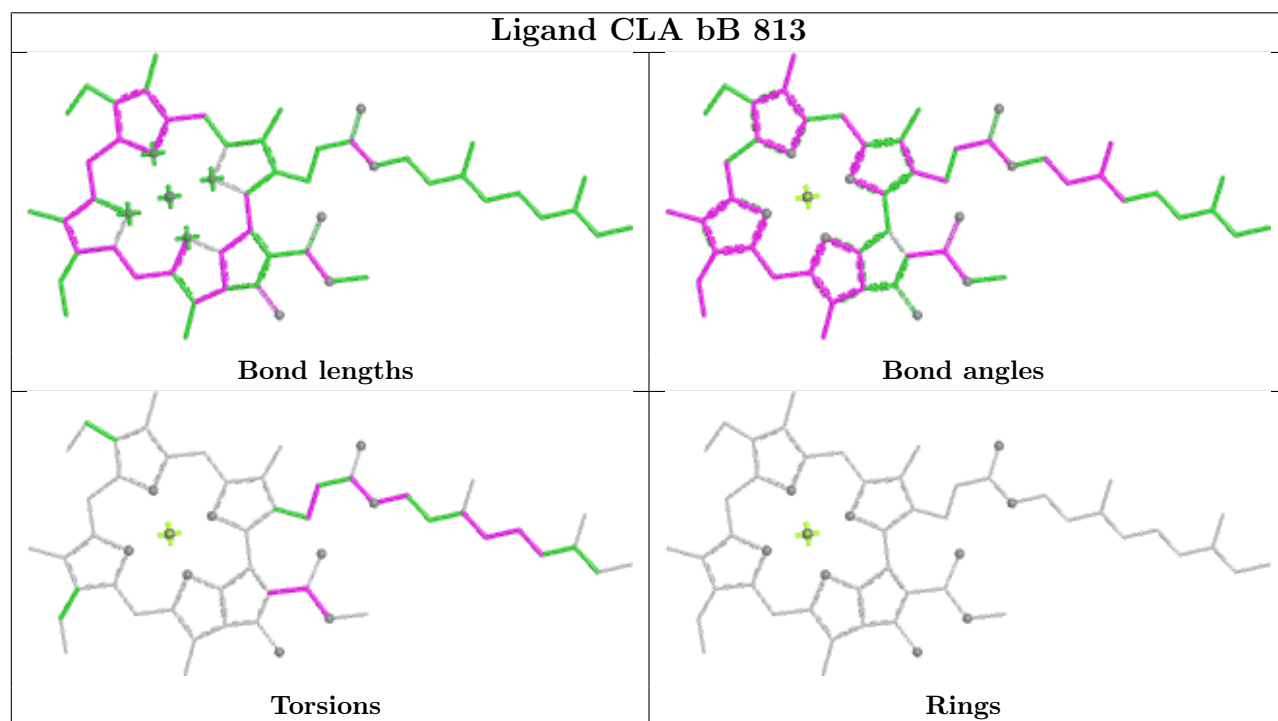
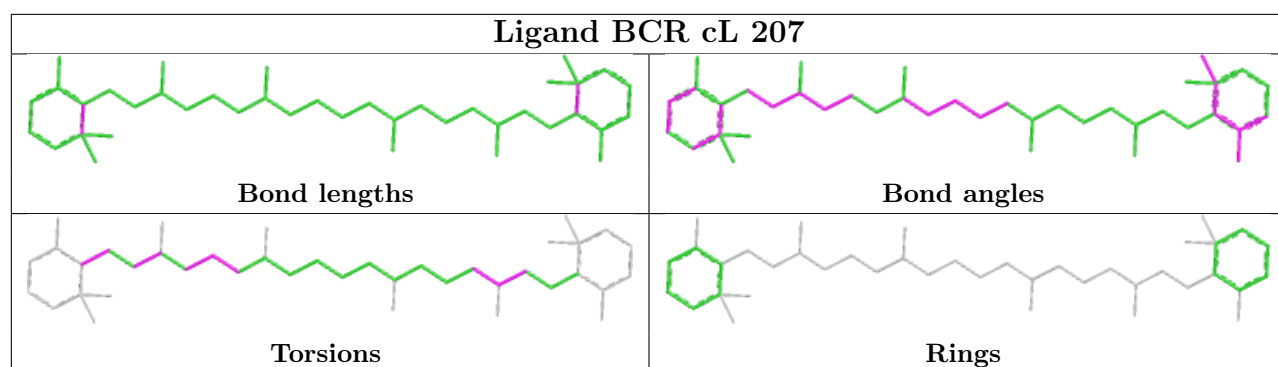
## Ligand CLA aB 827



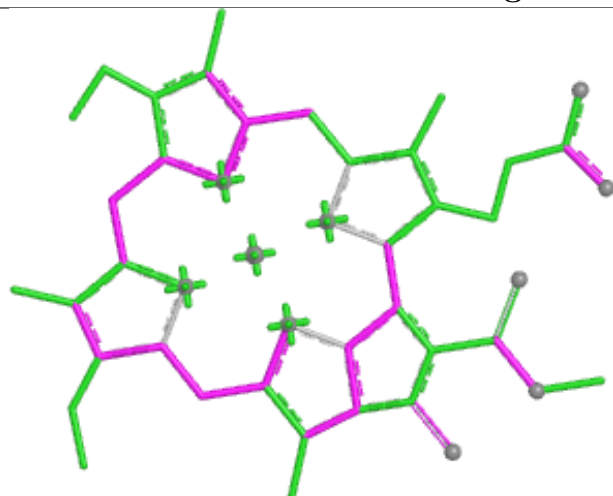




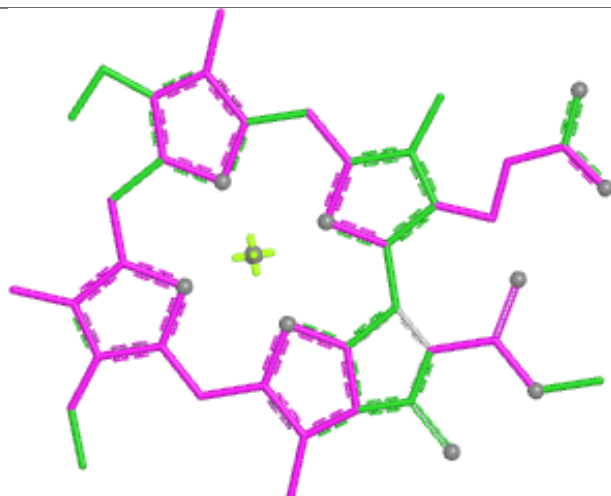




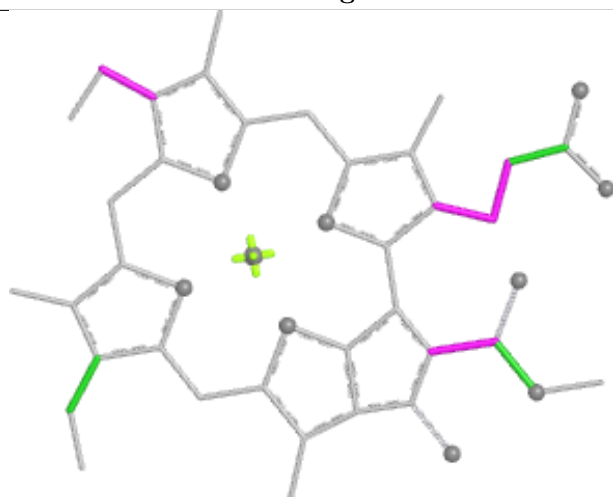
## Ligand CLA bB 829



Bond lengths



Bond angles

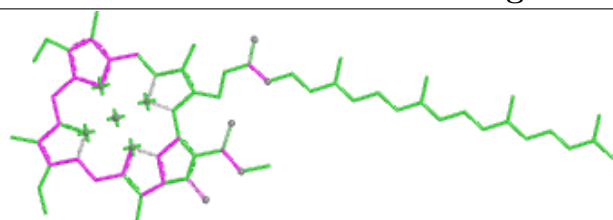


Torsions

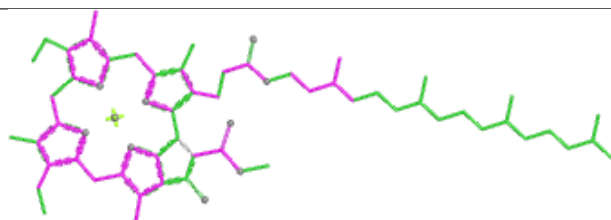


Rings

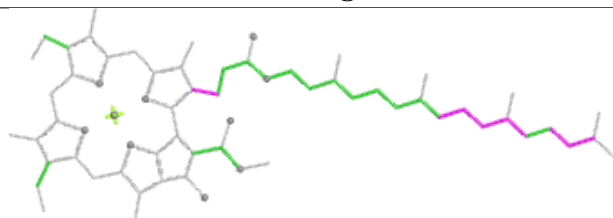
## Ligand CLA cB 825



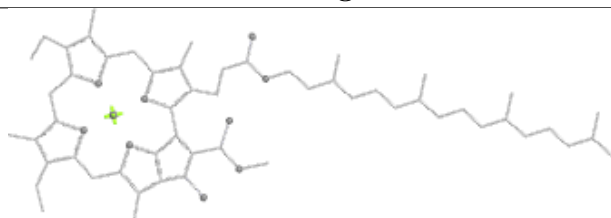
Bond lengths



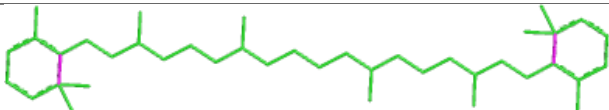
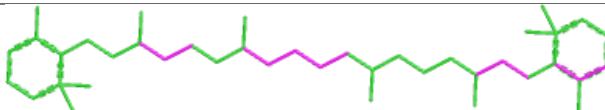
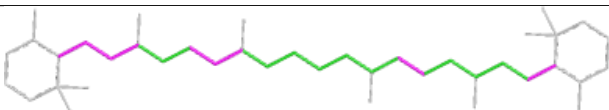
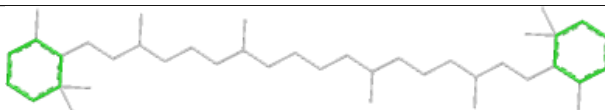
Bond angles

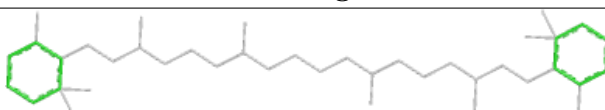


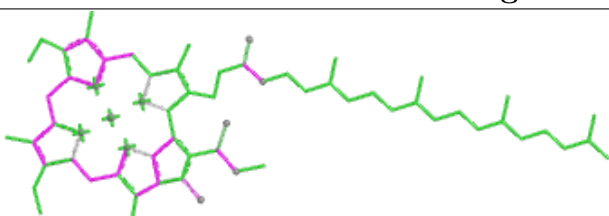
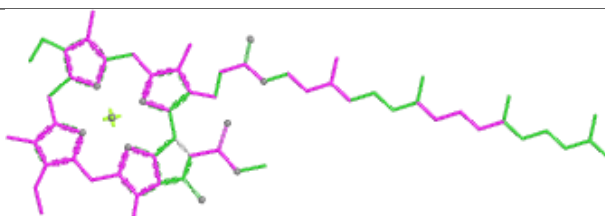
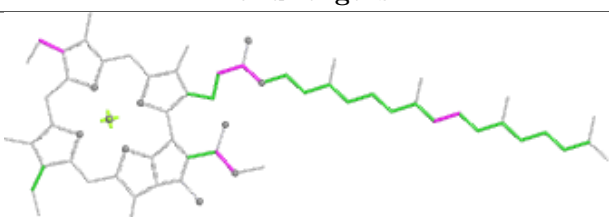
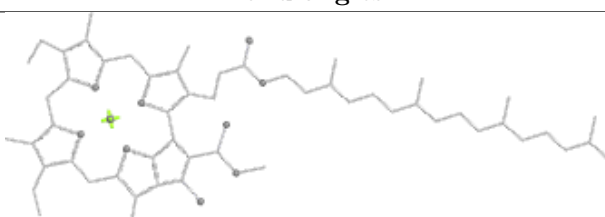
Torsions

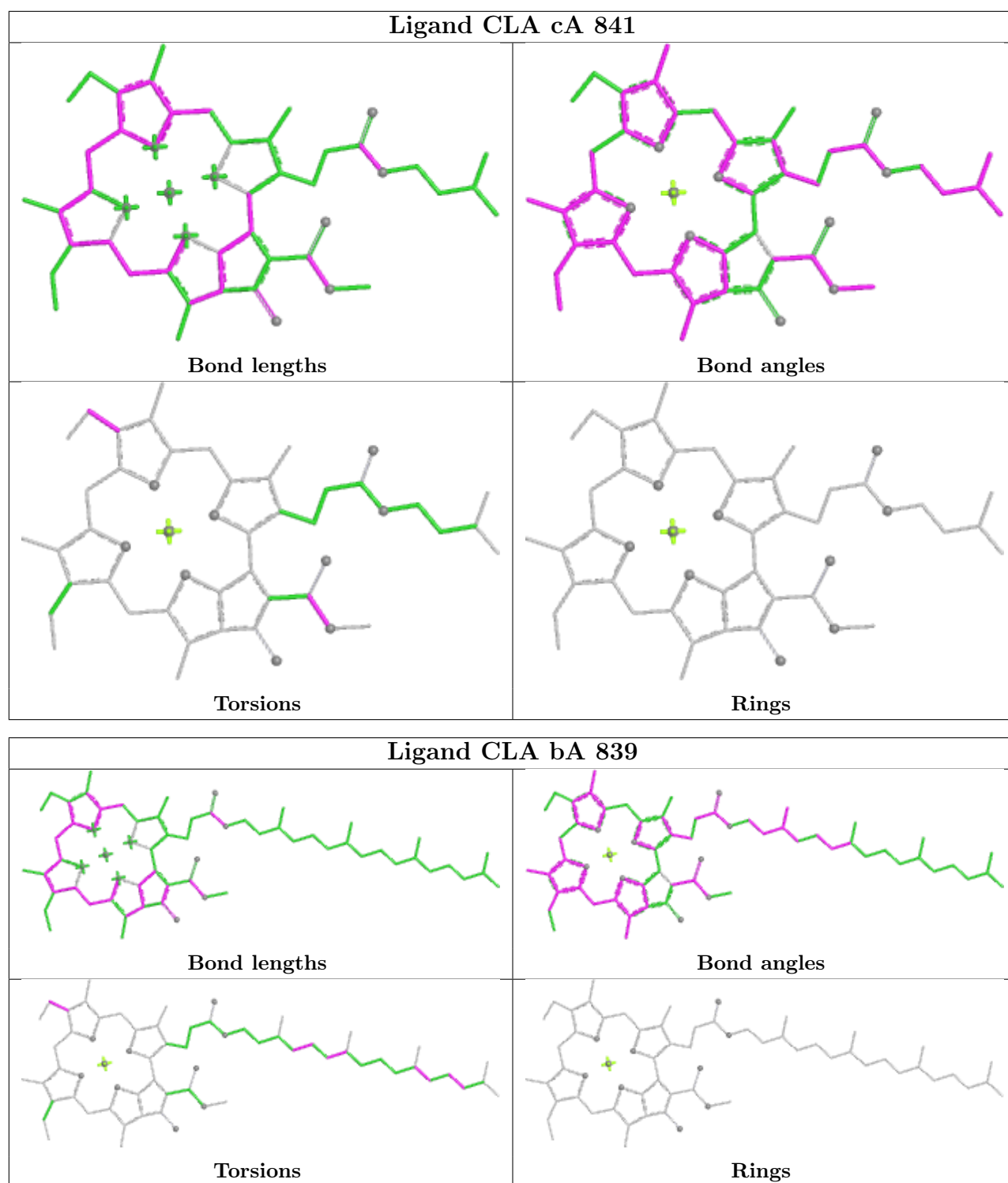


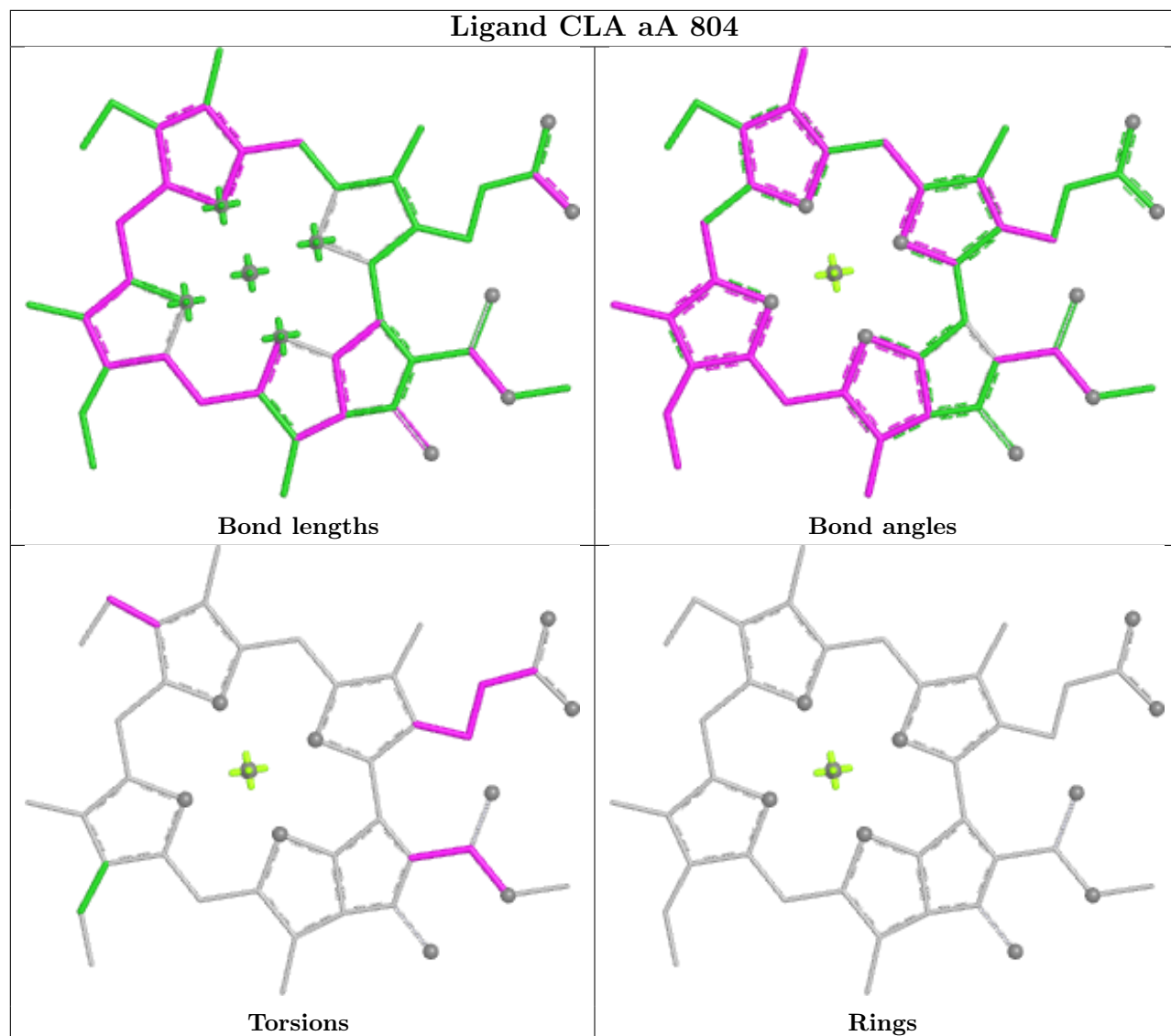
Rings

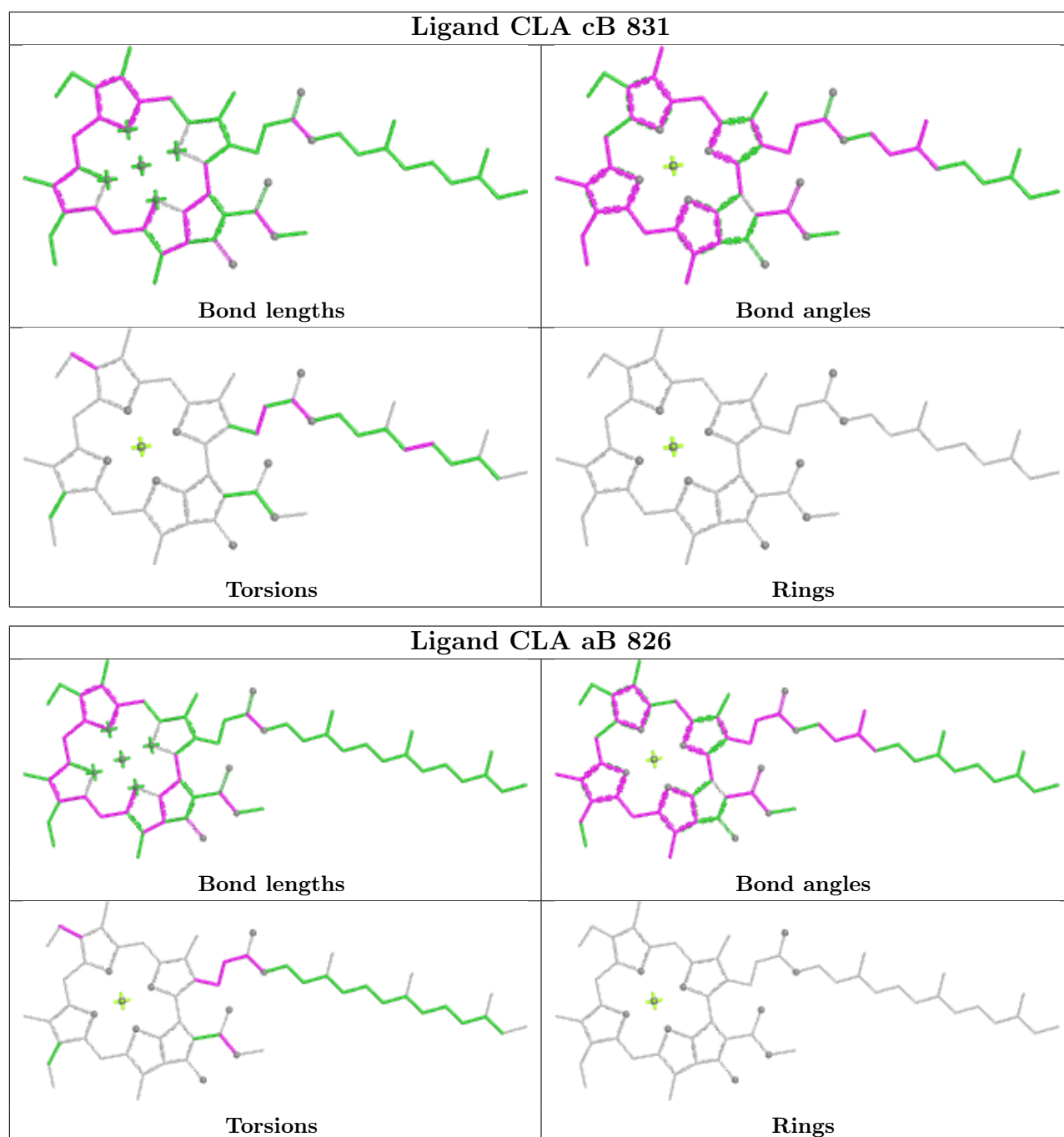
| Ligand BCR aB 845                                                                 |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

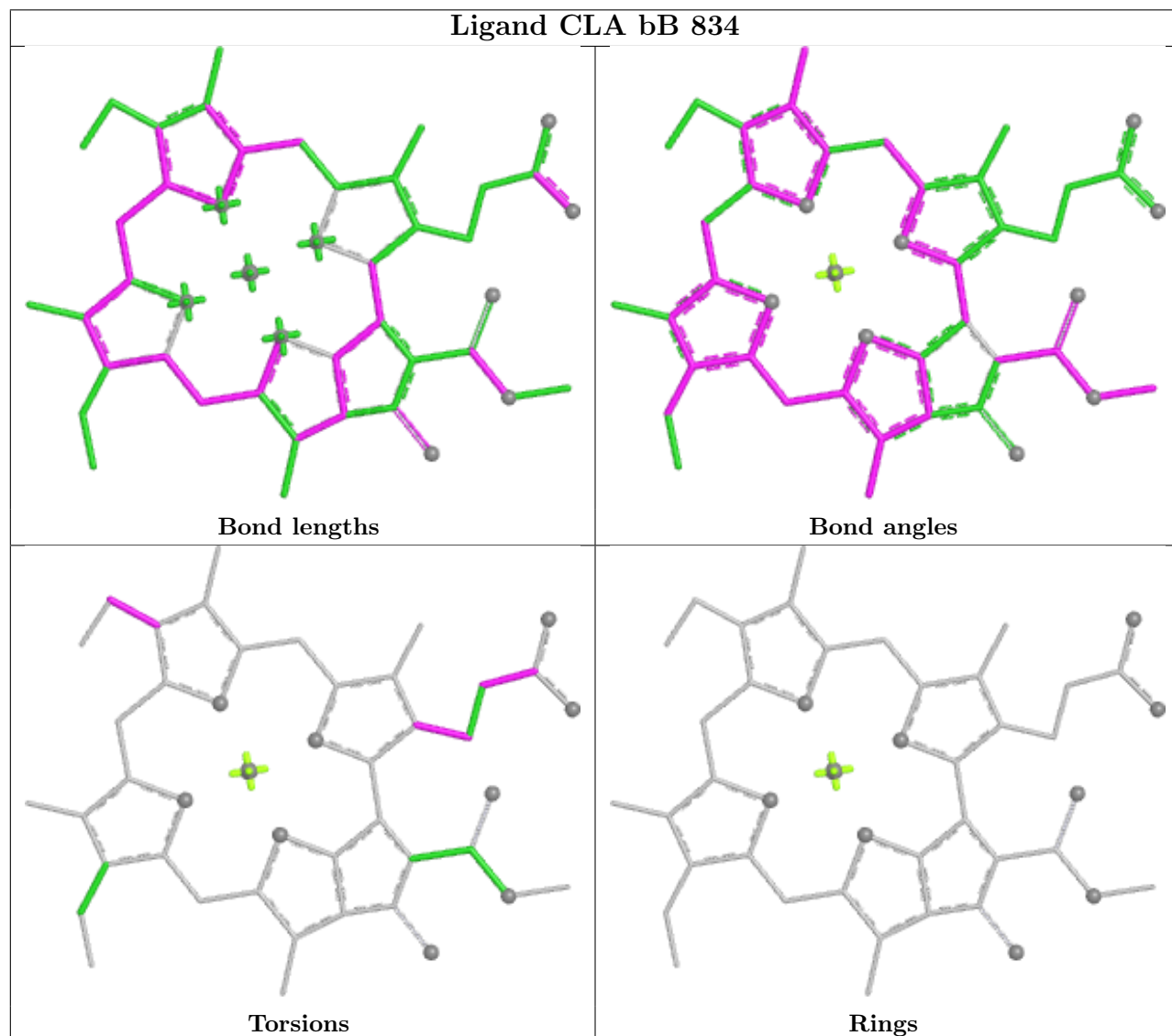
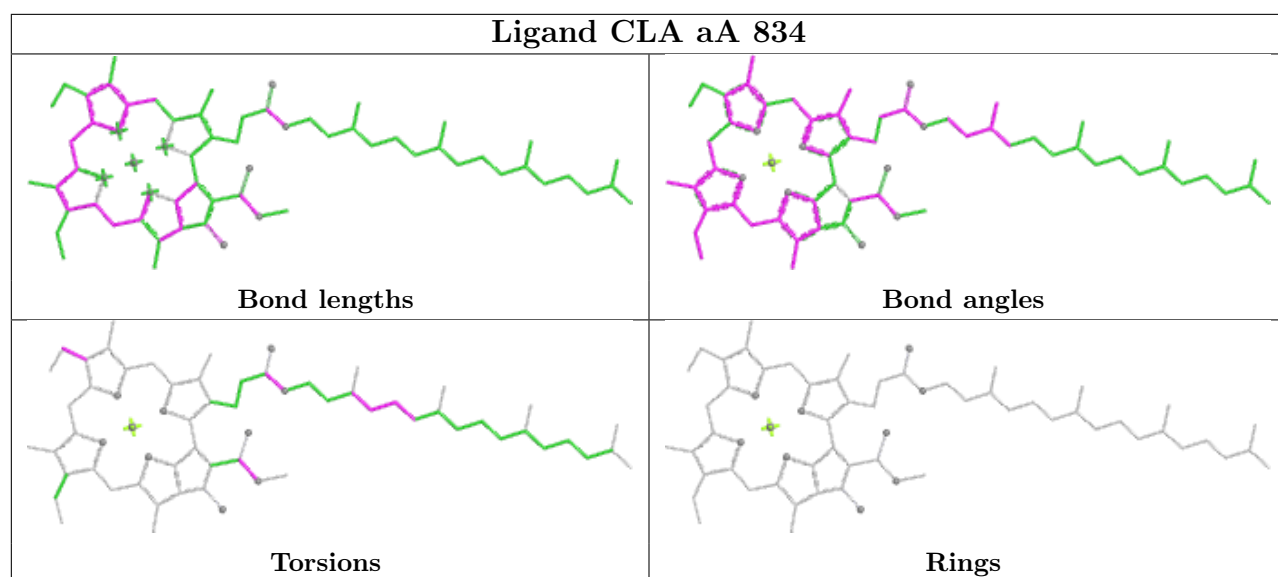
| Ligand BCR bB 844                                                                 |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

| Ligand CLA aB 801                                                                   |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

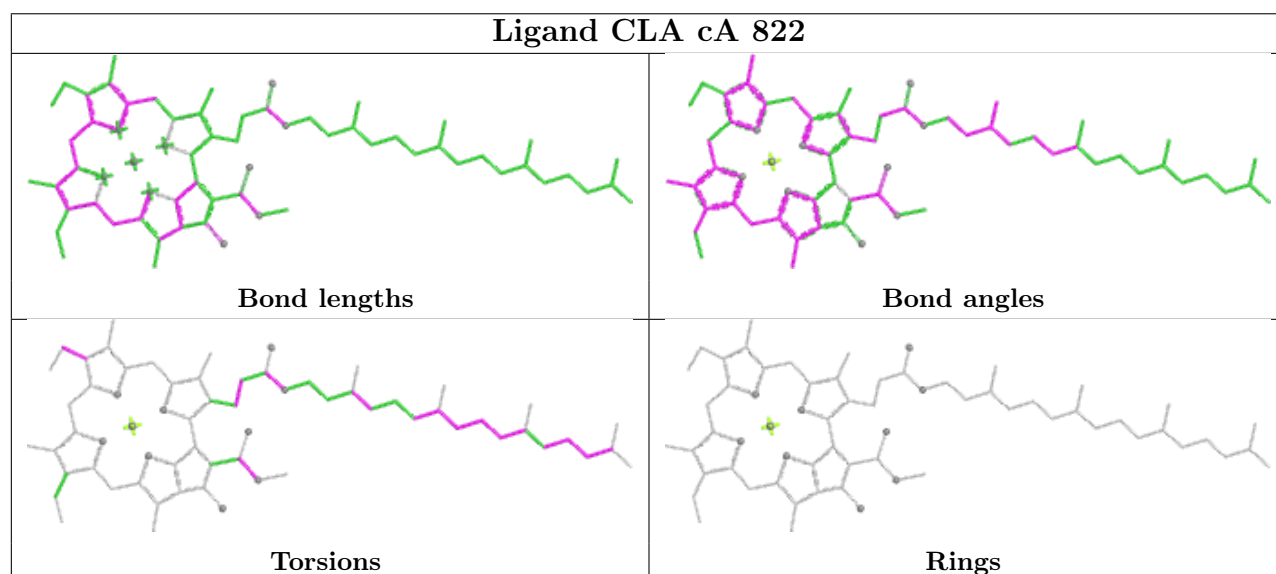
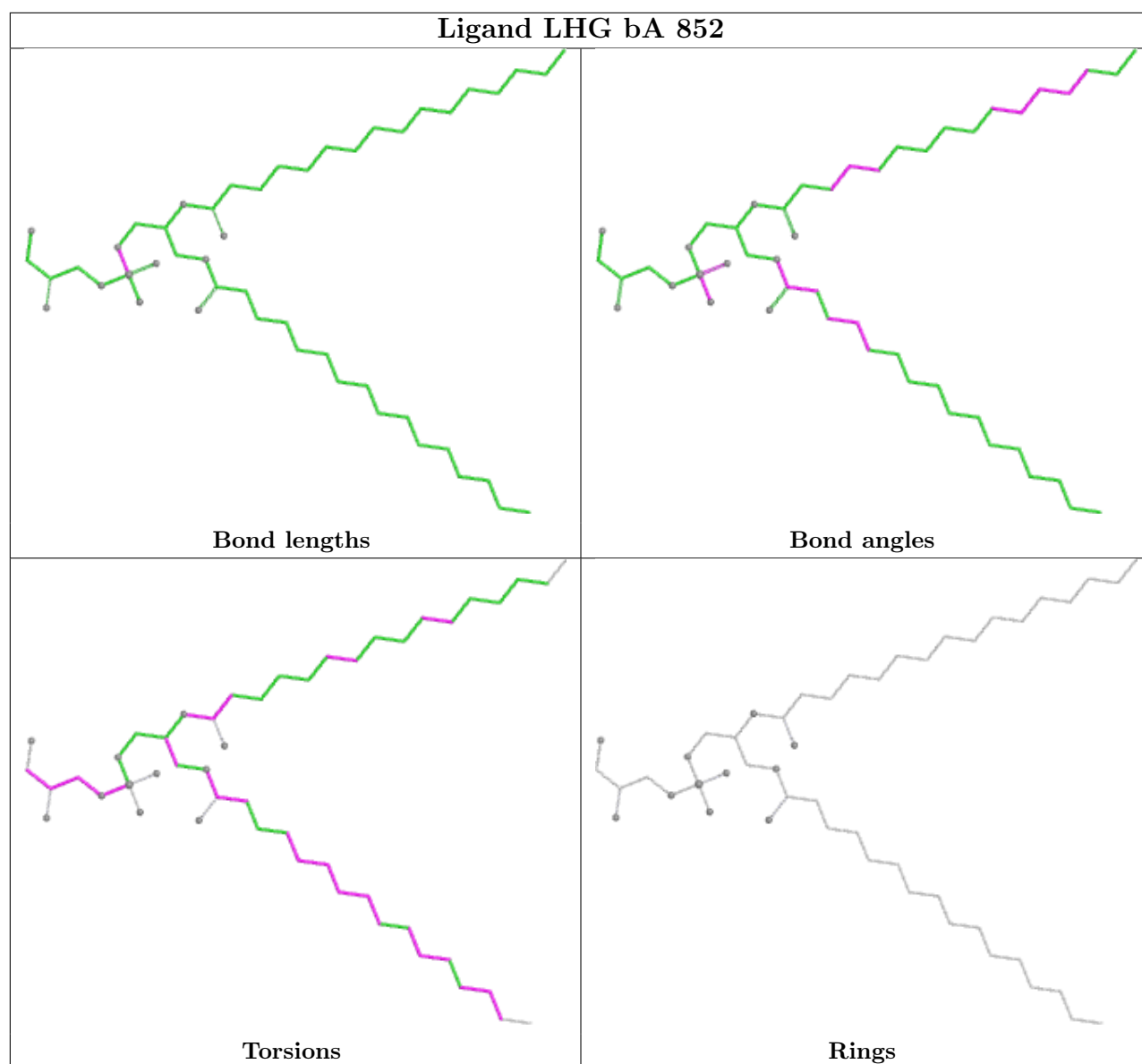




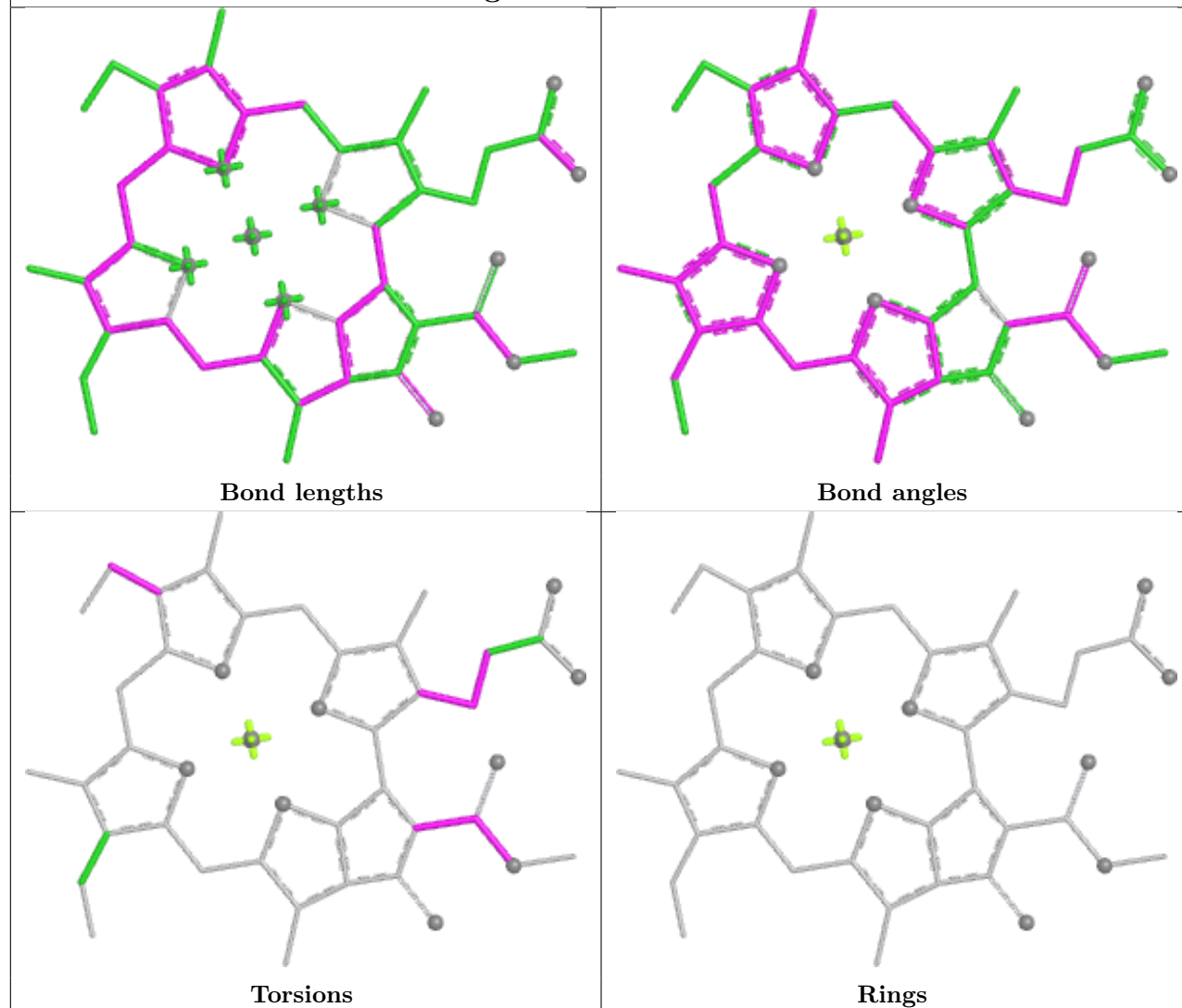




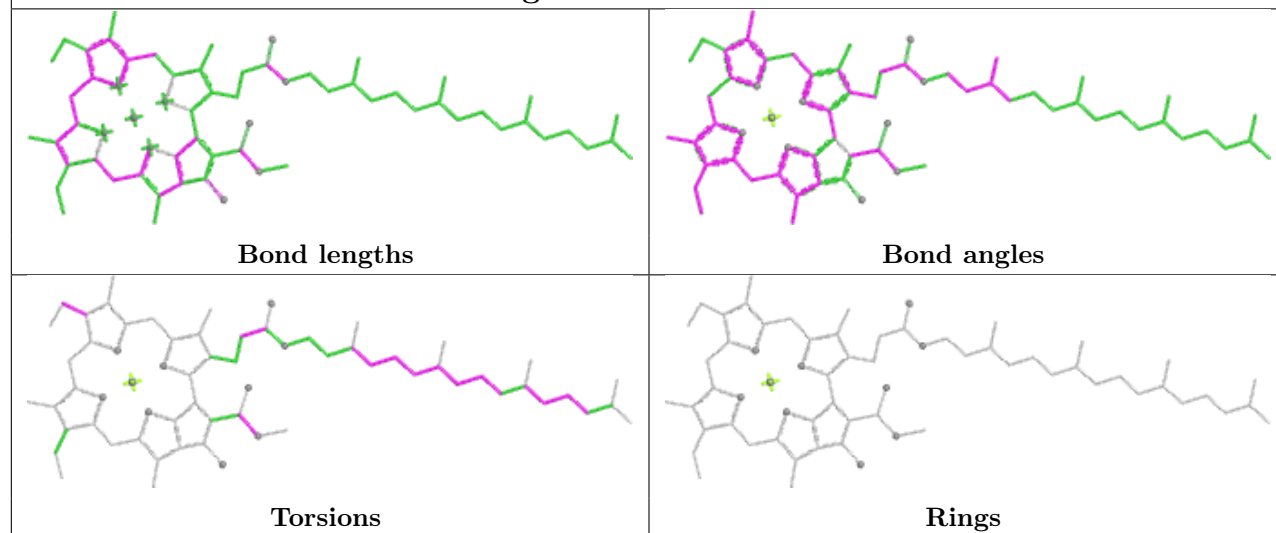


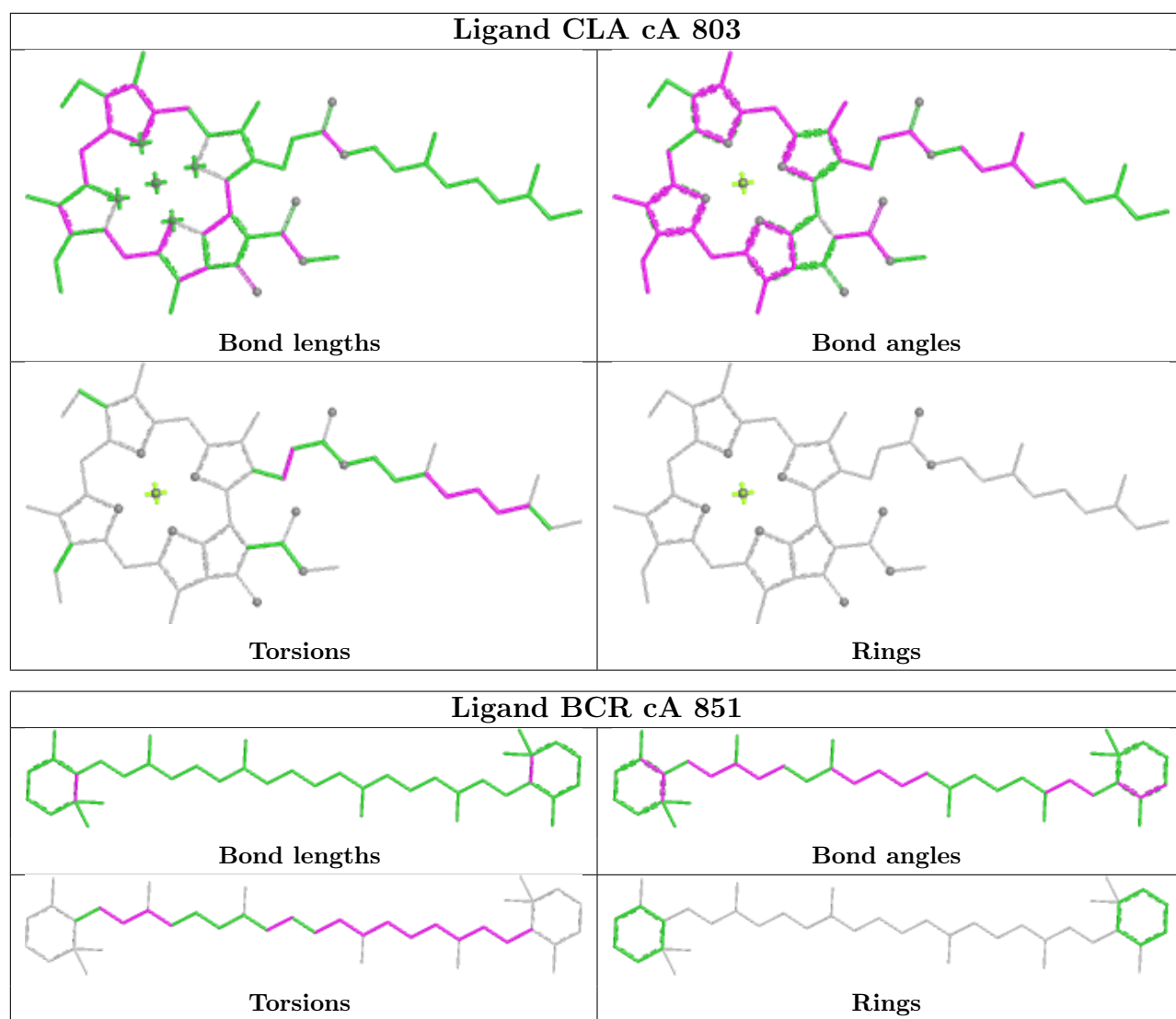


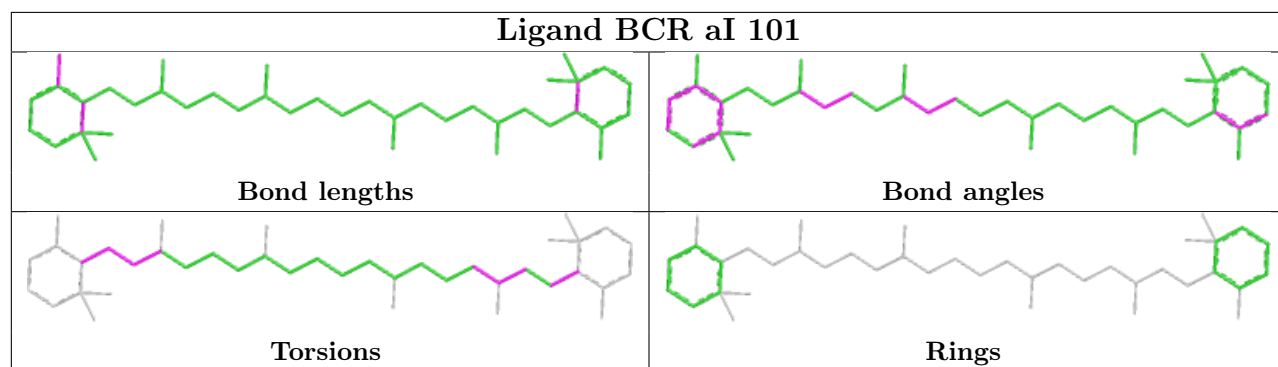
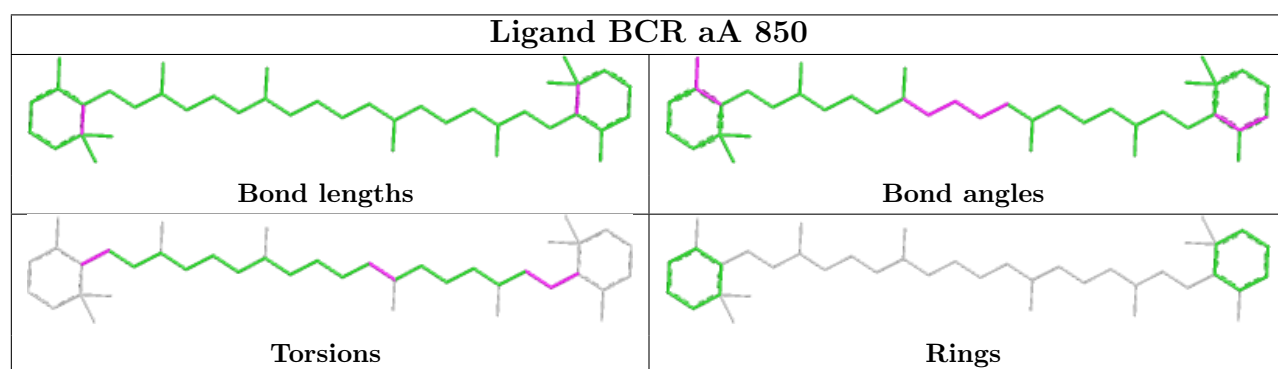
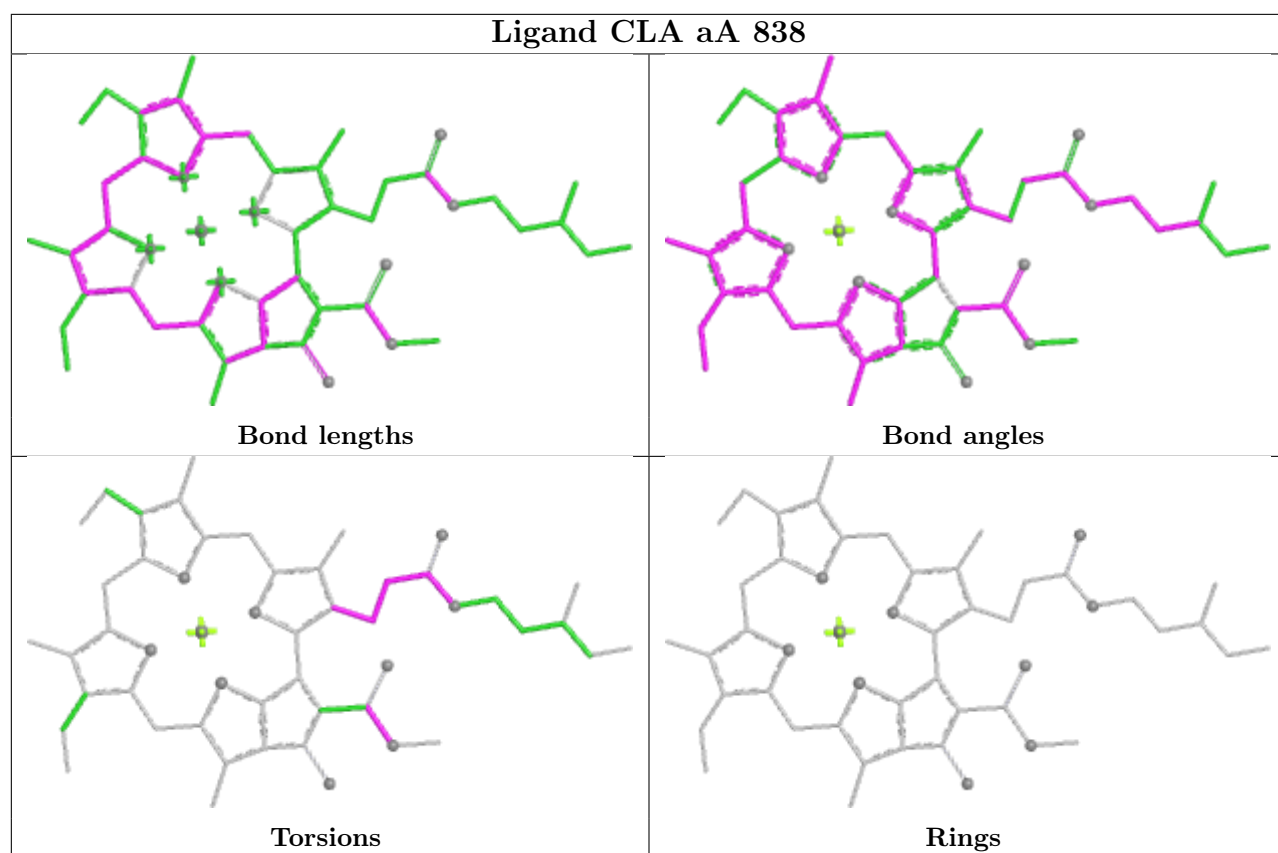
## Ligand CLA aA 809

