



## Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 03:48 AM JST

PDB ID : 7COY / pdb\_00007coy  
EMDB ID : EMD-30420  
Title : Structure of the far-red light utilizing photosystem I of *Acaryochloris marina*  
Authors : Kawakami, K.; Yonekura, K.; Hamaguchi, T.; Kashino, Y.; Shinzawa-Itoh, K.;  
Inoue-Kashino, N.; Itoh, S.; Ifuku, K.; Yamashita, E.  
Deposited on : 2020-08-05  
Resolution : 2.50 Å(reported)

This is a 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:

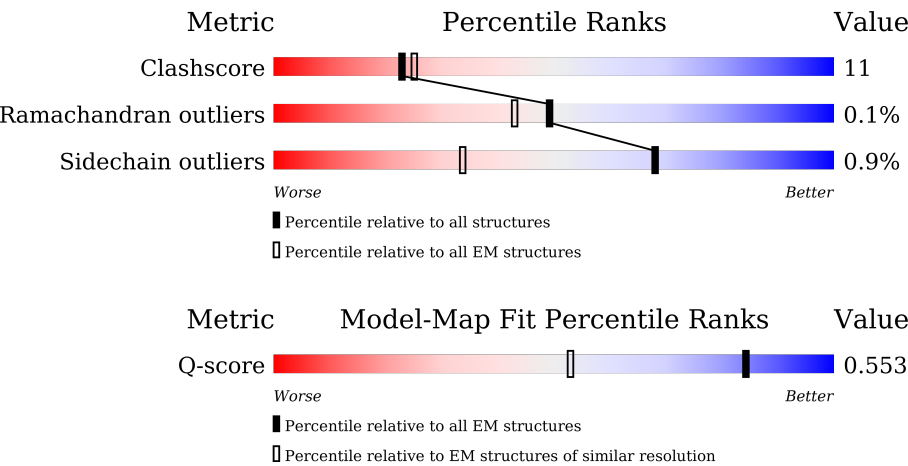
EMDB validation analysis : 0.0.1.dev133  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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) : 2.50

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.50 Å.

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



| Metric                | Whole archive<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                       | 7115 ( 2.00 - 3.00 )                                     |

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    | 753    |                  |
| 1   | bA    | 753    |                  |
| 1   | cA    | 753    |                  |
| 2   | aB    | 736    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2   | bB    | 736    |                  |
| 2   | cB    | 736    |                  |
| 3   | aC    | 81     |                  |
| 3   | bC    | 81     |                  |
| 3   | cC    | 81     |                  |
| 4   | aD    | 139    |                  |
| 4   | bD    | 139    |                  |
| 4   | cD    | 139    |                  |
| 5   | aE    | 89     |                  |
| 5   | bE    | 89     |                  |
| 5   | cE    | 89     |                  |
| 6   | aF    | 167    |                  |
| 6   | bF    | 167    |                  |
| 6   | cF    | 167    |                  |
| 7   | aI    | 34     |                  |
| 7   | bI    | 34     |                  |
| 7   | cI    | 34     |                  |
| 8   | aJ    | 51     |                  |
| 8   | bJ    | 51     |                  |
| 8   | cJ    | 51     |                  |
| 9   | aK    | 86     |                  |
| 9   | bK    | 86     |                  |
| 9   | cK    | 86     |                  |
| 10  | aL    | 153    |                  |
| 10  | bL    | 153    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 10  | cL    | 153    |                  |
| 11  | aM    | 31     |                  |
| 11  | bM    | 31     |                  |
| 11  | cM    | 31     |                  |