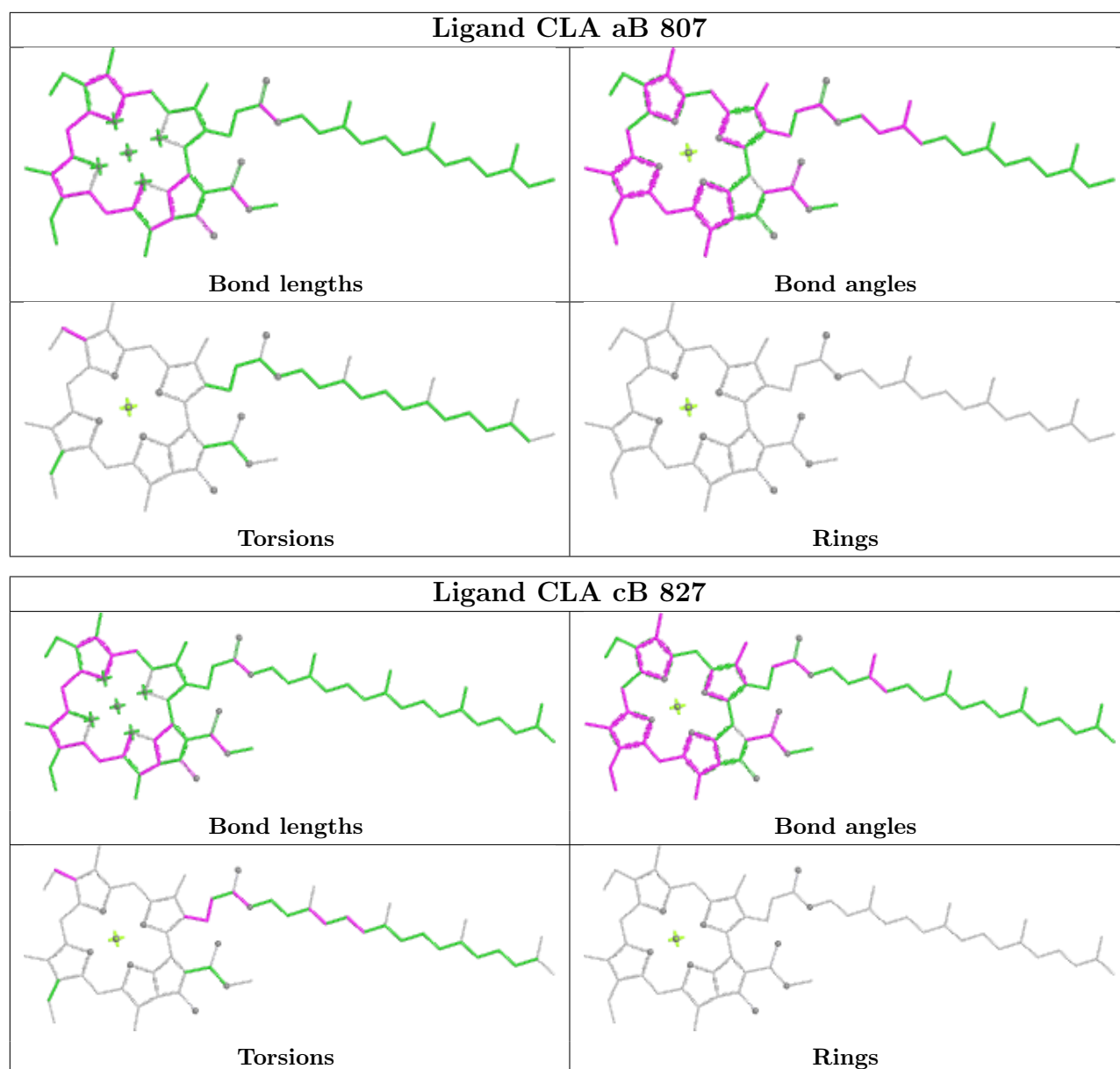


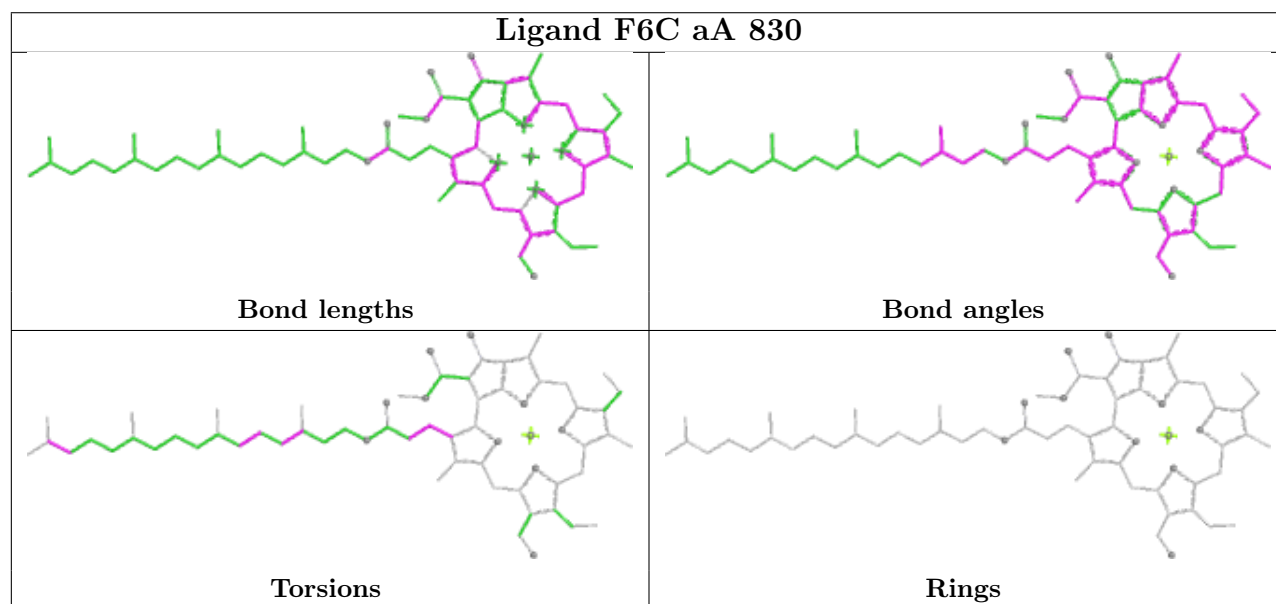
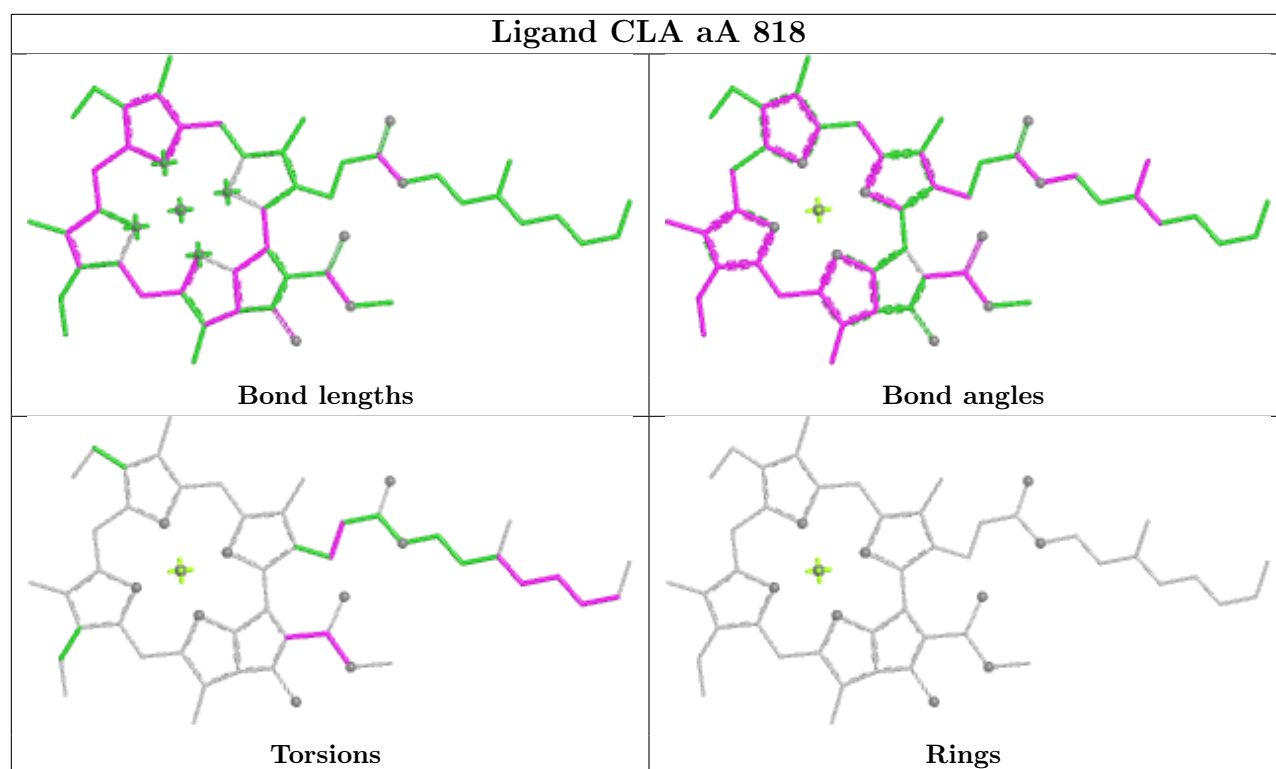
## Ligand CLA bB 806

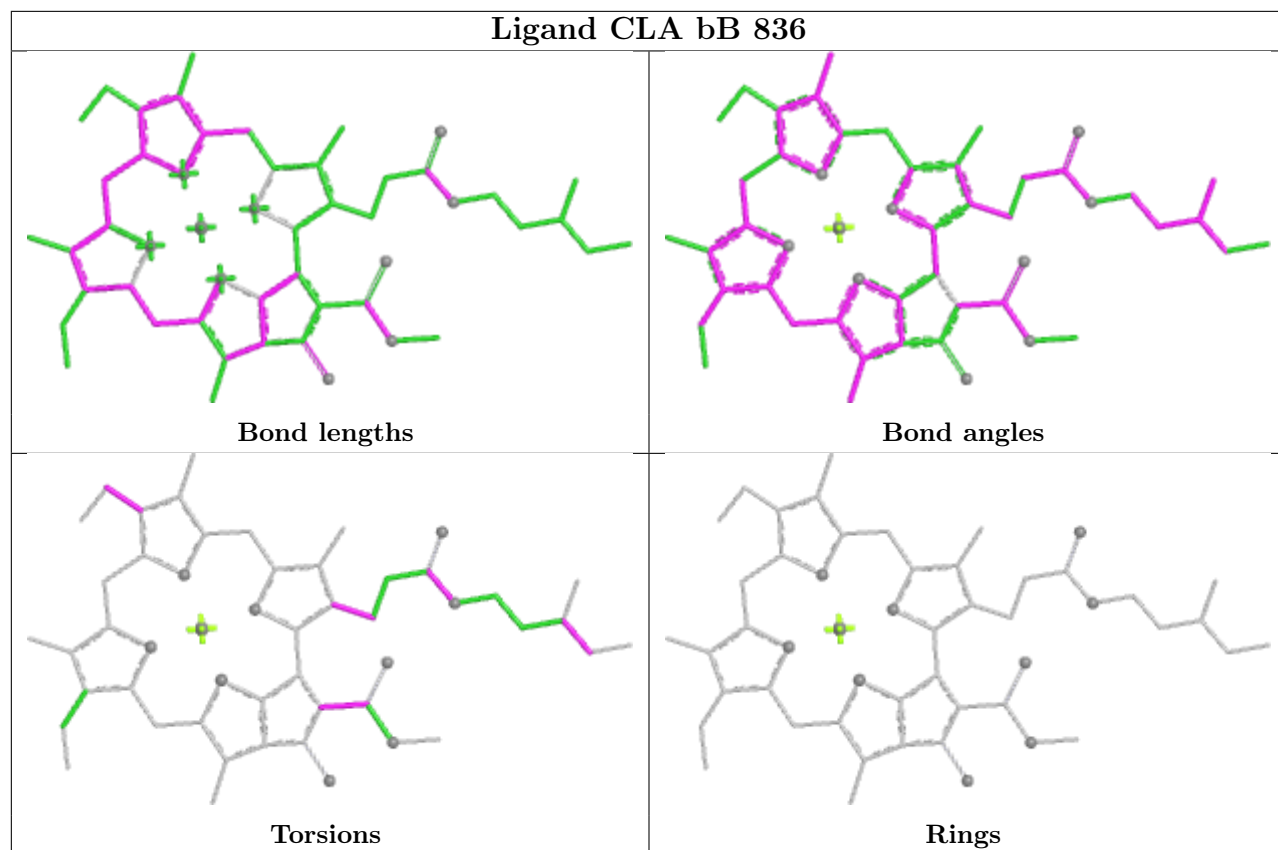




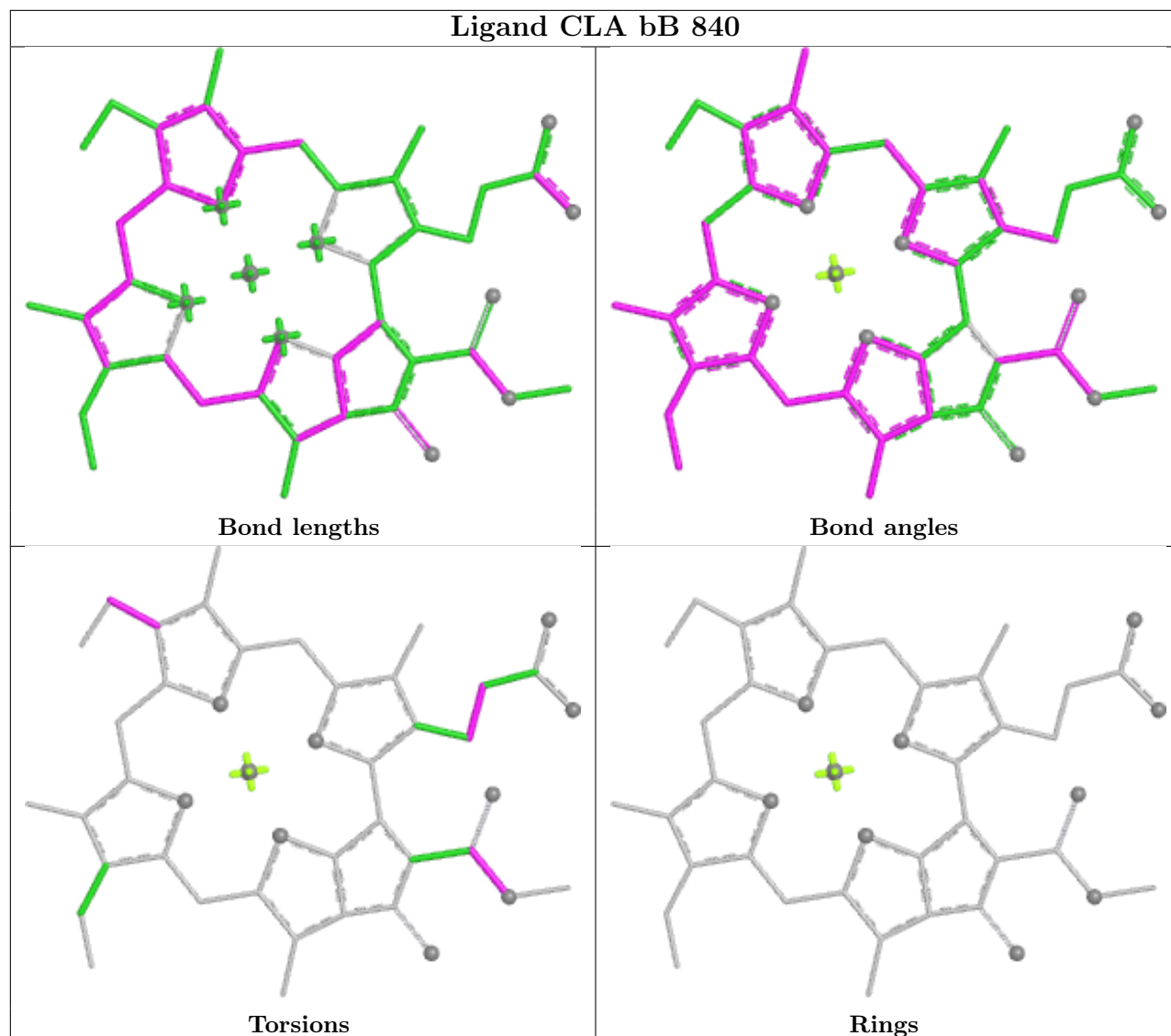




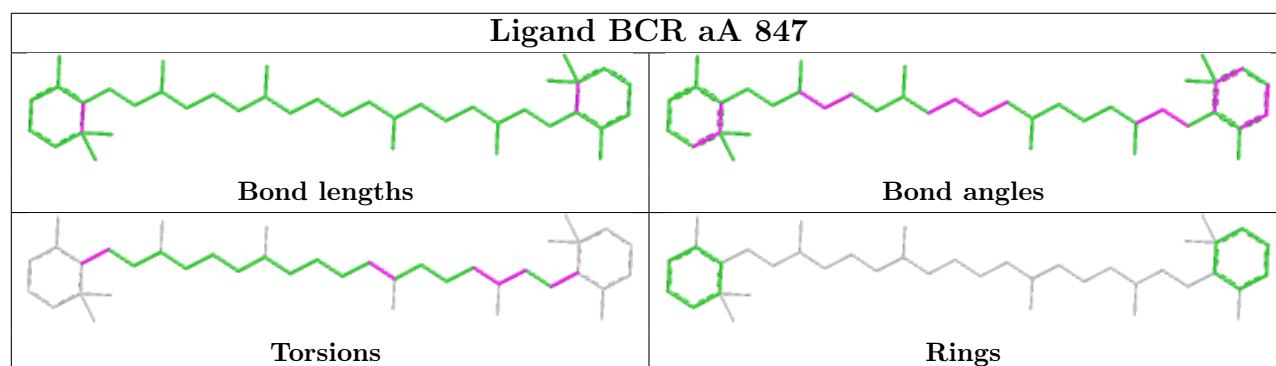




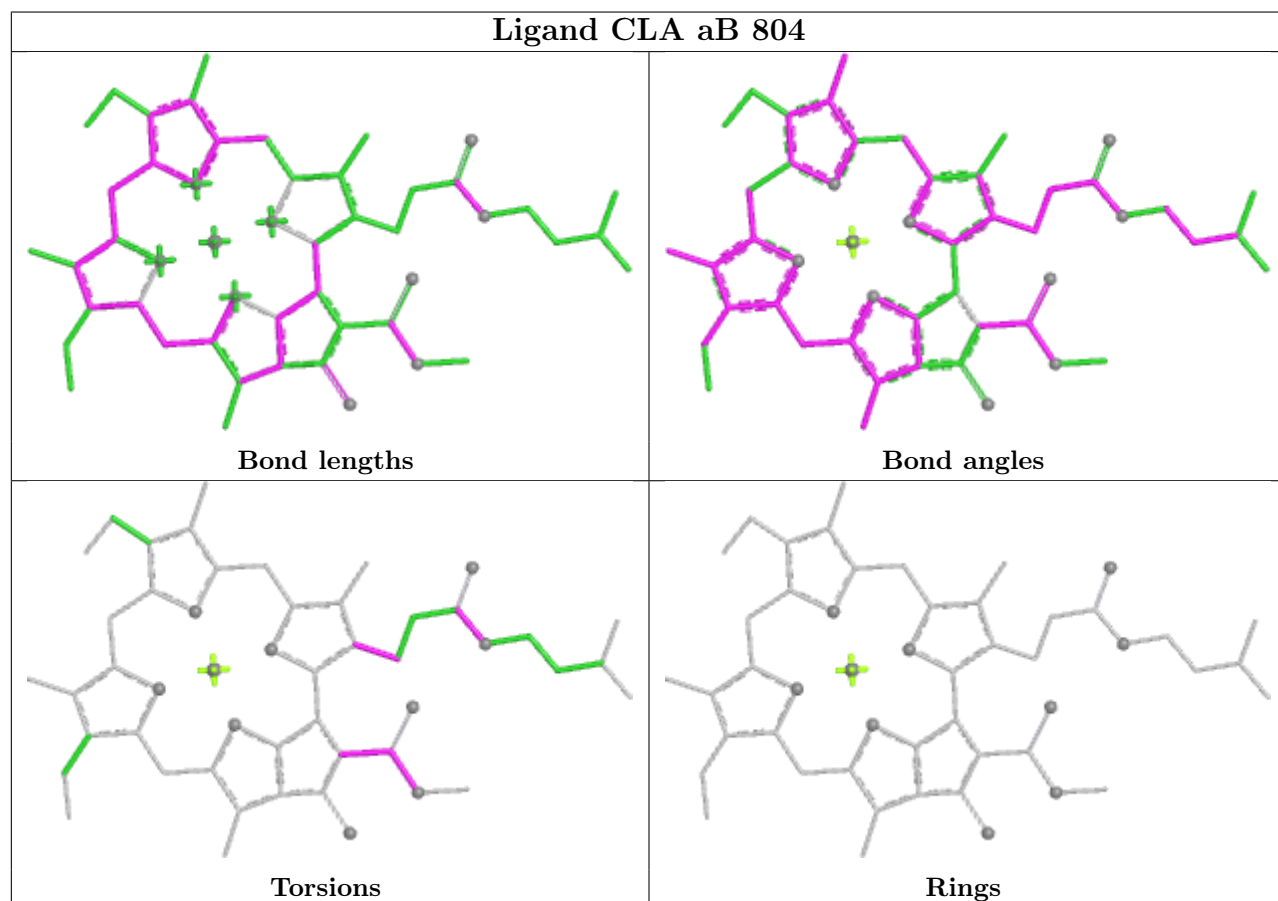
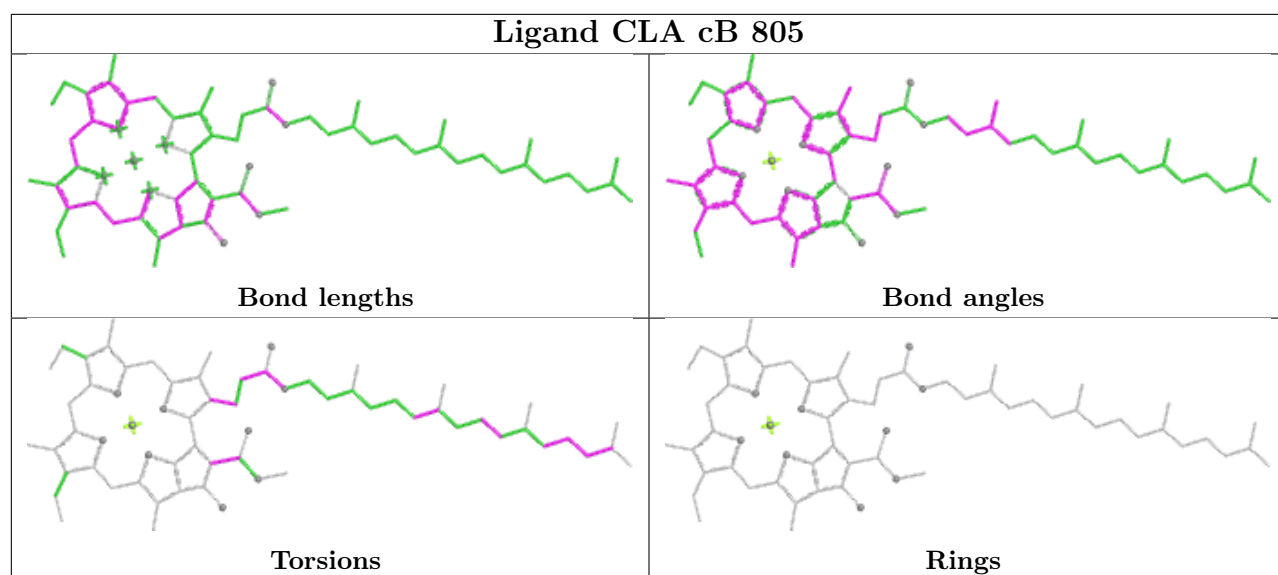
## Ligand CLA bB 840

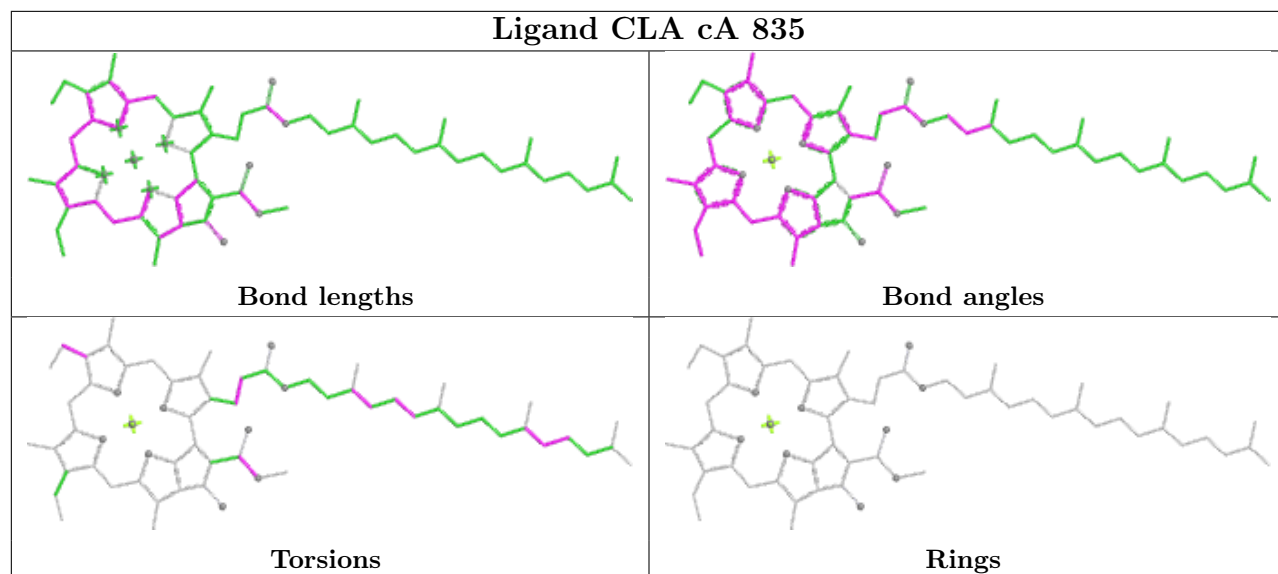
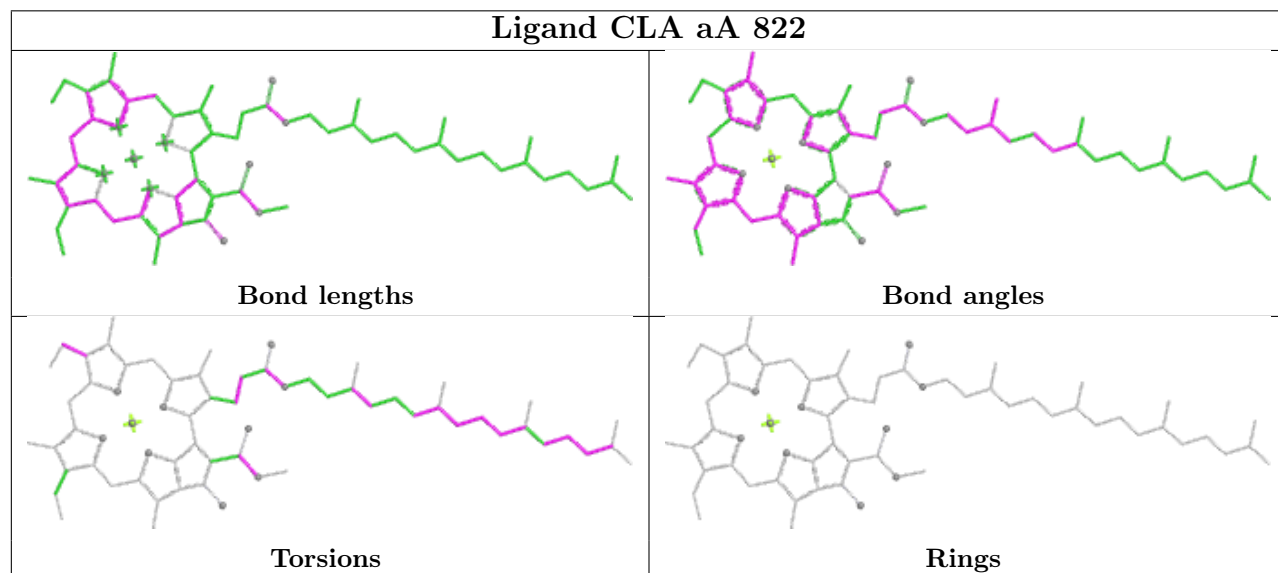


## Ligand BCR aA 847

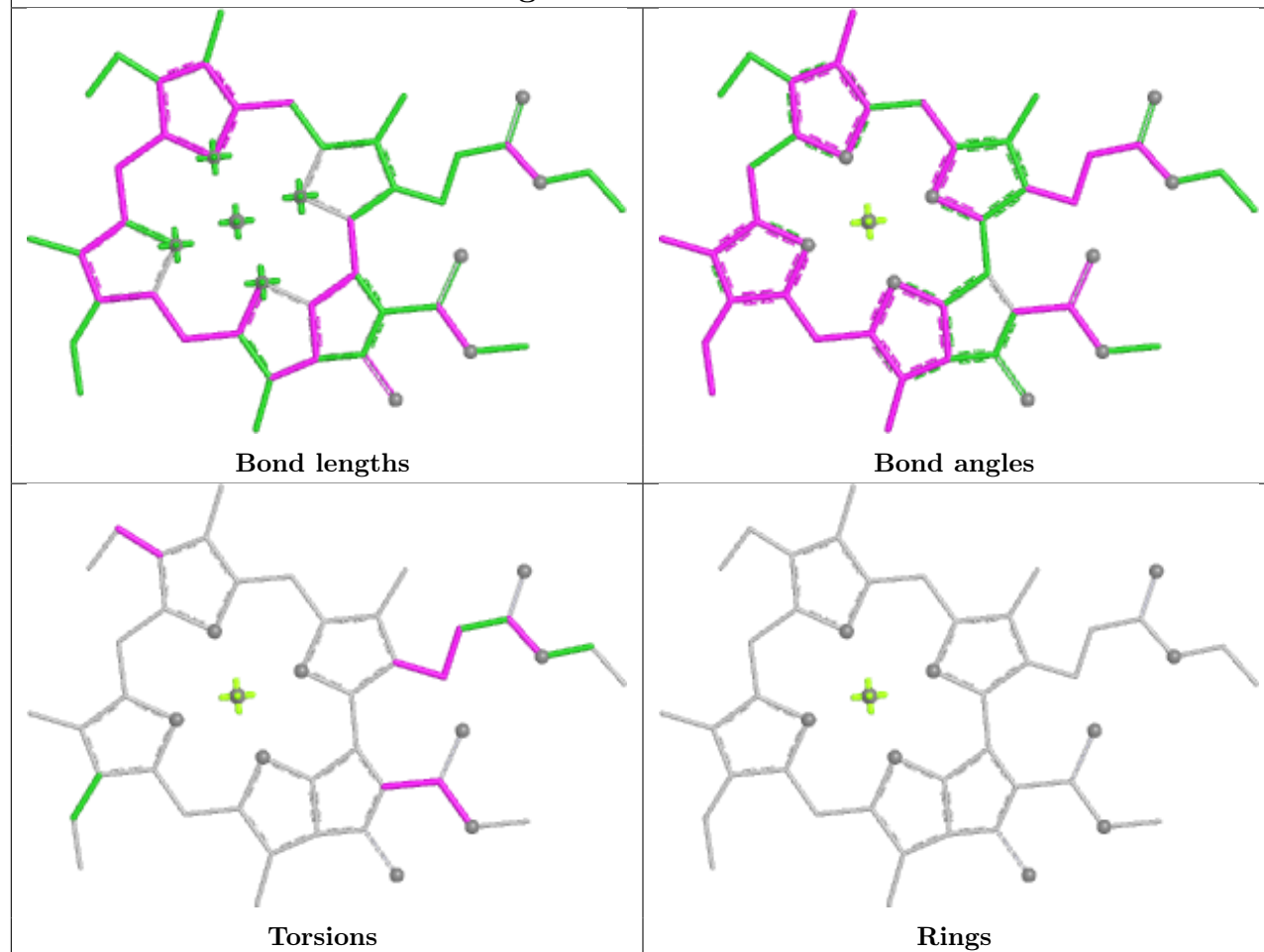




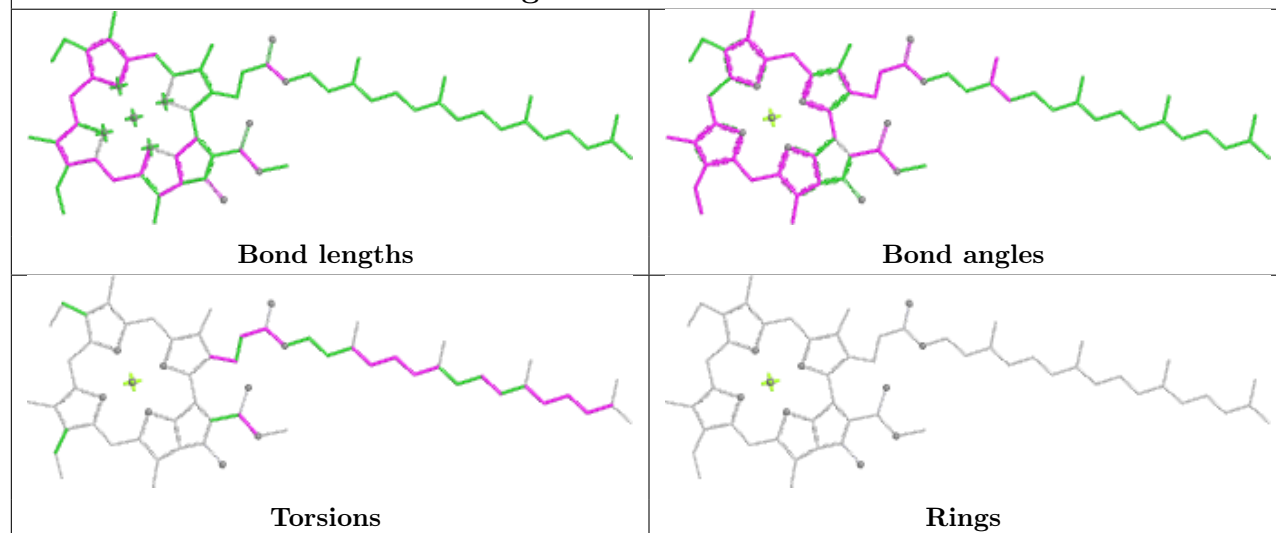


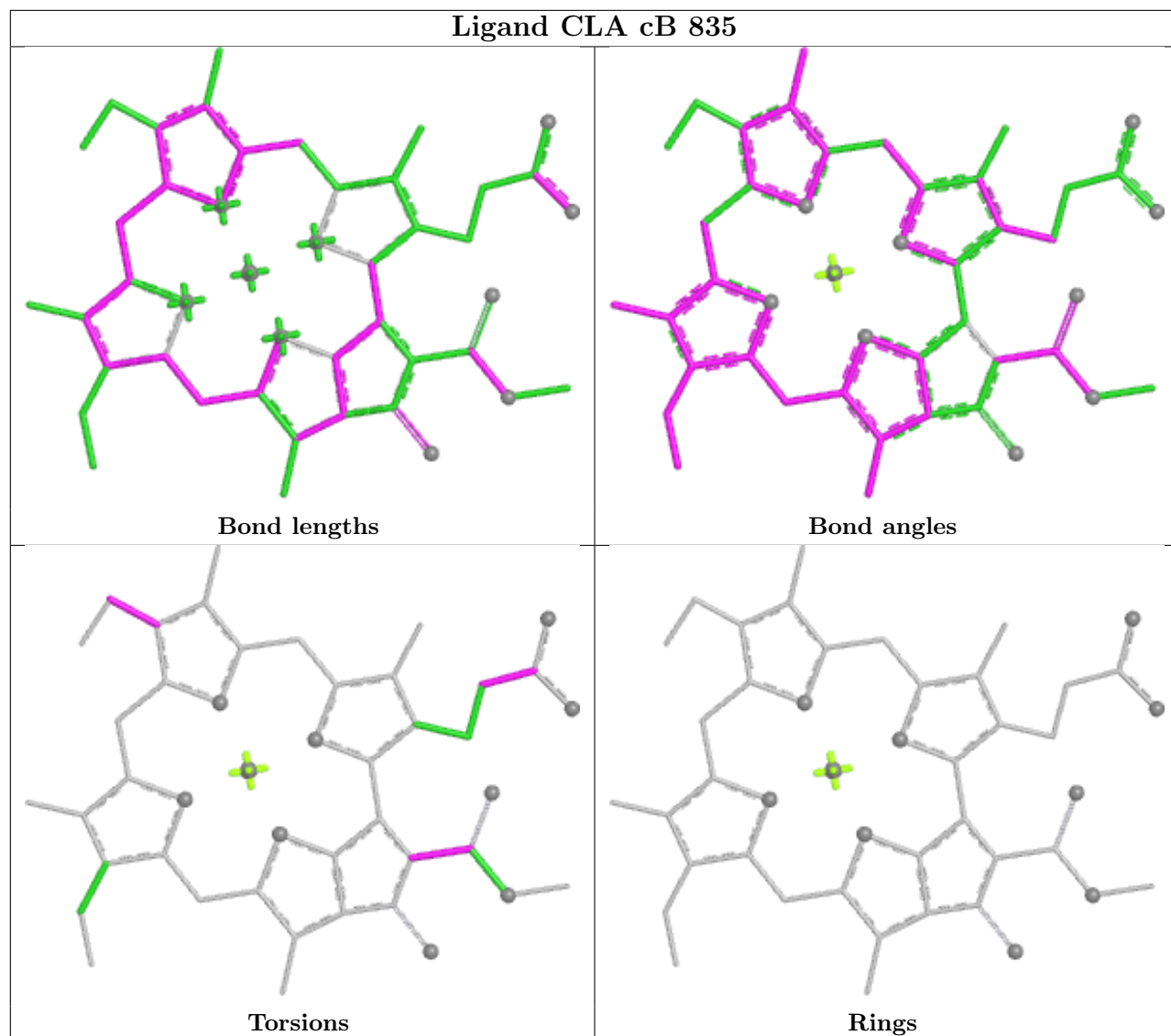
**Ligand CLA cA 835****Ligand CLA aA 822**