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

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 12  | G9R  | aA    | 3101 | X         | -        | -       | -                |
| 12  | G9R  | cA    | 3101 | X         | -        | -       | -                |
| 14  | CL7  | aA    | 3103 | X         | -        | -       | -                |
| 14  | CL7  | aA    | 3104 | X         | -        | -       | -                |
| 14  | CL7  | aA    | 3105 | X         | -        | -       | -                |
| 14  | CL7  | aA    | 3106 | X         | -        | -       | -                |
| 14  | CL7  | aA    | 3107 | X         | -        | -       | -                |
| 14  | CL7  | aA    | 3108 | X         | -        | -       | -                |
| 14  | CL7  | aA    | 3109 | X         | -        | -       | -                |
| 14  | CL7  | aA    | 3110 | X         | -        | -       | -                |
| 14  | CL7  | aA    | 3111 | X         | -        | -       | -                |
| 14  | CL7  | aA    | 3112 | X         | -        | -       | -                |
| 14  | CL7  | aA    | 3113 | X         | -        | -       | -                |
| 14  | CL7  | aA    | 3114 | X         | -        | -       | -                |
| 14  | CL7  | aA    | 3115 | X         | -        | -       | -                |
| 14  | CL7  | aA    | 3116 | X         | -        | -       | -                |
| 14  | CL7  | aA    | 3117 | X         | -        | -       | -                |
| 14  | CL7  | aA    | 3118 | X         | -        | -       | -                |
| 14  | CL7  | aA    | 3119 | X         | -        | -       | -                |
| 14  | CL7  | aA    | 3120 | X         | -        | -       | -                |
| 14  | CL7  | aA    | 3121 | X         | -        | -       | -                |
| 14  | CL7  | aA    | 3122 | X         | -        | -       | -                |
| 14  | CL7  | aA    | 3123 | X         | -        | -       | -                |
| 14  | CL7  | aA    | 3124 | X         | -        | -       | -                |
| 14  | CL7  | aA    | 3125 | X         | -        | -       | -                |
| 14  | CL7  | aA    | 3126 | X         | -        | -       | -                |
| 14  | CL7  | aA    | 3127 | X         | -        | -       | -                |
| 14  | CL7  | aA    | 3128 | X         | -        | -       | -                |
| 14  | CL7  | aA    | 3129 | X         | -        | -       | -                |
| 14  | CL7  | aA    | 3130 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 14  | CL7  | aA    | 3131 | X         | -        | -       | -                |
| 14  | CL7  | aA    | 3132 | X         | -        | -       | -                |
| 14  | CL7  | aA    | 3133 | X         | -        | -       | -                |
| 14  | CL7  | aA    | 3134 | X         | -        | -       | -                |
| 14  | CL7  | aA    | 3140 | X         | -        | -       | -                |
| 14  | CL7  | aA    | 3141 | X         | -        | -       | -                |
| 14  | CL7  | aA    | 3142 | X         | -        | -       | -                |
| 14  | CL7  | aA    | 3143 | X         | -        | -       | -                |
| 14  | CL7  | aA    | 3146 | X         | -        | -       | -                |
| 14  | CL7  | aB    | 3002 | X         | -        | -       | -                |
| 14  | CL7  | aB    | 3003 | X         | -        | -       | -                |
| 14  | CL7  | aB    | 3005 | X         | -        | -       | -                |
| 14  | CL7  | aB    | 3006 | X         | -        | -       | -                |
| 14  | CL7  | aB    | 3007 | X         | -        | -       | -                |
| 14  | CL7  | aB    | 3008 | X         | -        | -       | -                |
| 14  | CL7  | aB    | 3009 | X         | -        | -       | -                |
| 14  | CL7  | aB    | 3010 | X         | -        | -       | -                |
| 14  | CL7  | aB    | 3011 | X         | -        | -       | -                |
| 14  | CL7  | aB    | 3012 | X         | -        | -       | -                |
| 14  | CL7  | aB    | 3013 | X         | -        | -       | -                |
| 14  | CL7  | aB    | 3014 | X         | -        | -       | -                |
| 14  | CL7  | aB    | 3015 | X         | -        | -       | -                |
| 14  | CL7  | aB    | 3016 | X         | -        | -       | -                |
| 14  | CL7  | aB    | 3017 | X         | -        | -       | -                |
| 14  | CL7  | aB    | 3018 | X         | -        | -       | -                |
| 14  | CL7  | aB    | 3019 | X         | -        | -       | -                |
| 14  | CL7  | aB    | 3020 | X         | -        | -       | -                |
| 14  | CL7  | aB    | 3021 | X         | -        | -       | -                |
| 14  | CL7  | aB    | 3022 | X         | -        | -       | -                |
| 14  | CL7  | aB    | 3023 | X         | -        | -       | -                |
| 14  | CL7  | aB    | 3024 | X         | -        | -       | -                |
| 14  | CL7  | aB    | 3025 | X         | -        | -       | -                |
| 14  | CL7  | aB    | 3026 | X         | -        | -       | -                |
| 14  | CL7  | aB    | 3030 | X         | -        | -       | -                |
| 14  | CL7  | aB    | 3031 | X         | -        | -       | -                |
| 14  | CL7  | aB    | 3032 | X         | -        | -       | -                |
| 14  | CL7  | aF    | 201  | X         | -        | -       | -                |
| 14  | CL7  | aJ    | 101  | X         | -        | -       | -                |
| 14  | CL7  | aK    | 101  | X         | -        | -       | -                |
| 14  | CL7  | aL    | 202  | X         | -        | -       | -                |
| 14  | CL7  | aL    | 203  | X         | -        | -       | -                |
| 14  | CL7  | aL    | 204  | X         | -        | -       | -                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 14  | CL7  | bA    | 3102 | X         | -        | -       | -                |
| 14  | CL7  | bA    | 3103 | X         | -        | -       | -                |
| 14  | CL7  | bA    | 3104 | X         | -        | -       | -                |
| 14  | CL7  | bA    | 3105 | X         | -        | -       | -                |
| 14  | CL7  | bA    | 3106 | X         | -        | -       | -                |
| 14  | CL7  | bA    | 3107 | X         | -        | -       | -                |
| 14  | CL7  | bA    | 3108 | X         | -        | -       | -                |
| 14  | CL7  | bA    | 3109 | X         | -        | -       | -                |
| 14  | CL7  | bA    | 3110 | X         | -        | -       | -                |
| 14  | CL7  | bA    | 3111 | X         | -        | -       | -                |
| 14  | CL7  | bA    | 3112 | X         | -        | -       | -                |
| 14  | CL7  | bA    | 3113 | X         | -        | -       | -                |
| 14  | CL7  | bA    | 3114 | X         | -        | -       | -                |
| 14  | CL7  | bA    | 3115 | X         | -        | -       | -                |
| 14  | CL7  | bA    | 3116 | X         | -        | -       | -                |
| 14  | CL7  | bA    | 3117 | X         | -        | -       | -                |
| 14  | CL7  | bA    | 3118 | X         | -        | -       | -                |
| 14  | CL7  | bA    | 3119 | X         | -        | -       | -                |
| 14  | CL7  | bA    | 3120 | X         | -        | -       | -                |
| 14  | CL7  | bA    | 3121 | X         | -        | -       | -                |
| 14  | CL7  | bA    | 3122 | X         | -        | -       | -                |
| 14  | CL7  | bA    | 3123 | X         | -        | -       | -                |
| 14  | CL7  | bA    | 3124 | X         | -        | -       | -                |
| 14  | CL7  | bA    | 3125 | X         | -        | -       | -                |
| 14  | CL7  | bA    | 3126 | X         | -        | -       | -                |
| 14  | CL7  | bA    | 3127 | X         | -        | -       | -                |
| 14  | CL7  | bA    | 3128 | X         | -        | -       | -                |
| 14  | CL7  | bA    | 3129 | X         | -        | -       | -                |
| 14  | CL7  | bA    | 3130 | X         | -        | -       | -                |
| 14  | CL7  | bA    | 3131 | X         | -        | -       | -                |
| 14  | CL7  | bA    | 3132 | X         | -        | -       | -                |
| 14  | CL7  | bA    | 3133 | X         | -        | -       | -                |
| 14  | CL7  | bA    | 3139 | X         | -        | -       | -                |
| 14  | CL7  | bA    | 3140 | X         | -        | -       | -                |
| 14  | CL7  | bA    | 3141 | X         | -        | -       | -                |
| 14  | CL7  | bA    | 3142 | X         | -        | -       | -                |
| 14  | CL7  | bA    | 3145 | X         | -        | -       | -                |
| 14  | CL7  | bB    | 803  | X         | -        | -       | -                |
| 14  | CL7  | bB    | 804  | X         | -        | -       | -                |
| 14  | CL7  | bB    | 806  | X         | -        | -       | -                |
| 14  | CL7  | bB    | 807  | X         | -        | -       | -                |
| 14  | CL7  | bB    | 808  | X         | -        | -       | -                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 14  | CL7  | bB    | 809  | X         | -        | -       | -                |
| 14  | CL7  | bB    | 810  | X         | -        | -       | -                |
| 14  | CL7  | bB    | 811  | X         | -        | -       | -                |
| 14  | CL7  | bB    | 812  | X         | -        | -       | -                |
| 14  | CL7  | bB    | 813  | X         | -        | -       | -                |
| 14  | CL7  | bB    | 814  | X         | -        | -       | -                |
| 14  | CL7  | bB    | 815  | X         | -        | -       | -                |
| 14  | CL7  | bB    | 816  | X         | -        | -       | -                |
| 14  | CL7  | bB    | 817  | X         | -        | -       | -                |
| 14  | CL7  | bB    | 818  | X         | -        | -       | -                |
| 14  | CL7  | bB    | 819  | X         | -        | -       | -                |
| 14  | CL7  | bB    | 820  | X         | -        | -       | -                |
| 14  | CL7  | bB    | 821  | X         | -        | -       | -                |
| 14  | CL7  | bB    | 822  | X         | -        | -       | -                |
| 14  | CL7  | bB    | 823  | X         | -        | -       | -                |
| 14  | CL7  | bB    | 824  | X         | -        | -       | -                |
| 14  | CL7  | bB    | 825  | X         | -        | -       | -                |
| 14  | CL7  | bB    | 826  | X         | -        | -       | -                |
| 14  | CL7  | bB    | 827  | X         | -        | -       | -                |
| 14  | CL7  | bB    | 831  | X         | -        | -       | -                |
| 14  | CL7  | bB    | 832  | X         | -        | -       | -                |
| 14  | CL7  | bB    | 833  | X         | -        | -       | -                |
| 14  | CL7  | bF    | 201  | X         | -        | -       | -                |
| 14  | CL7  | bJ    | 101  | X         | -        | -       | -                |
| 14  | CL7  | bK    | 101  | X         | -        | -       | -                |
| 14  | CL7  | bL    | 203  | X         | -        | -       | -                |