## Ligand CLA aB 819

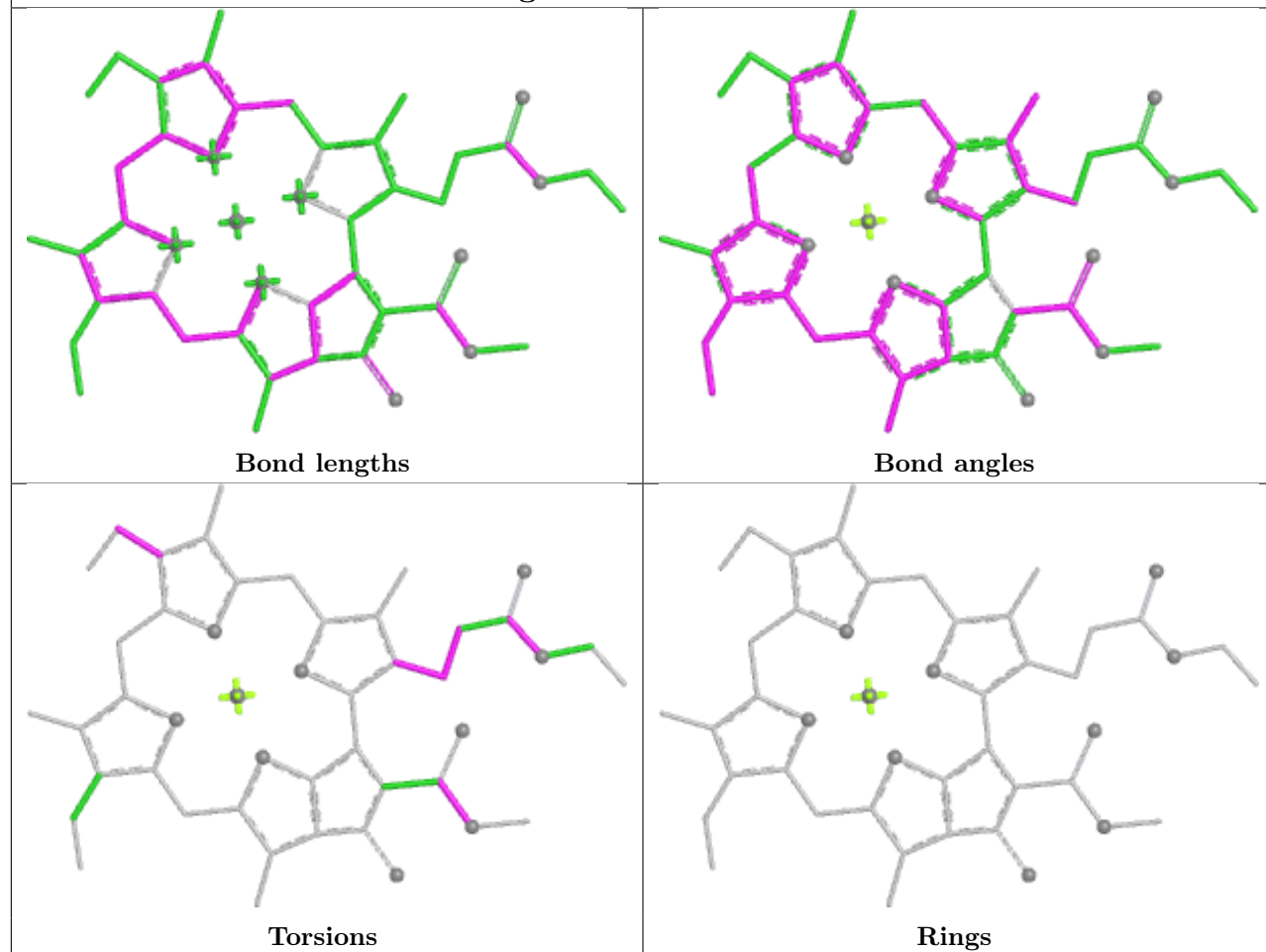


## Ligand CLA bA 840

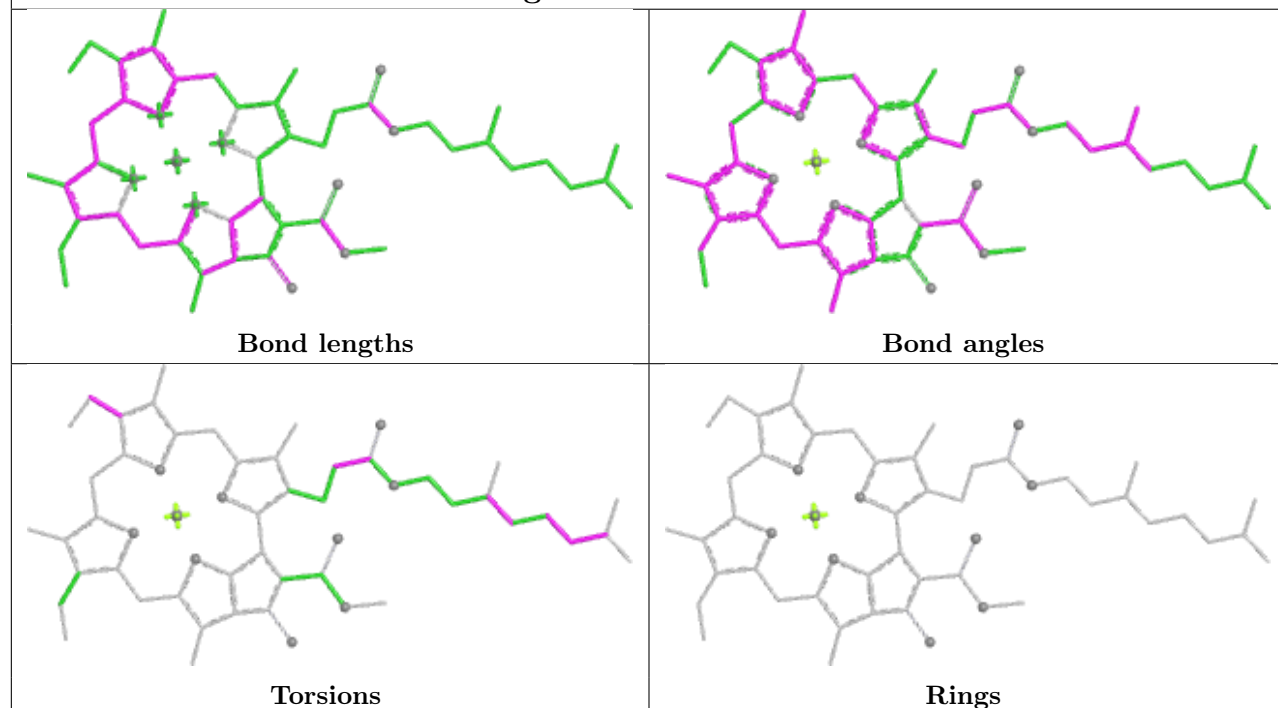


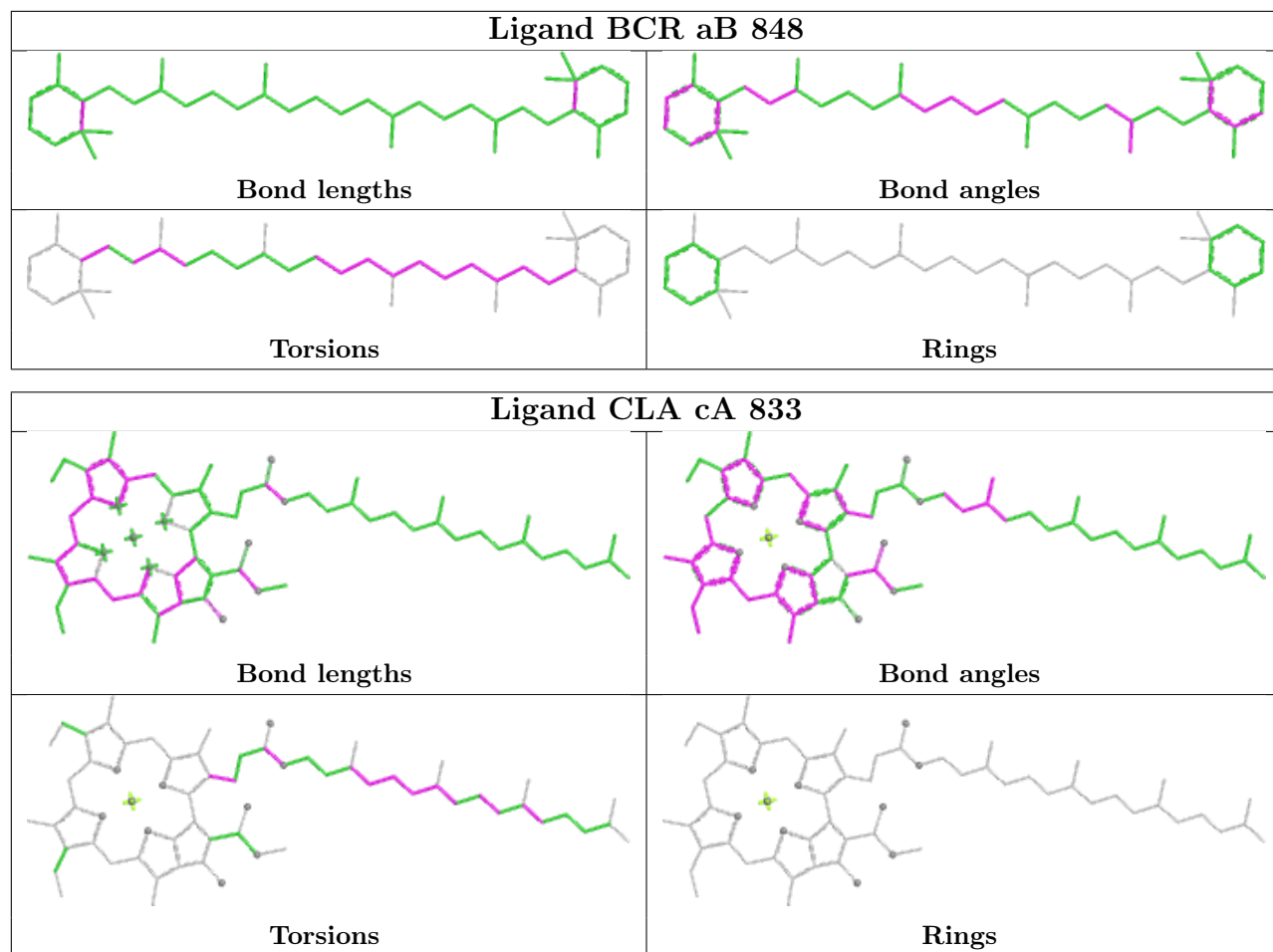


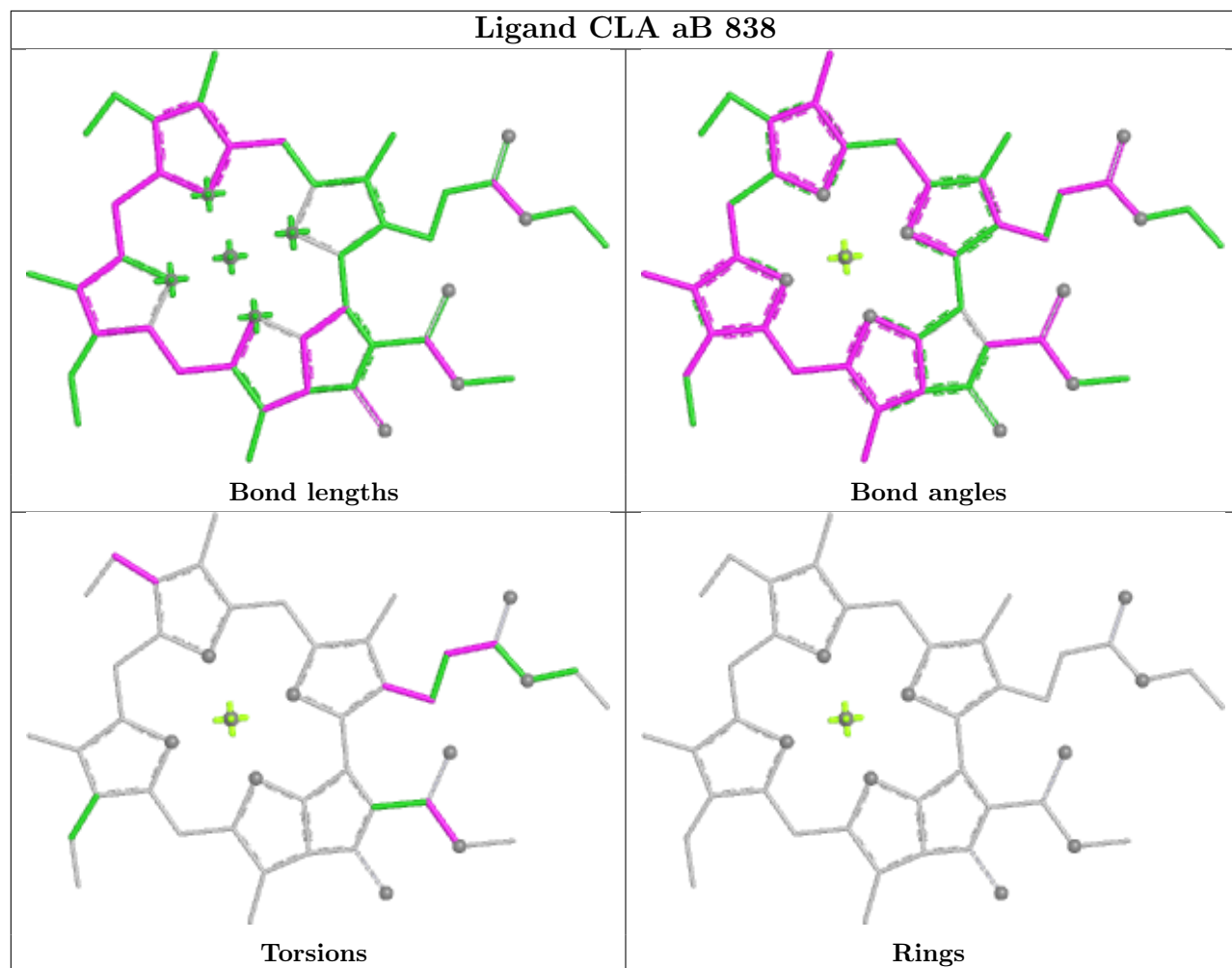
## Ligand CLA aB 809

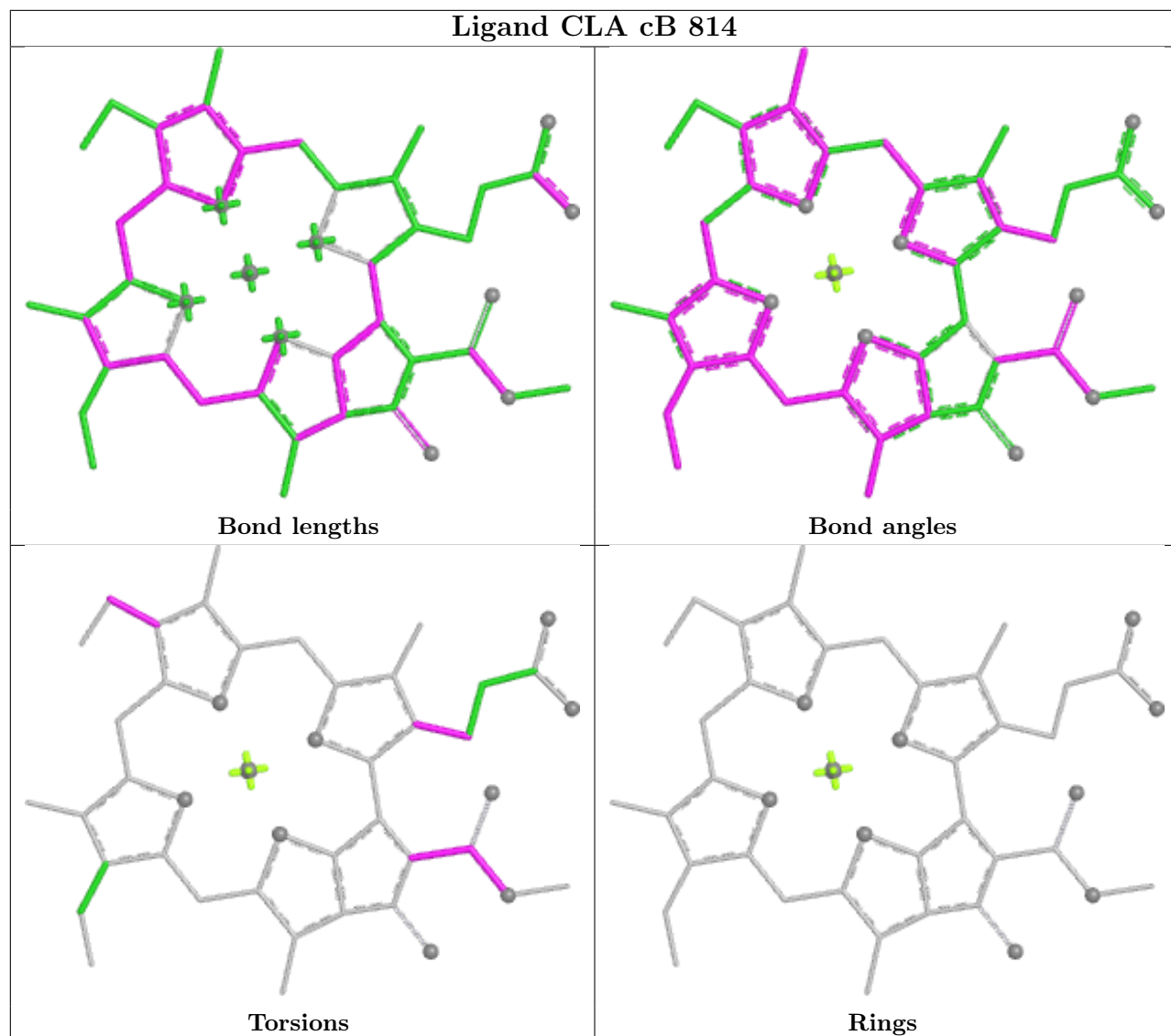


## Ligand CLA aB 837

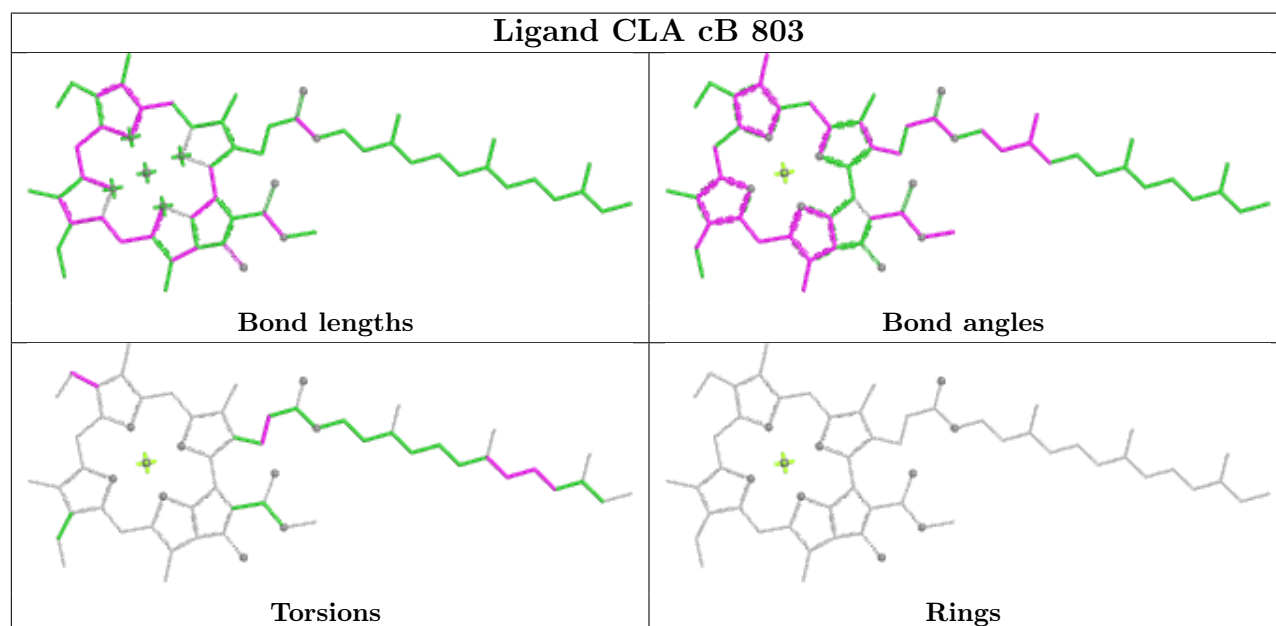
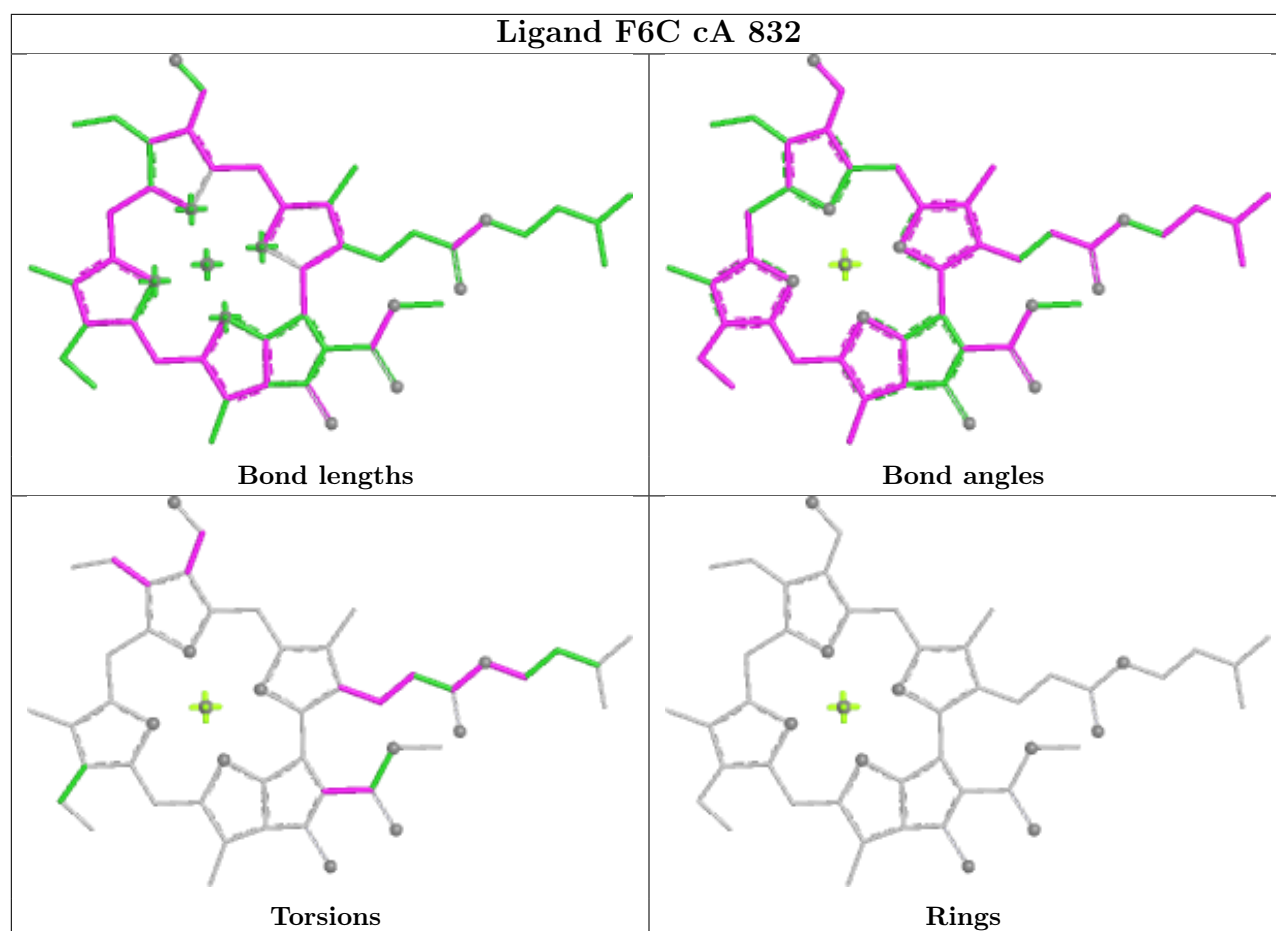


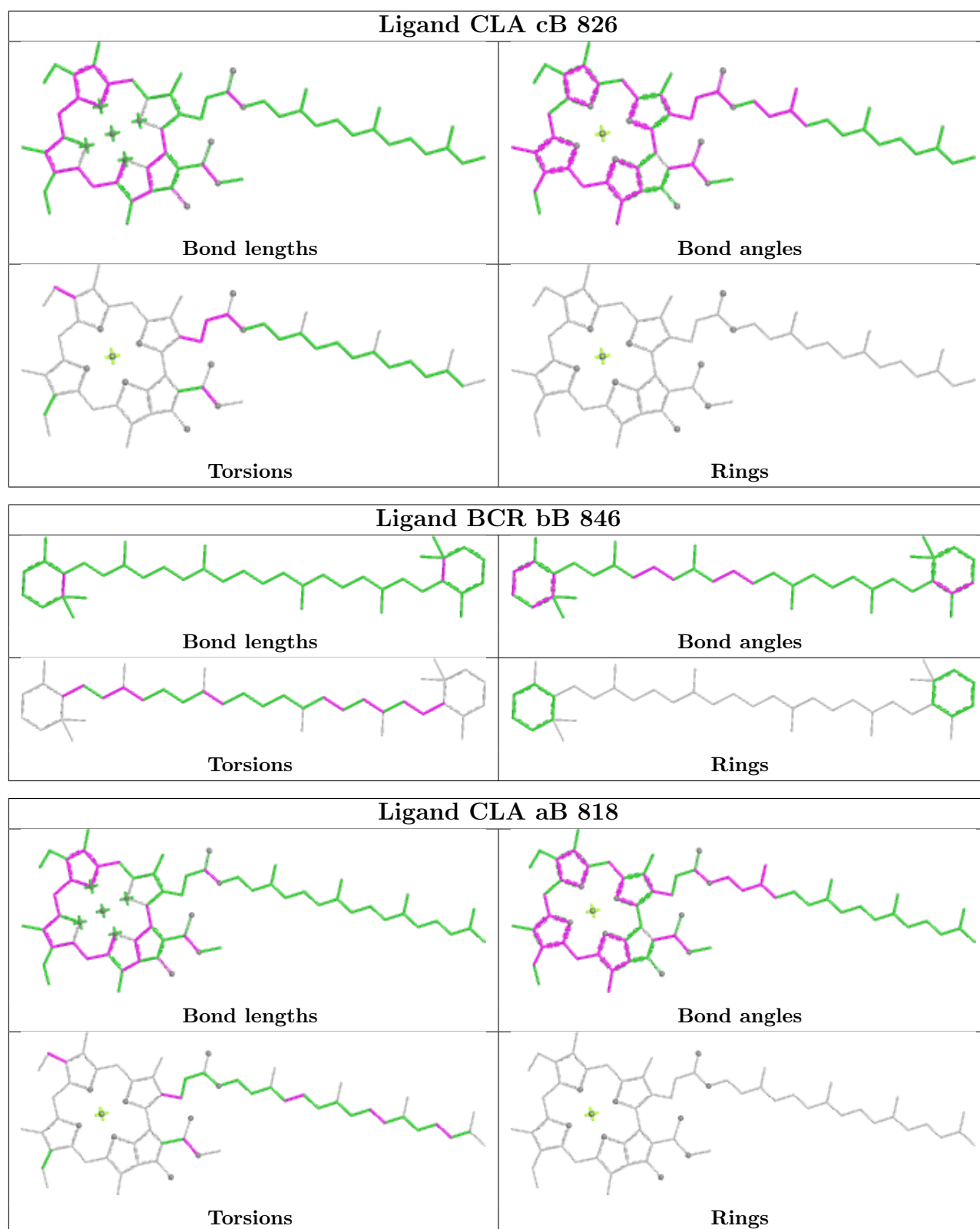


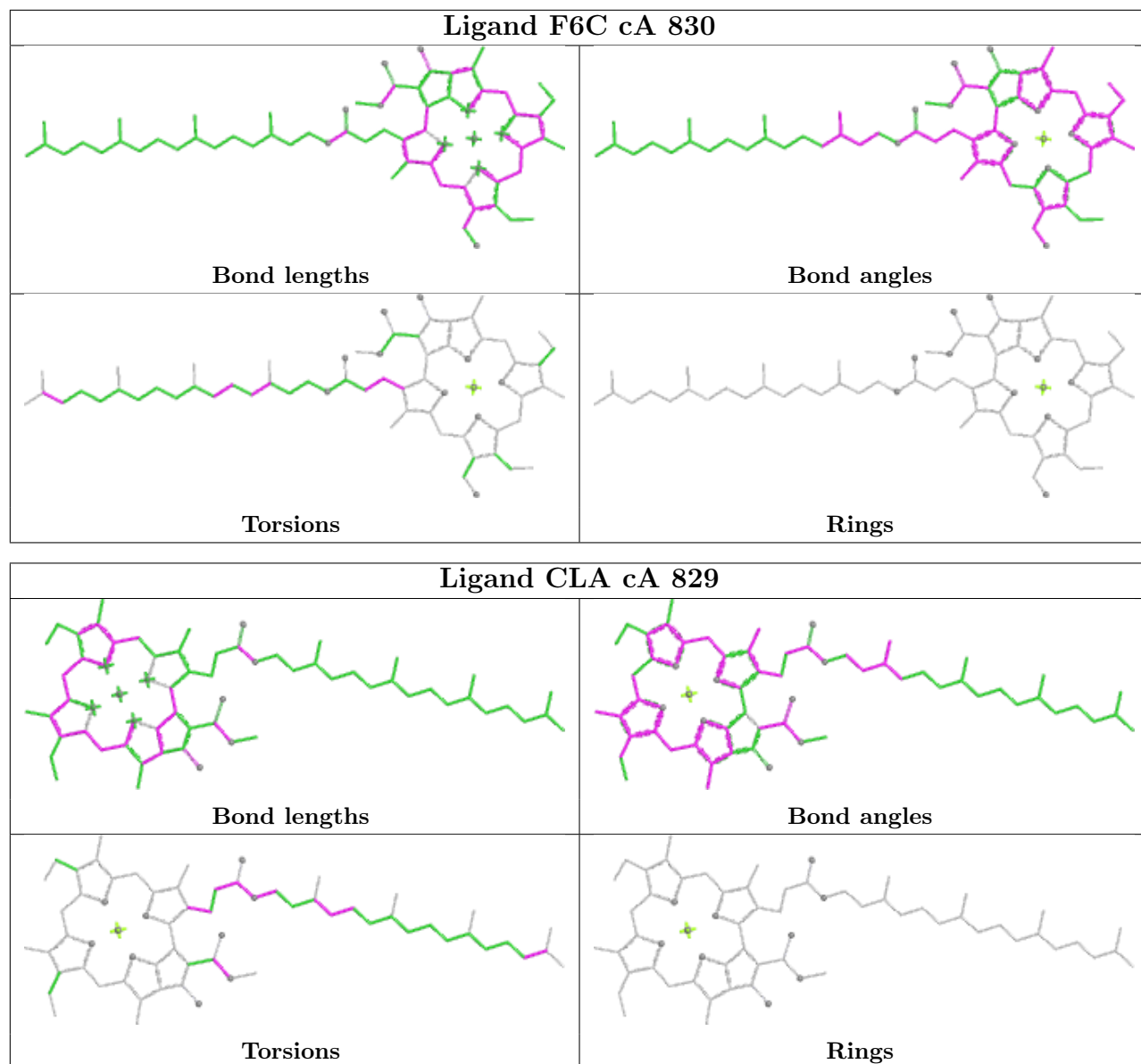


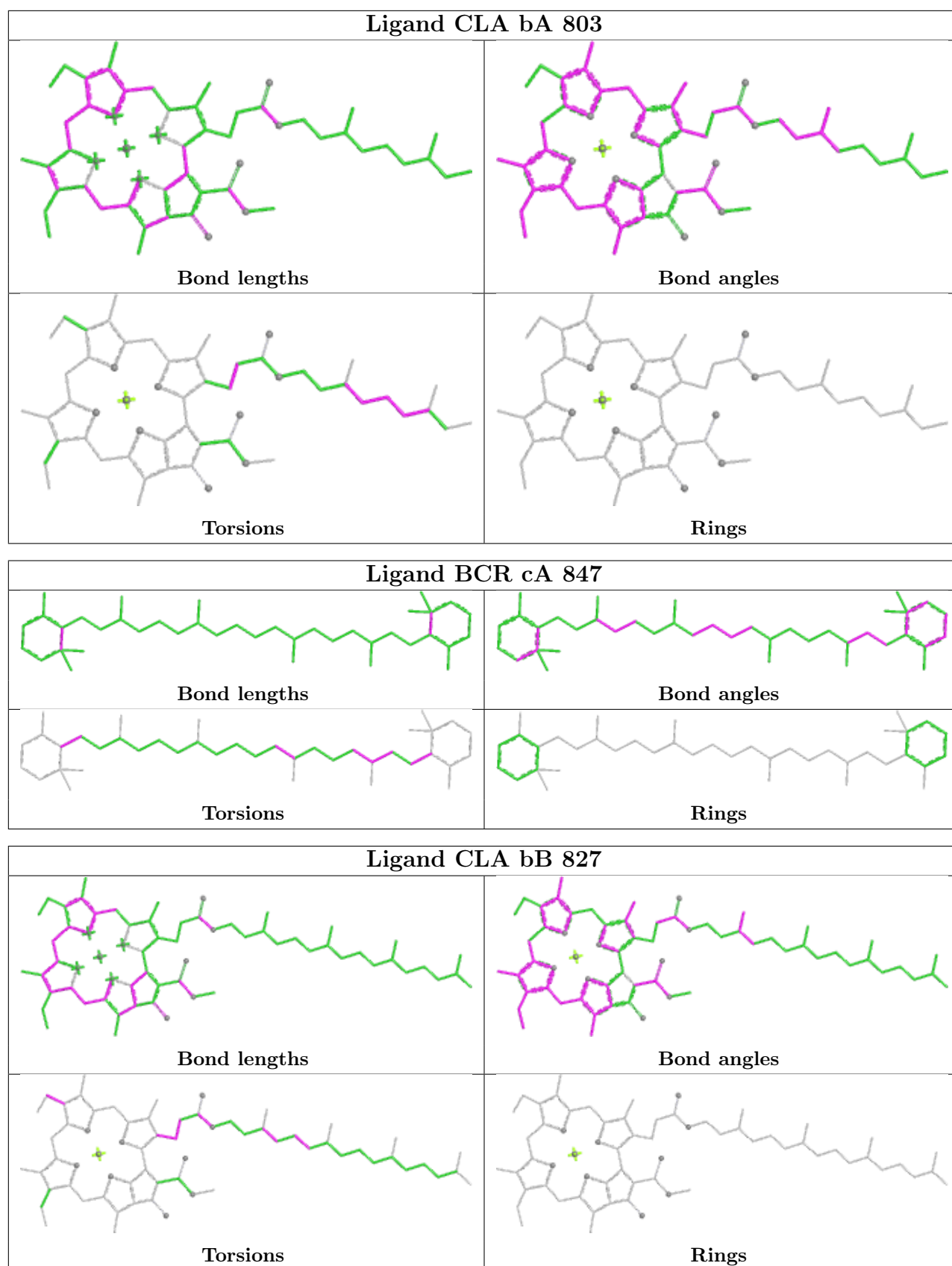




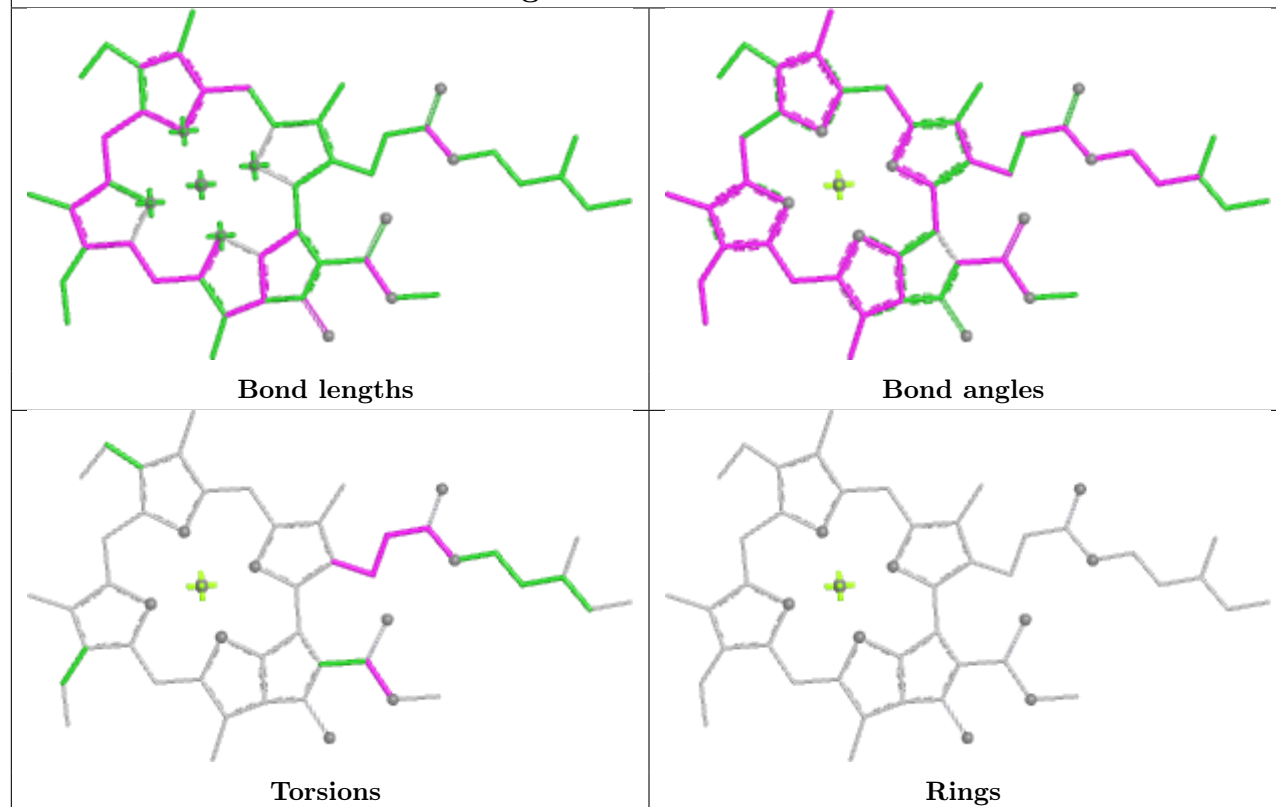




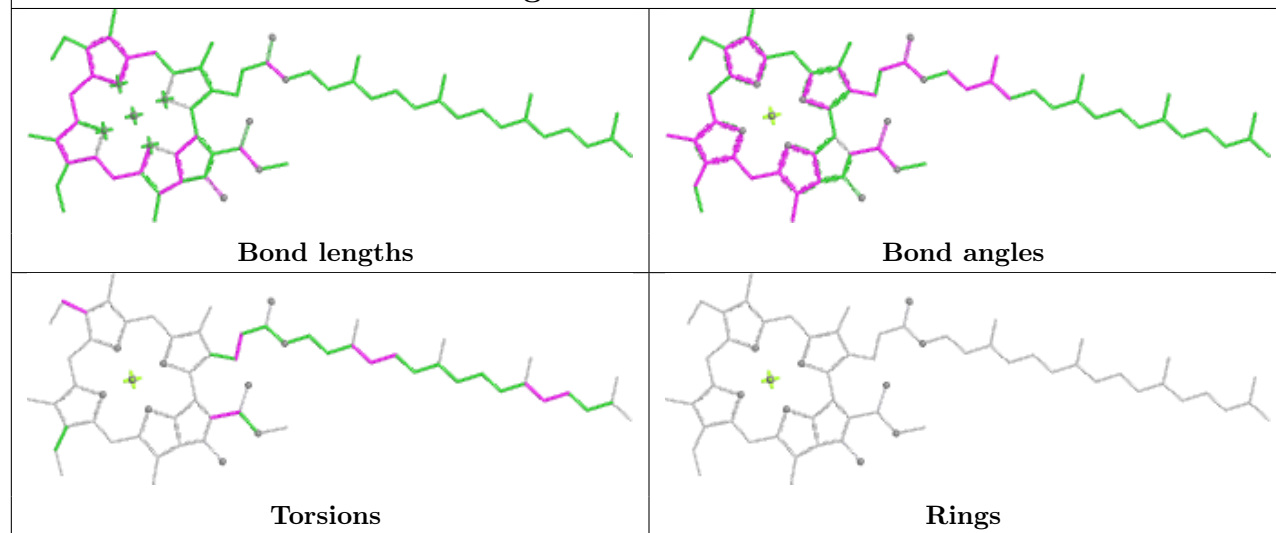


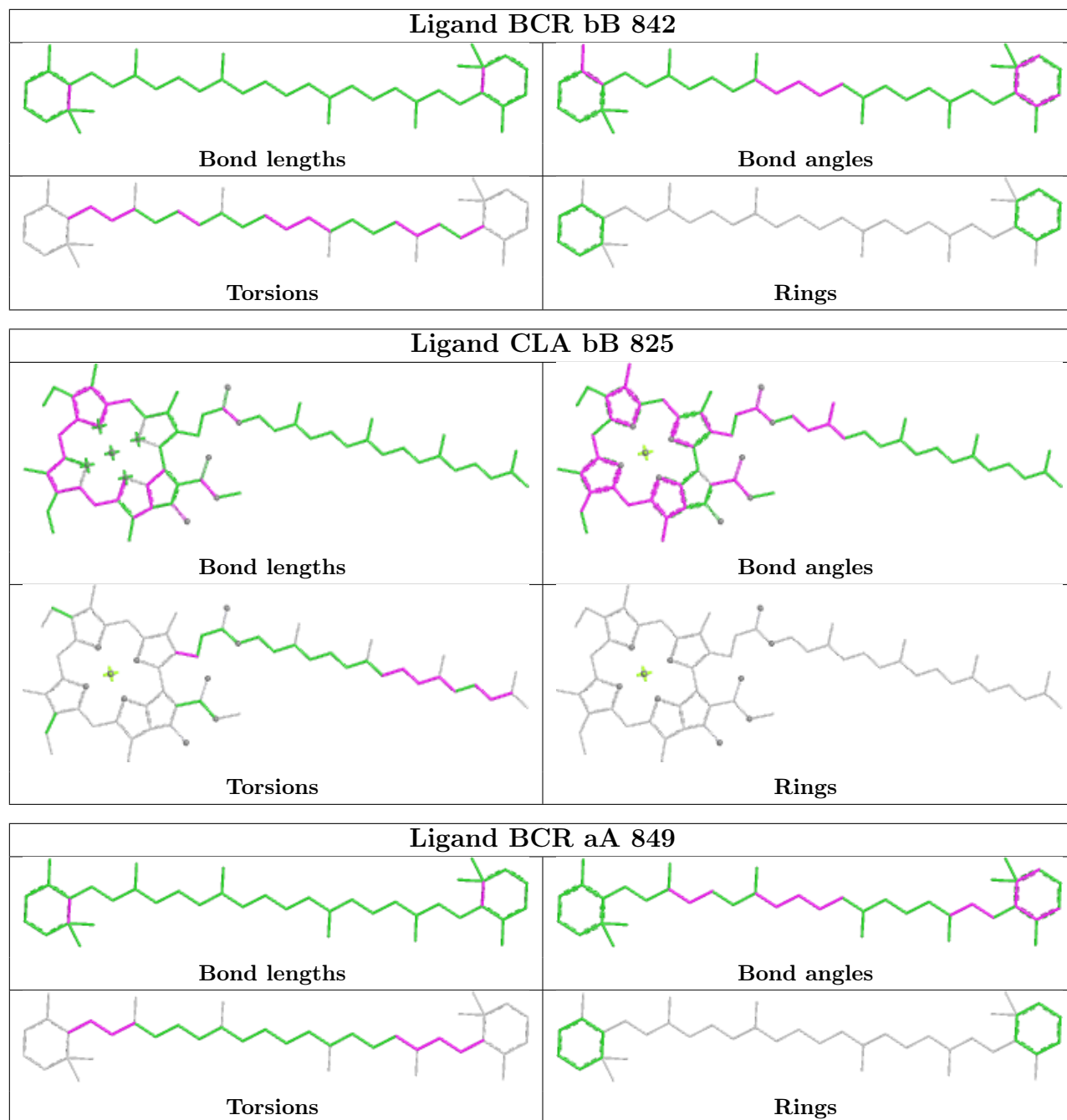


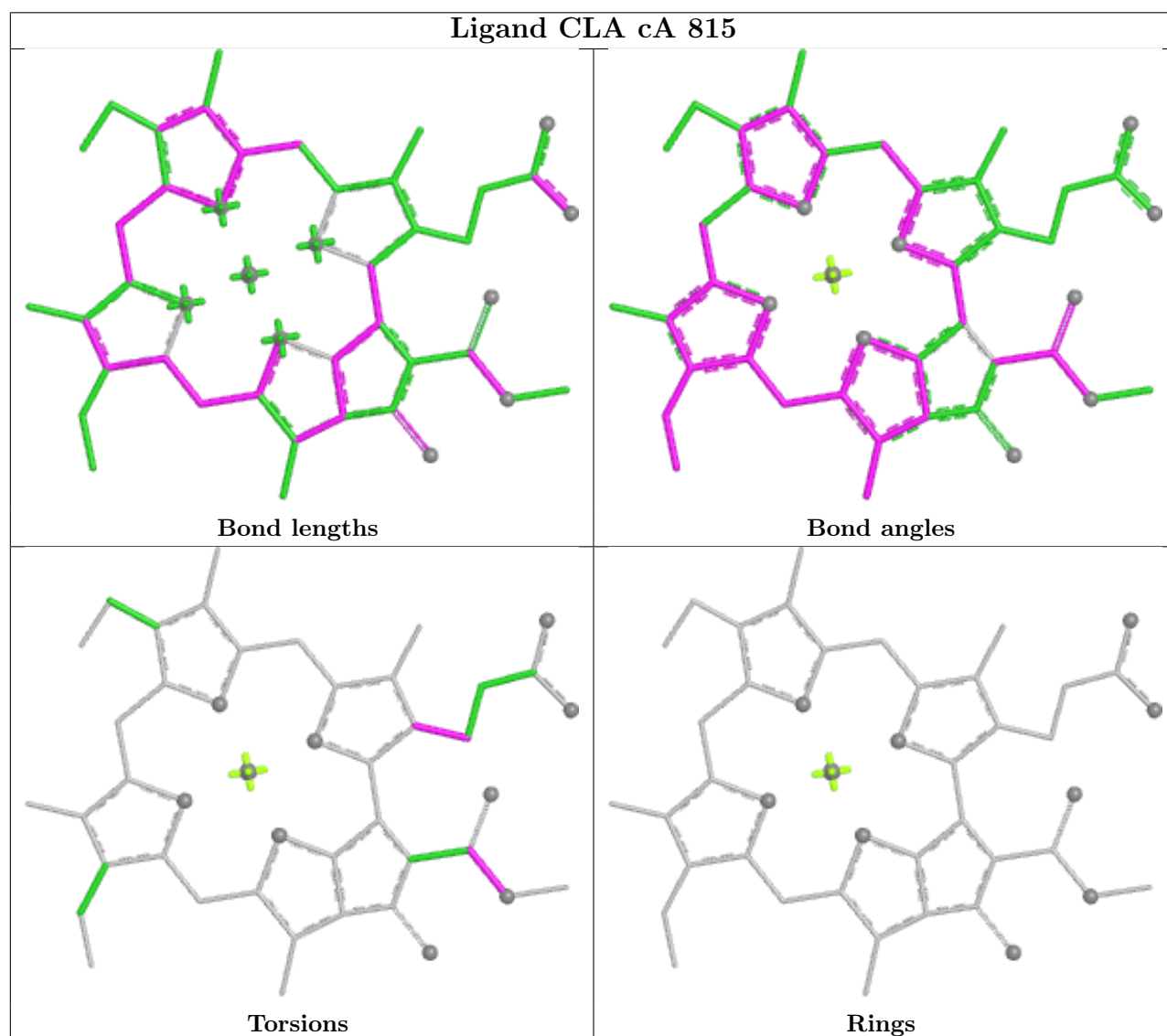
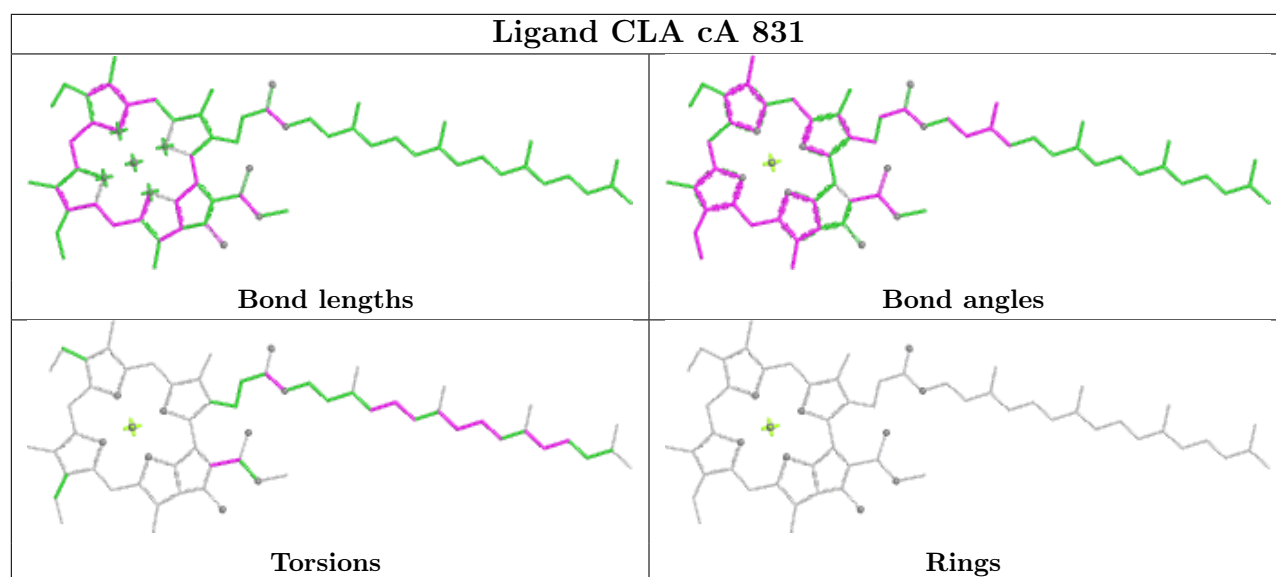
## Ligand CLA bA 838

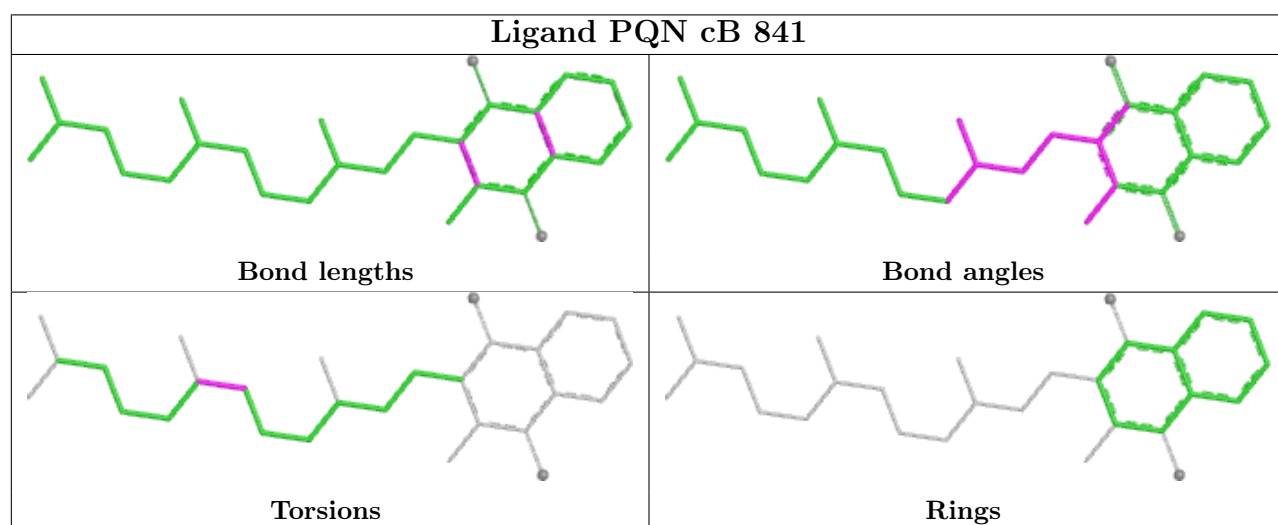
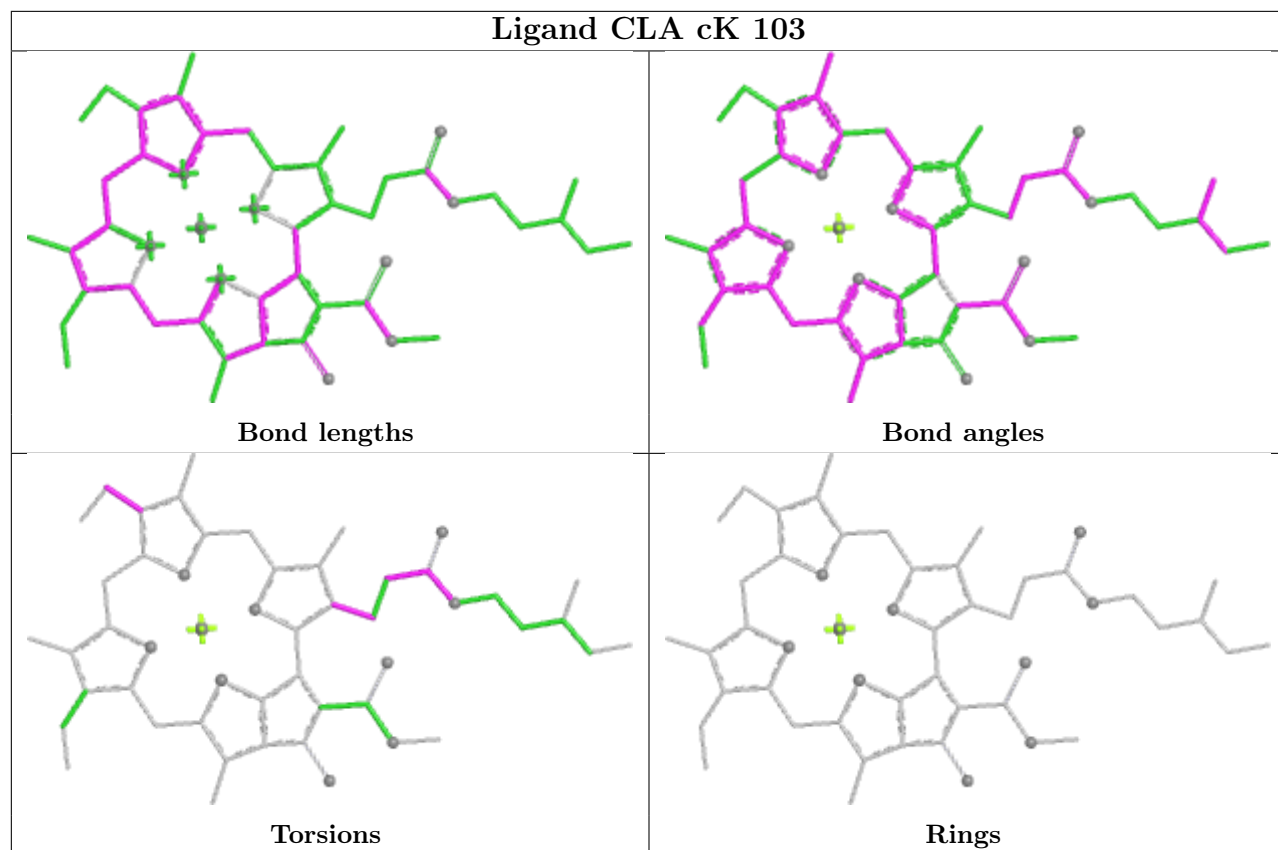


## Ligand CLA aB 839



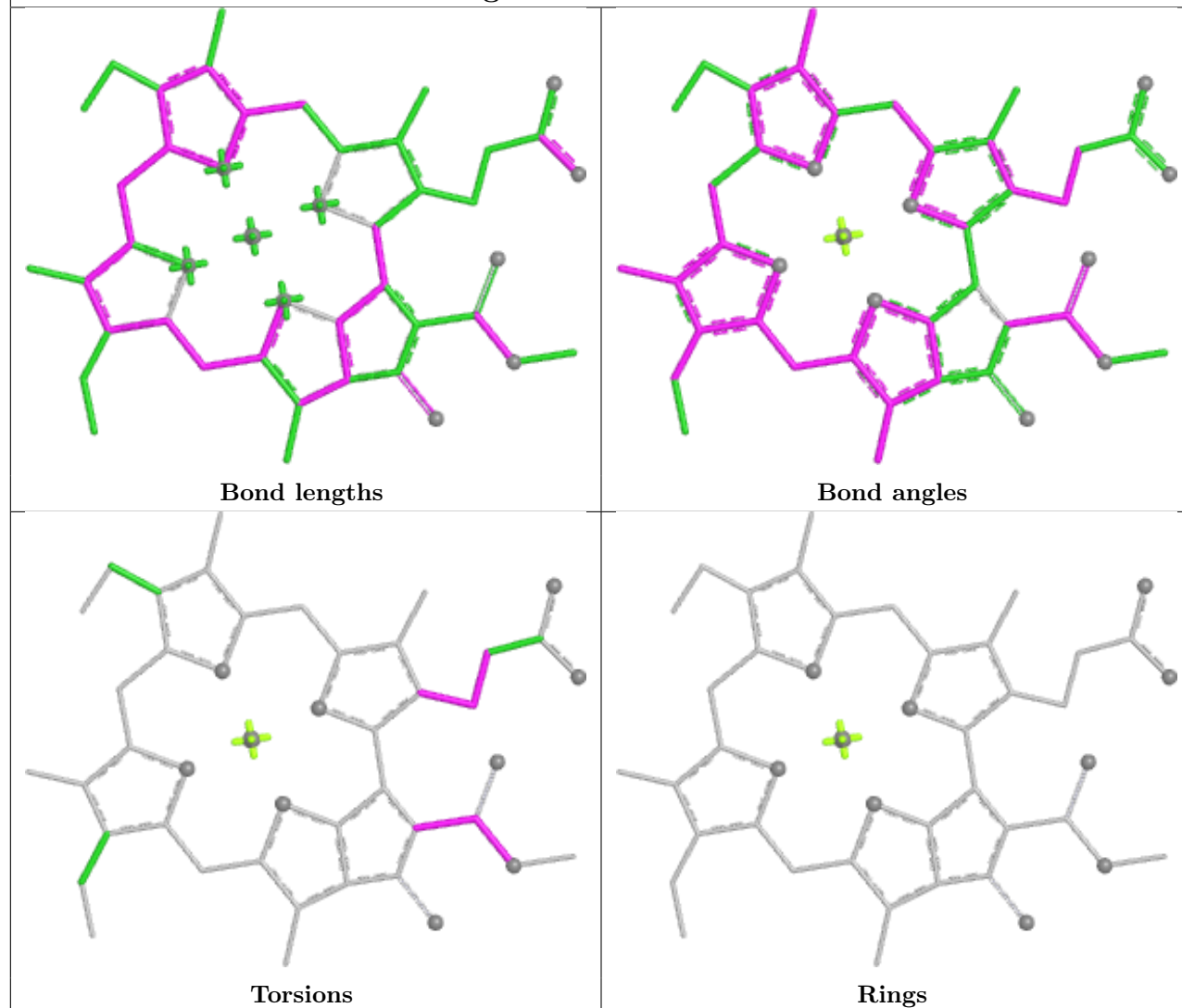




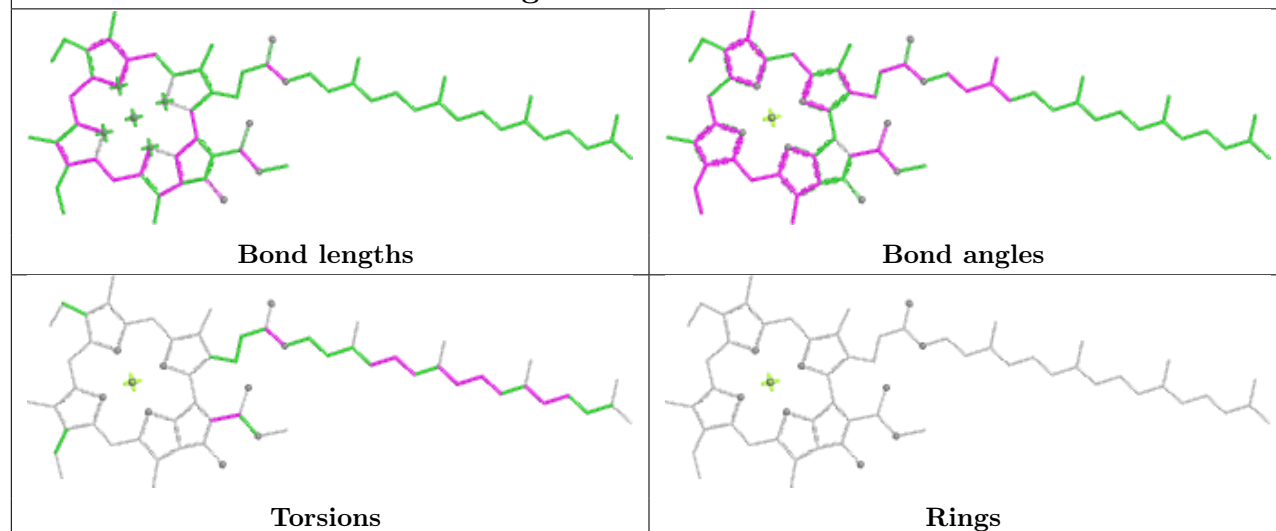


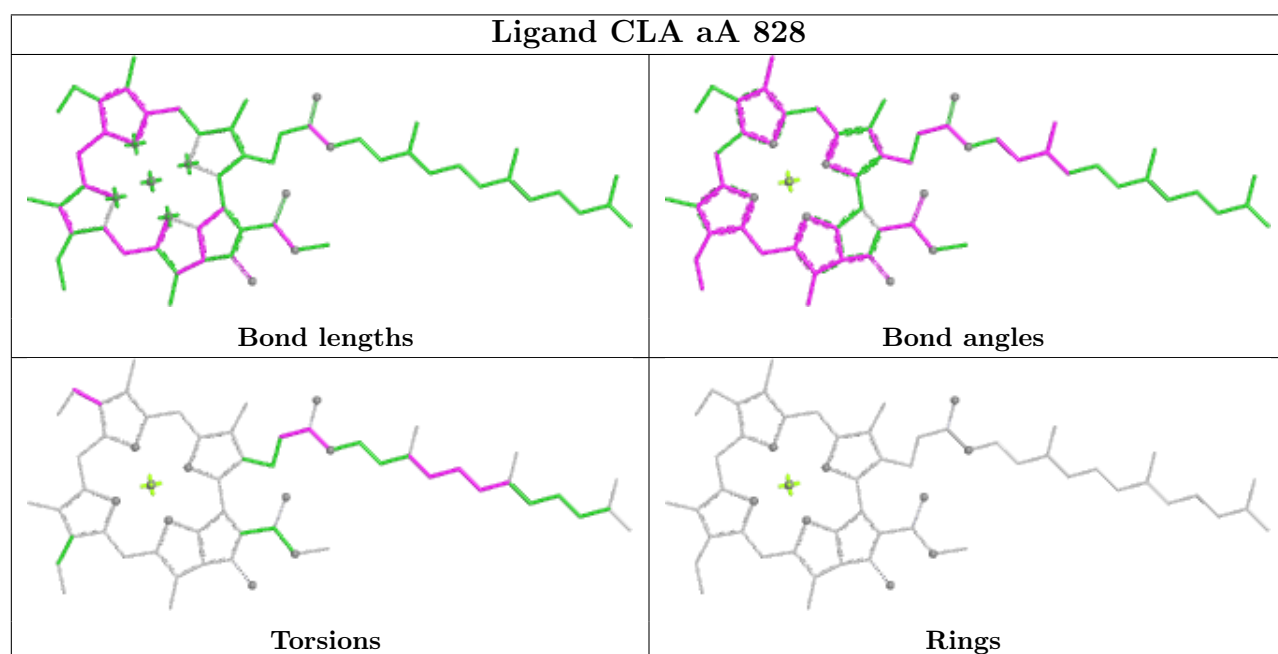
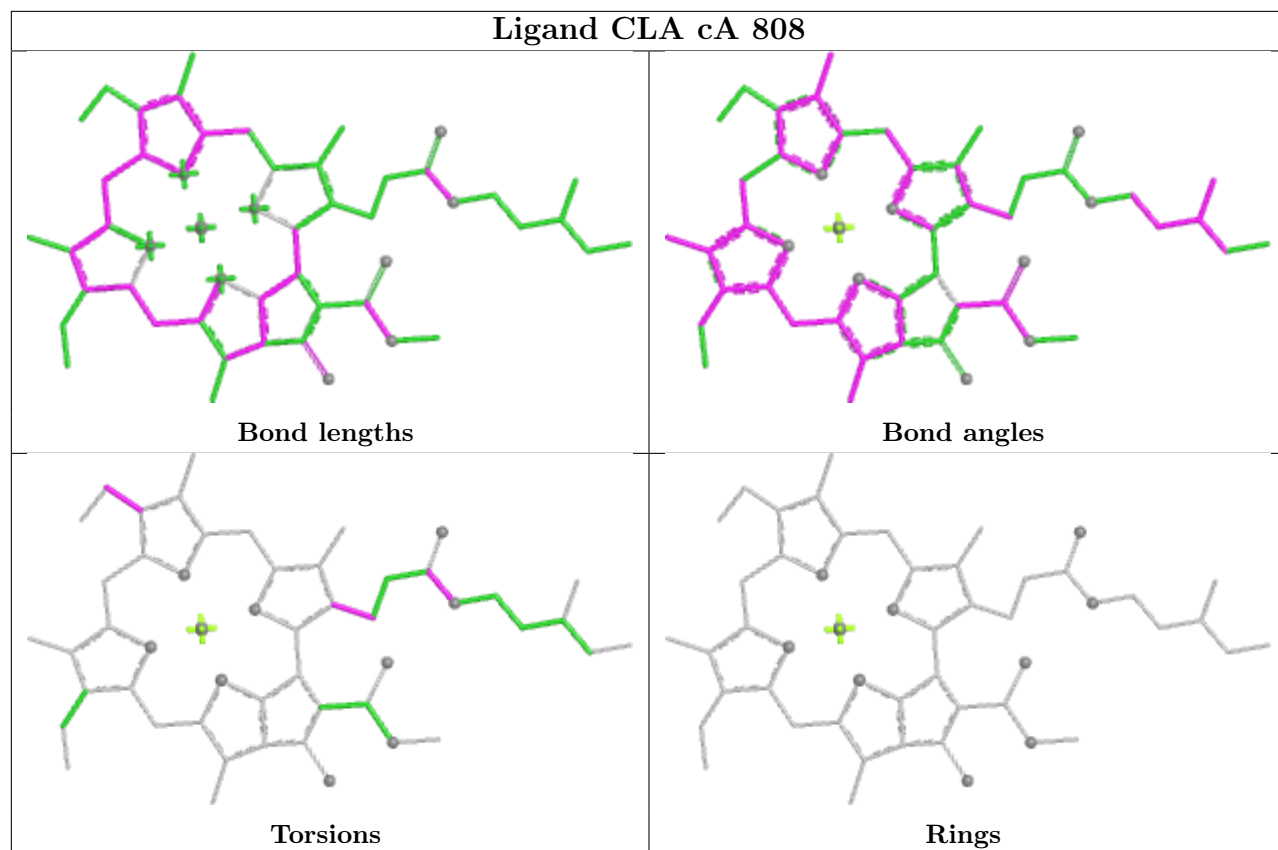


## Ligand CLA bA 809

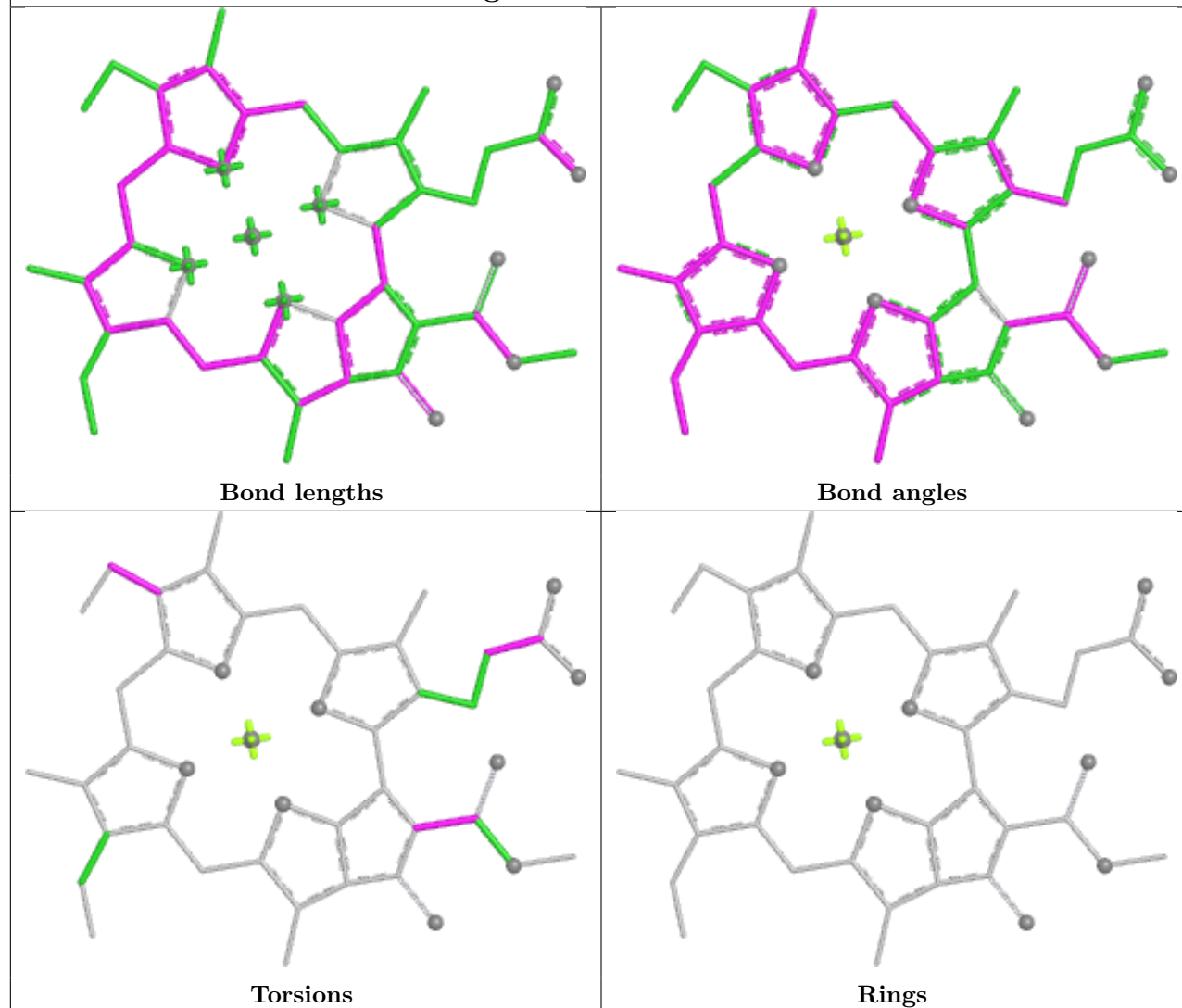


## Ligand CLA bA 831

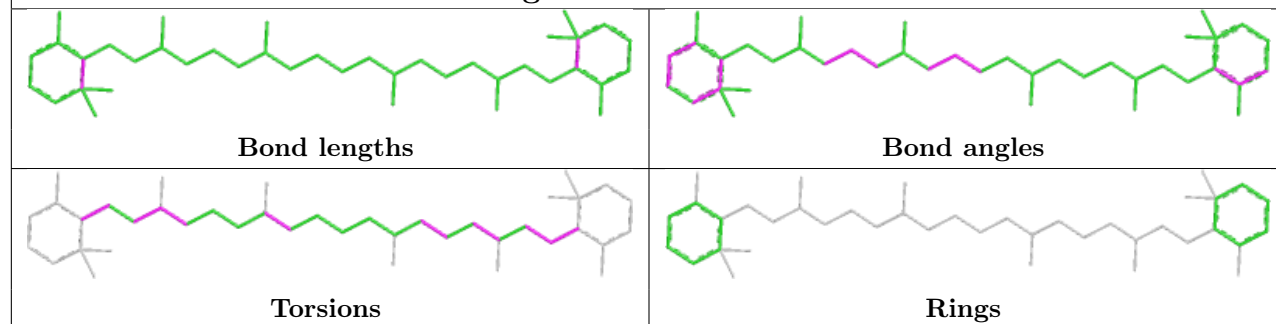


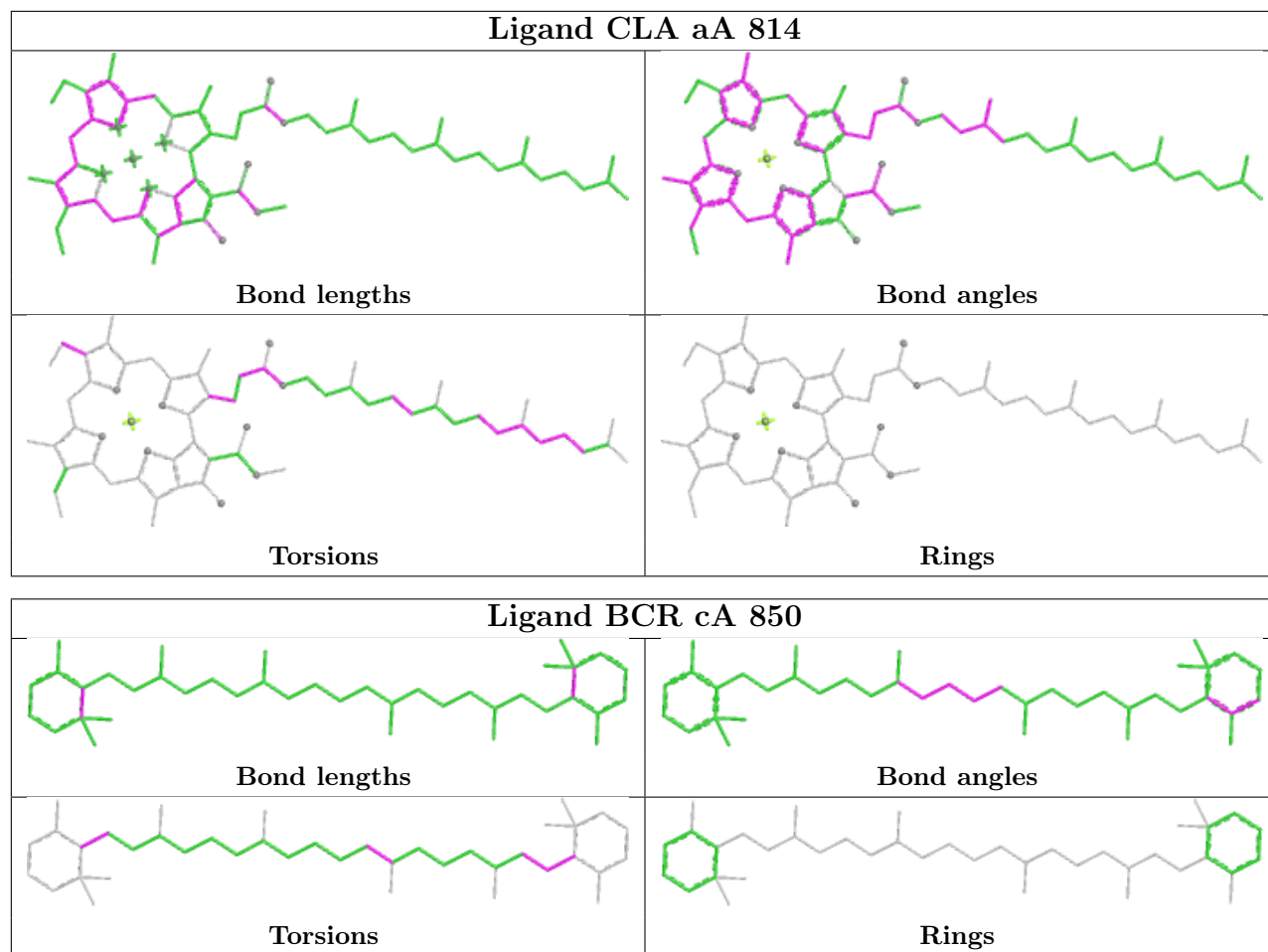


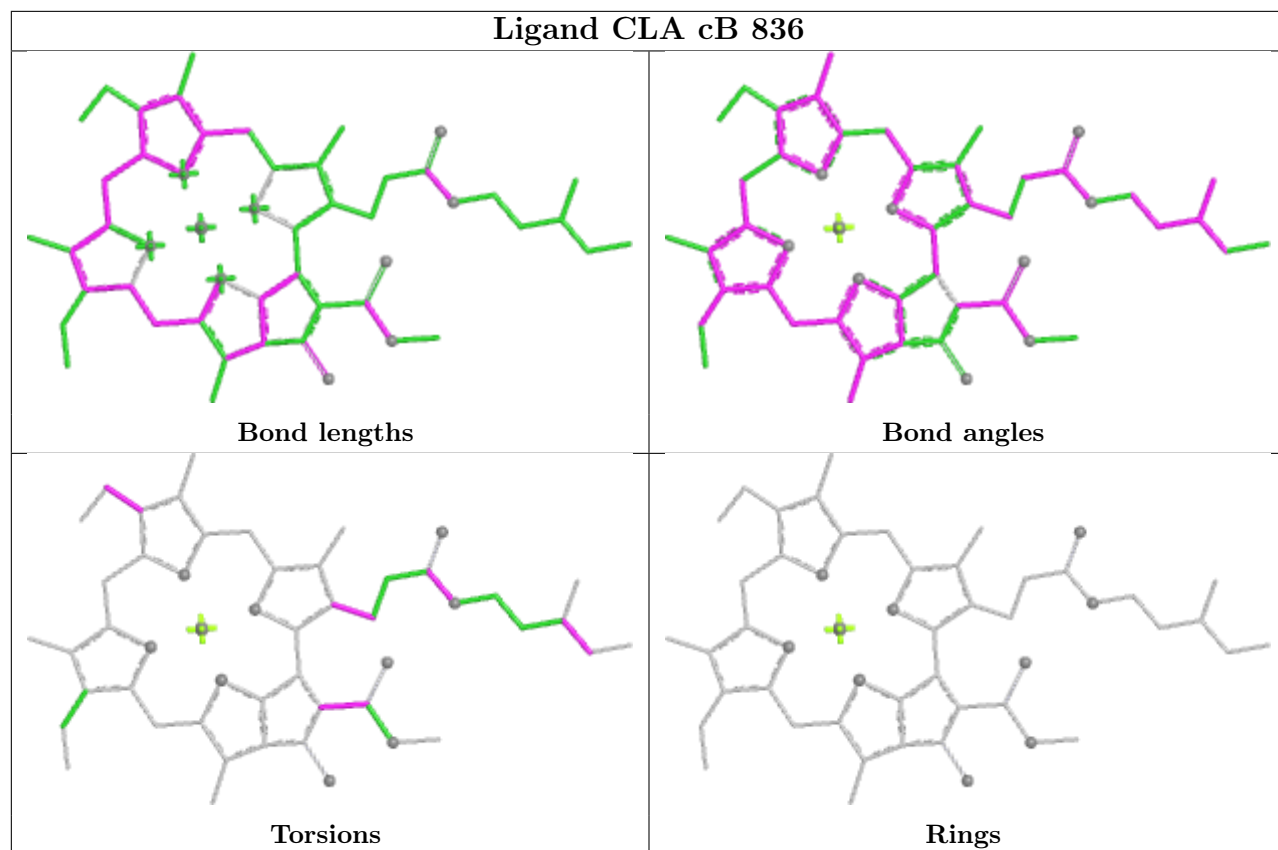
## Ligand CLA bB 835



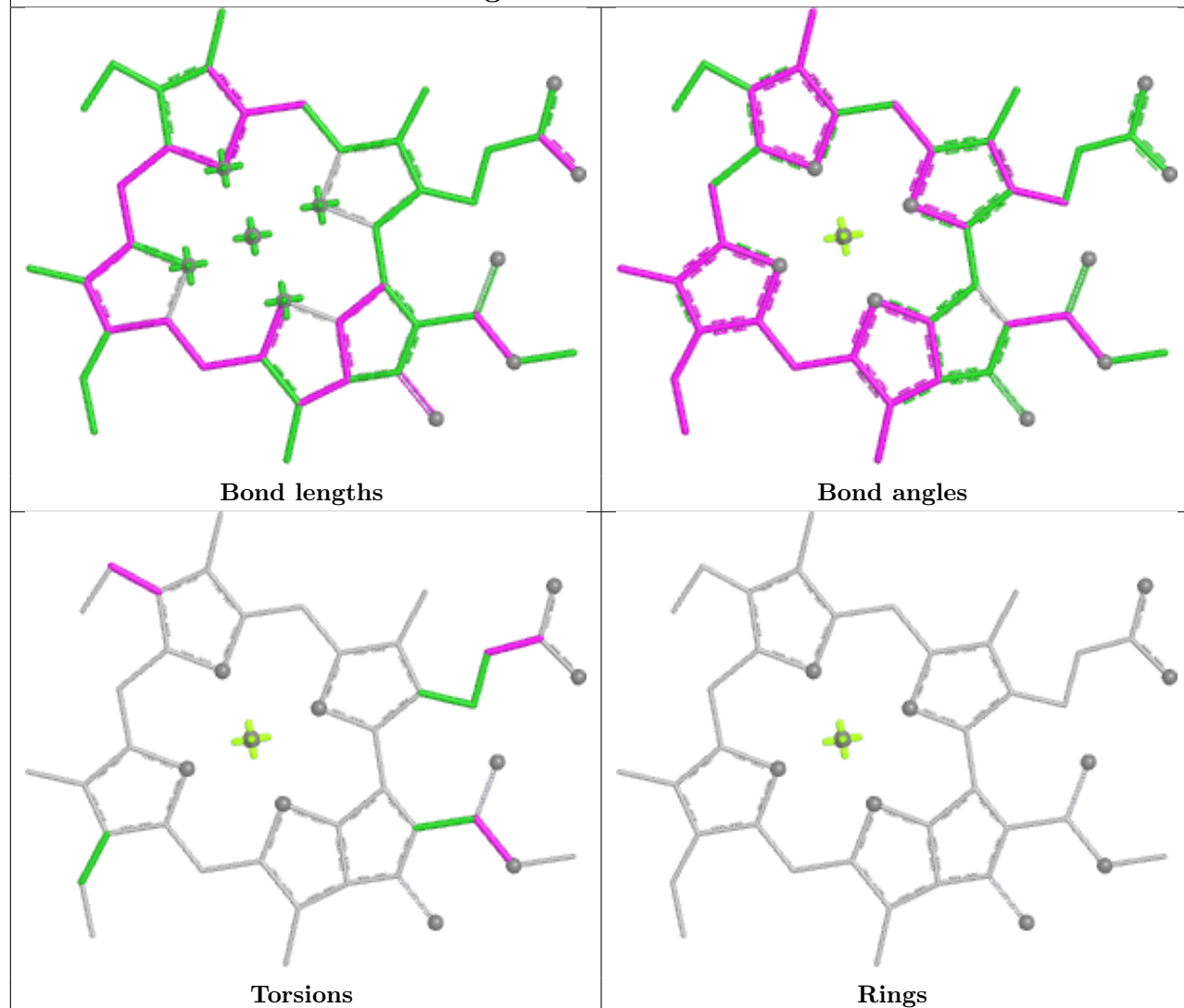
## Ligand BCR cB 846



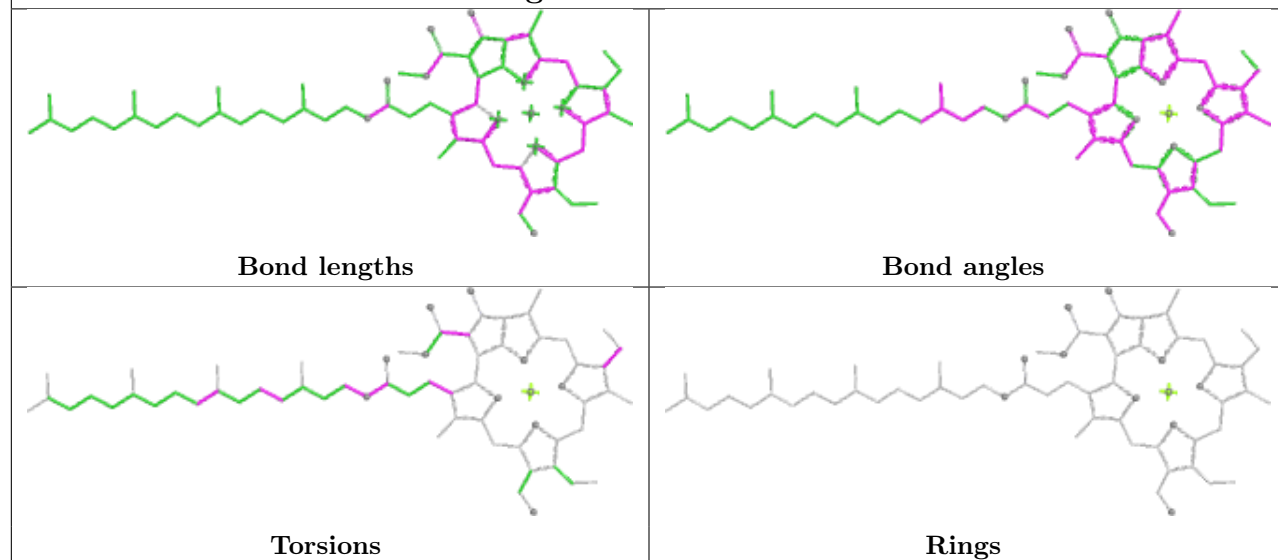


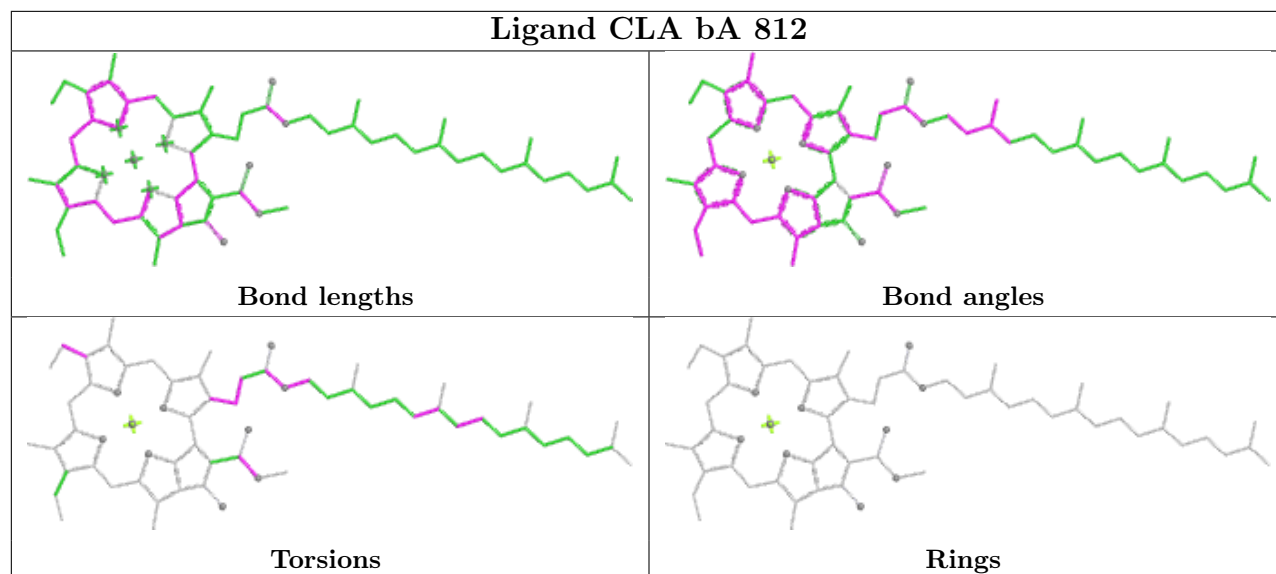
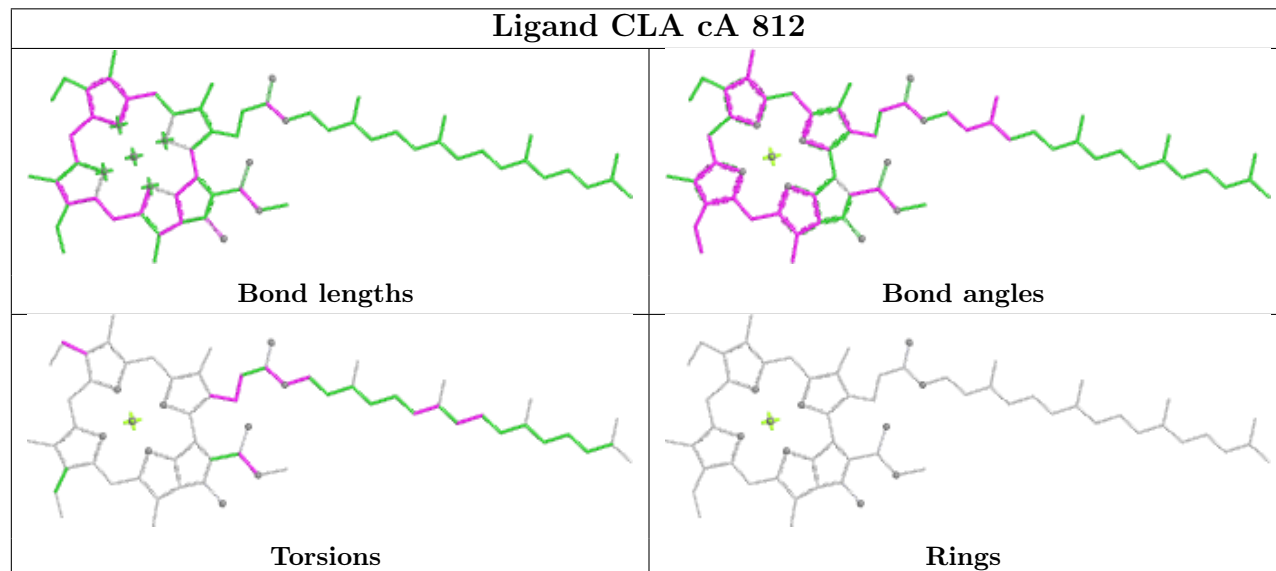


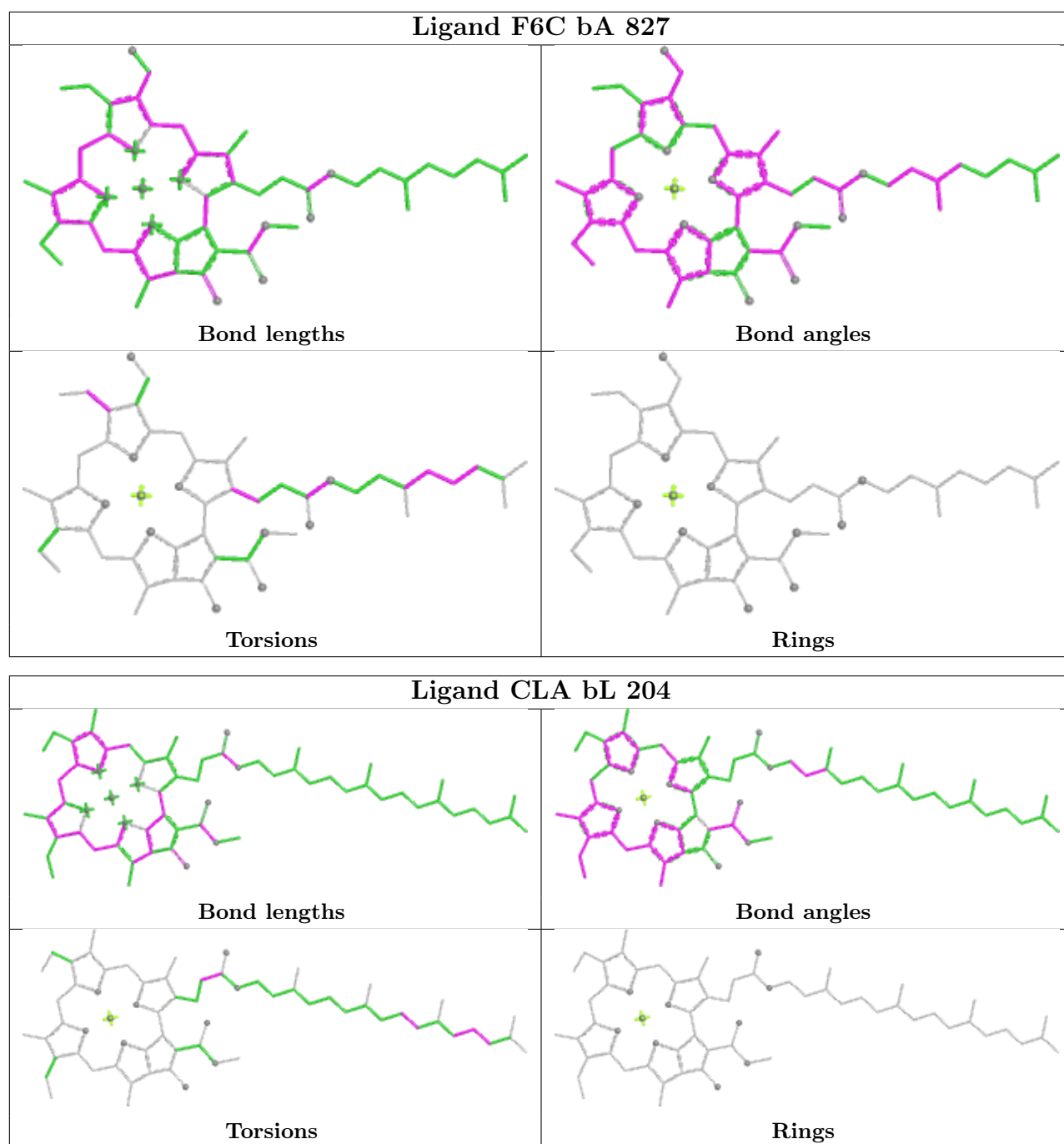
## Ligand CLA aA 836



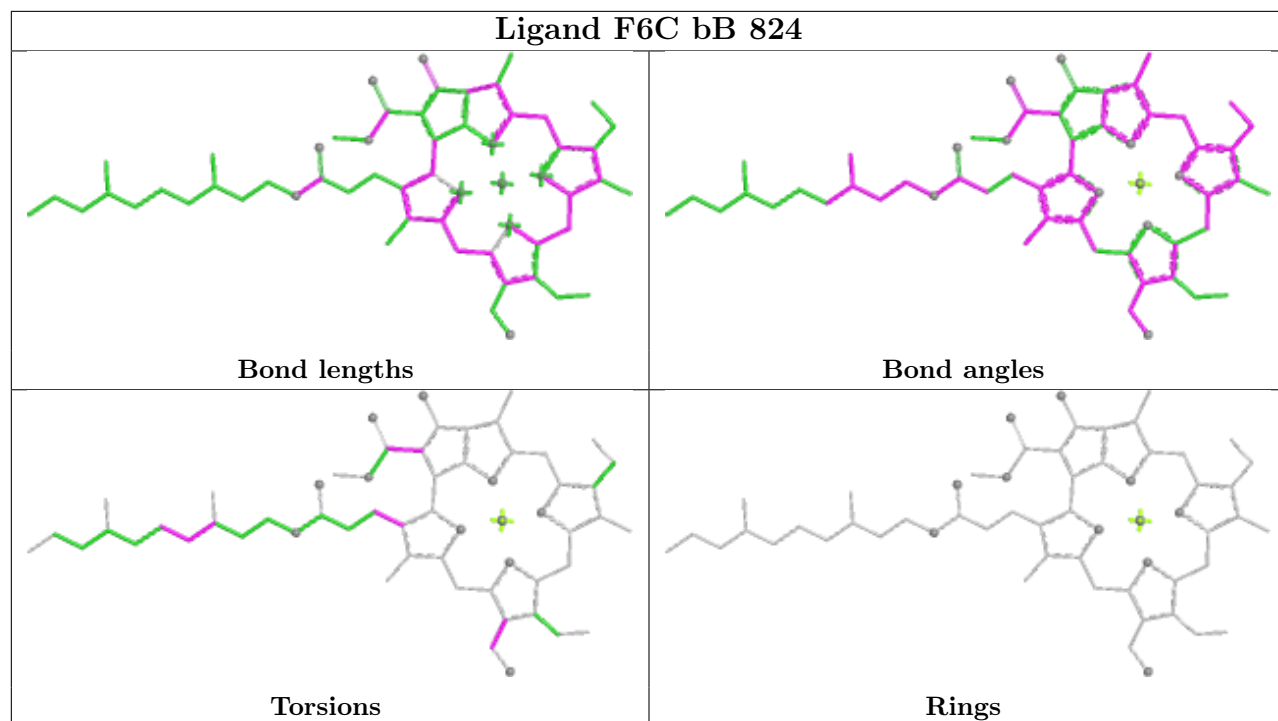
## Ligand F6C bA 826



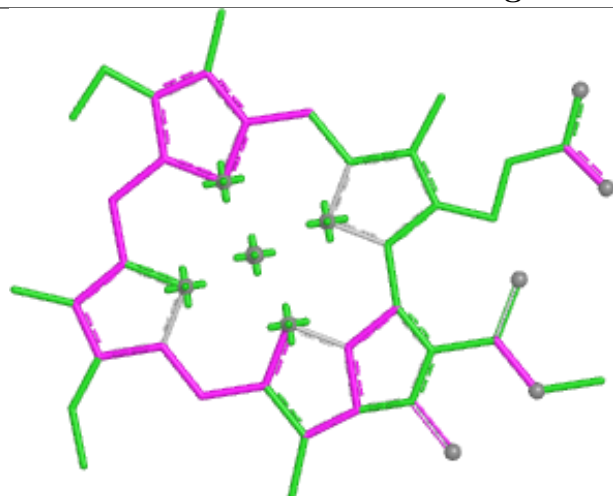
**Ligand CLA bA 812****Ligand CLA cA 812**



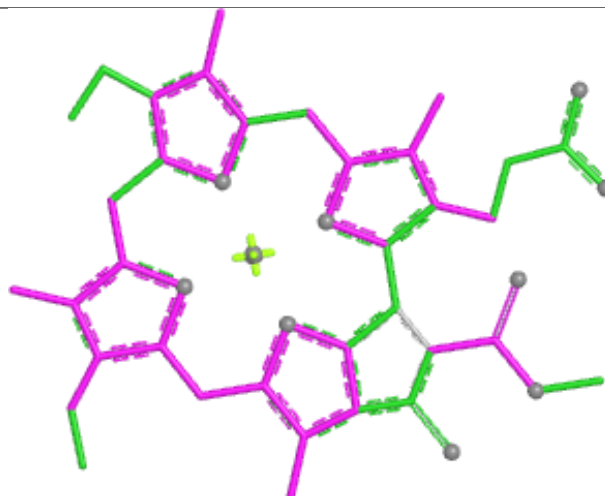




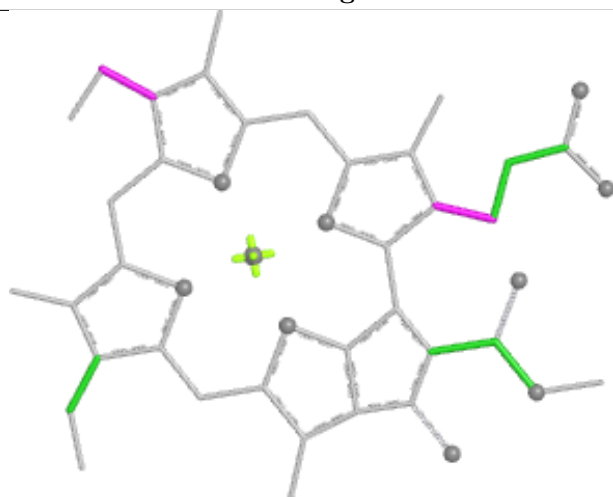
## Ligand CLA bB 833



Bond lengths



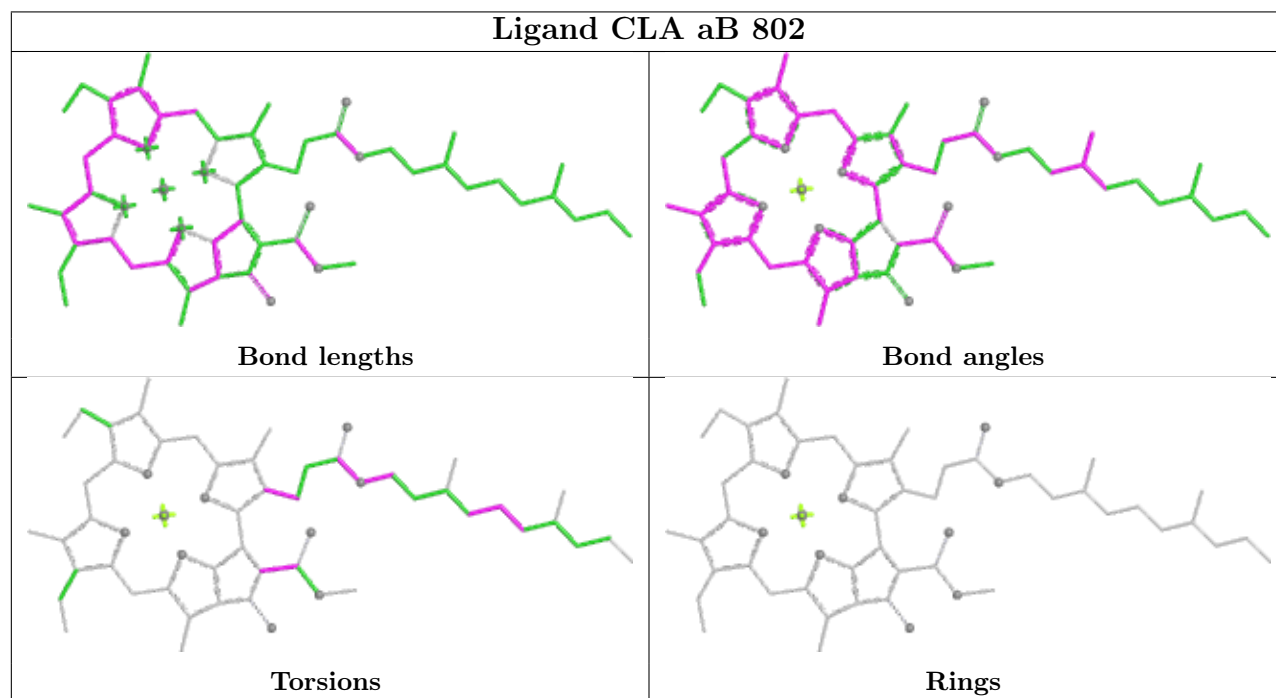
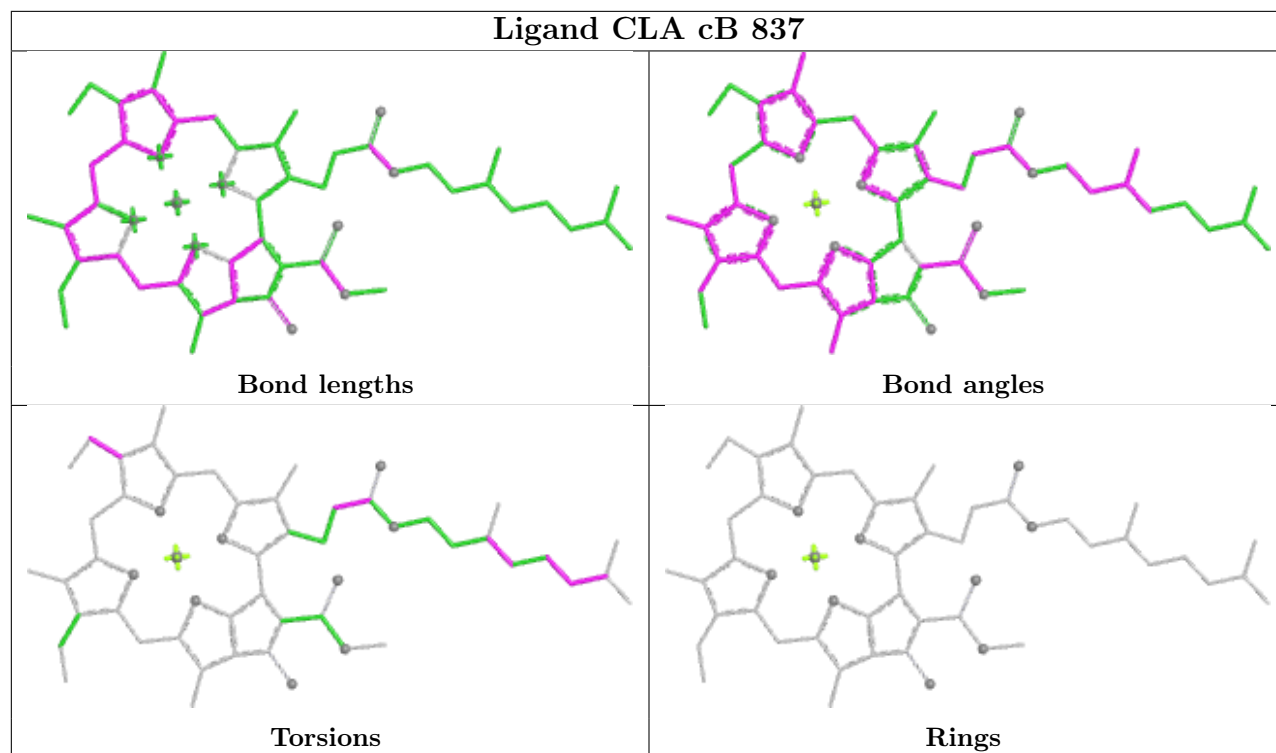
Bond angles

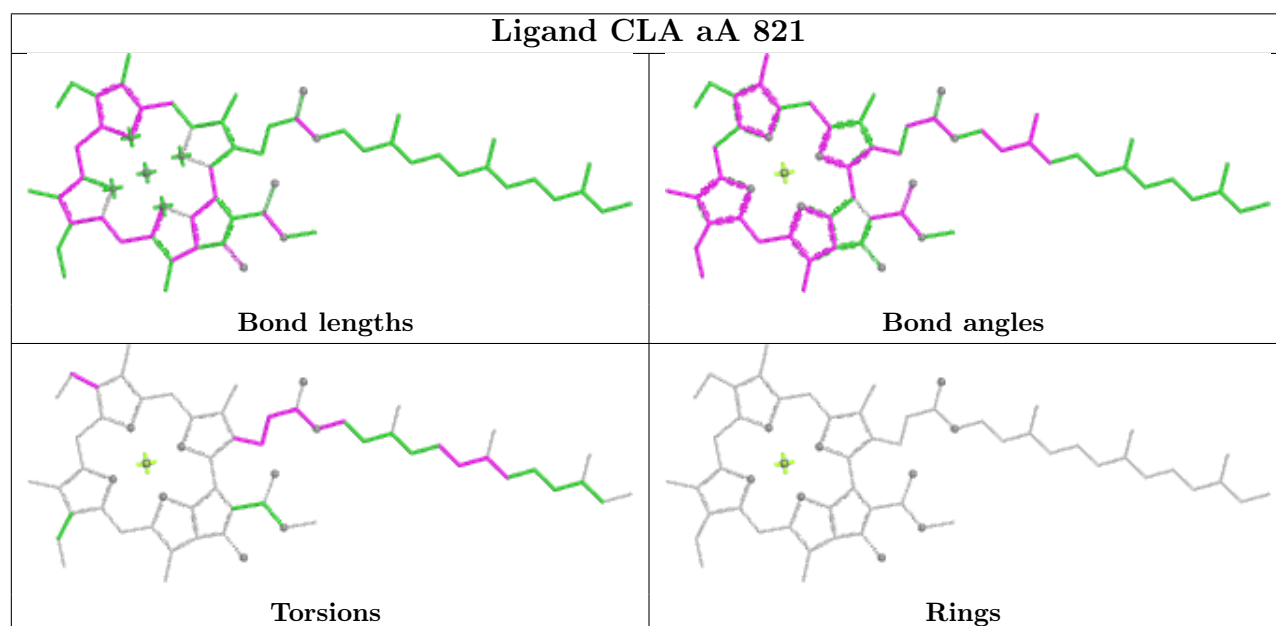
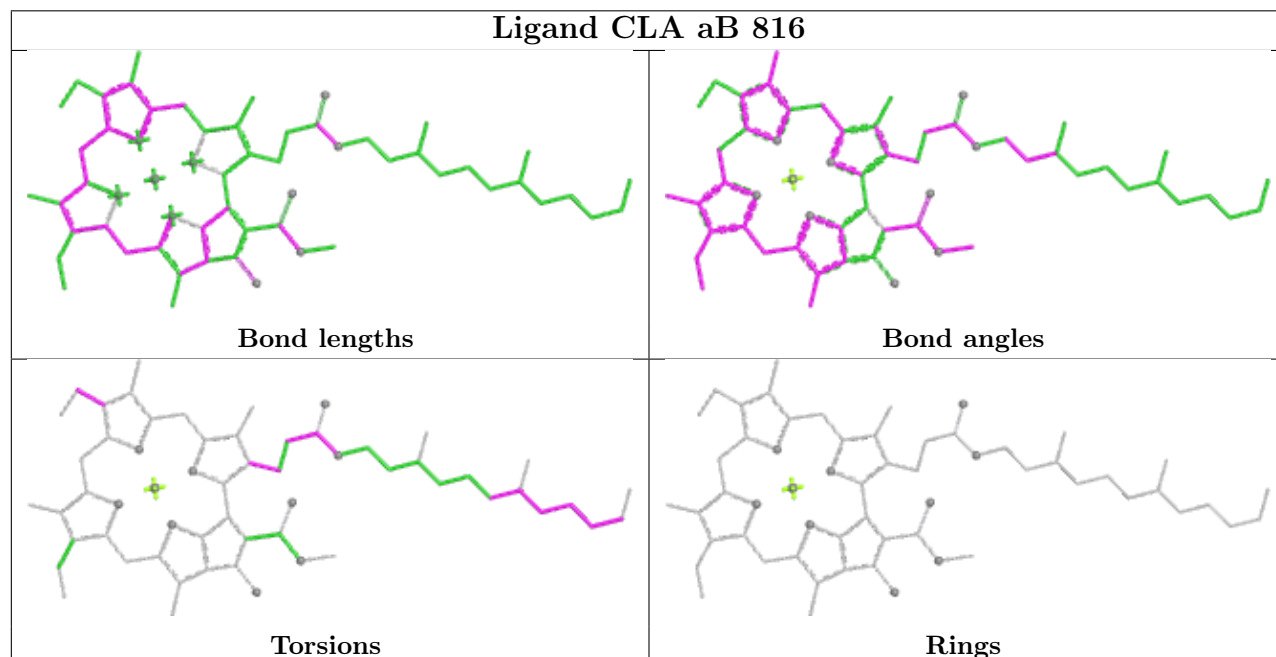
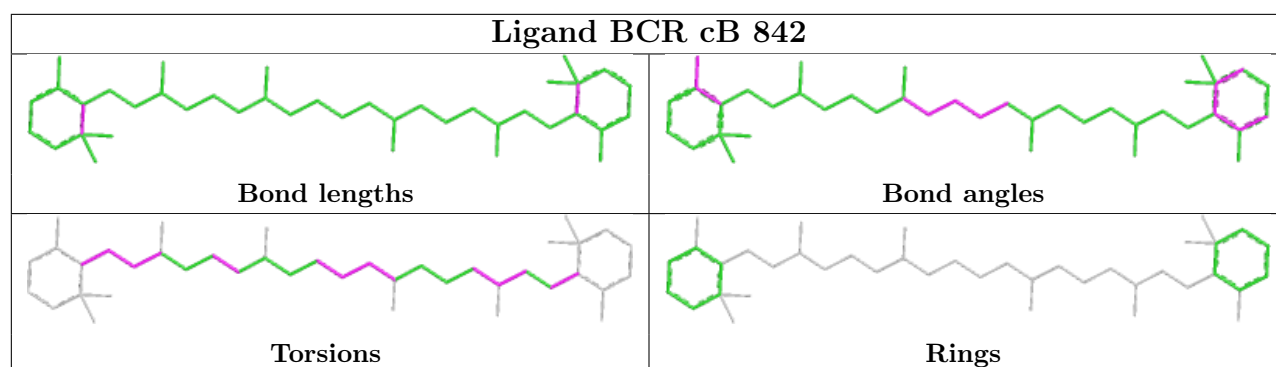


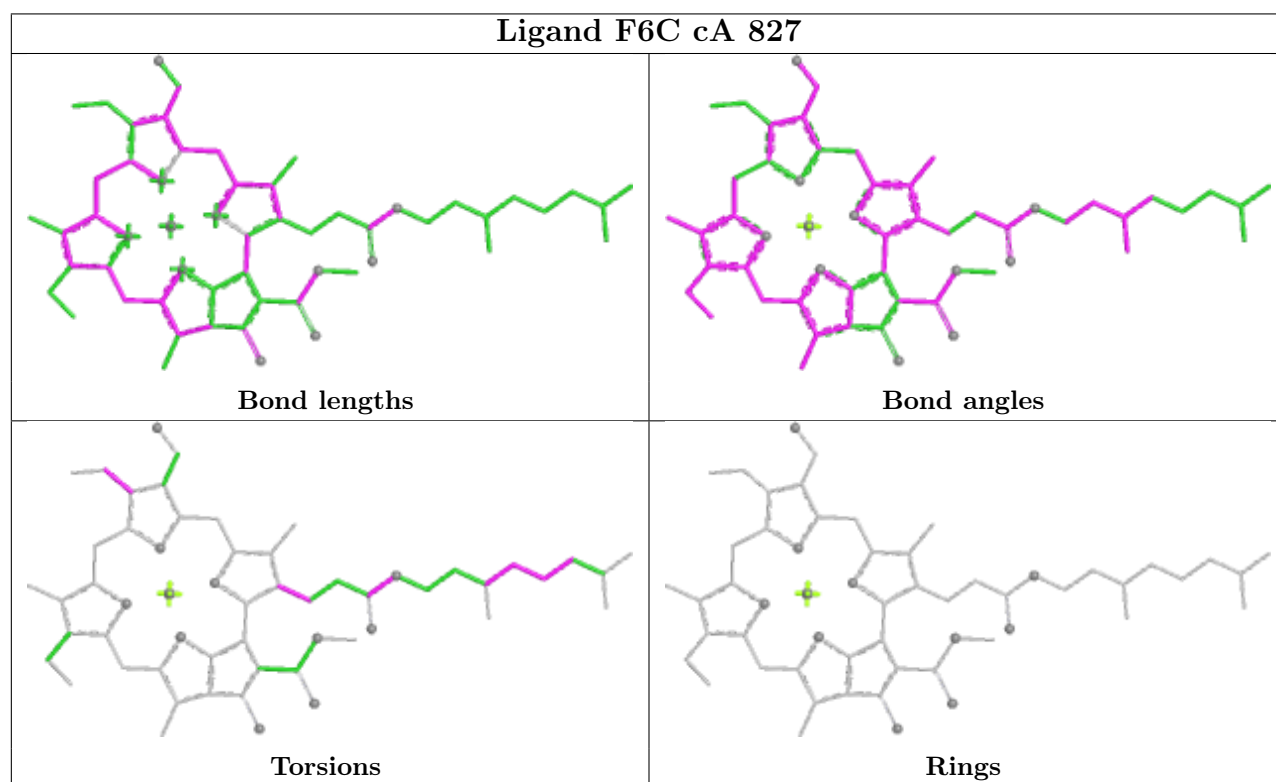
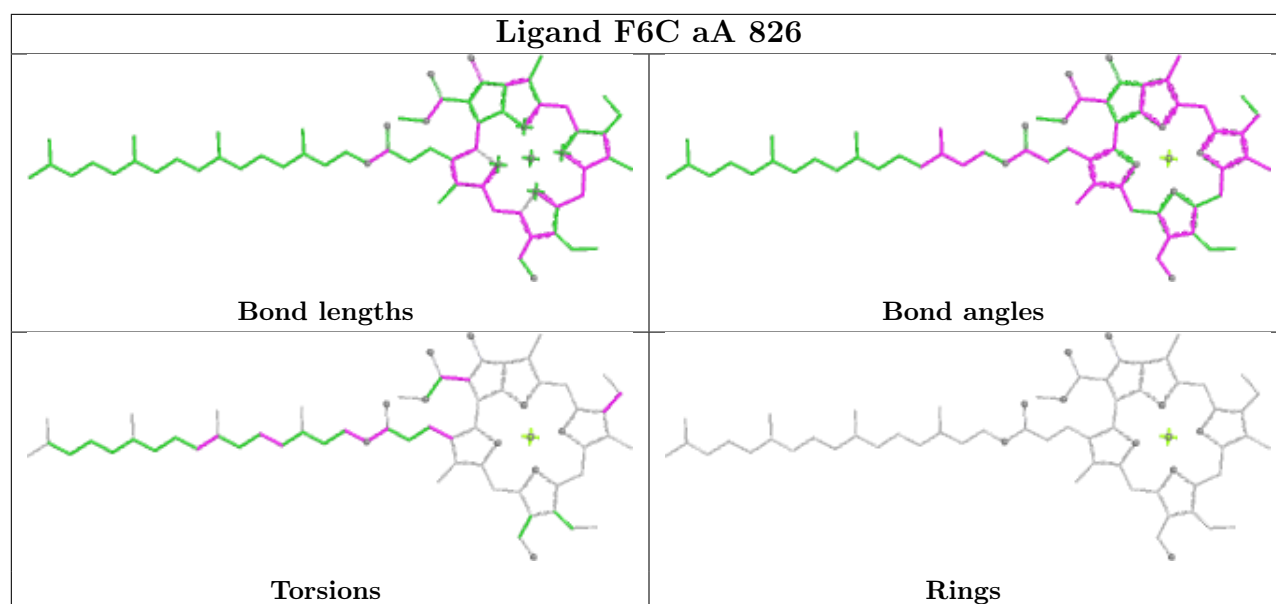
Torsions