| 14  | CL7  | bL    | 204  | X         | -        | -       | -                |
| 14  | CL7  | bL    | 205  | X         | -        | -       | -                |
| 14  | CL7  | cA    | 3102 | X         | -        | -       | -                |
| 14  | CL7  | cA    | 3103 | X         | -        | -       | -                |
| 14  | CL7  | cA    | 3104 | X         | -        | -       | -                |
| 14  | CL7  | cA    | 3105 | X         | -        | -       | -                |
| 14  | CL7  | cA    | 3106 | X         | -        | -       | -                |
| 14  | CL7  | cA    | 3107 | X         | -        | -       | -                |
| 14  | CL7  | cA    | 3108 | X         | -        | -       | -                |
| 14  | CL7  | cA    | 3109 | X         | -        | -       | -                |
| 14  | CL7  | cA    | 3110 | X         | -        | -       | -                |
| 14  | CL7  | cA    | 3111 | X         | -        | -       | -                |
| 14  | CL7  | cA    | 3112 | X         | -        | -       | -                |
| 14  | CL7  | cA    | 3113 | X         | -        | -       | -                |
| 14  | CL7  | cA    | 3114 | X         | -        | -       | -                |
| 14  | CL7  | cA    | 3115 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 14  | CL7  | cA    | 3116 | X         | -        | -       | -                |
| 14  | CL7  | cA    | 3117 | X         | -        | -       | -                |
| 14  | CL7  | cA    | 3118 | X         | -        | -       | -                |
| 14  | CL7  | cA    | 3119 | X         | -        | -       | -                |
| 14  | CL7  | cA    | 3120 | X         | -        | -       | -                |
| 14  | CL7  | cA    | 3121 | X         | -        | -       | -                |
| 14  | CL7  | cA    | 3122 | X         | -        | -       | -                |
| 14  | CL7  | cA    | 3123 | X         | -        | -       | -                |
| 14  | CL7  | cA    | 3124 | X         | -        | -       | -                |
| 14  | CL7  | cA    | 3125 | X         | -        | -       | -                |
| 14  | CL7  | cA    | 3126 | X         | -        | -       | -                |
| 14  | CL7  | cA    | 3127 | X         | -        | -       | -                |
| 14  | CL7  | cA    | 3128 | X         | -        | -       | -                |
| 14  | CL7  | cA    | 3129 | X         | -        | -       | -                |
| 14  | CL7  | cA    | 3130 | X         | -        | -       | -                |
| 14  | CL7  | cA    | 3131 | X         | -        | -       | -                |
| 14  | CL7  | cA    | 3132 | X         | -        | -       | -                |
| 14  | CL7  | cA    | 3133 | X         | -        | -       | -                |
| 14  | CL7  | cA    | 3139 | X         | -        | -       | -                |
| 14  | CL7  | cA    | 3140 | X         | -        | -       | -                |
| 14  | CL7  | cA    | 3141 | X         | -        | -       | -                |
| 14  | CL7  | cA    | 3142 | X         | -        | -       | -                |
| 14  | CL7  | cA    | 3144 | X         | -        | -       | -                |
| 14  | CL7  | cB    | 803  | X         | -        | -       | -                |
| 14  | CL7  | cB    | 804  | X         | -        | -       | -                |
| 14  | CL7  | cB    | 806  | X         | -        | -       | -                |
| 14  | CL7  | cB    | 807  | X         | -        | -       | -                |
| 14  | CL7  | cB    | 808  | X         | -        | -       | -                |
| 14  | CL7  | cB    | 809  | X         | -        | -       | -                |
| 14  | CL7  | cB    | 810  | X         | -        | -       | -                |
| 14  | CL7  | cB    | 811  | X         | -        | -       | -                |
| 14  | CL7  | cB    | 812  | X         | -        | -       | -                |
| 14  | CL7  | cB    | 813  | X         | -        | -       | -                |
| 14  | CL7  | cB    | 814  | X         | -        | -       | -                |
| 14  | CL7  | cB    | 815  | X         | -        | -       | -                |
| 14  | CL7  | cB    | 816  | X         | -        | -       | -                |
| 14  | CL7  | cB    | 817  | X         | -        | -       | -                |
| 14  | CL7  | cB    | 818  | X         | -        | -       | -                |
| 14  | CL7  | cB    | 819  | X         | -        | -       | -                |
| 14  | CL7  | cB    | 820  | X         | -        | -       | -                |
| 14  | CL7  | cB    | 821  | X         | -        | -       | -                |
| 14  | CL7  | cB    | 822  | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 14  | CL7  | cB    | 823 | X         | -        | -       | -                |
| 14  | CL7  | cB    | 824 | X         | -        | -       | -                |
| 14  | CL7  | cB    | 825 | X         | -        | -       | -                |
| 14  | CL7  | cB    | 826 | X         | -        | -       | -                |
| 14  | CL7  | cB    | 827 | X         | -        | -       | -                |
| 14  | CL7  | cB    | 831 | X         | -        | -       | -                |
| 14  | CL7  | cB    | 832 | X         | -        | -       | -                |
| 14  | CL7  | cB    | 833 | X         | -        | -       | -                |
| 14  | CL7  | cF    | 201 | X         | -        | -       | -                |
| 14  | CL7  | cJ    | 101 | X         | -        | -       | -                |
| 14  | CL7  | cK    | 101 | X         | -        | -       | -                |
| 14  | CL7  | cL    | 203 | X         | -        | -       | -                |
| 14  | CL7  | cL    | 204 | X         | -        | -       | -                |
| 14  | CL7  | cL    | 205 | X         | -        | -       | -                |