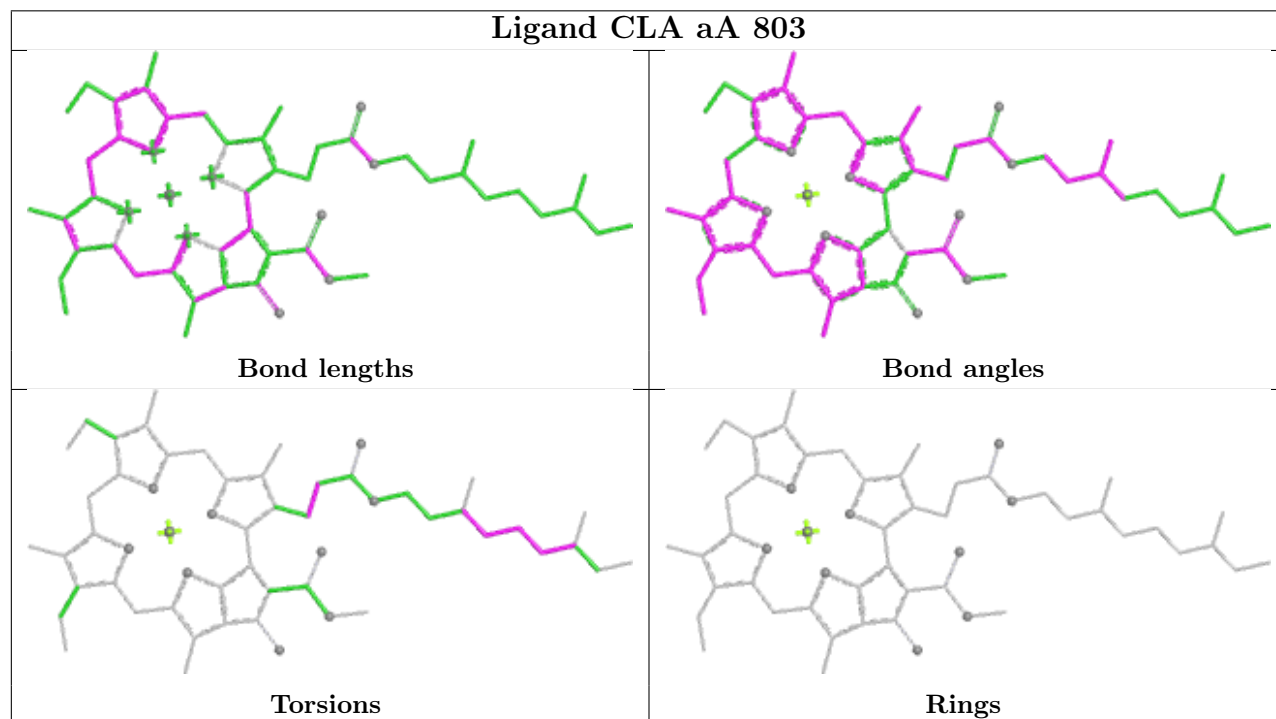
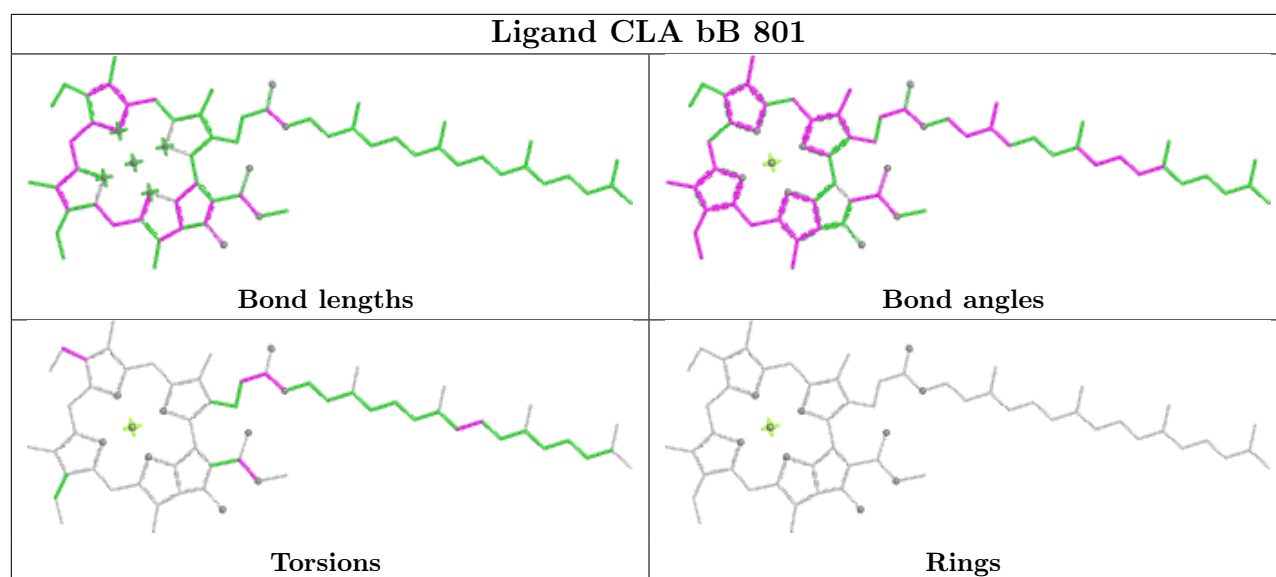


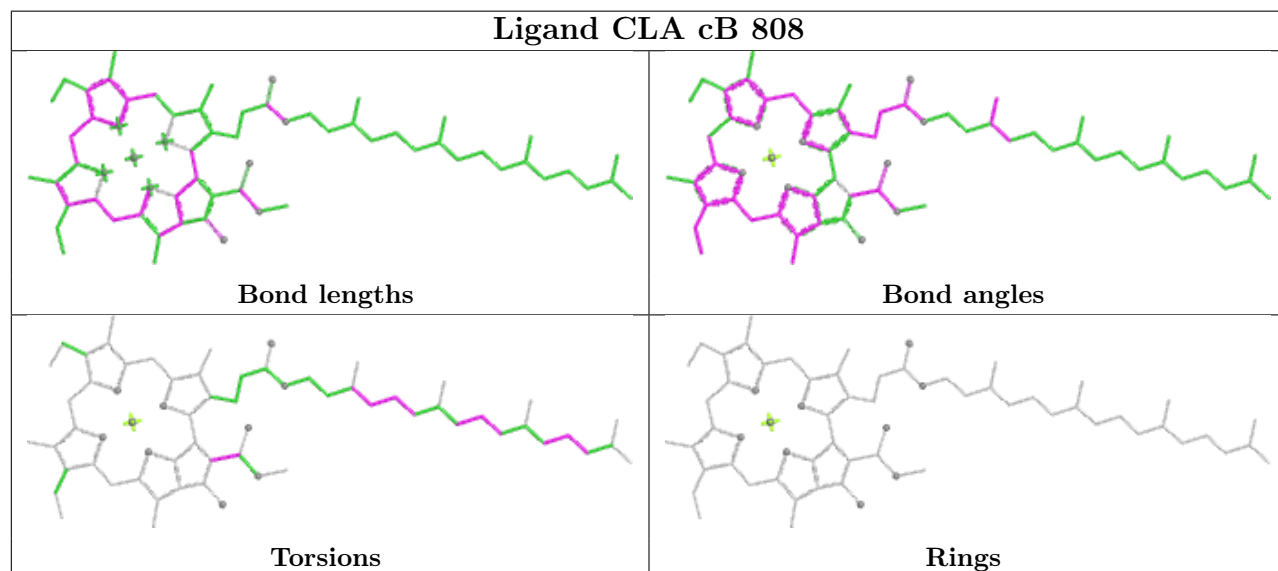
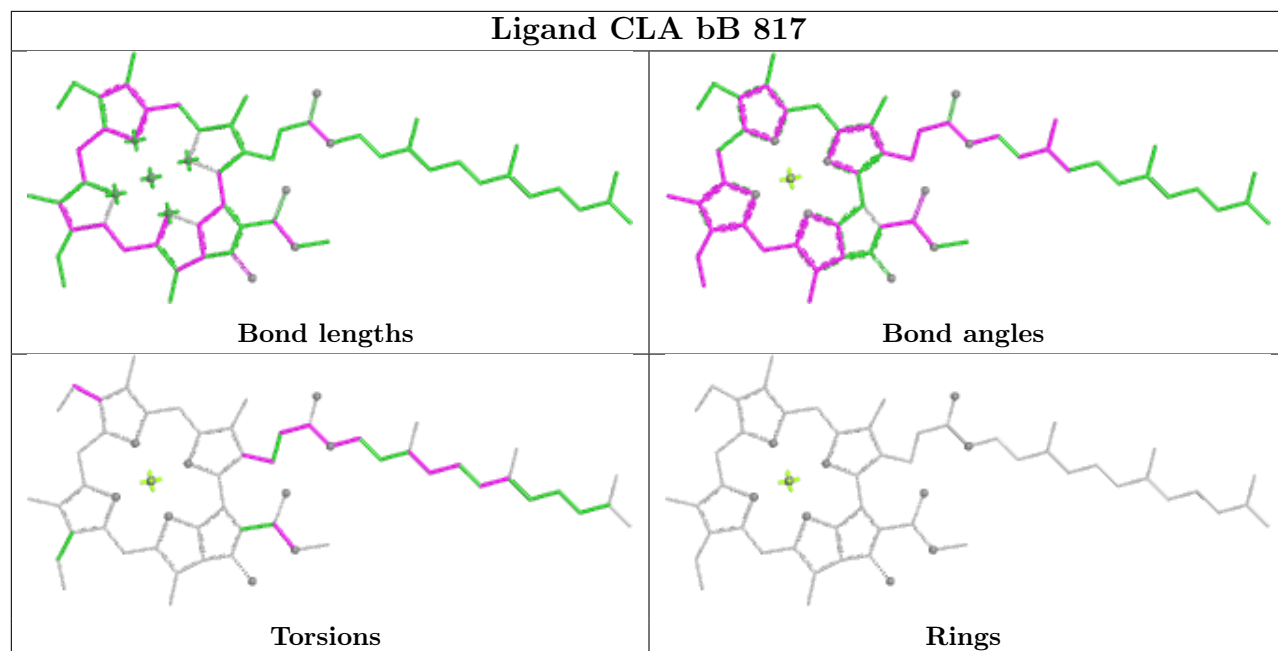
Rings



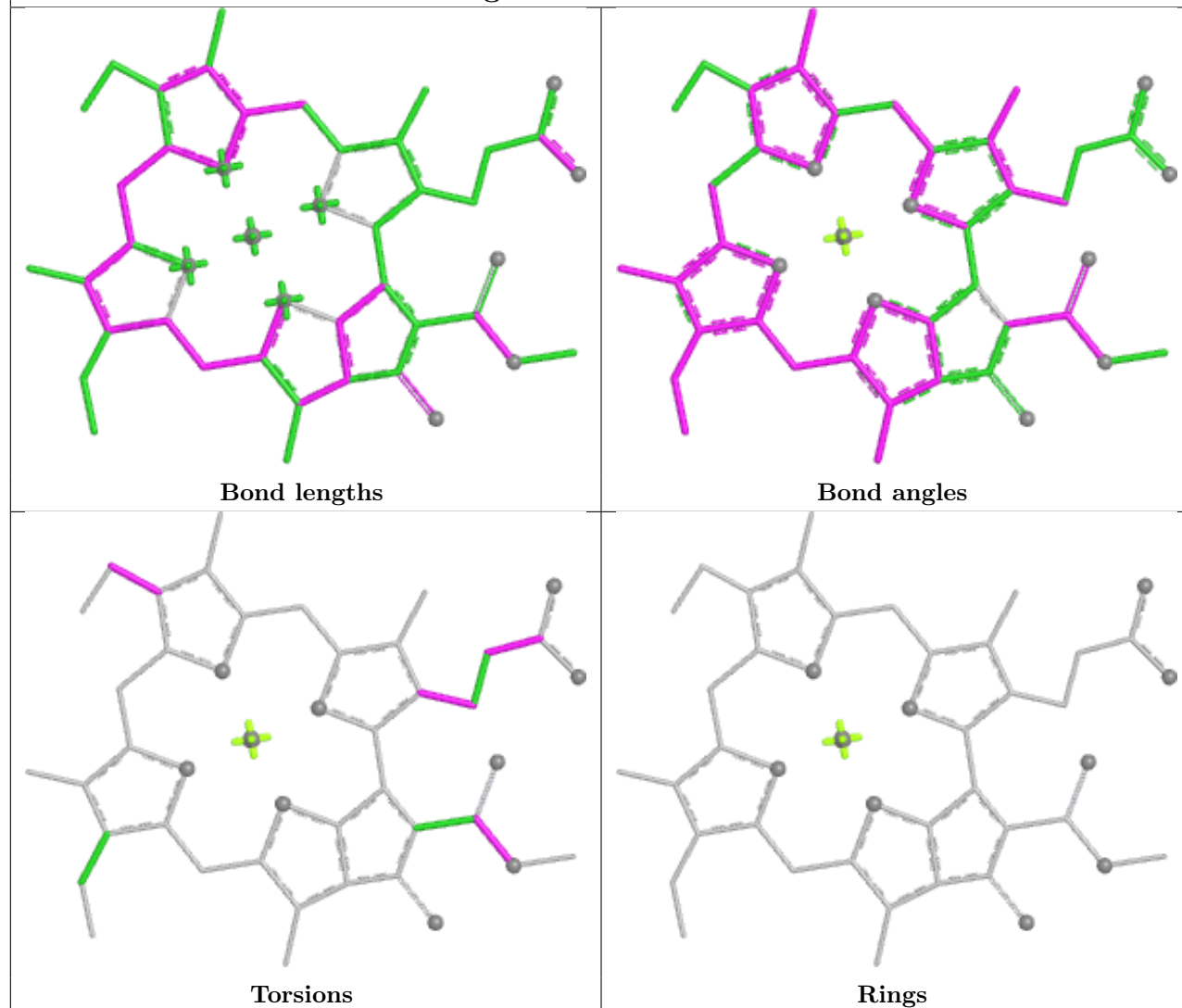




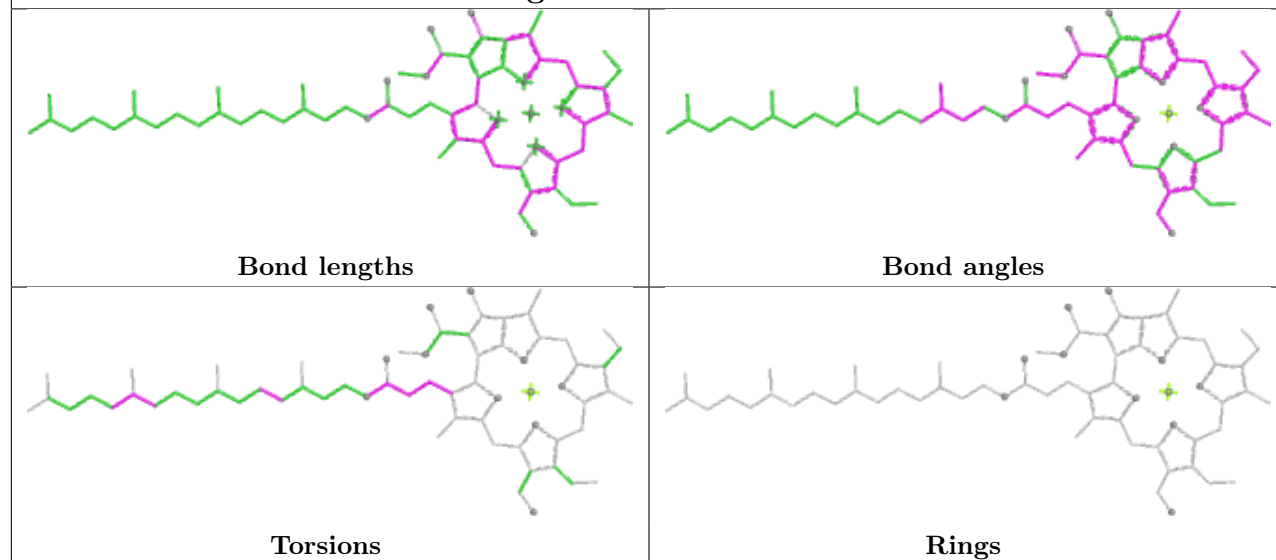




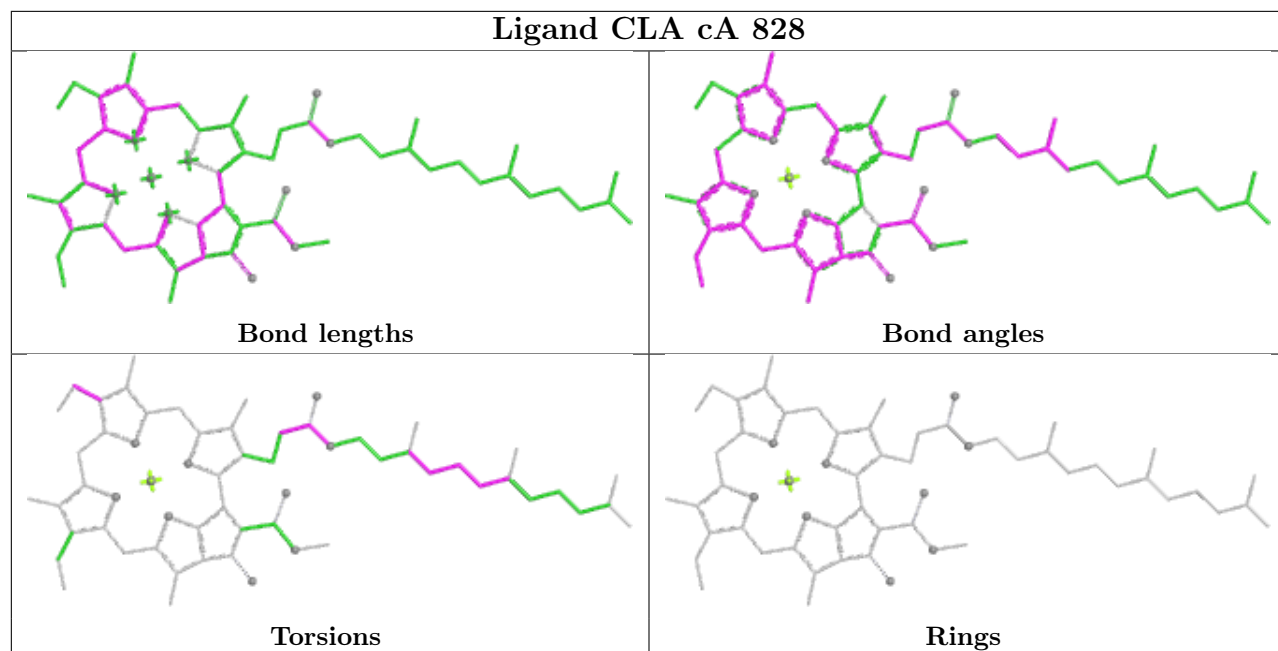
## Ligand CLA bB 810



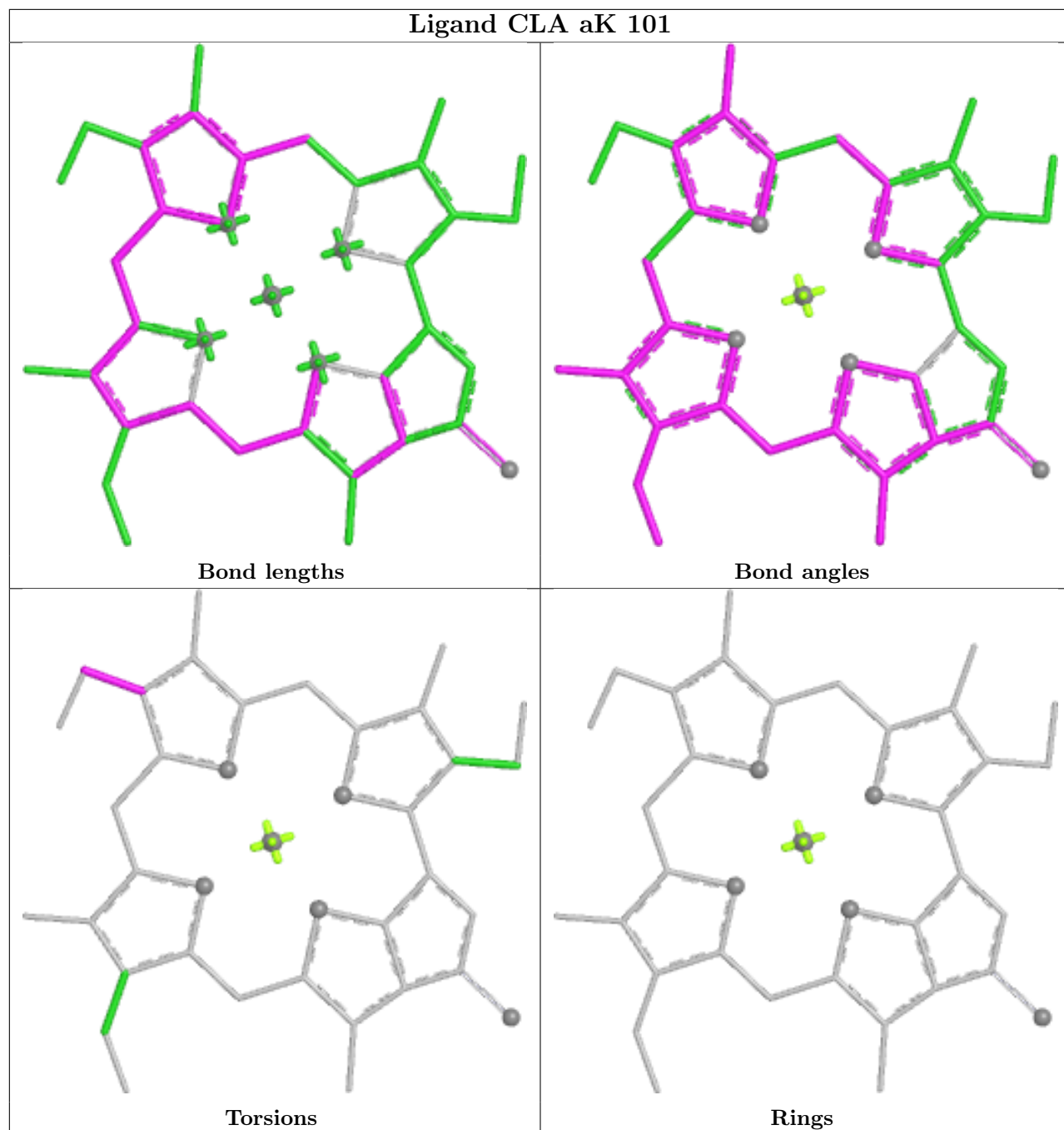
## Ligand F6C aA 844

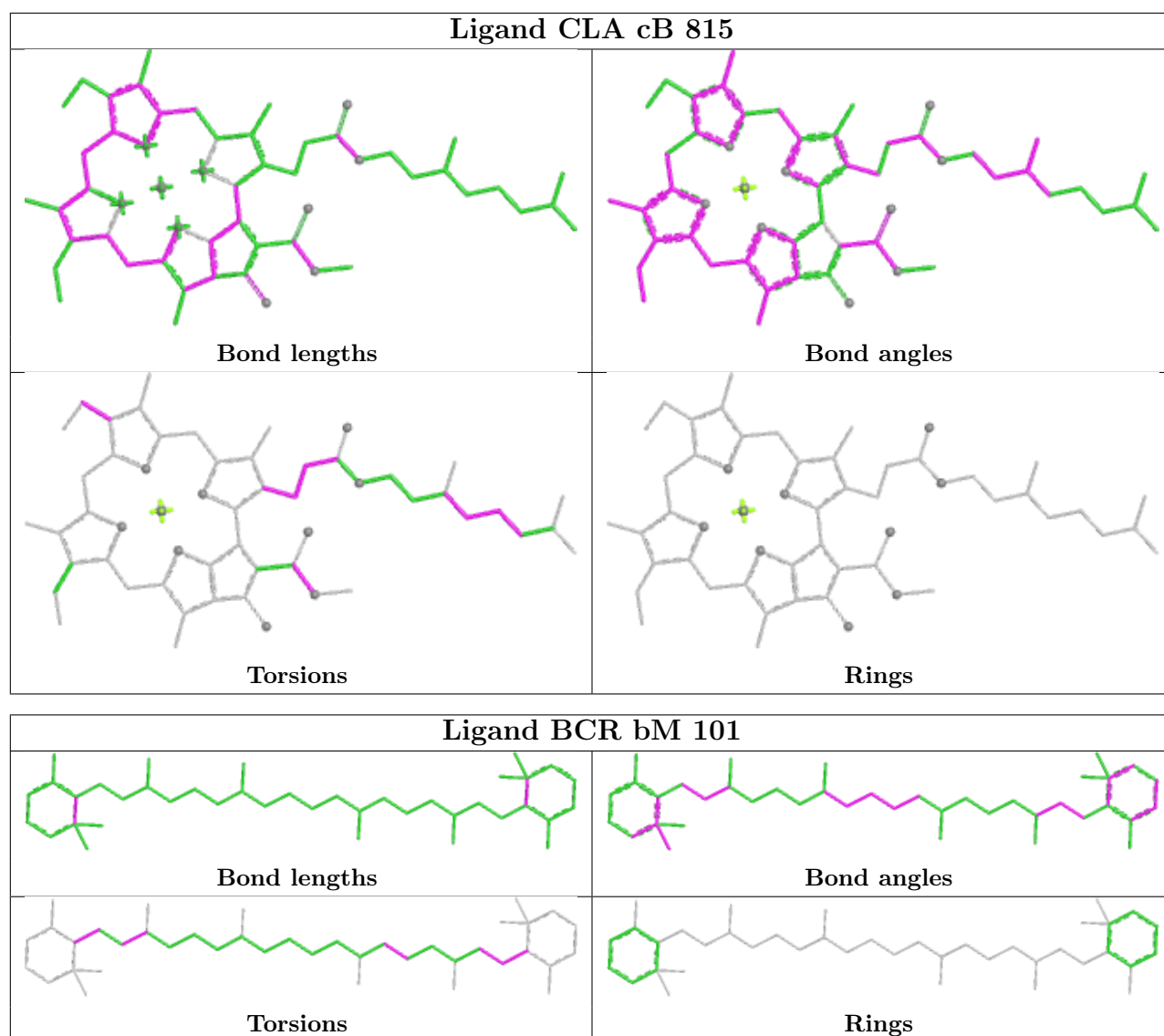




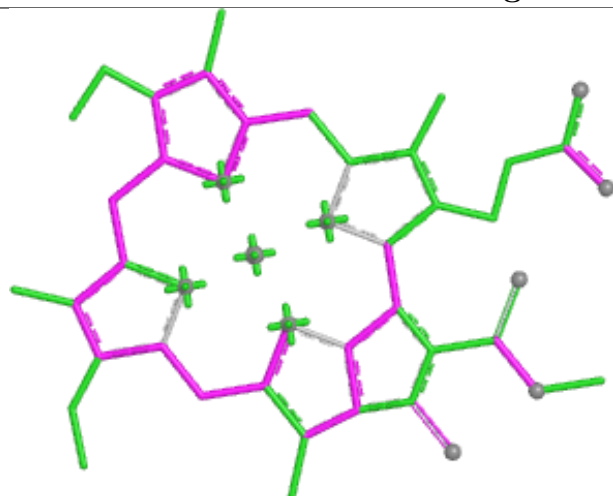


## Ligand CLA aK 101

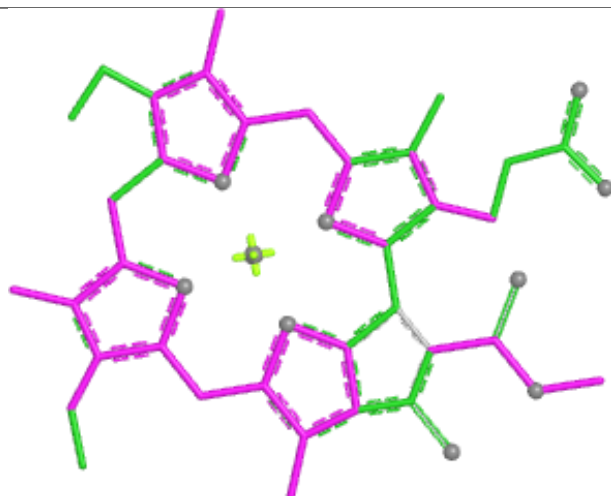




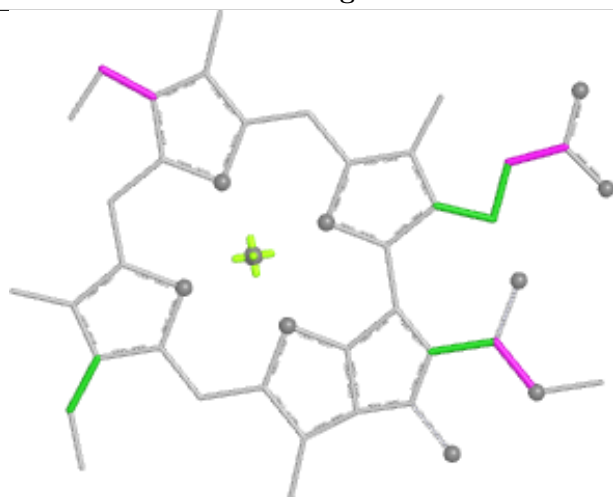
## Ligand CLA bA 842



Bond lengths



Bond angles

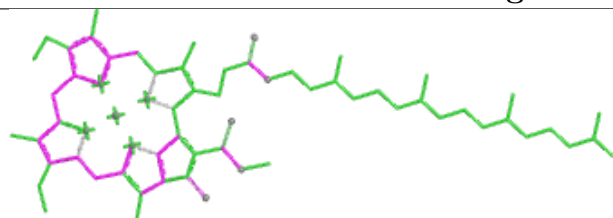


Torsions

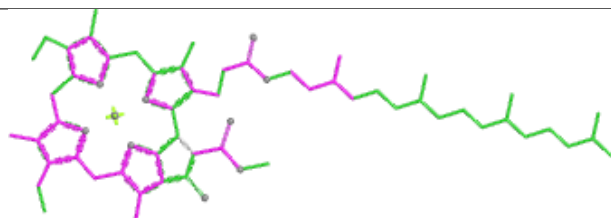


Rings

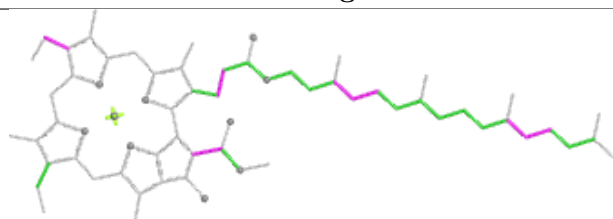
## Ligand CLA cB 839



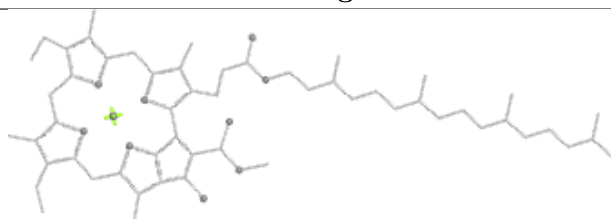
Bond lengths



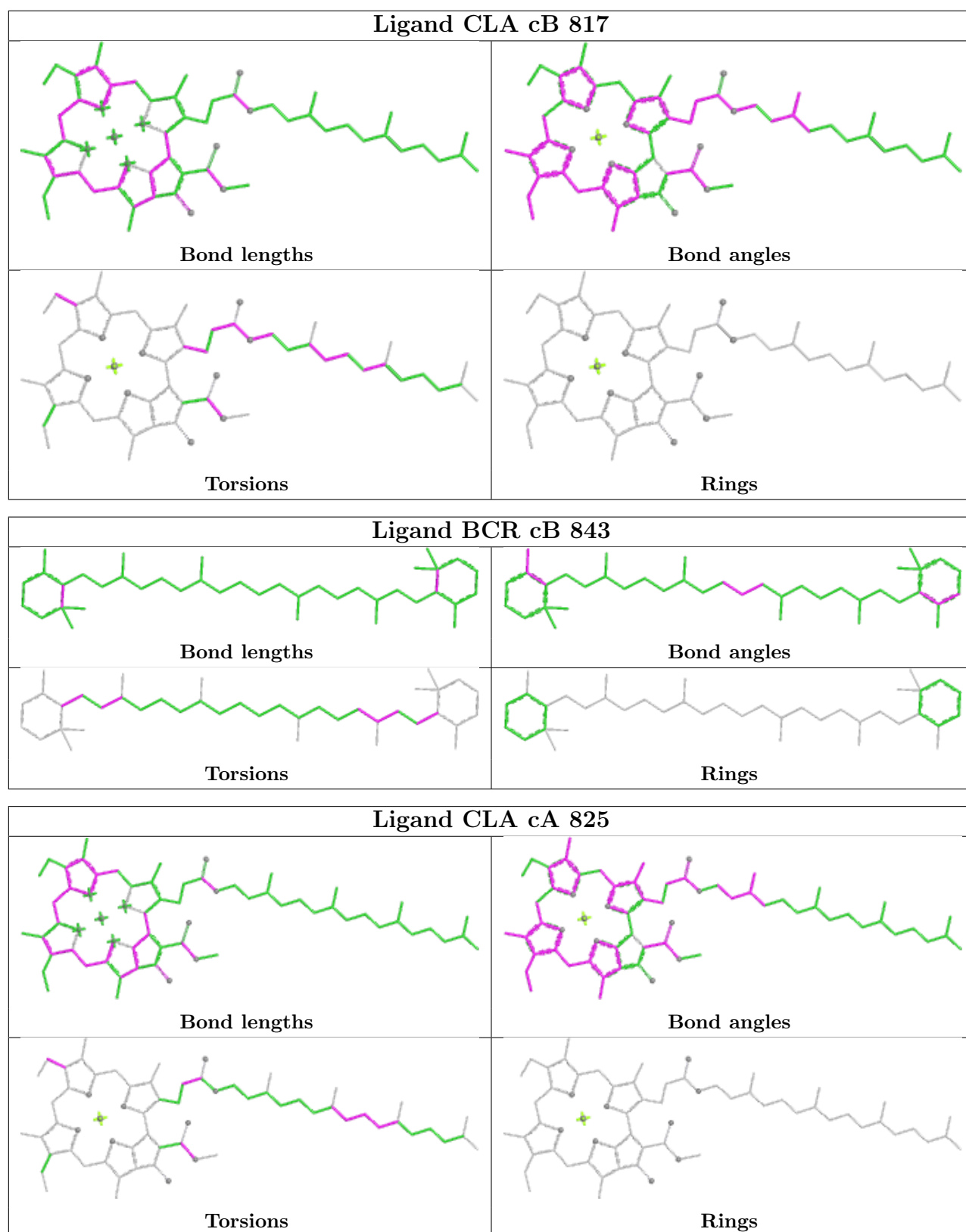
Bond angles



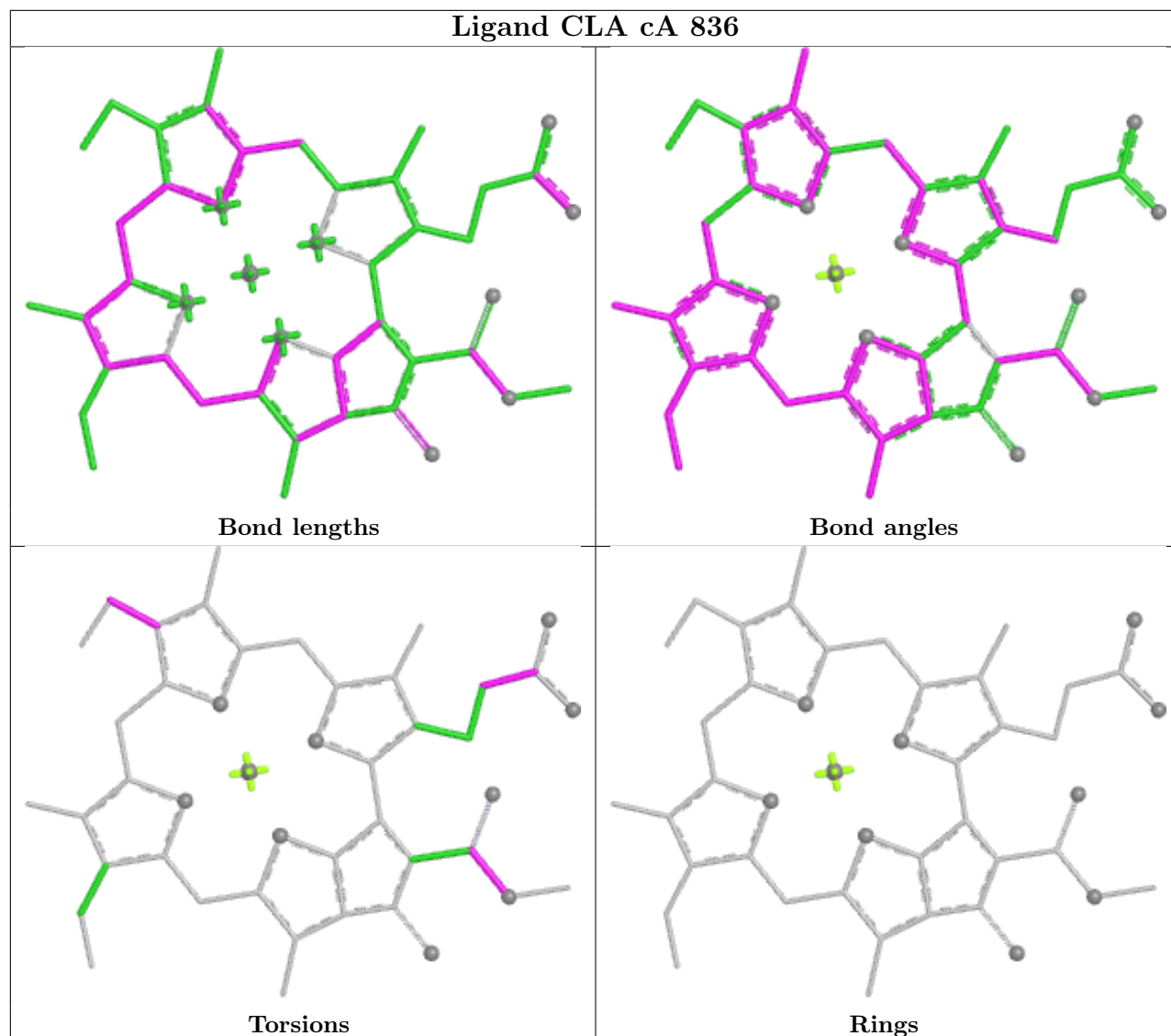
Torsions



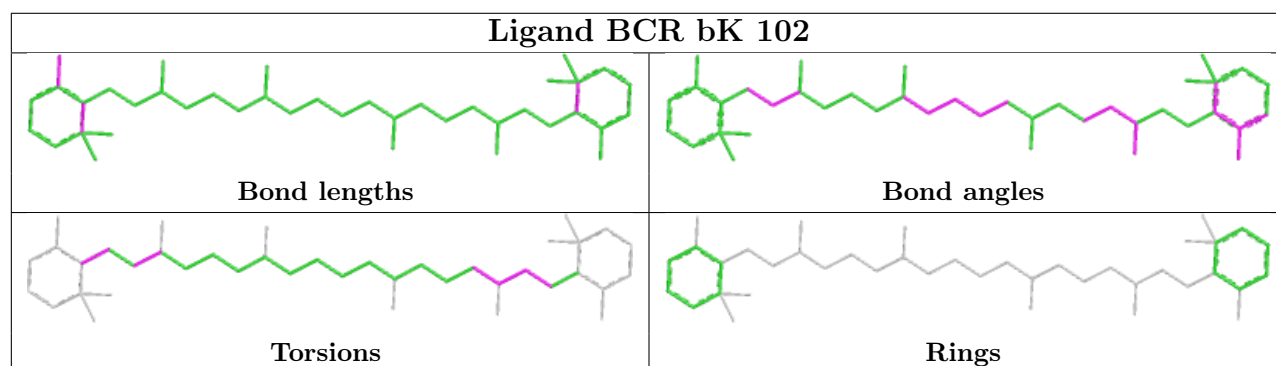
Rings

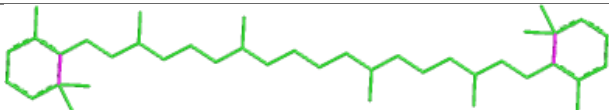
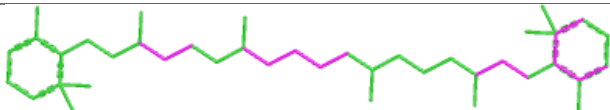
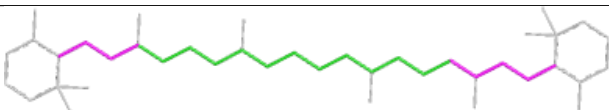
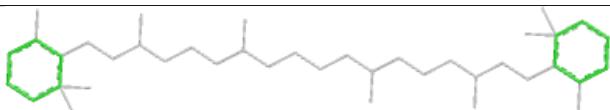


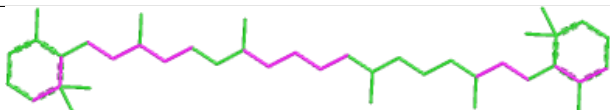
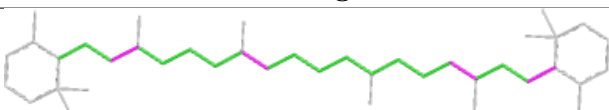
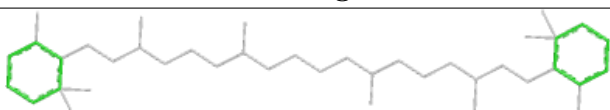
## Ligand CLA cA 836

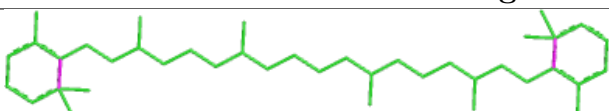
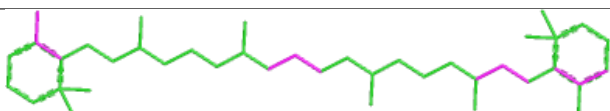
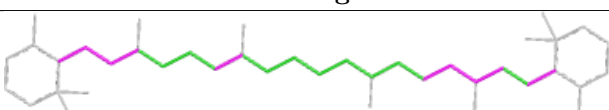
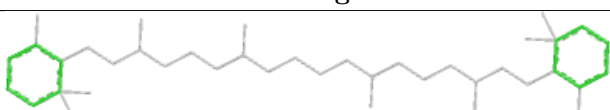


## Ligand BCR bK 102

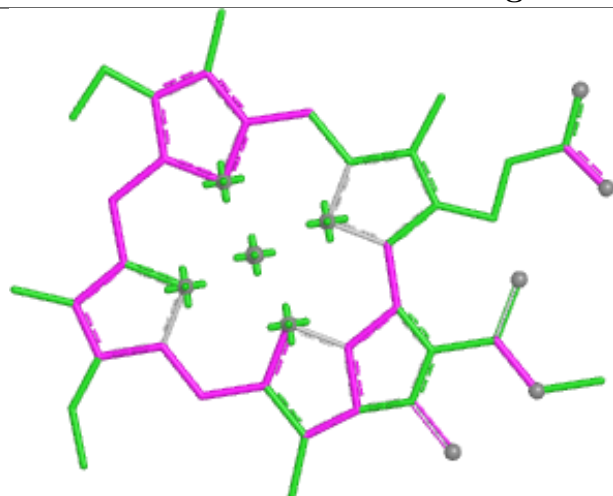


| Ligand BCR bA 849                                                                 |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

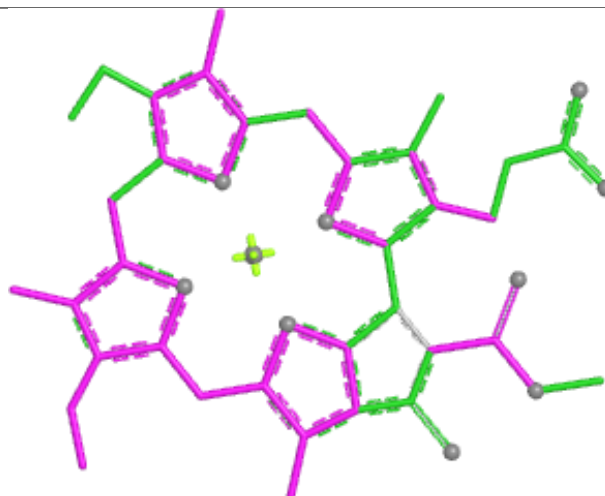
| Ligand BCR bL 208                                                                 |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

| Ligand BCR cA 848                                                                   |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

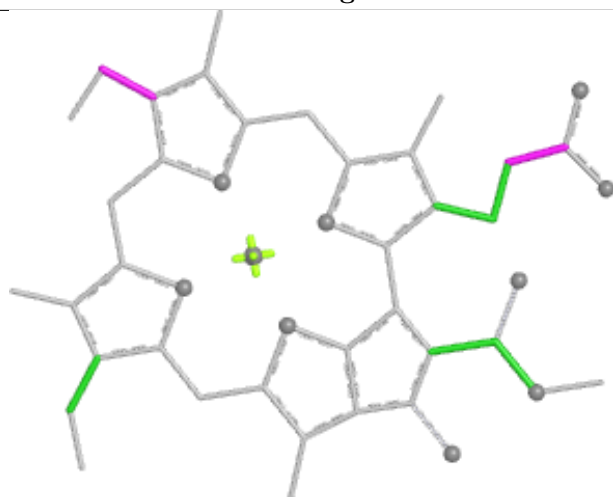
## Ligand CLA aB 835



Bond lengths



Bond angles

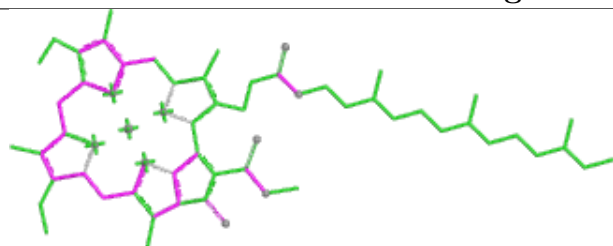


Torsions

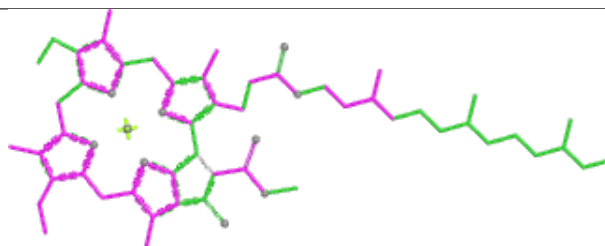


Rings

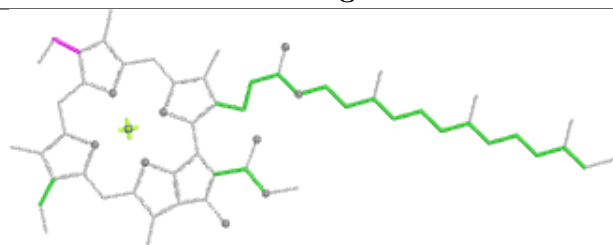
## Ligand CLA bB 807



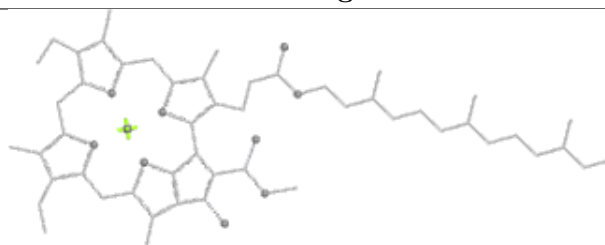
Bond lengths



Bond angles

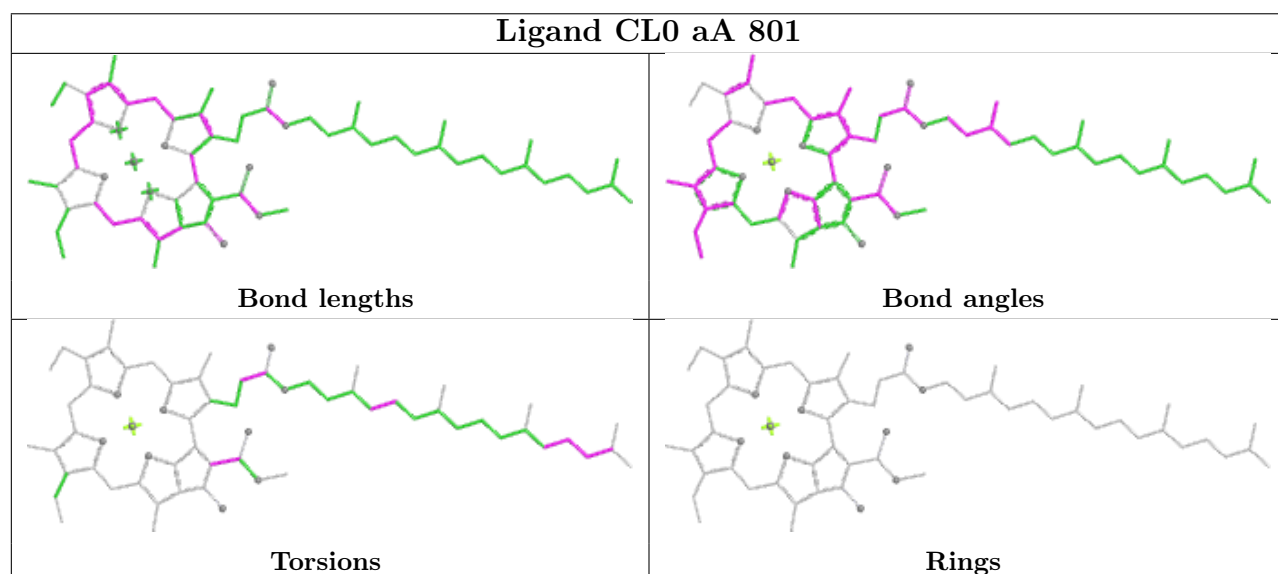
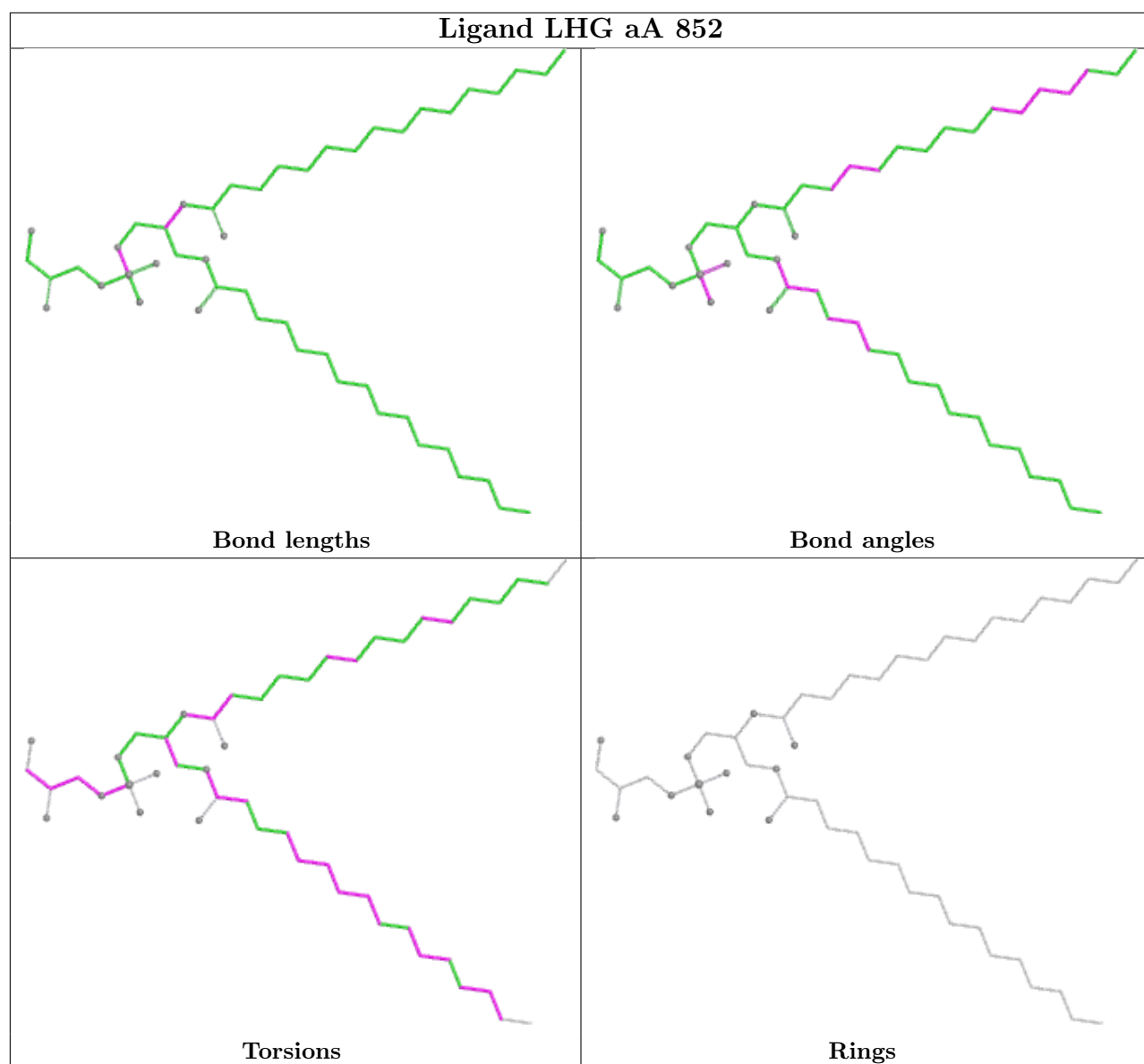