## 2 Entry composition

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 7 is a protein called Photosystem I protein Psa27.

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

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

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

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

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

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

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

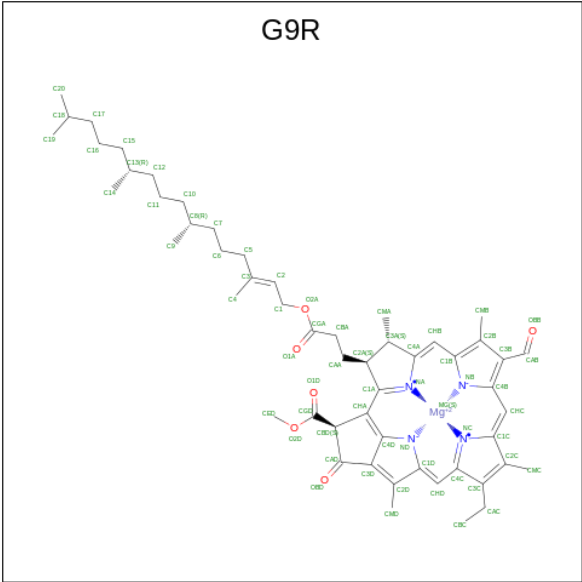
| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | aL    | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 999   | 638 | 168 | 189 | 4 |         |       |
|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

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

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

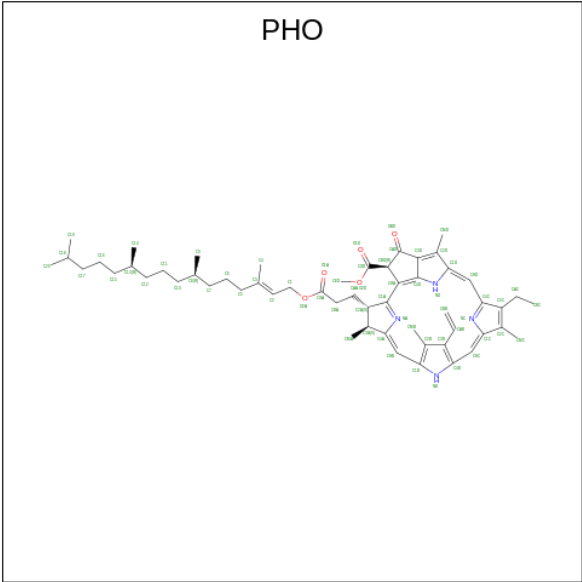
- Molecule 12 is CHLOROPHYLL D ISOMER (CCD ID: G9R) (formula:  $C_{54}H_{70}MgN_4O_6$ ) (labeled as "Ligand of Interest" by depositor).





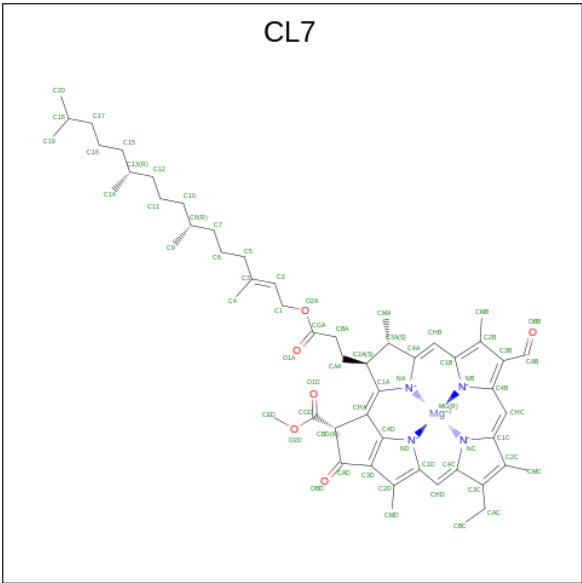
| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 12  | aA    | 1        | Total<br>65 | C<br>54 | Mg<br>1 | N<br>4 | O<br>6 | 0       |
| 12  | bA    | 1        | Total<br>65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

- Molecule 13 is PHEOPHYTIN A (CCD ID: PHO) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 14 is CHLOROPHYLL D (CCD ID: CL7) (formula: C<sub>54</sub>H<sub>70</sub>MgN<sub>4</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



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

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

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

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

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

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

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

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

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

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

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

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

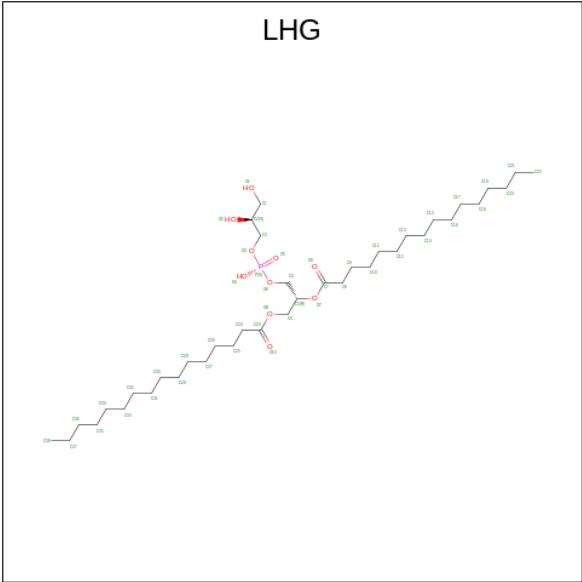
| Mol | Chain | Residues | Atoms |     | AltConf |
|-----|-------|----------|-------|-----|---------|
| 15  | aA    | 4        | Total | C   | 0       |
|     |       |          | 150   | 150 |         |
| 15  | aB    | 3        | Total | C   | 0       |
|     |       |          | 120   | 120 |     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