Torsions

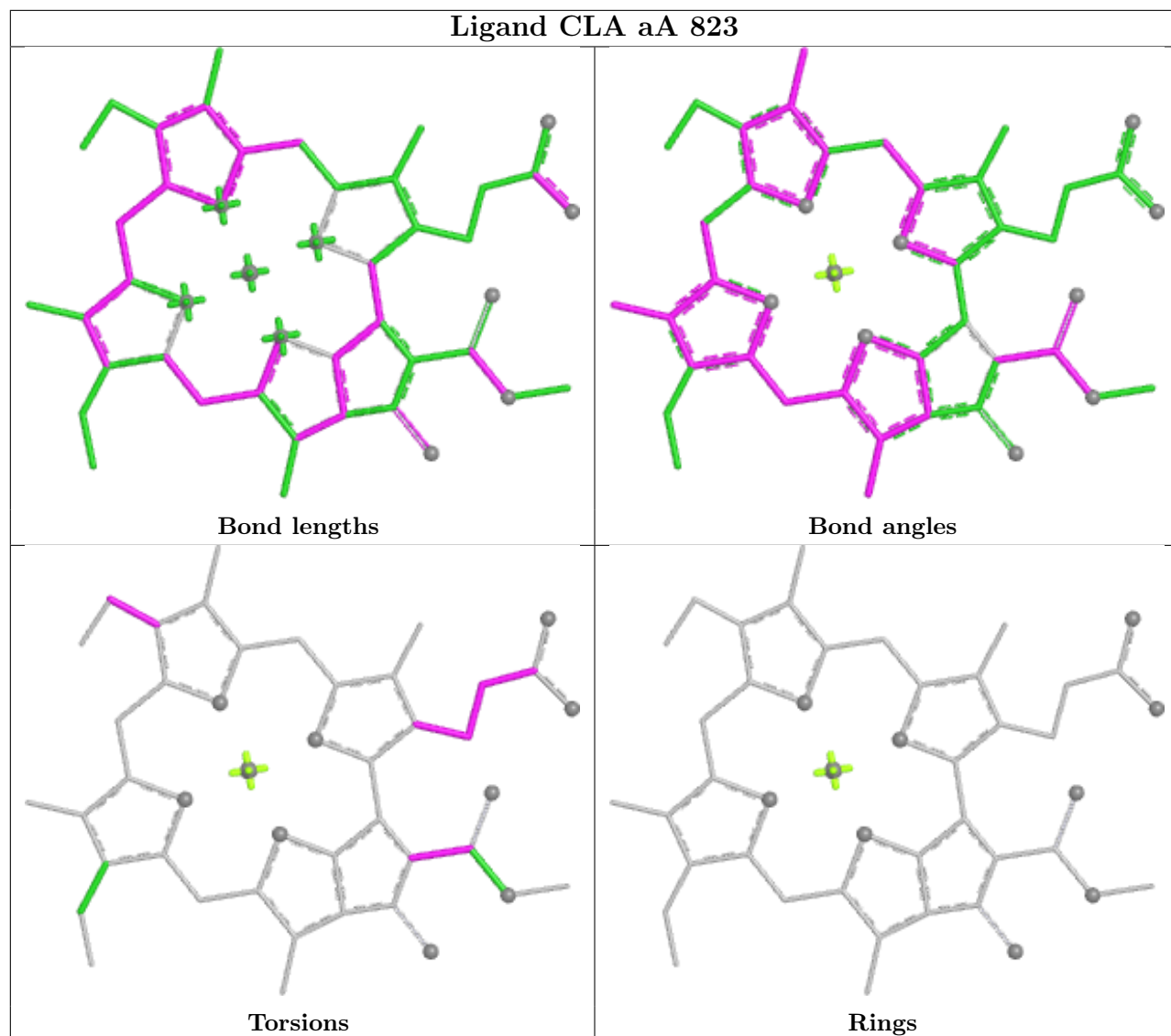


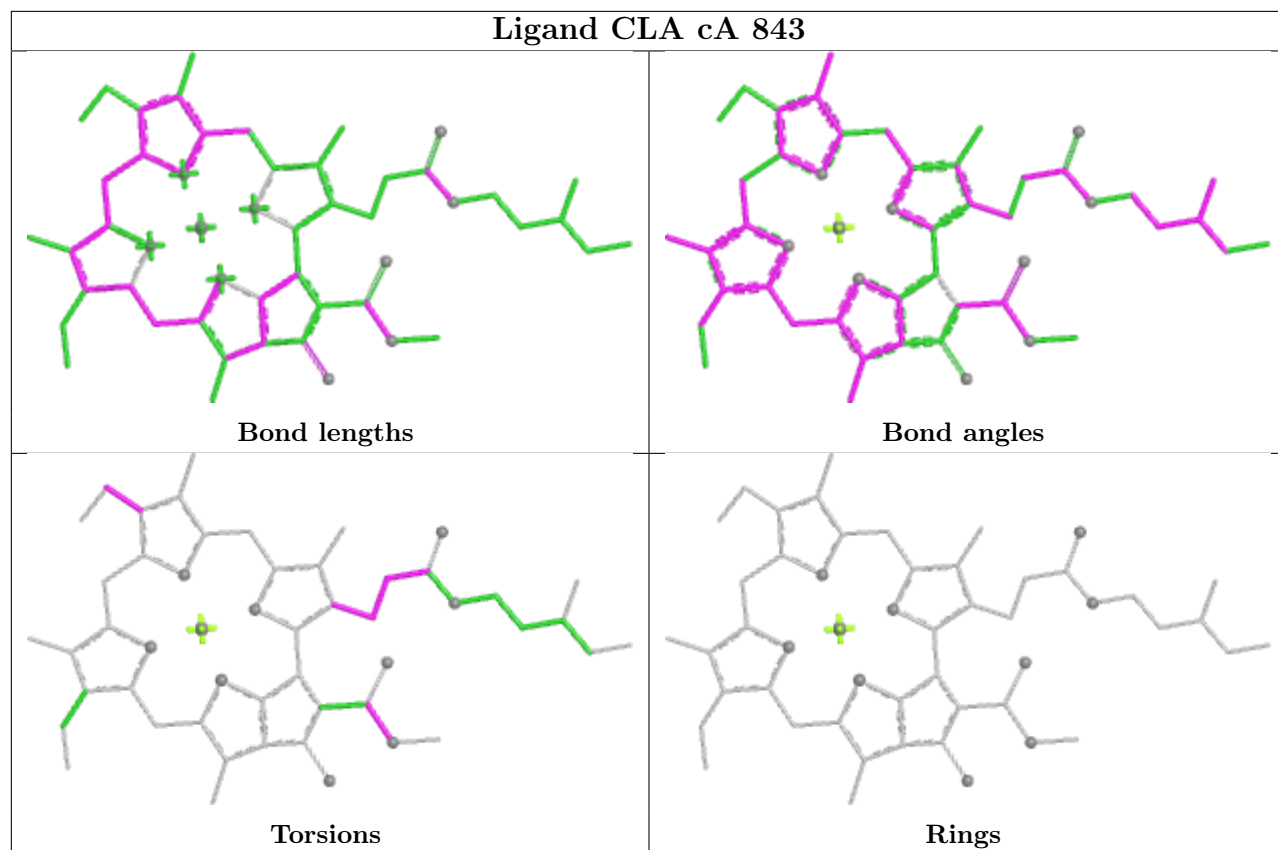
Rings

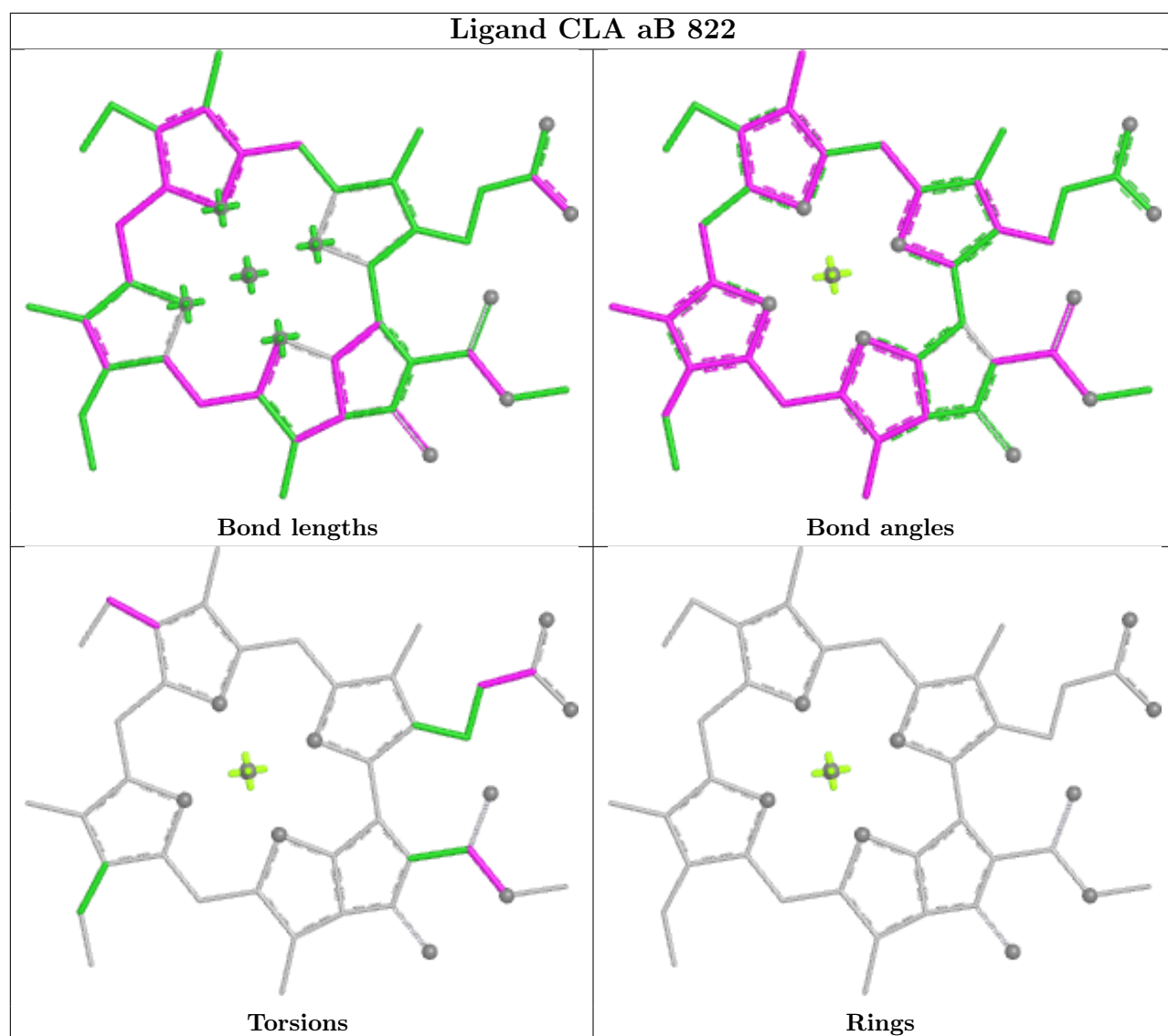


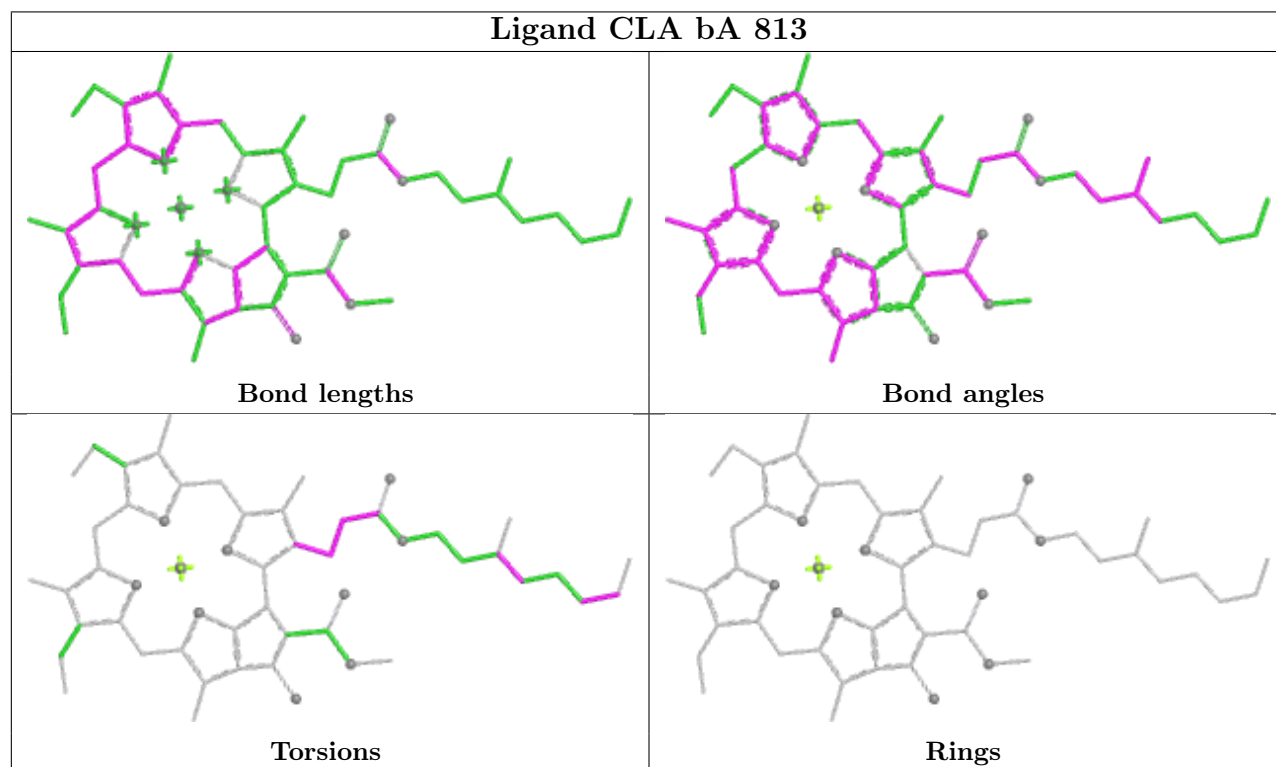
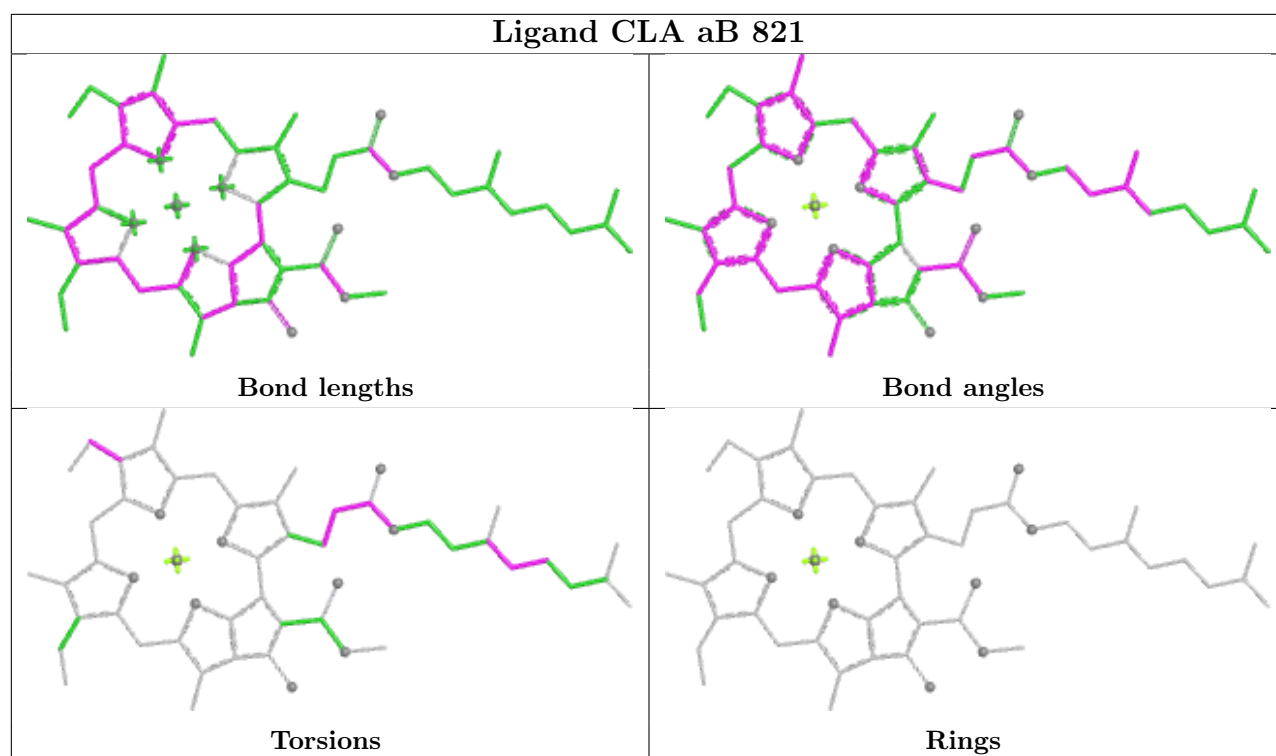


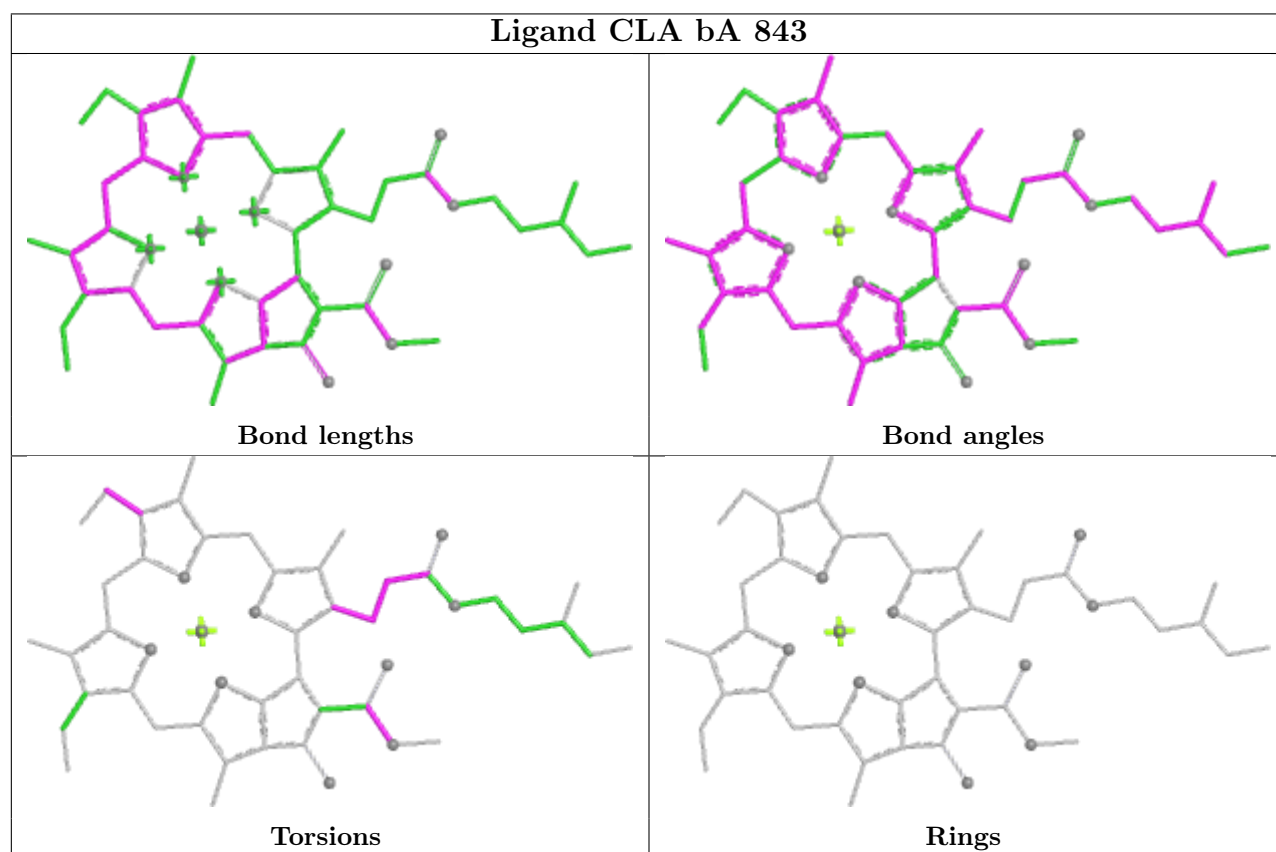
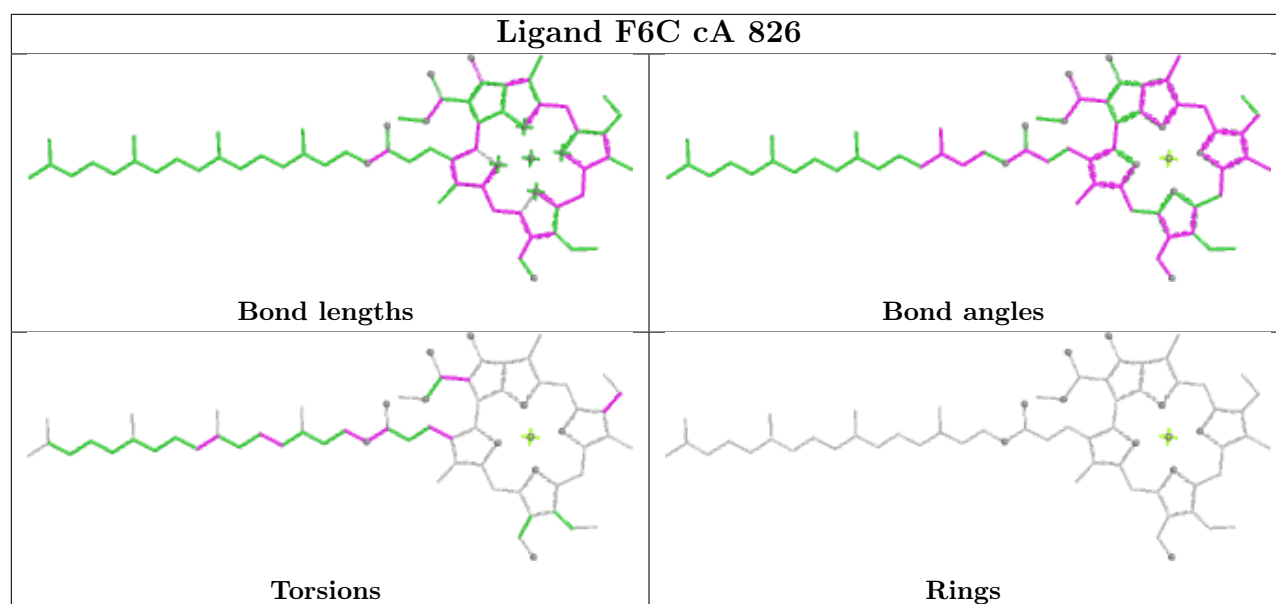
## Ligand CLA aA 823

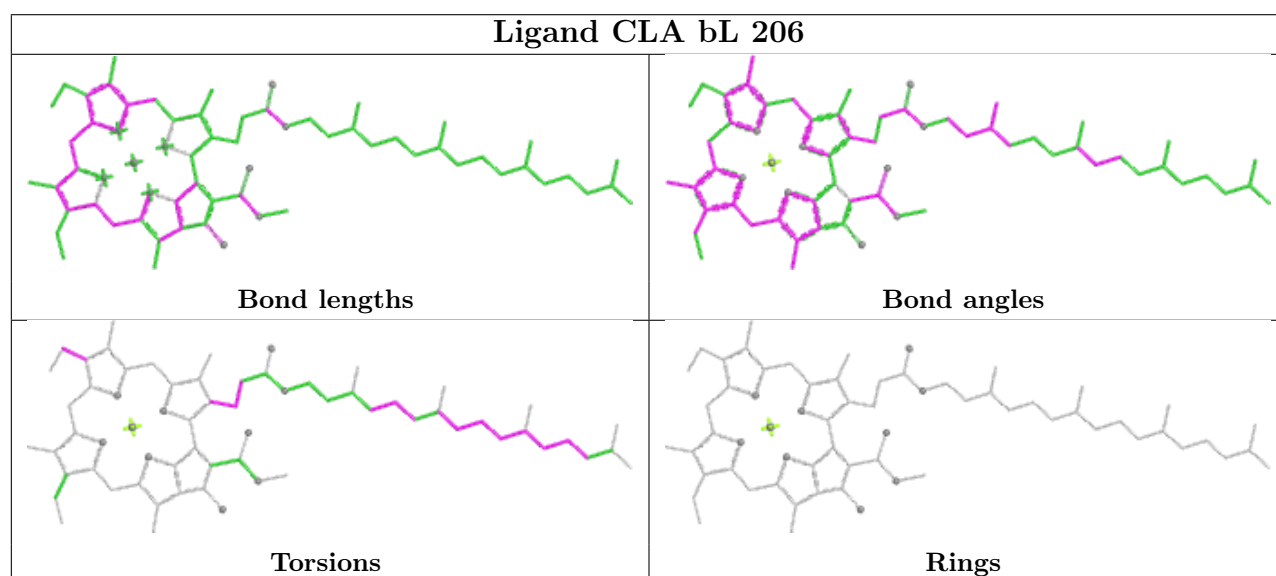
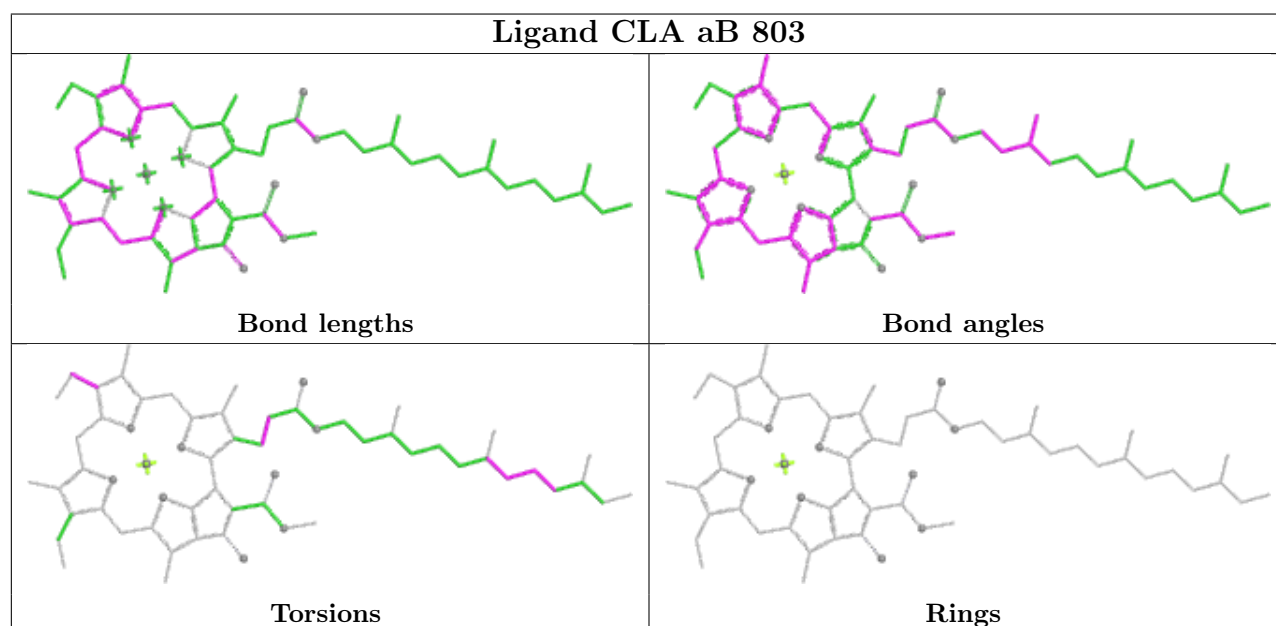
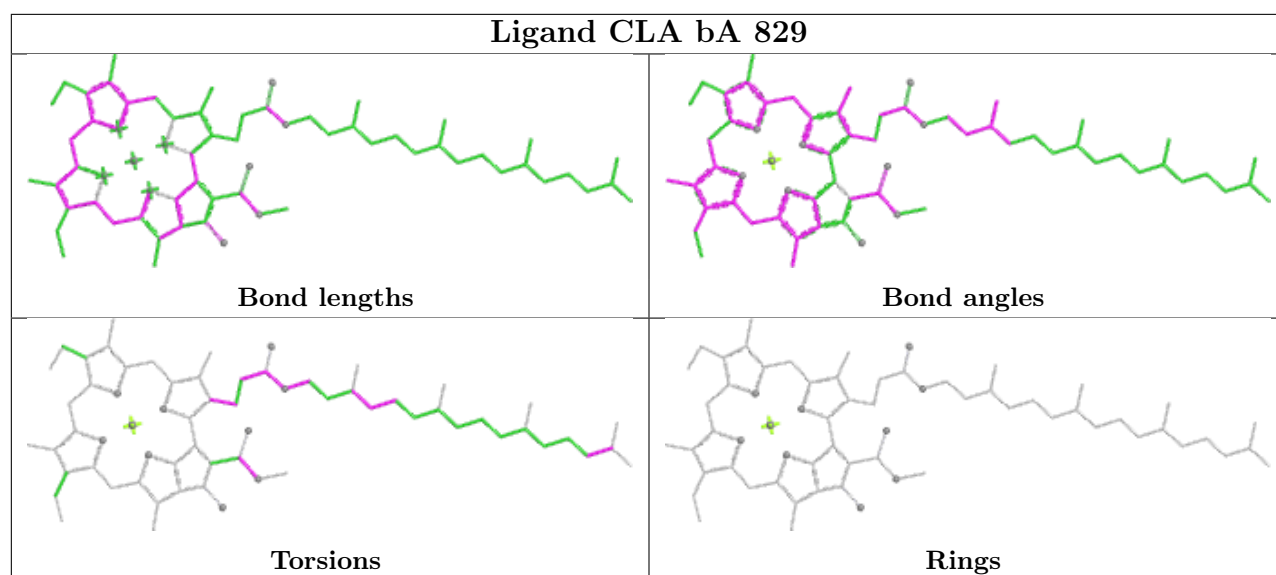




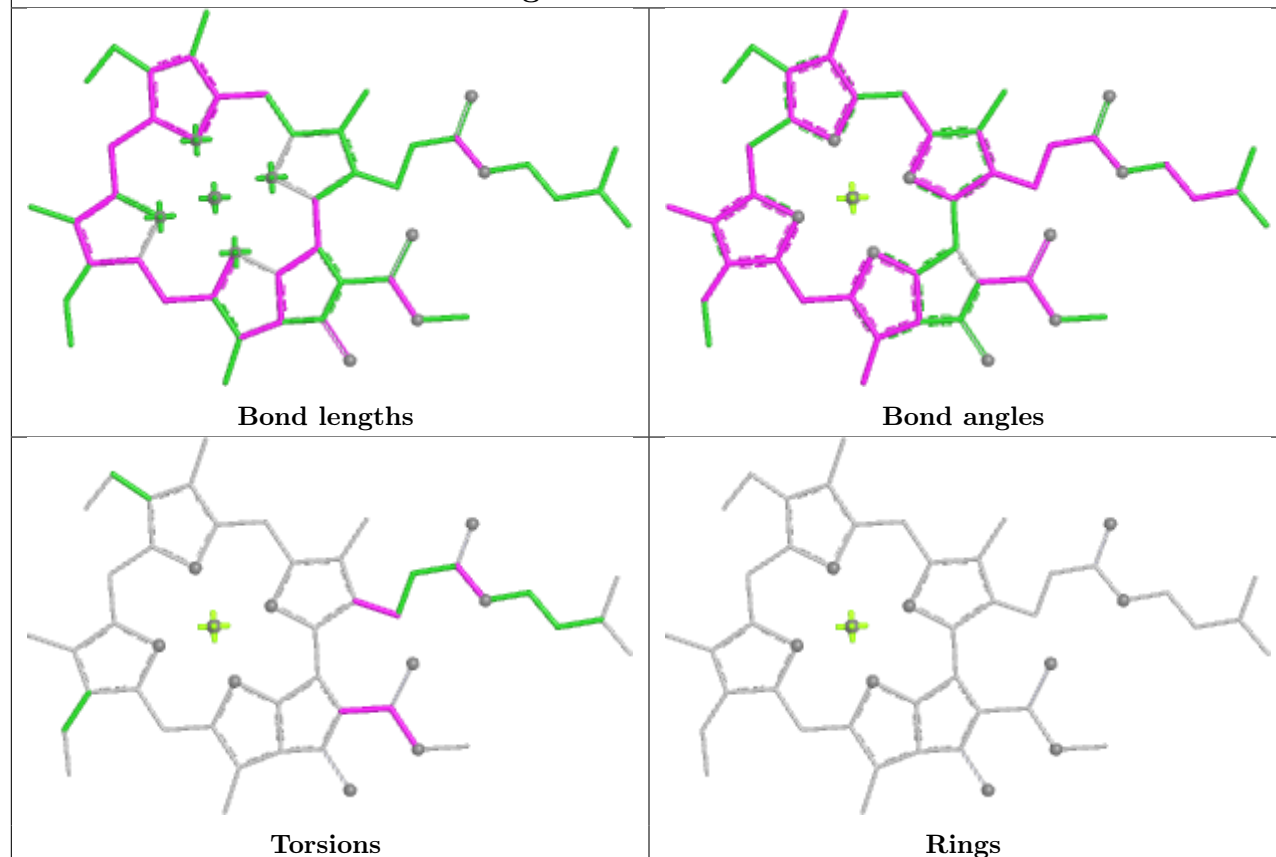




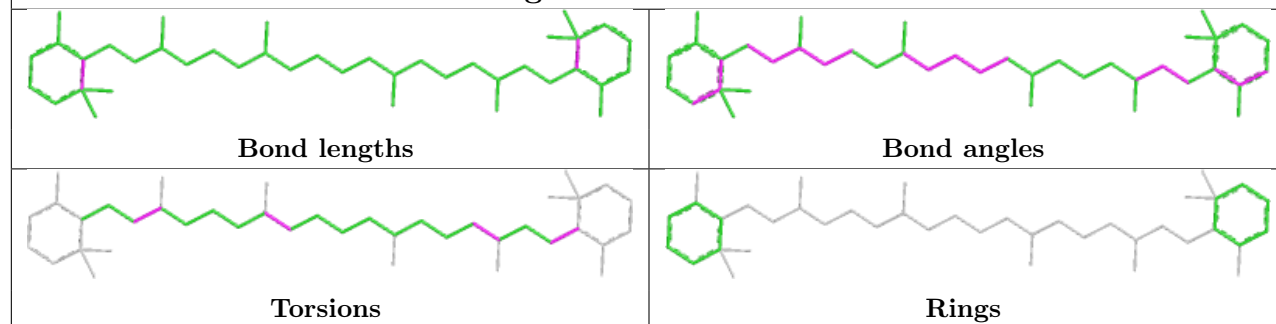




## Ligand CLA bB 804

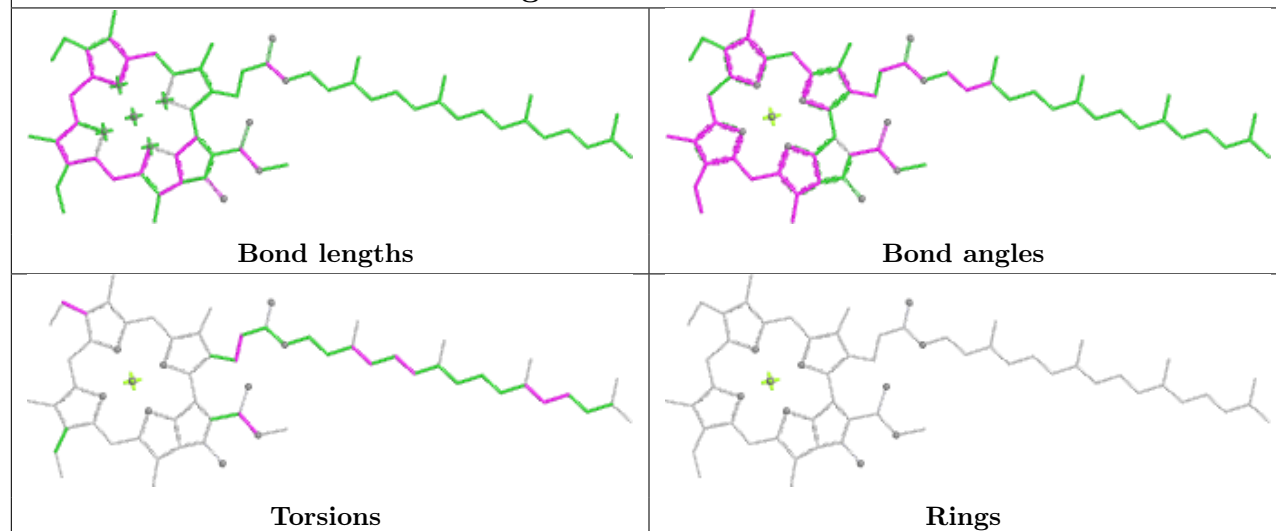


## Ligand BCR cL 208

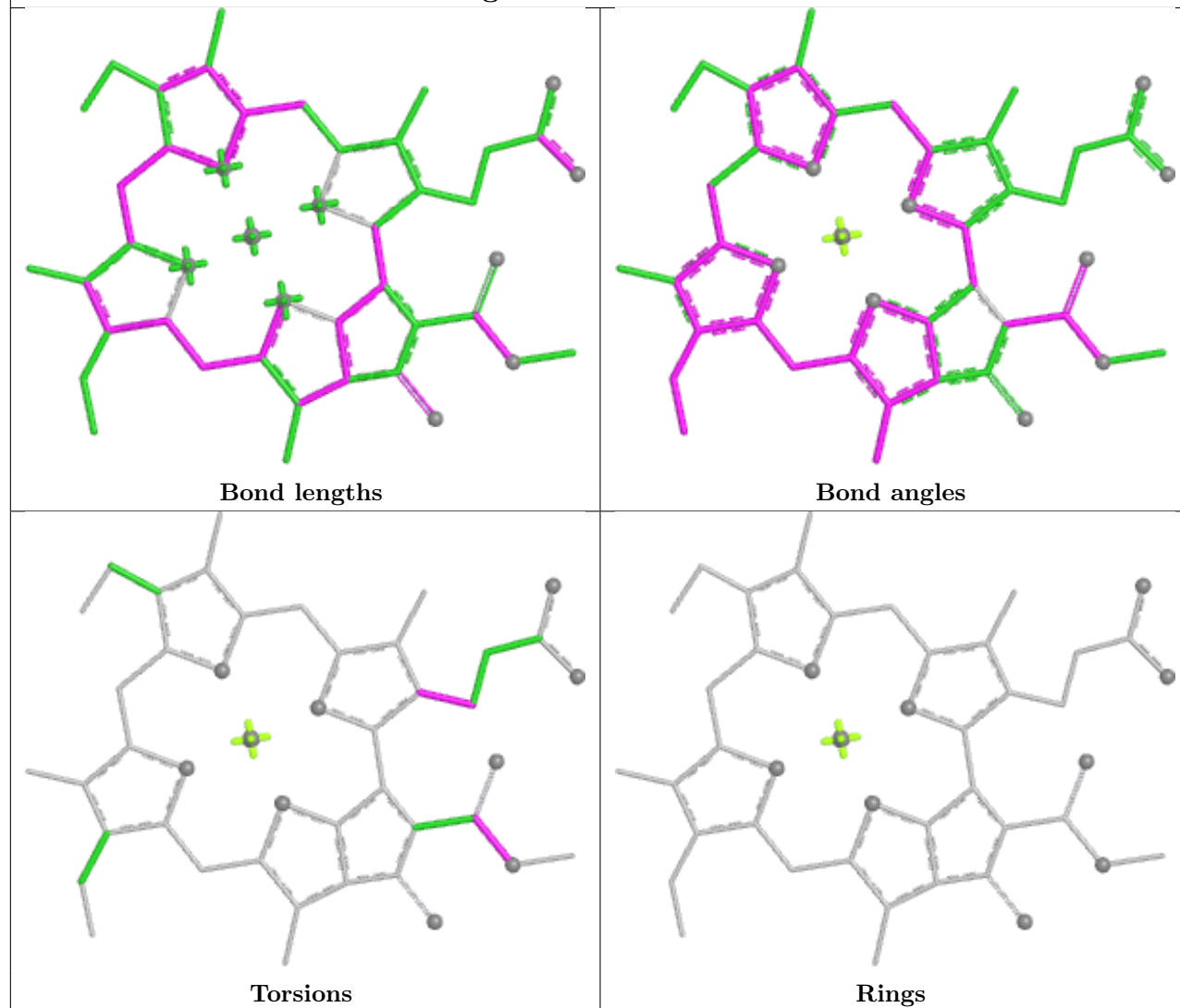




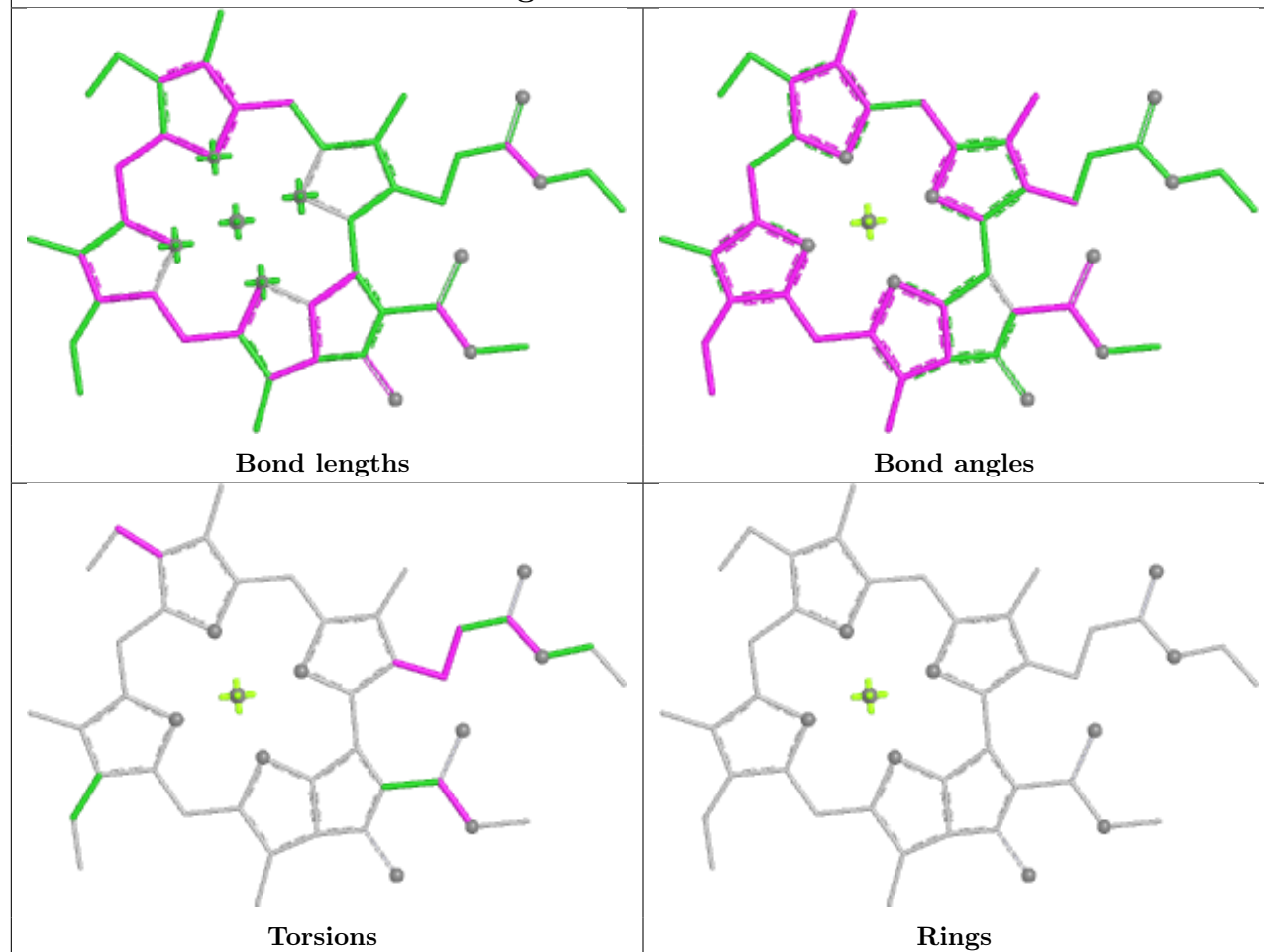
## Ligand CLA ba 835



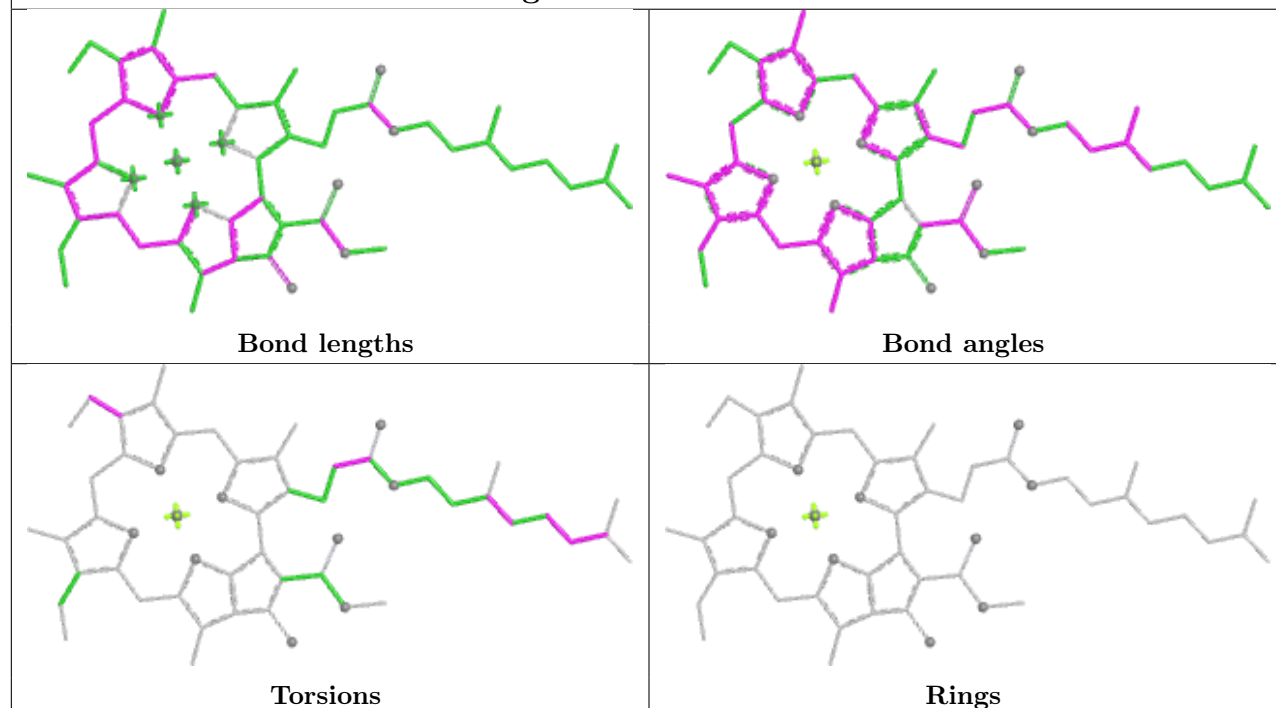
## Ligand CLA ba 815

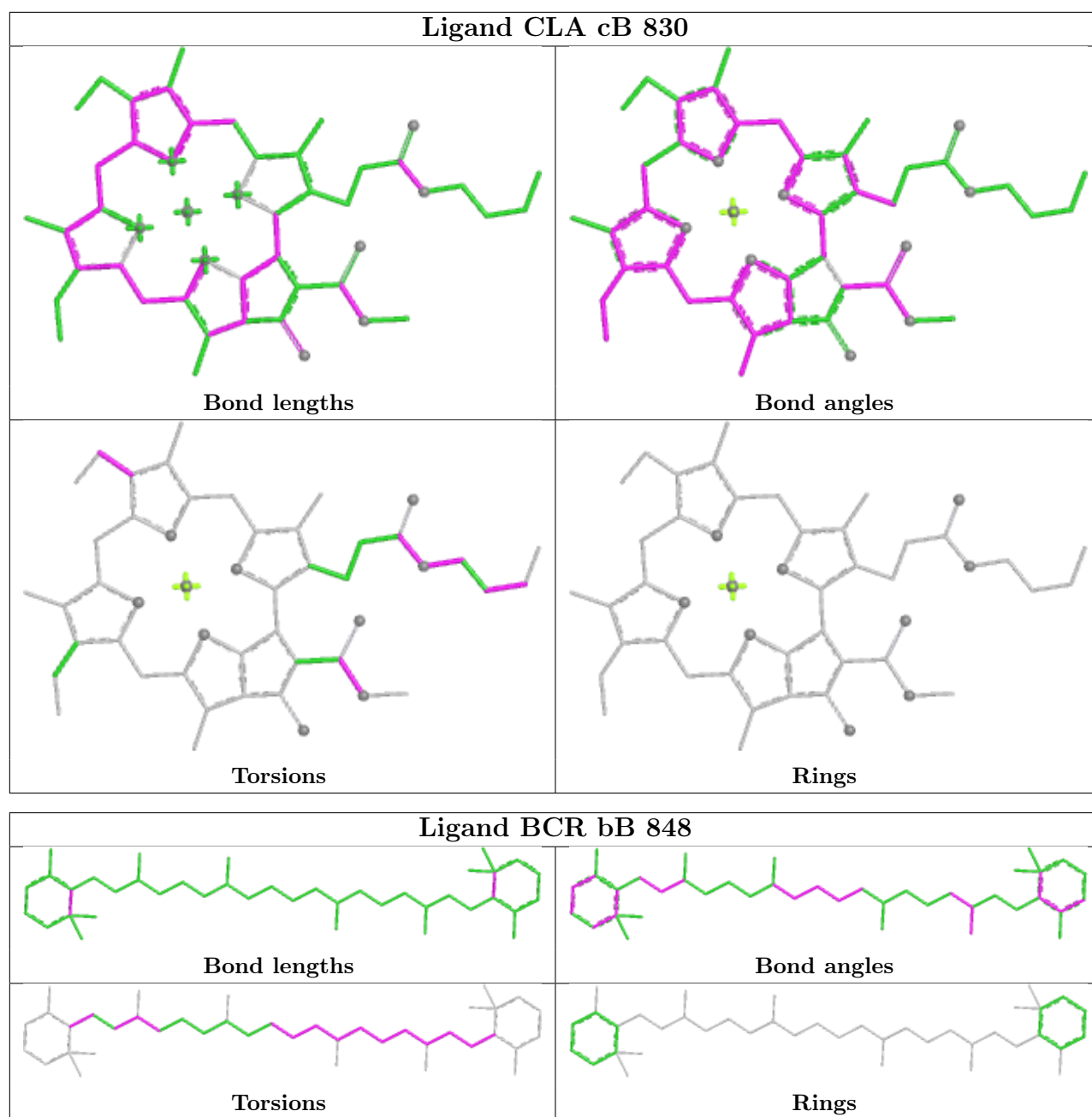


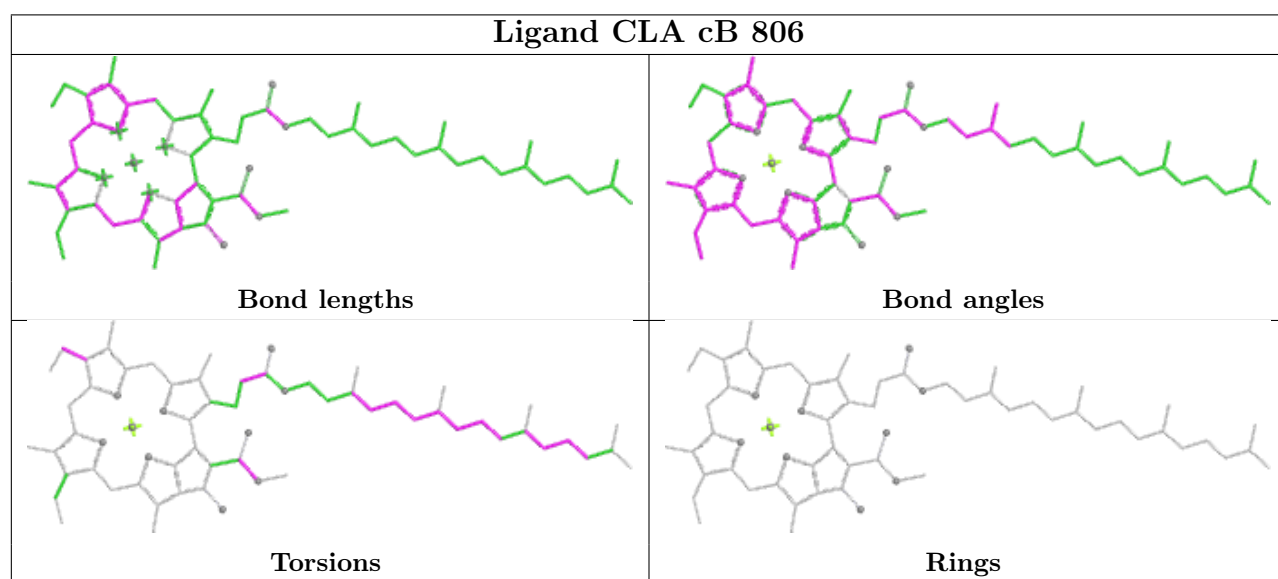
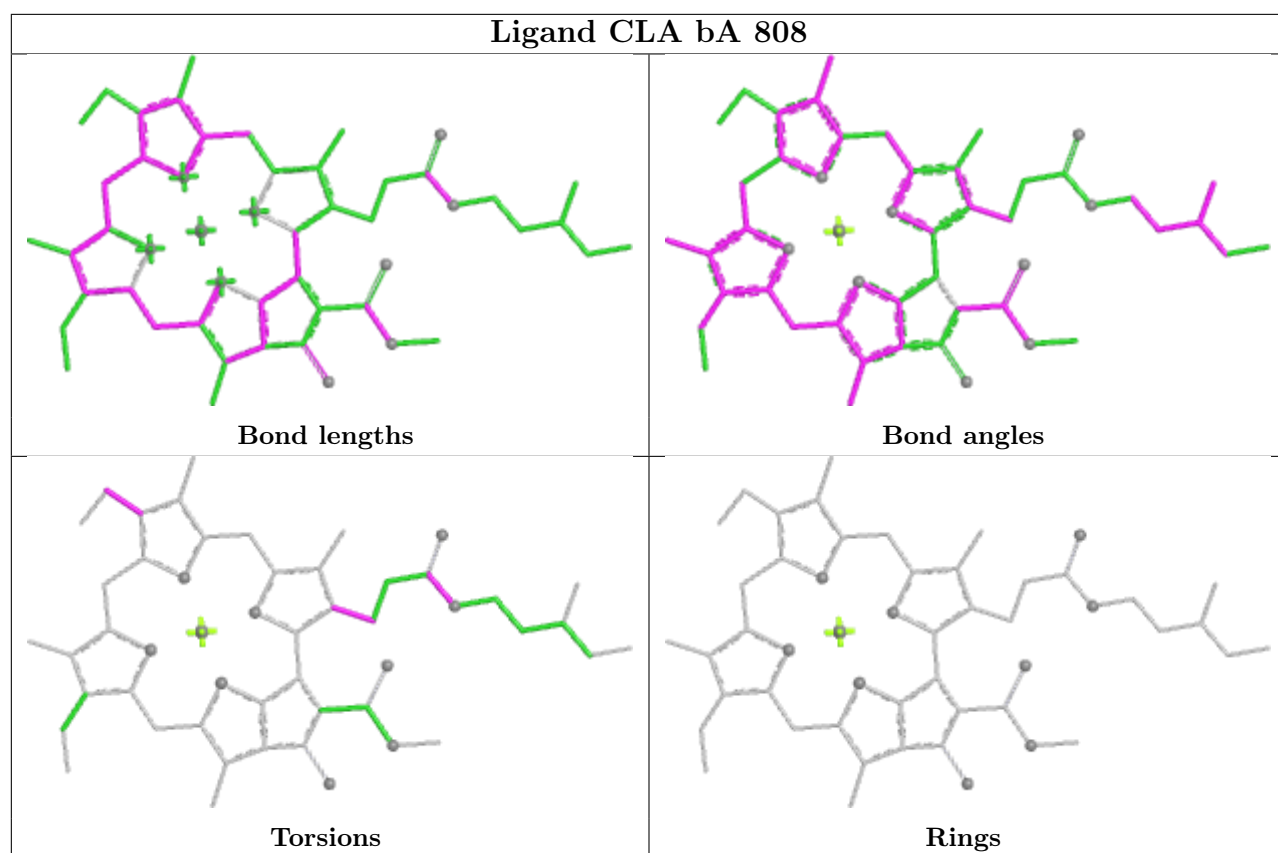
## Ligand CLA bB 809

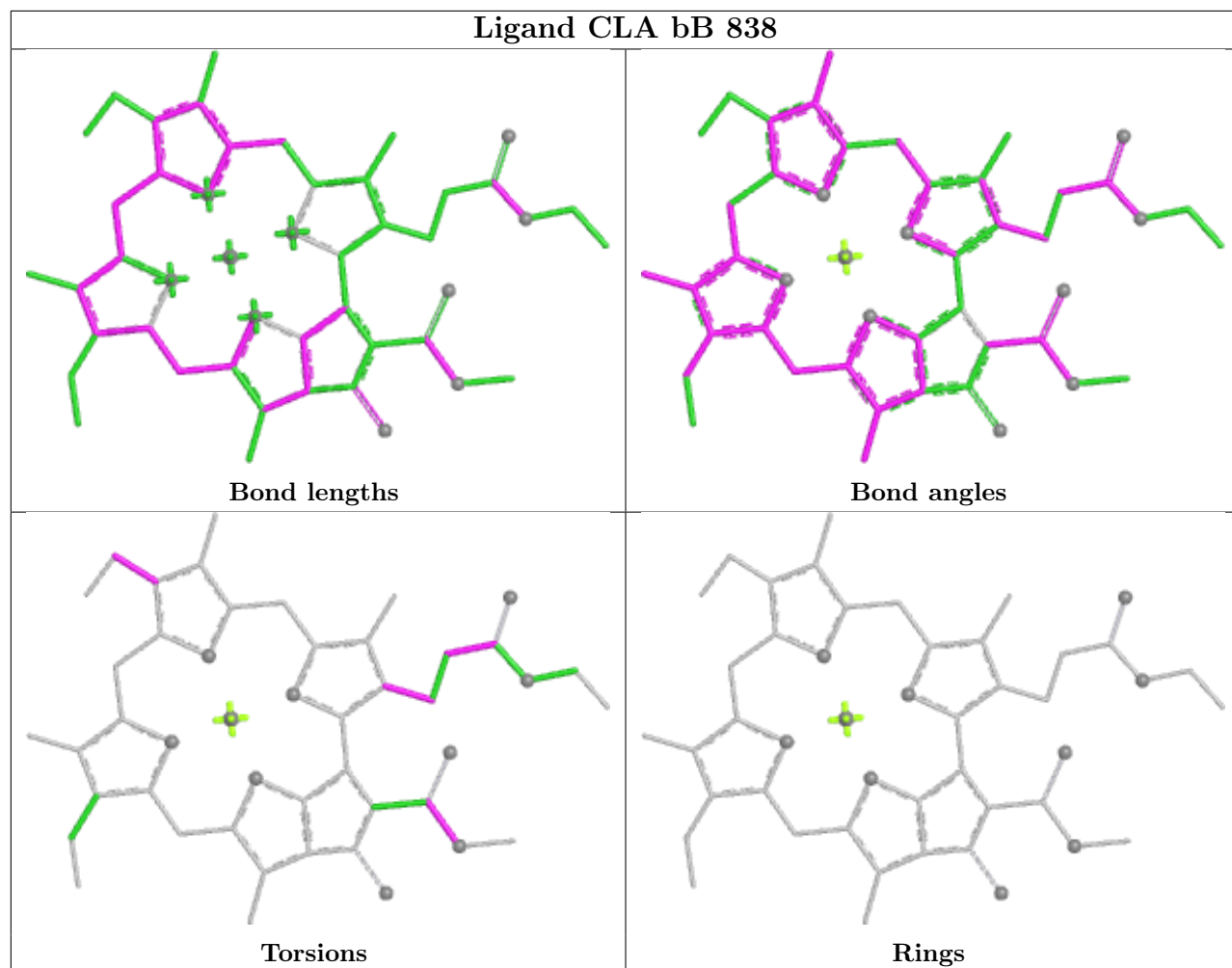


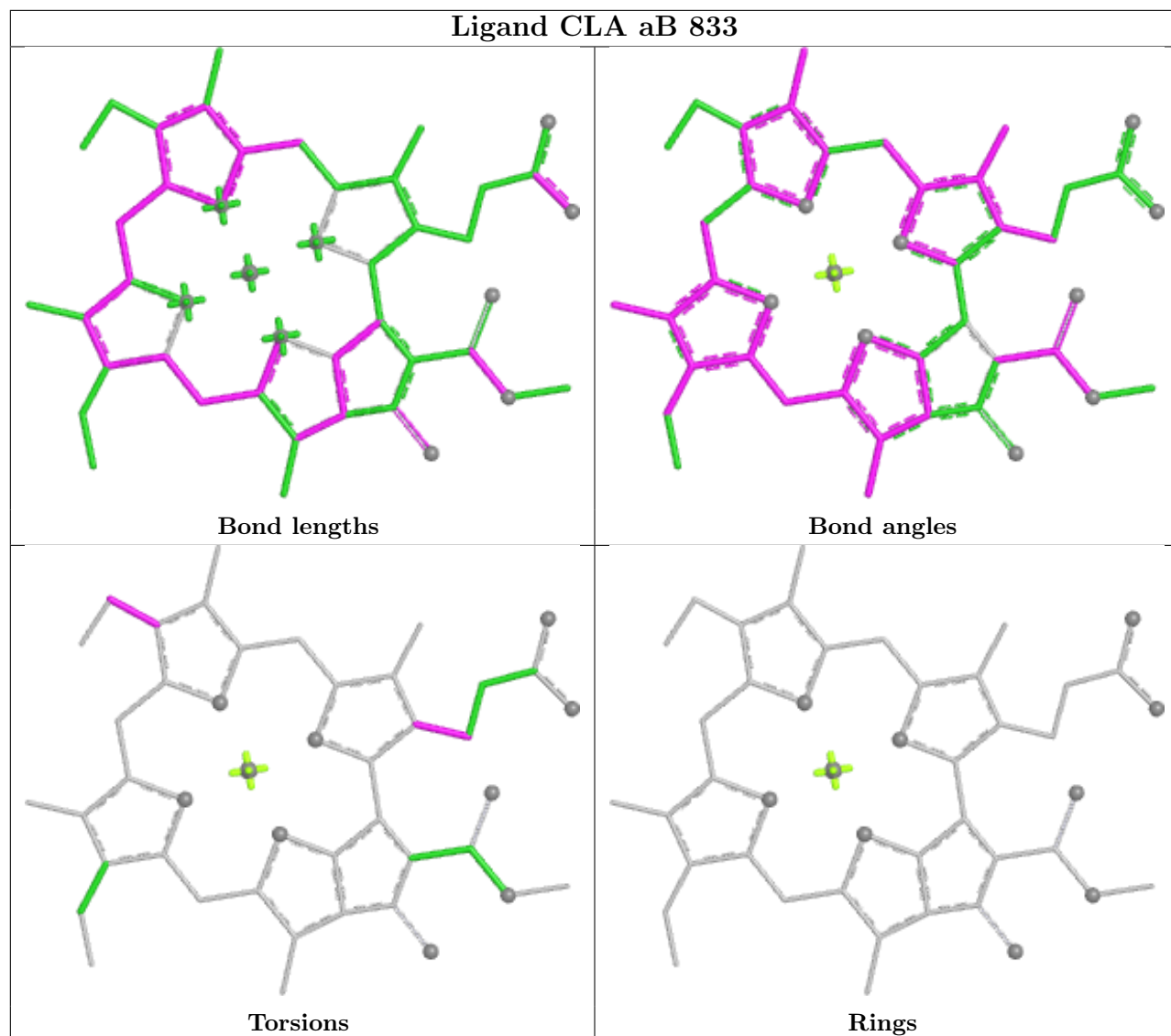
## Ligand CLA bB 837



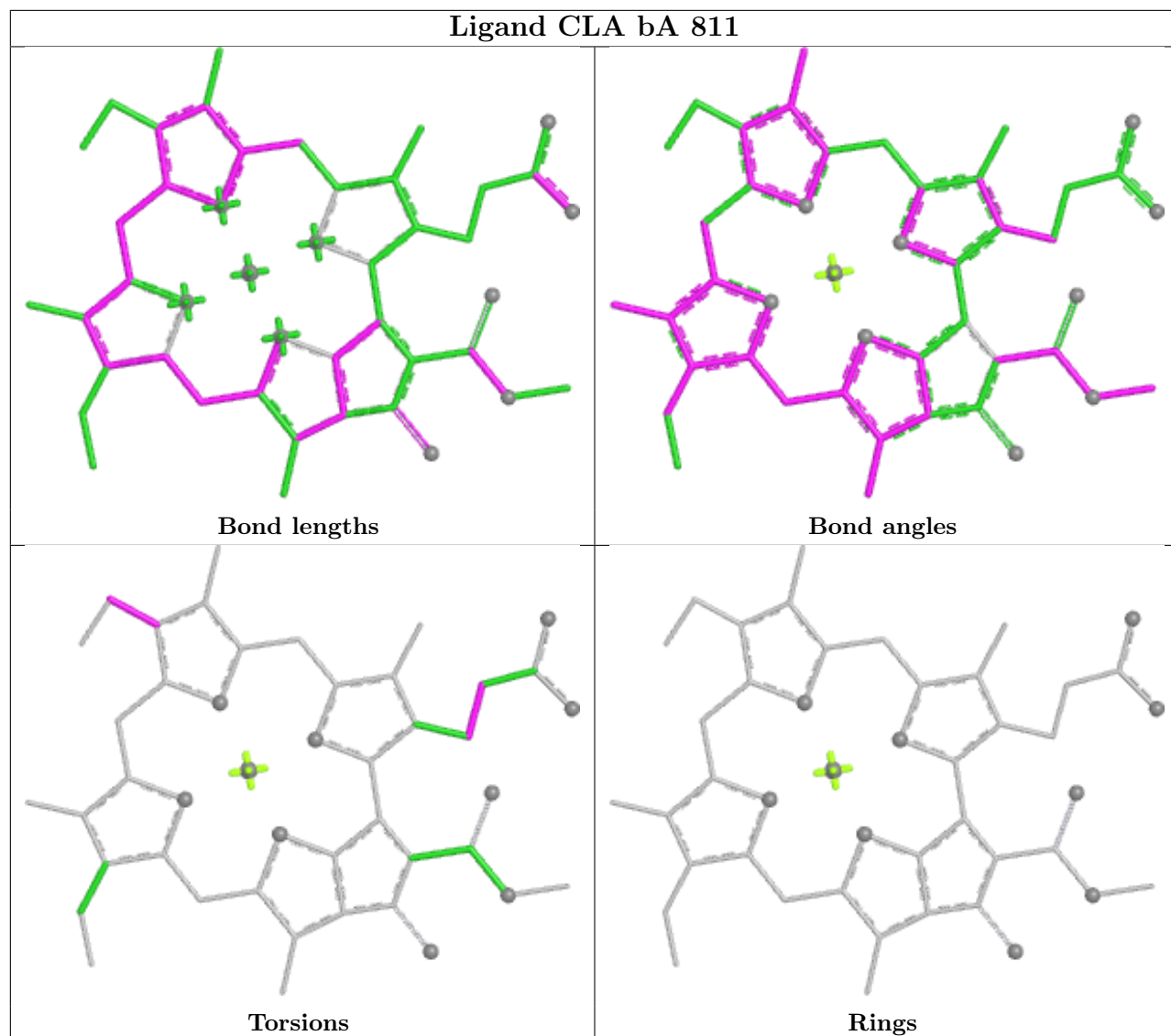


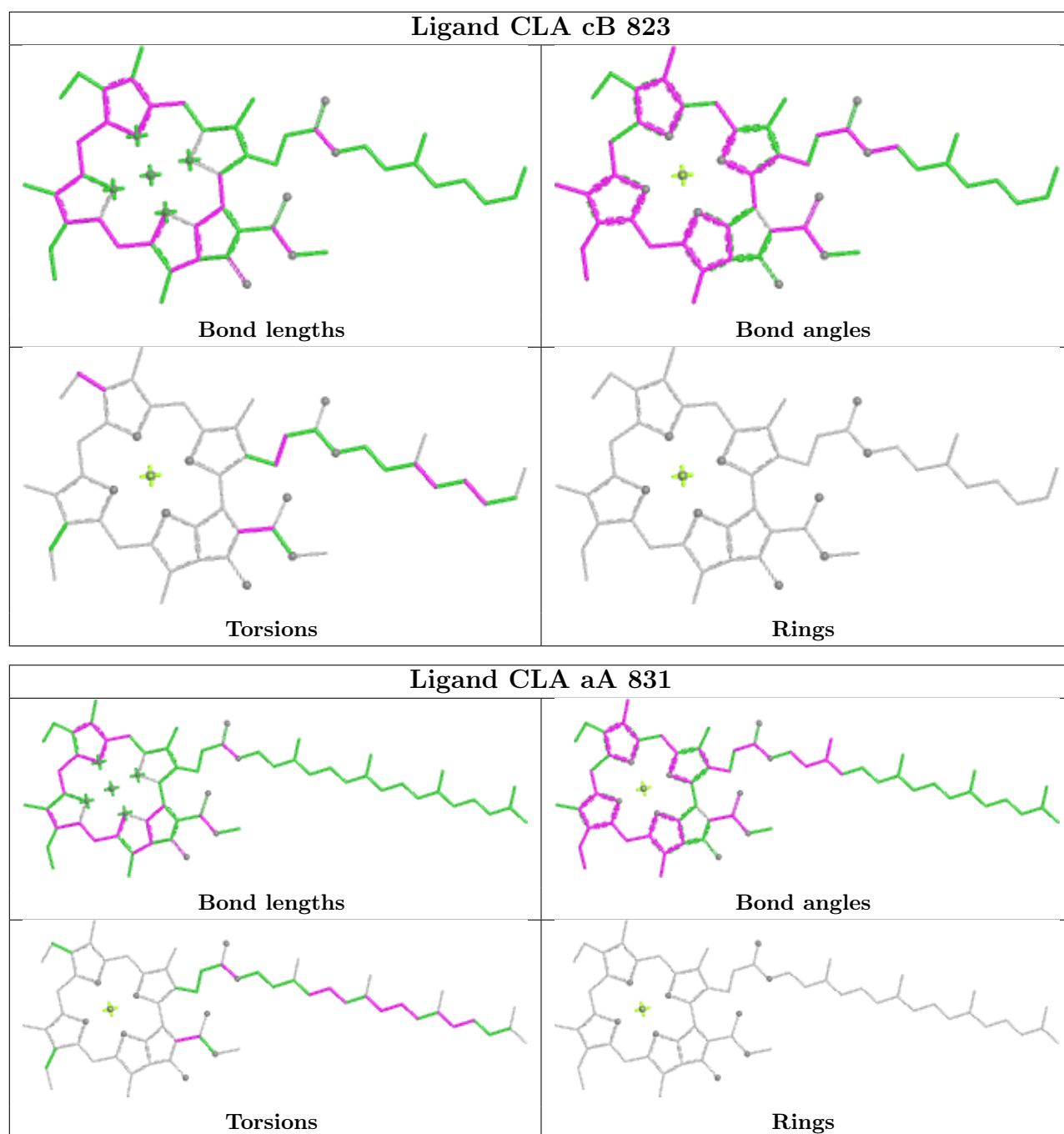




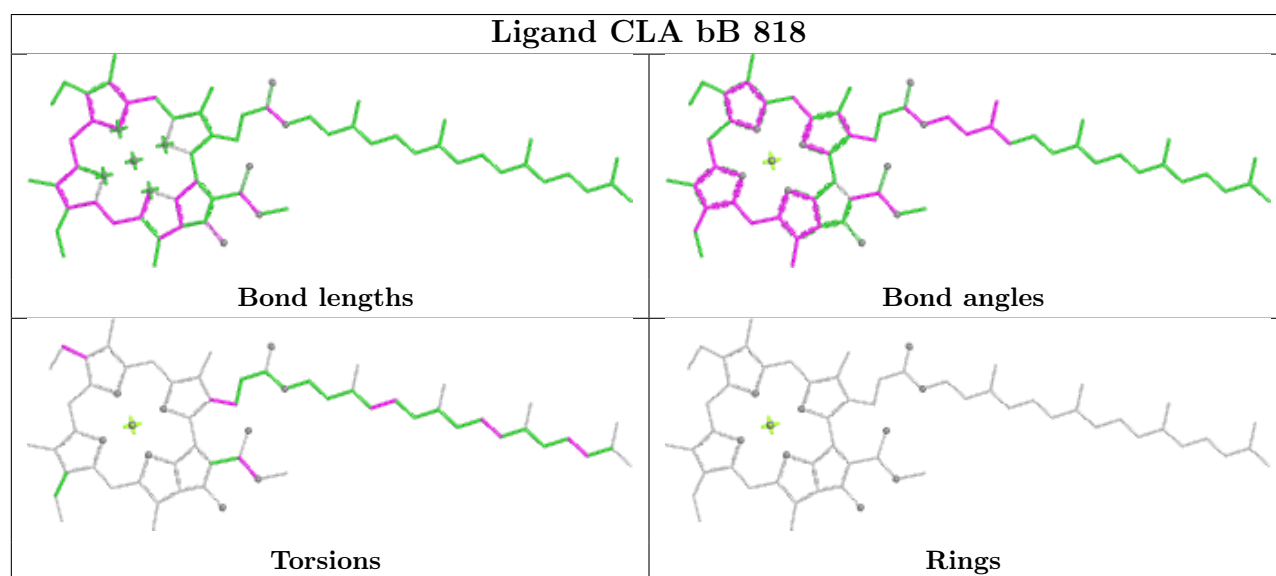
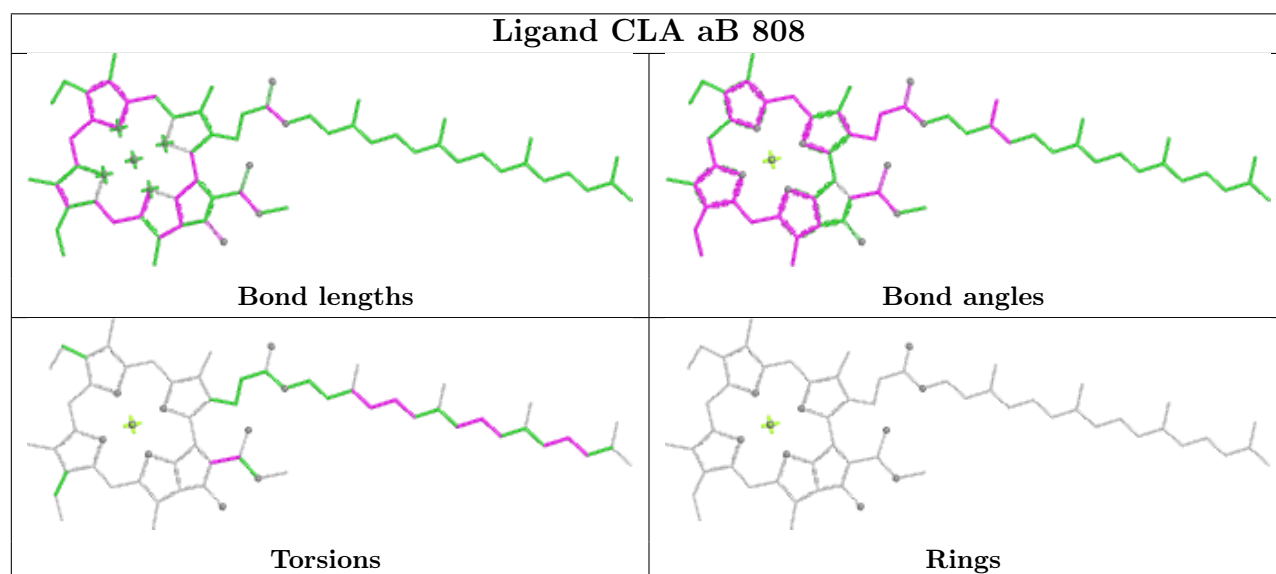
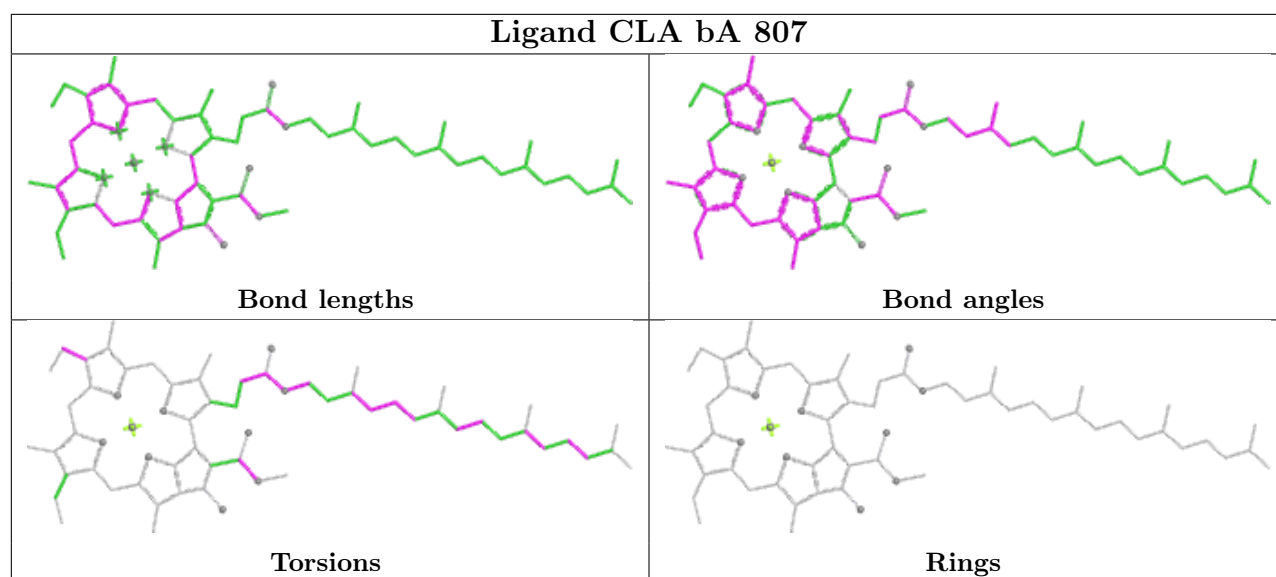


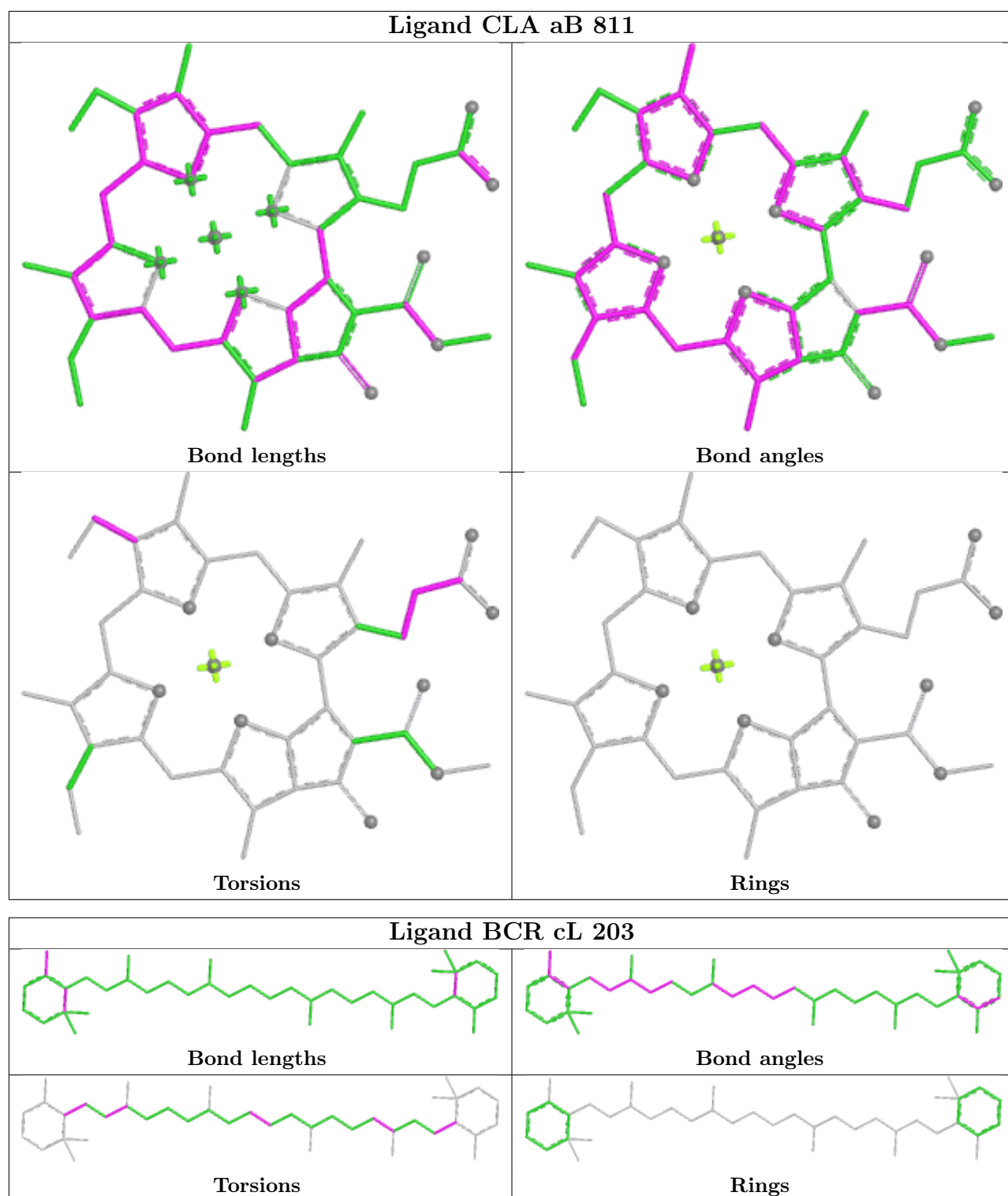
## Ligand CLA bA 811



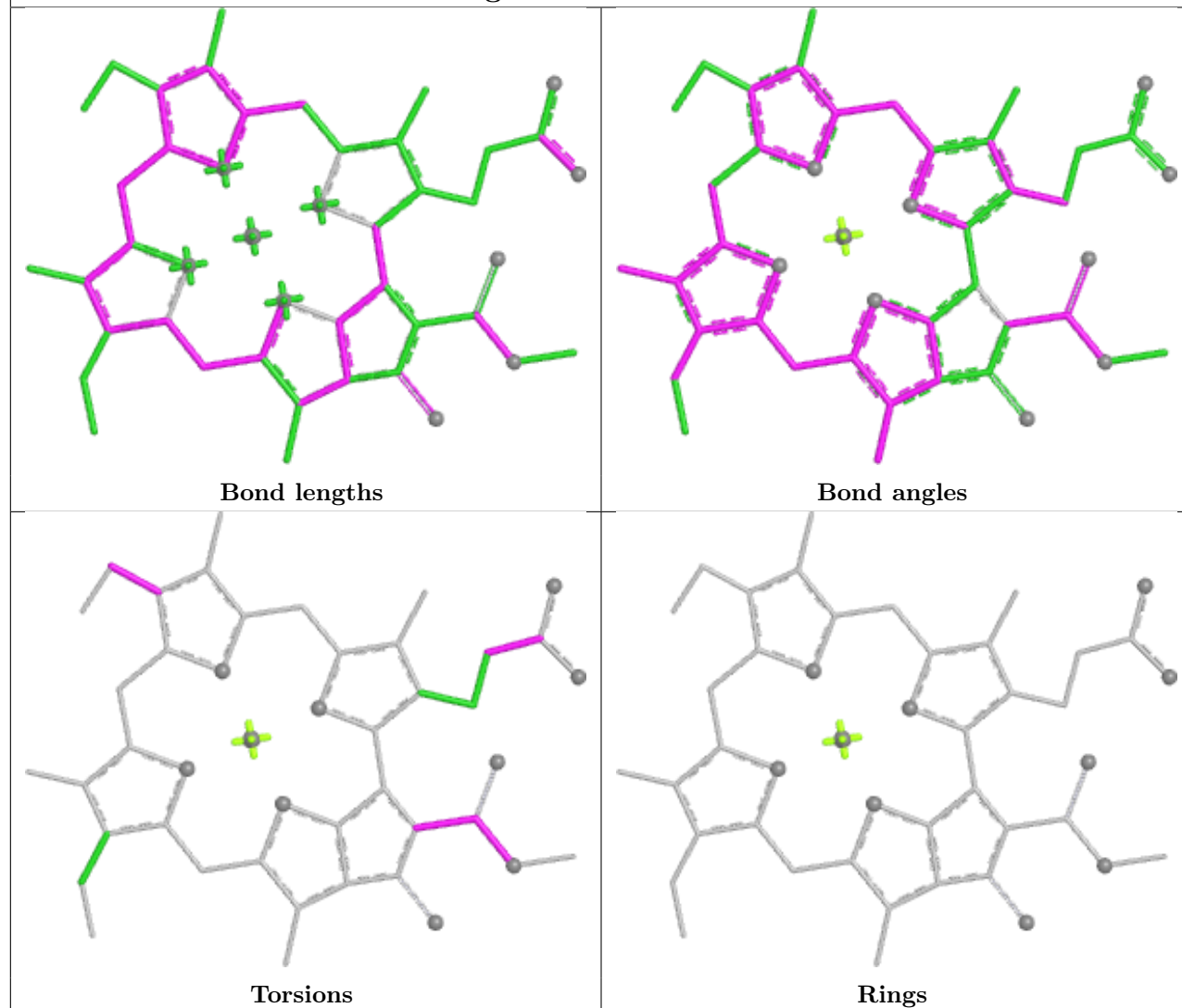




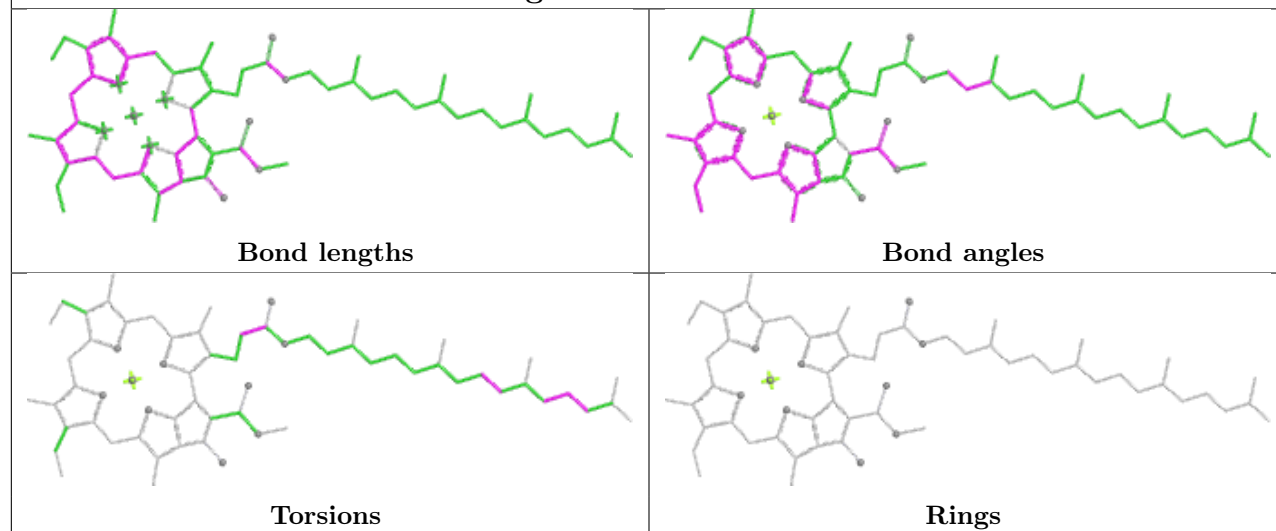




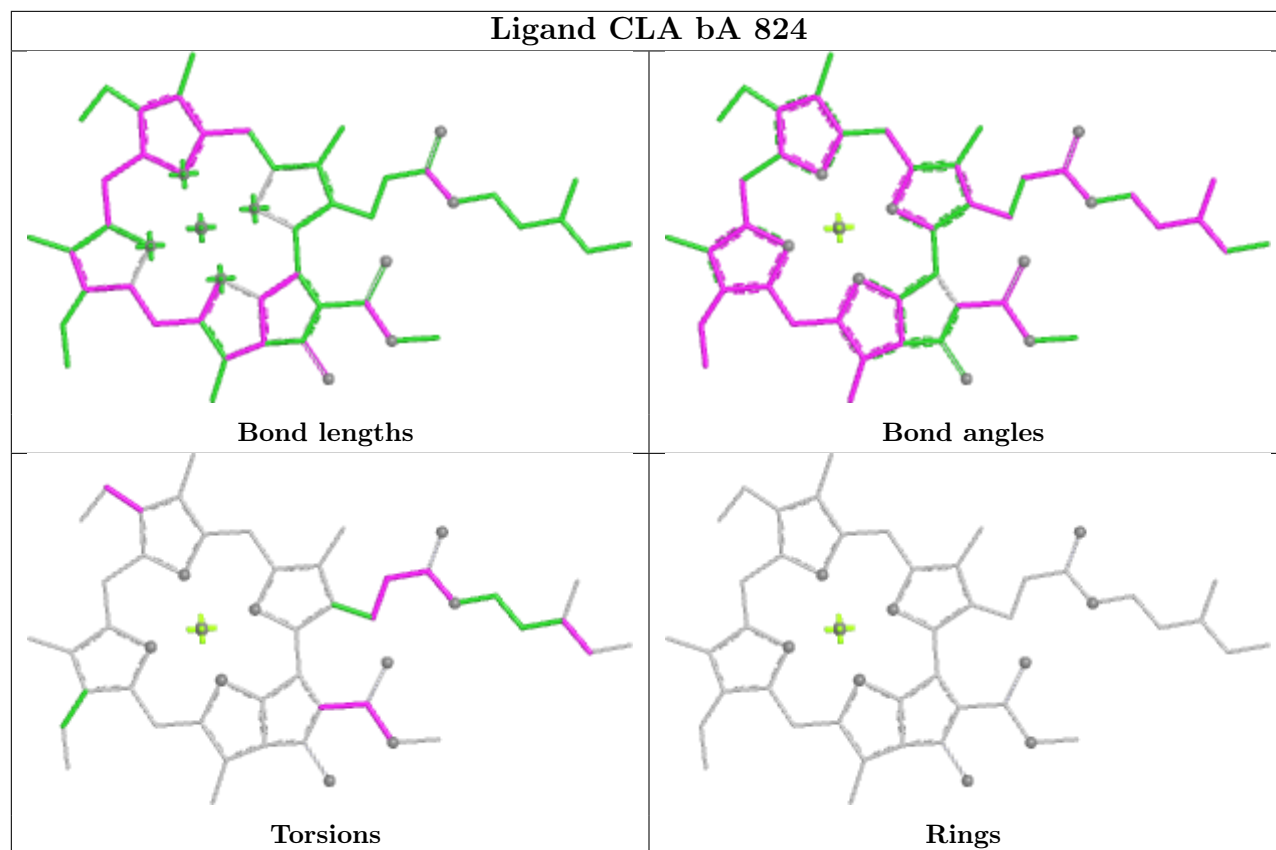
## Ligand CLA cA 805



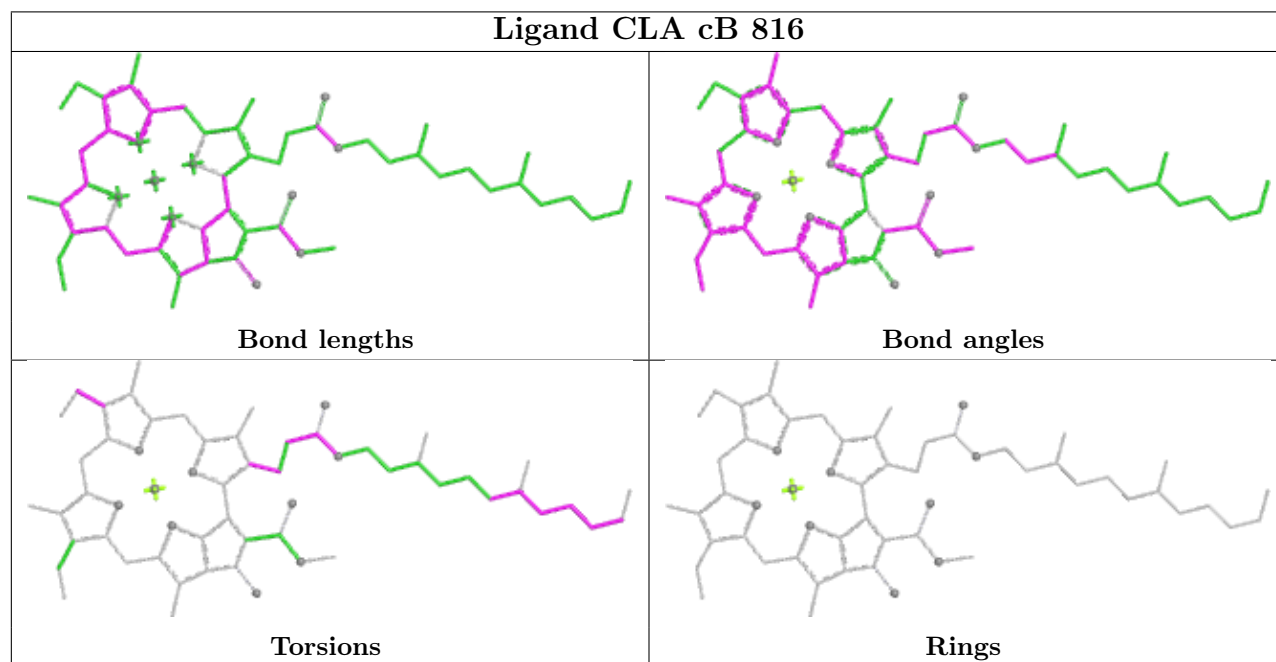
## Ligand CLA aL 204



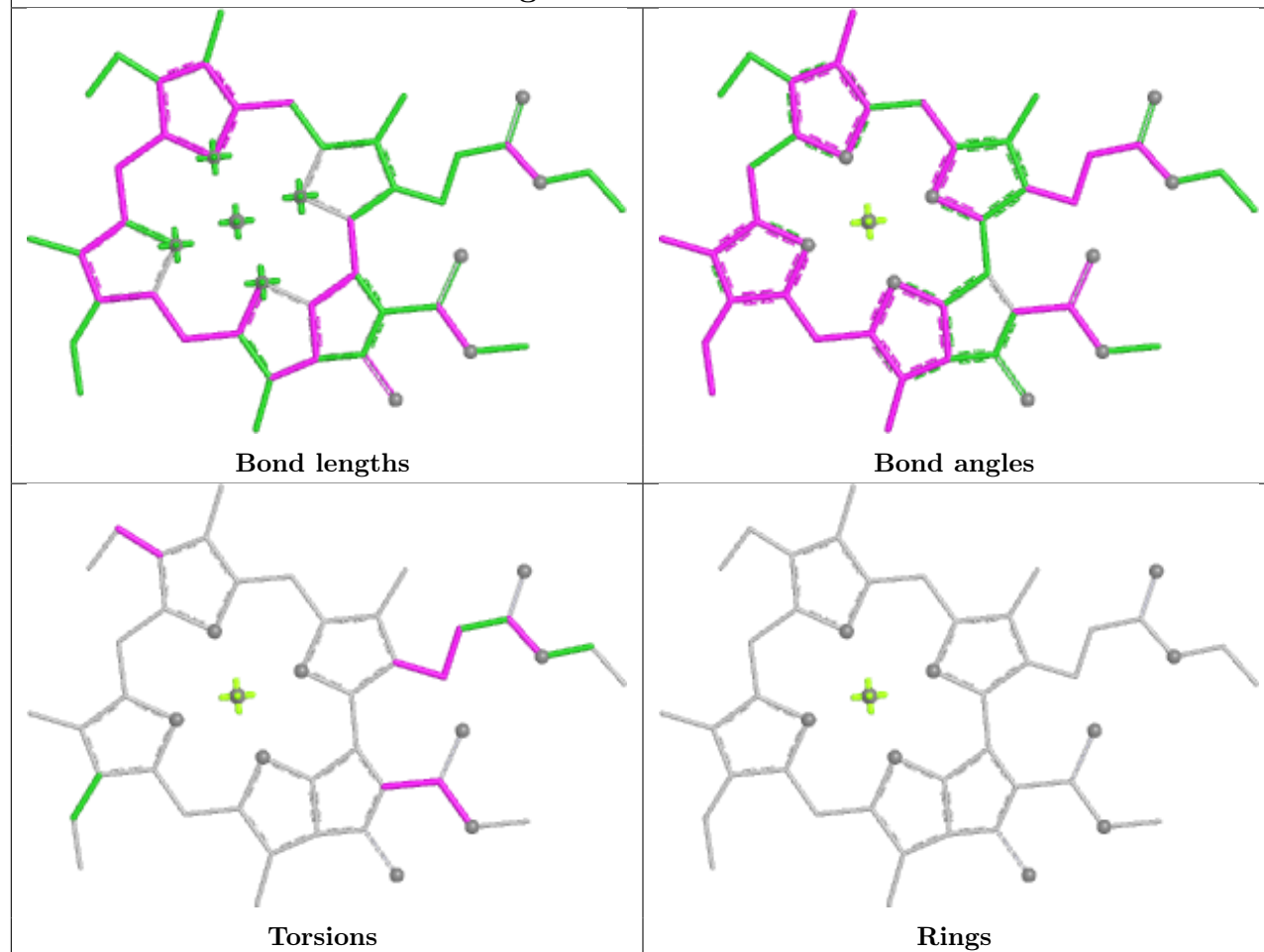
## Ligand CLA bA 824



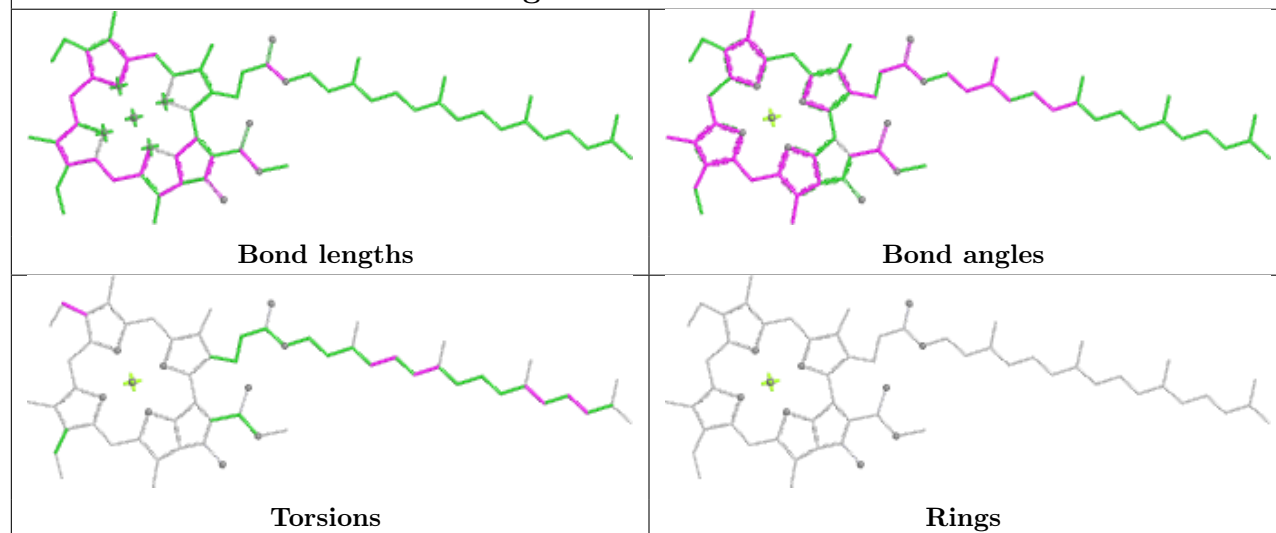
## Ligand CLA cB 816

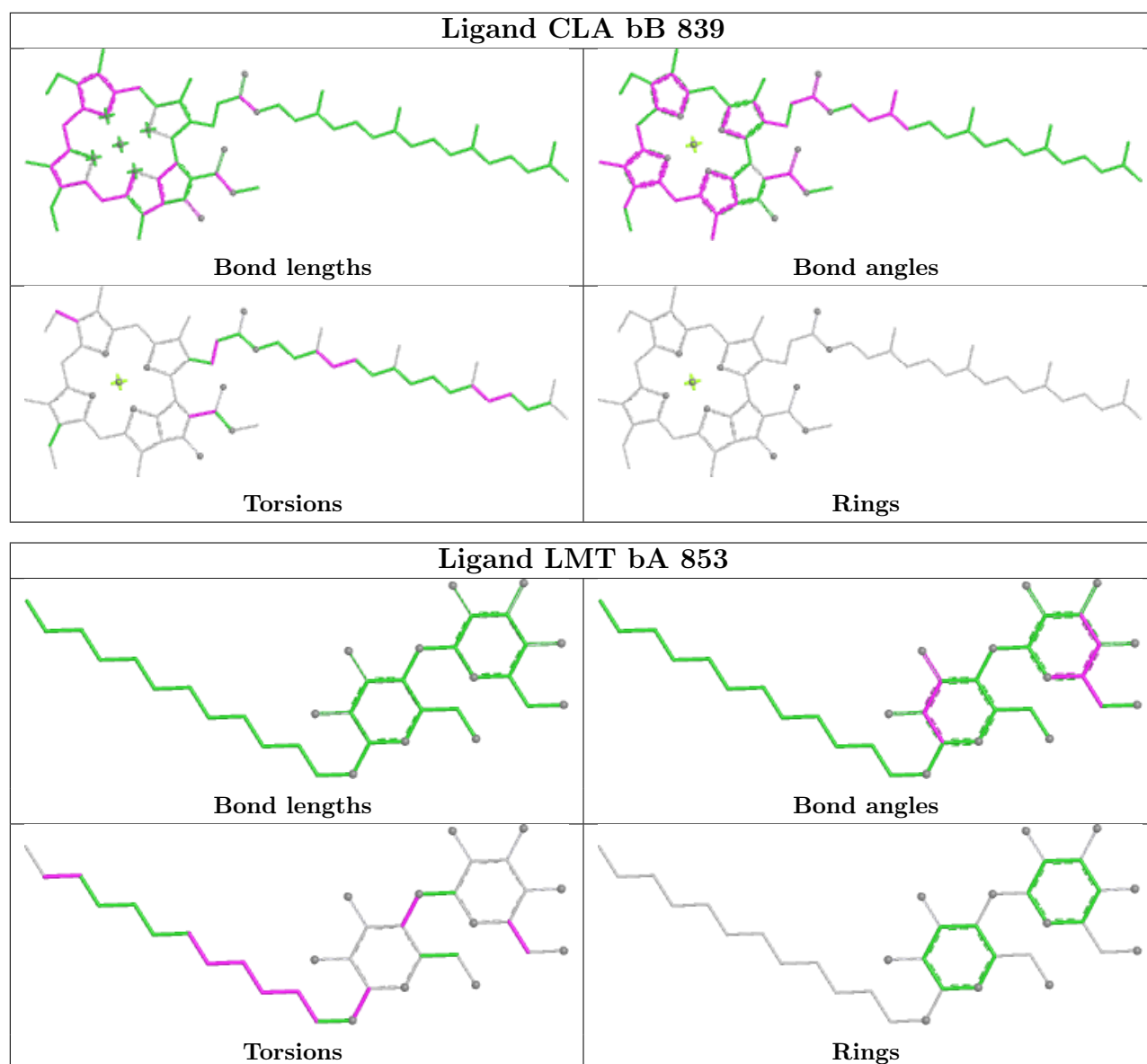


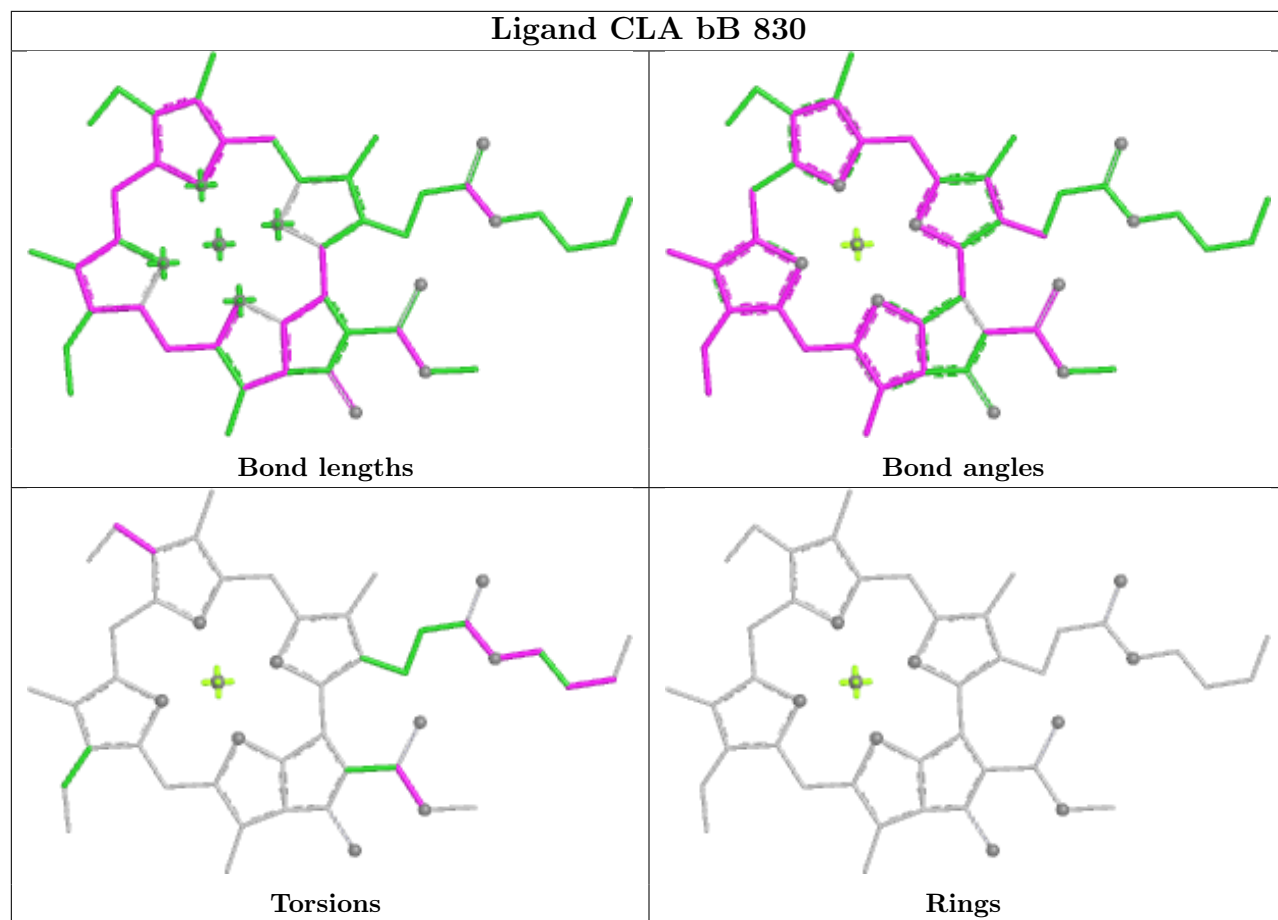
## Ligand CLA cB 819



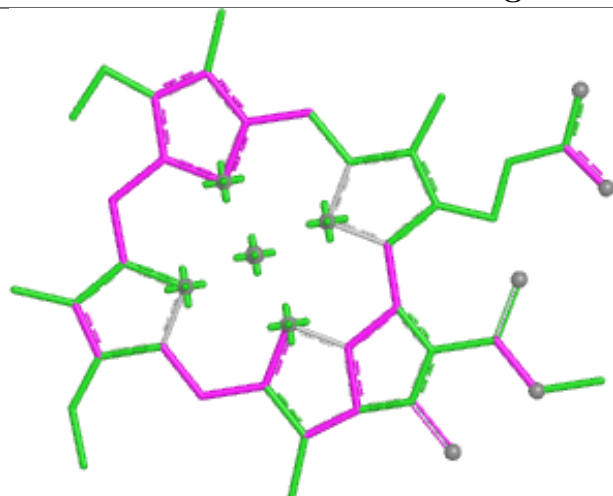
## Ligand CLA aA 839



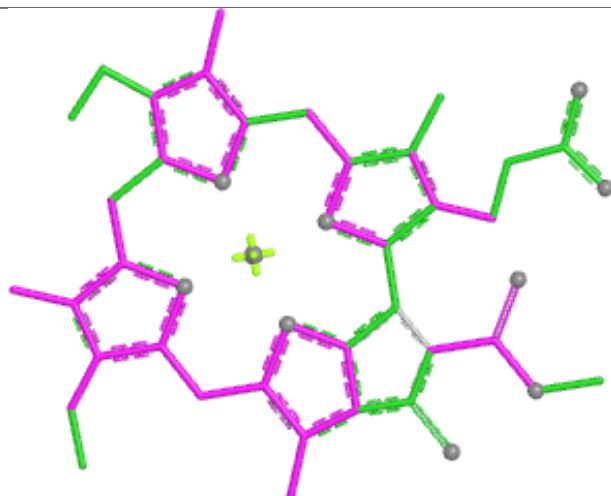




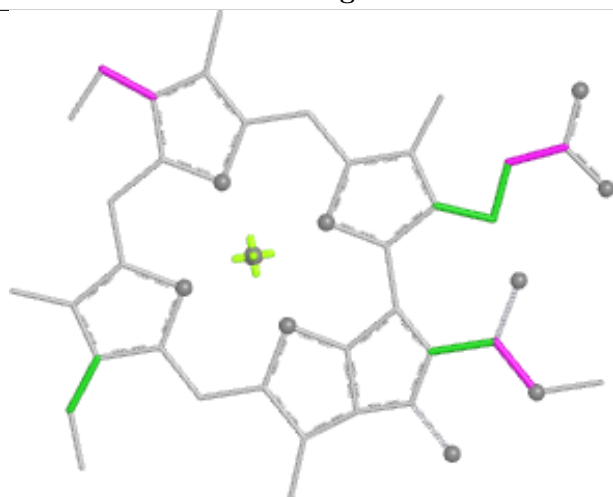
## Ligand CLA bB 822



Bond lengths



Bond angles

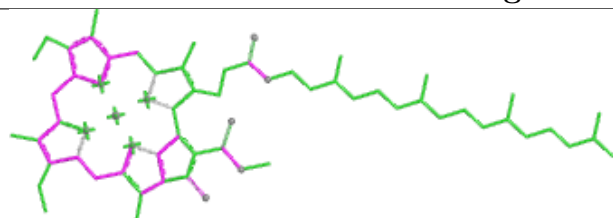


Torsions

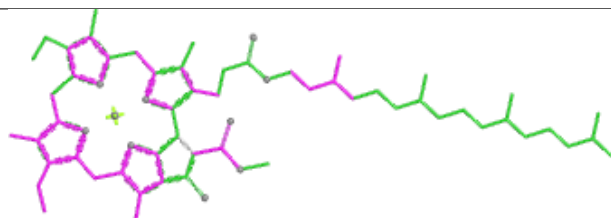


Rings

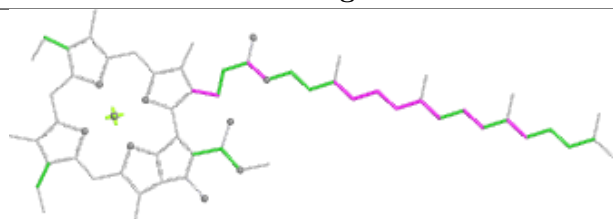
## Ligand CLA bA 833



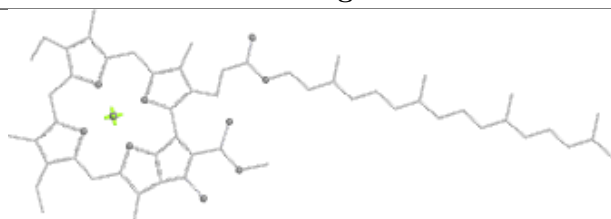
Bond lengths



Bond angles

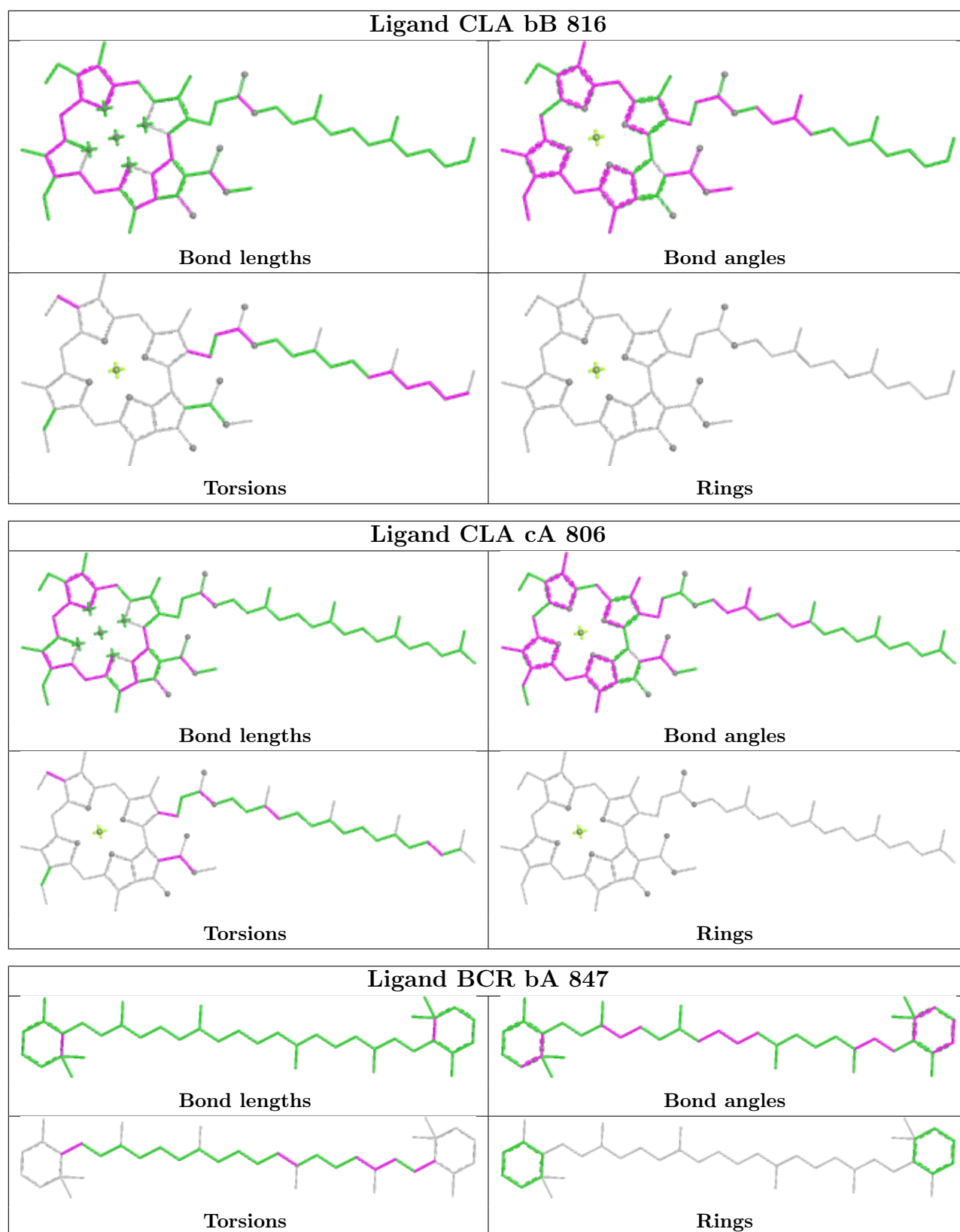


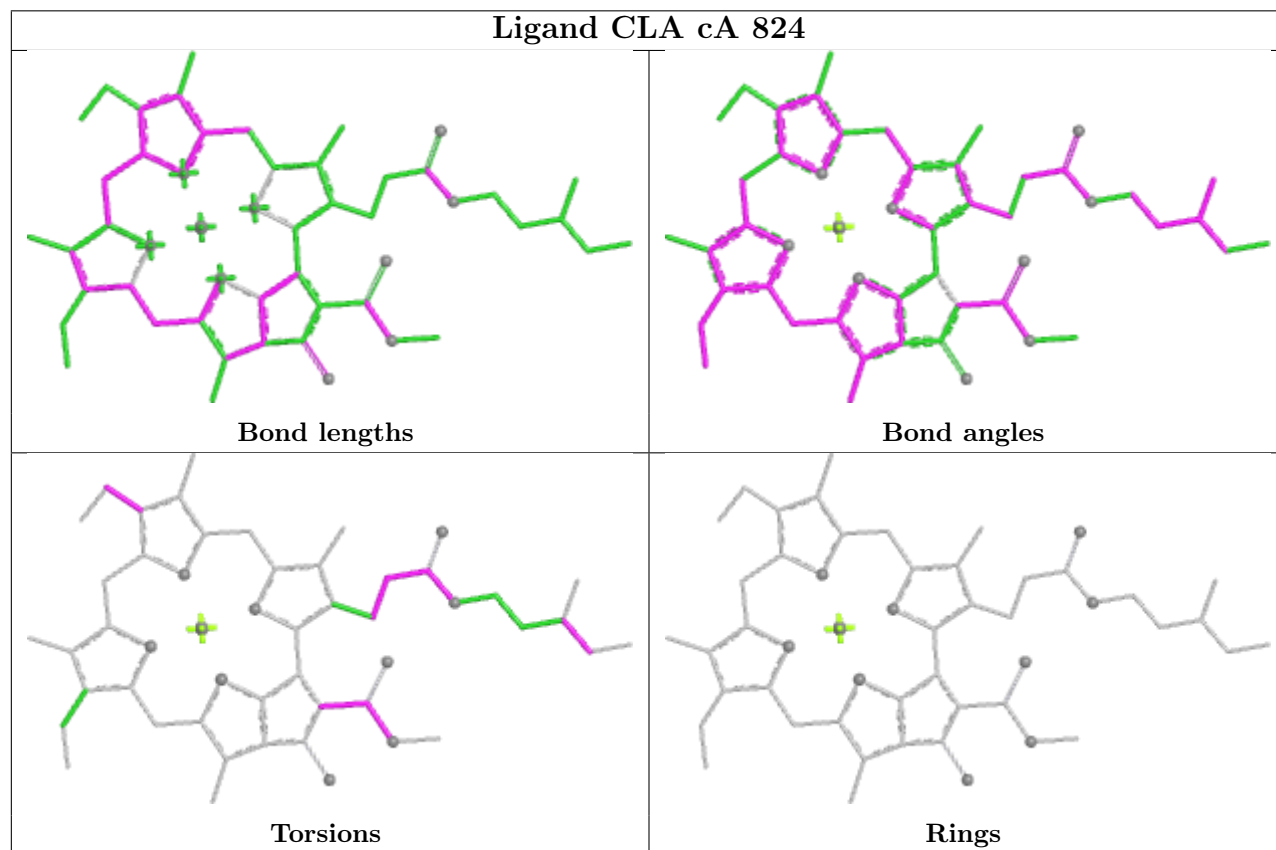
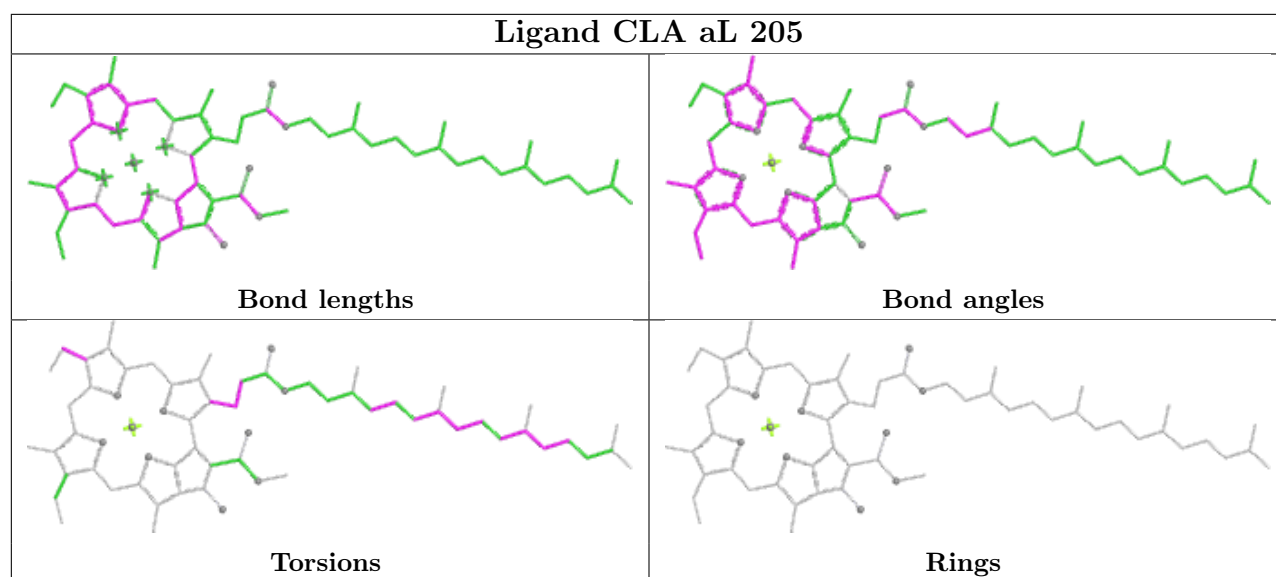
Torsions

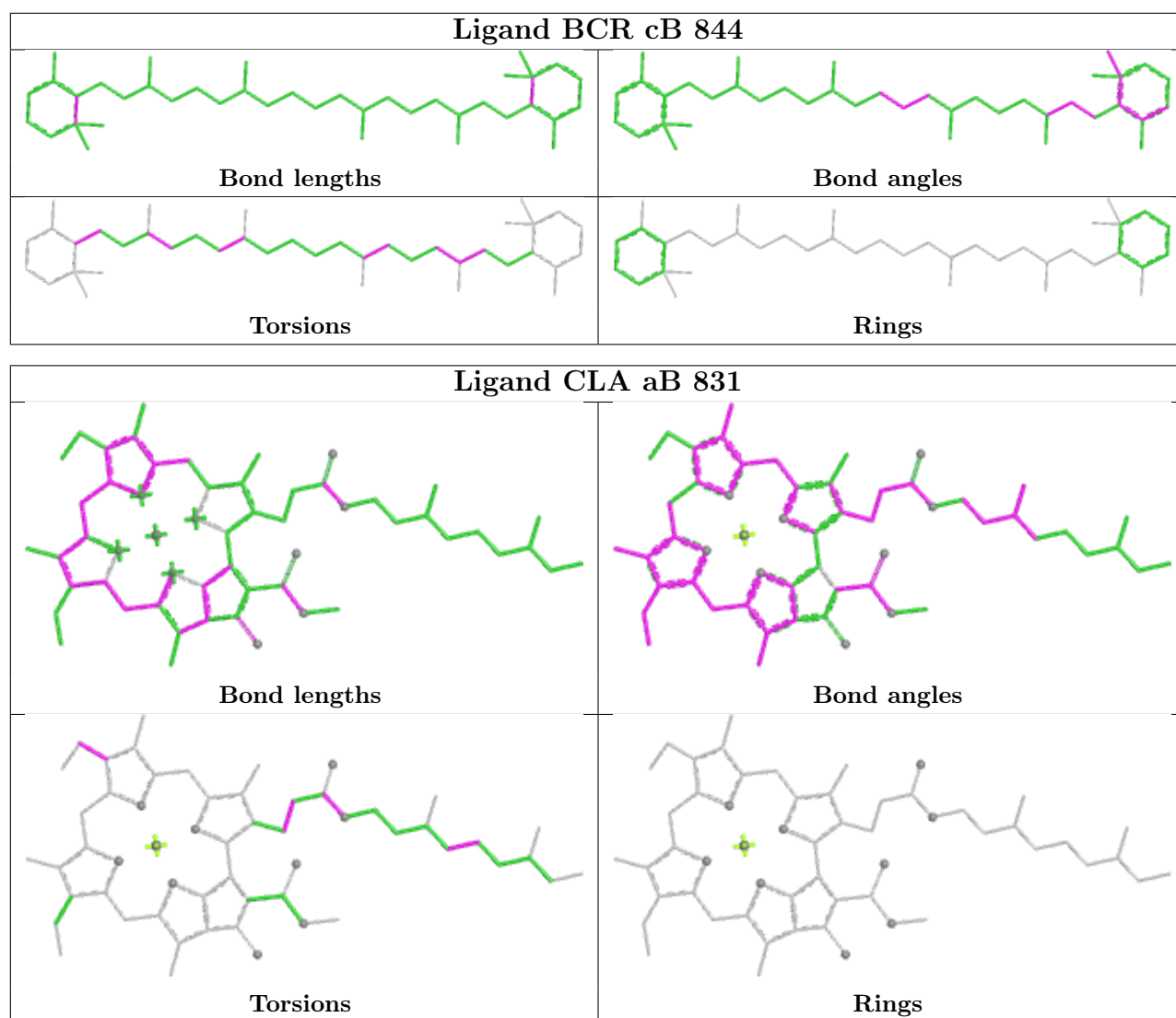


Rings









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

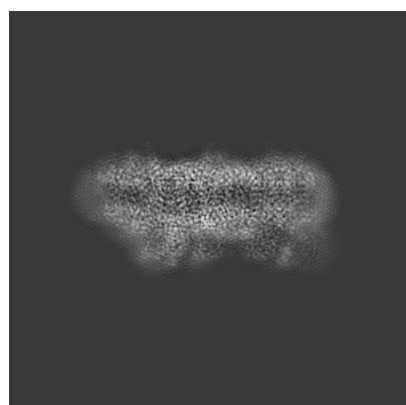
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0727. These allow visual inspection of the internal detail of the map and identification of artifacts.

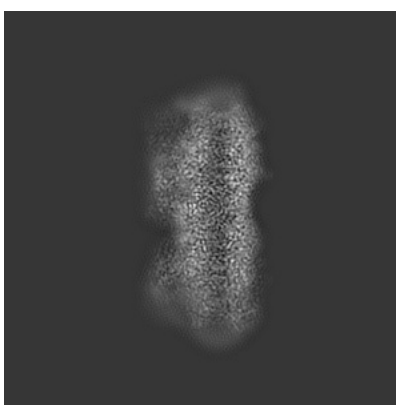
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

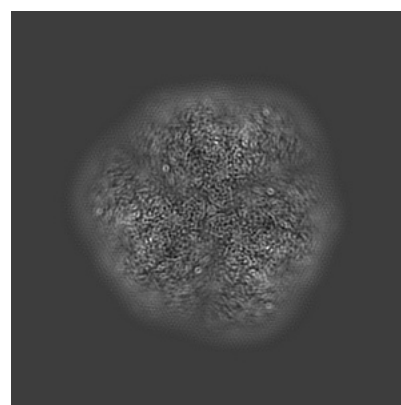
#### 6.1.1 Primary map



X



Y



Z

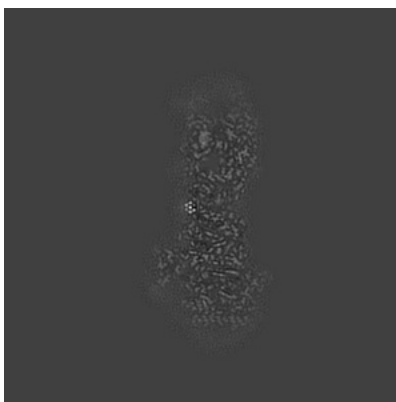
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

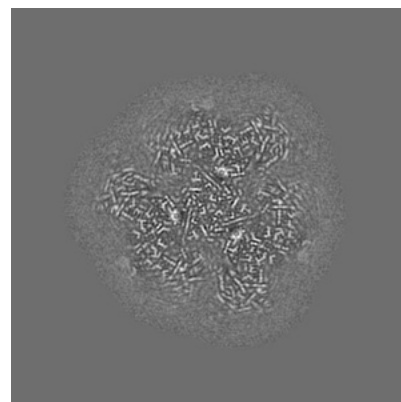
#### 6.2.1 Primary map



X Index: 180



Y Index: 180

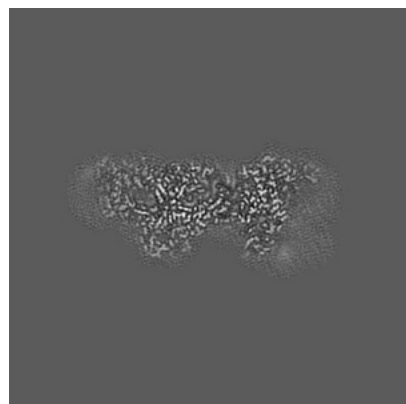


Z Index: 180

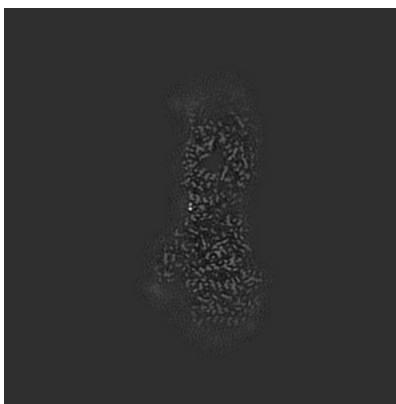
The images above show central slices of the map in three orthogonal directions.

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

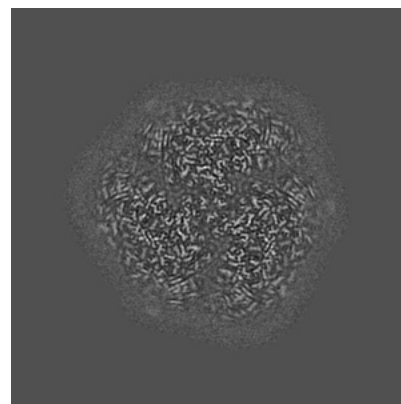
### 6.3.1 Primary map



X Index: 200



Y Index: 176

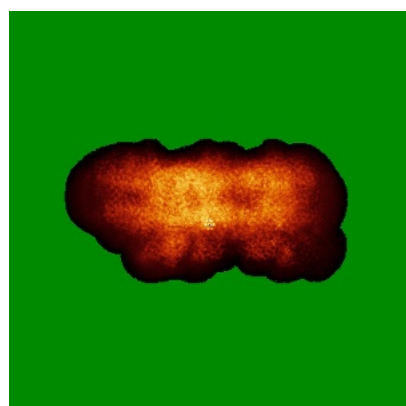


Z Index: 204

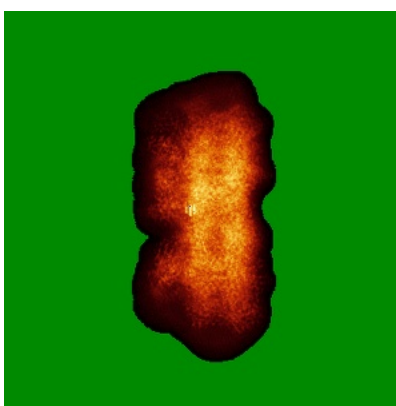
The images above show the largest variance slices of the map in three orthogonal directions.

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

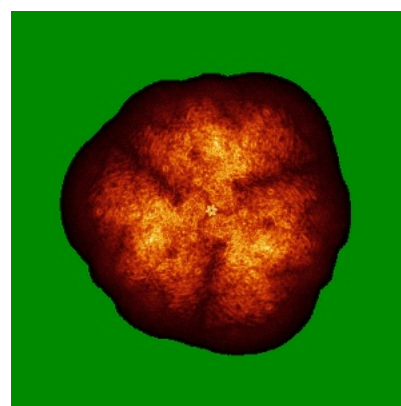
### 6.4.1 Primary map



X



Y

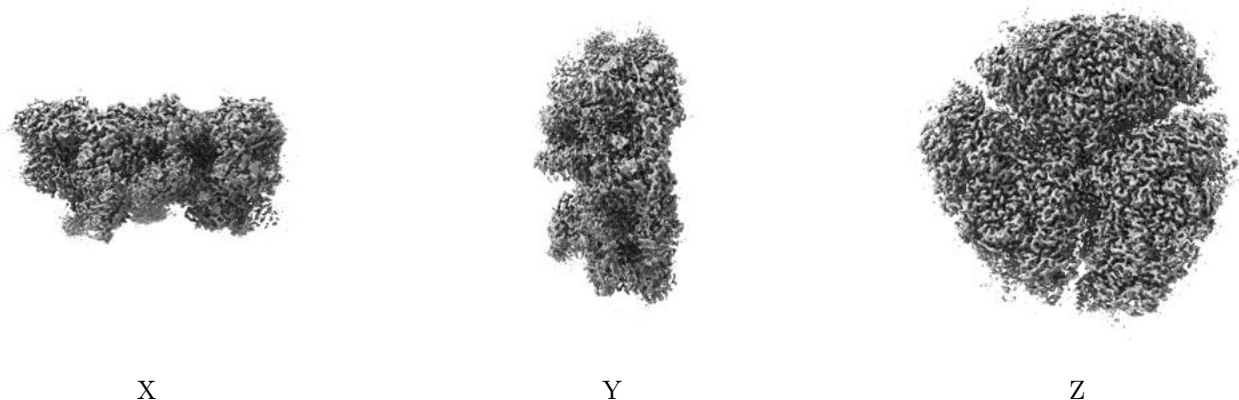


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

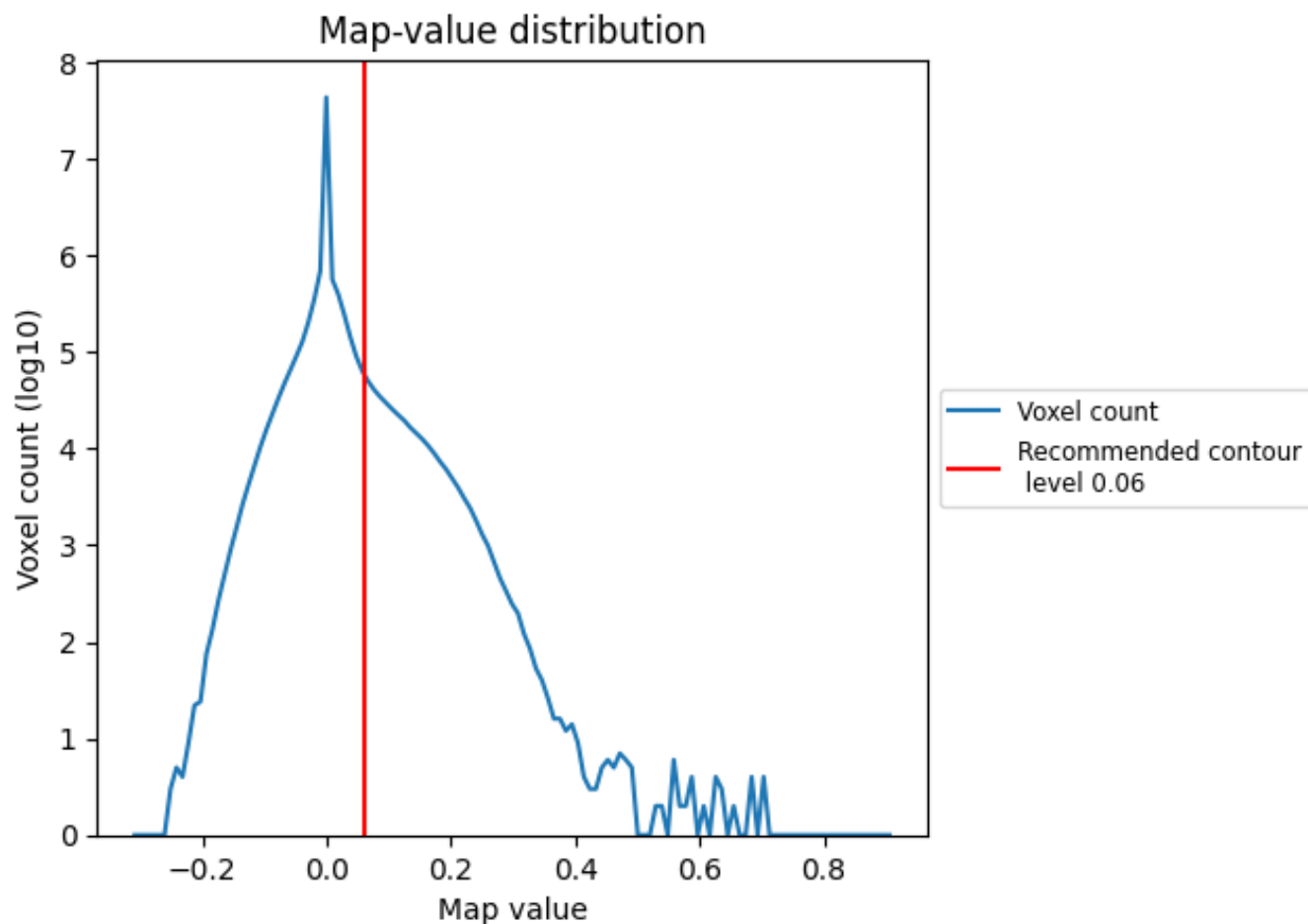
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

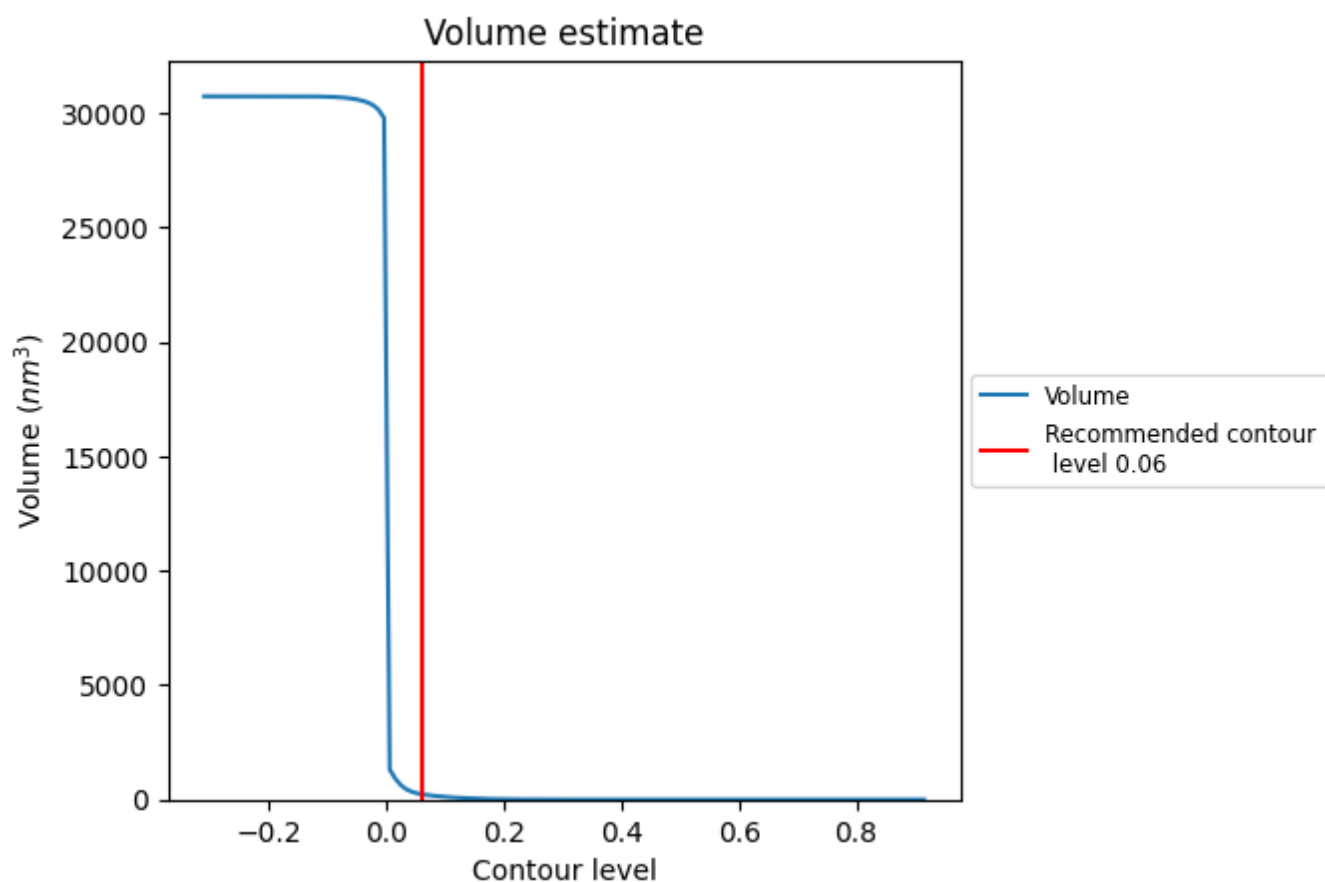
This section contains the results of statistical analysis of the map.

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



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

## 7.2 Volume estimate [i](#)

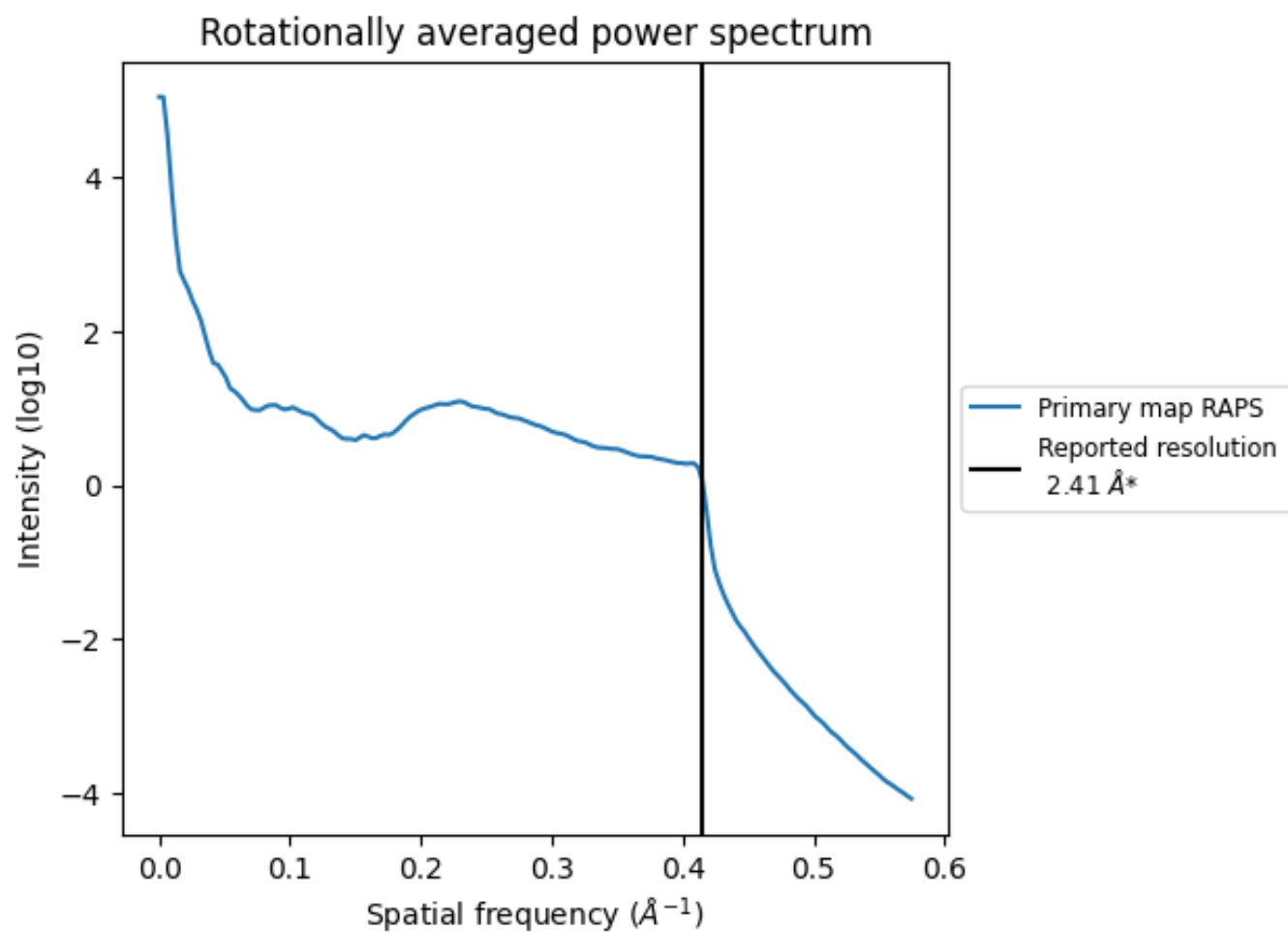


The volume at the recommended contour level is 239 nm<sup>3</sup>; this corresponds to an approximate mass of 215 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.



### 7.3 Rotationally averaged power spectrum ⓘ

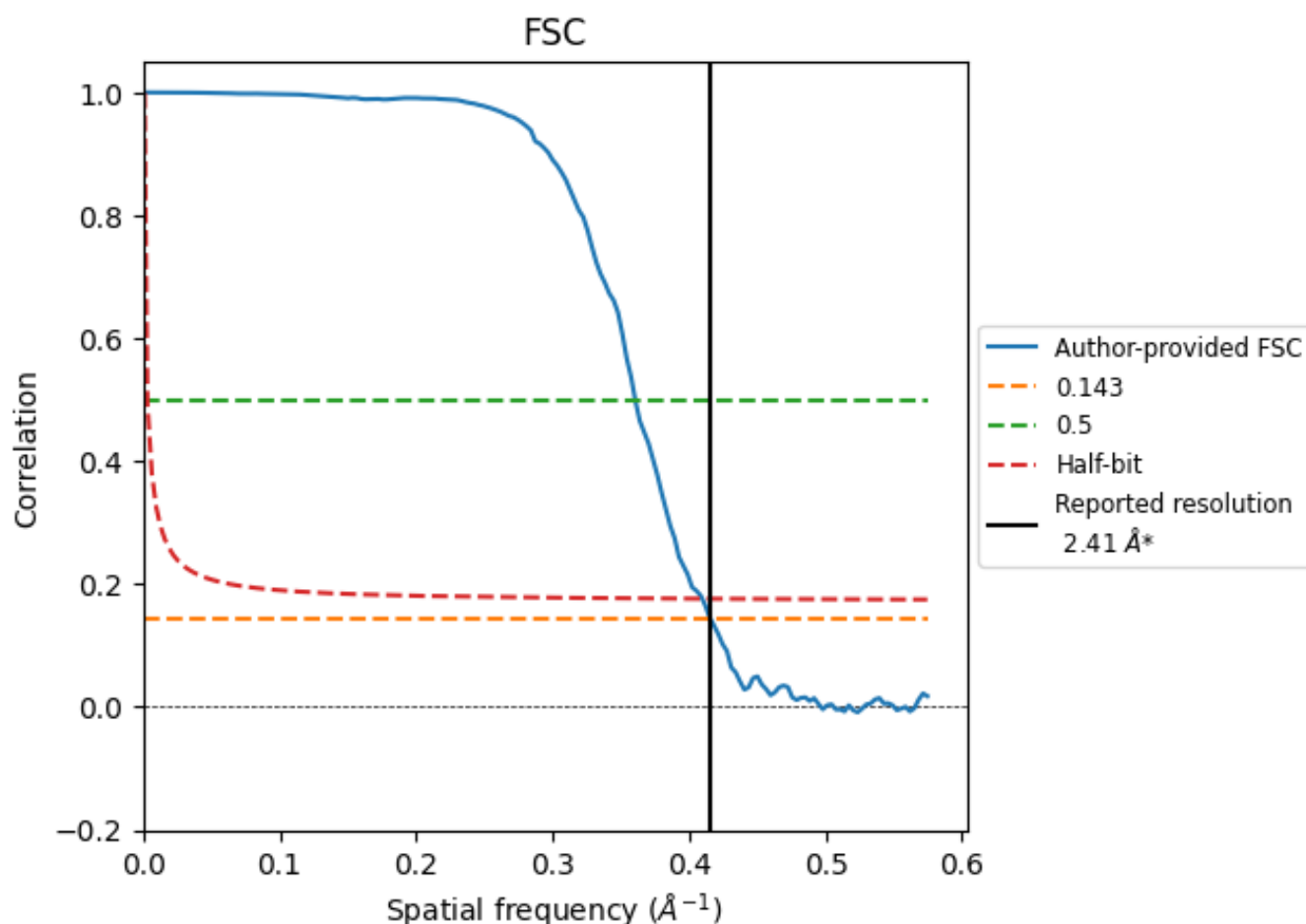


\*Reported resolution corresponds to spatial frequency of 0.415 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.415 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

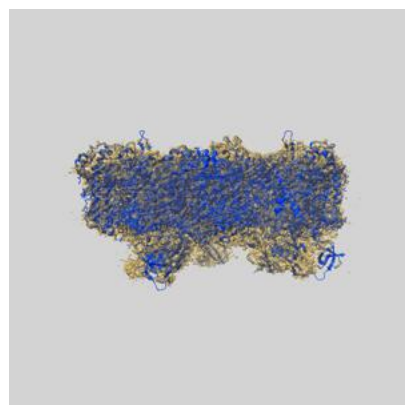
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.41                               | -    | -        |
| Author-provided FSC curve | 2.41                               | 2.77 | 2.44     |
| Unmasked-calculated*      | -                                  | -    | -        |

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

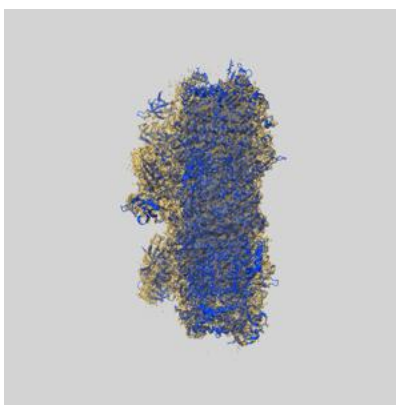
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0727 and PDB model 6KMX. Per-residue inclusion information can be found in section [3](#) on page [36](#).

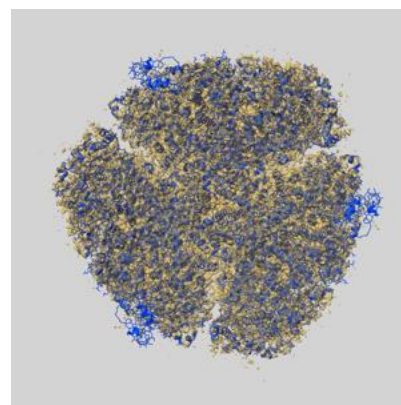
### 9.1 Map-model overlay [i](#)



X



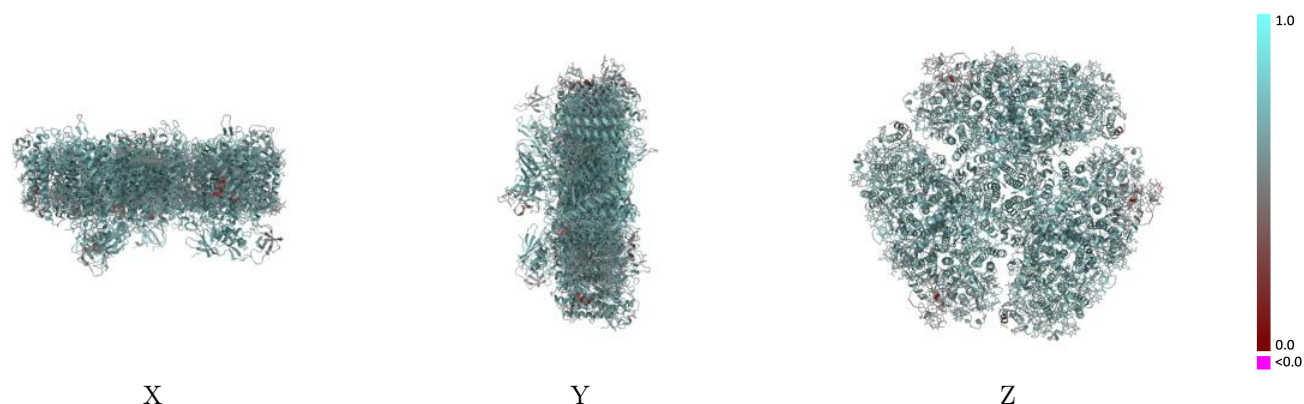
Y



Z

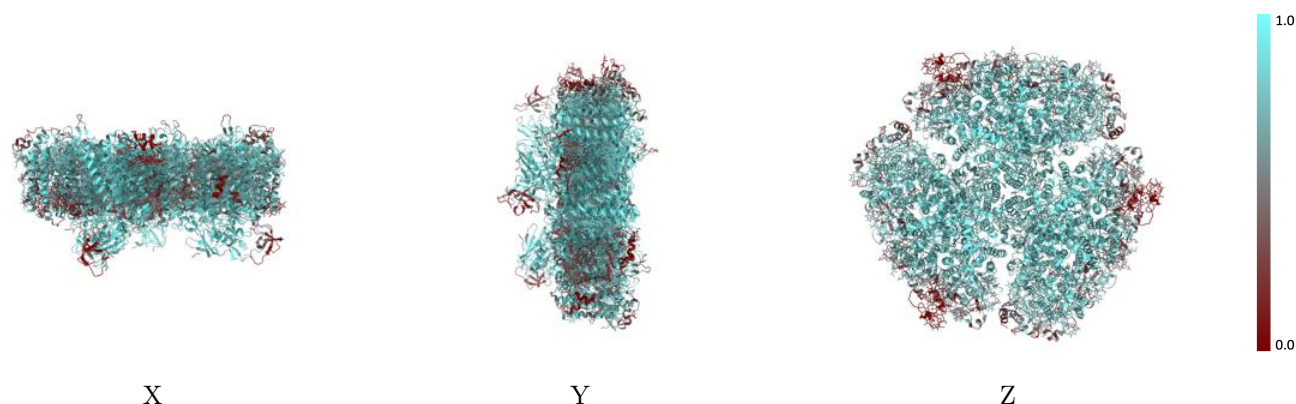
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



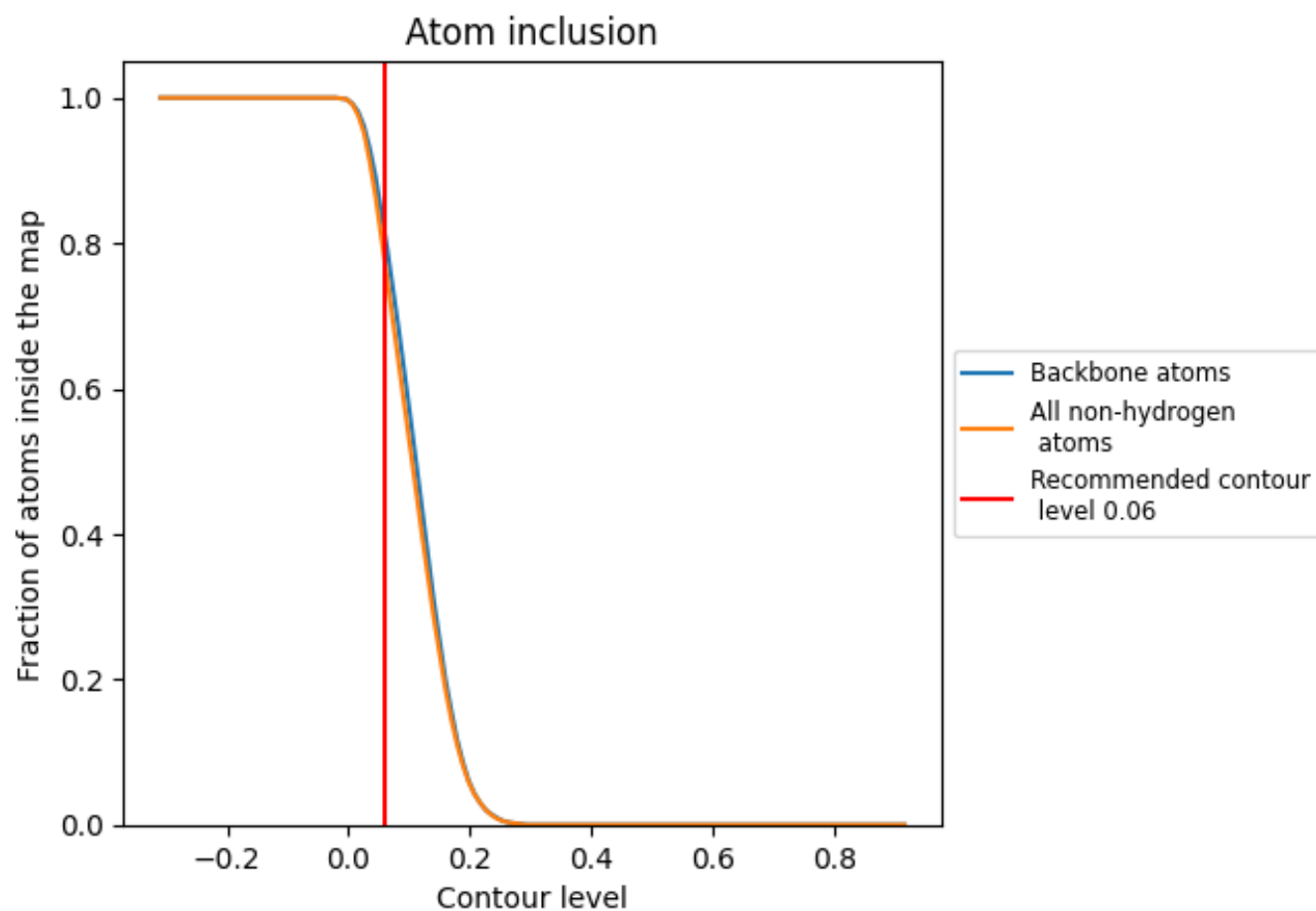
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 81% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

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

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.7730   |  0.6490   |
| aA    |  0.7920   |  0.6560   |
| aB    |  0.7450   |  0.6400   |
| aC    |  0.9000   |  0.6780   |
| aD    |  0.8630   |  0.6760   |
| aE    |  0.3350   |  0.5280   |
| aI    |  0.8930   |  0.6970   |
| aK    |  0.3490   |  0.5080   |
| aL    |  0.9090   |  0.6980   |
| aM    |  0.7880   |  0.6400   |
| bA    |  0.7920   |  0.6570   |
| bB    |  0.7500   |  0.6400   |
| bC    |  0.9010   |  0.6780   |
| bD    |  0.8730   |  0.6760   |
| bE    |  0.3310  |  0.5280  |
| bI    |  0.8930 |  0.6980 |
| bK    |  0.3430 |  0.5070 |
| bL    |  0.9130 |  0.6970 |
| bM    |  0.7840 |  0.6440 |
| cA    |  0.7920 |  0.6560 |
| cB    |  0.7490 |  0.6410 |
| cC    |  0.8960 |  0.6800 |
| cD    |  0.8700 |  0.6740 |
| cE    |  0.3240 |  0.5240 |
| cI    |  0.8800 |  0.6940 |
| cK    |  0.3330 |  0.5040 |
| cL    |  0.9140 |  0.6970 |
| cM    |  0.7880 |  0.6400 |