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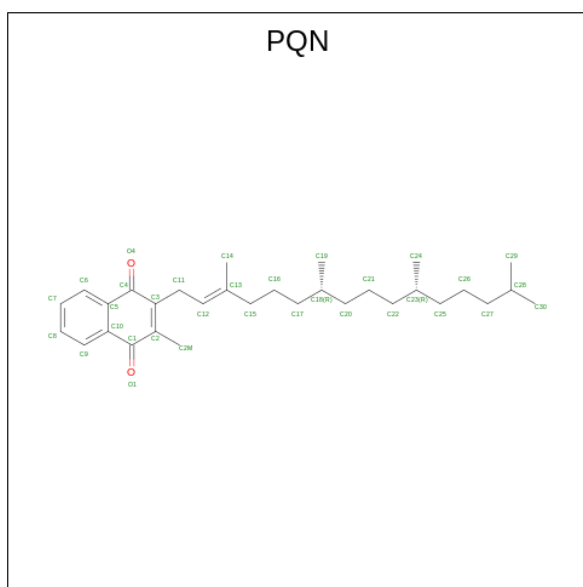
| Mol | Chain | Residues | Atoms        |          | AltConf |
|-----|-------|----------|--------------|----------|---------|
| 15  | aJ    | 1        | Total<br>40  | C<br>40  | 0       |
| 15  | aL    | 2        | Total<br>80  | C<br>80  | 0       |
| 15  | bA    | 4        | Total<br>150 | C<br>150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

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



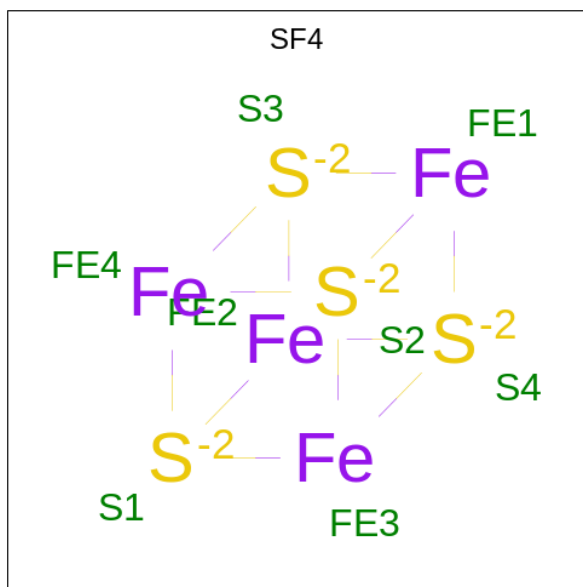
| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 16  | aA    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 16  | aA    | 1        | Total | C  | O  | P | 0       |
|    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

- Molecule 17 is PHYLLOQUINONE (CCD ID: PQN) (formula: C<sub>31</sub>H<sub>46</sub>O<sub>2</sub>) (labeled as "Lig- and of Interest" by depositor).



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

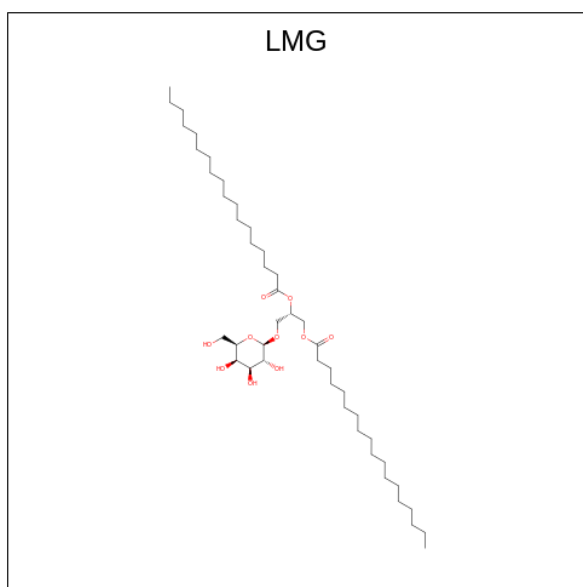
- Molecule 18 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 19 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>) (labeled as "Ligand of Interest" by depositor).





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

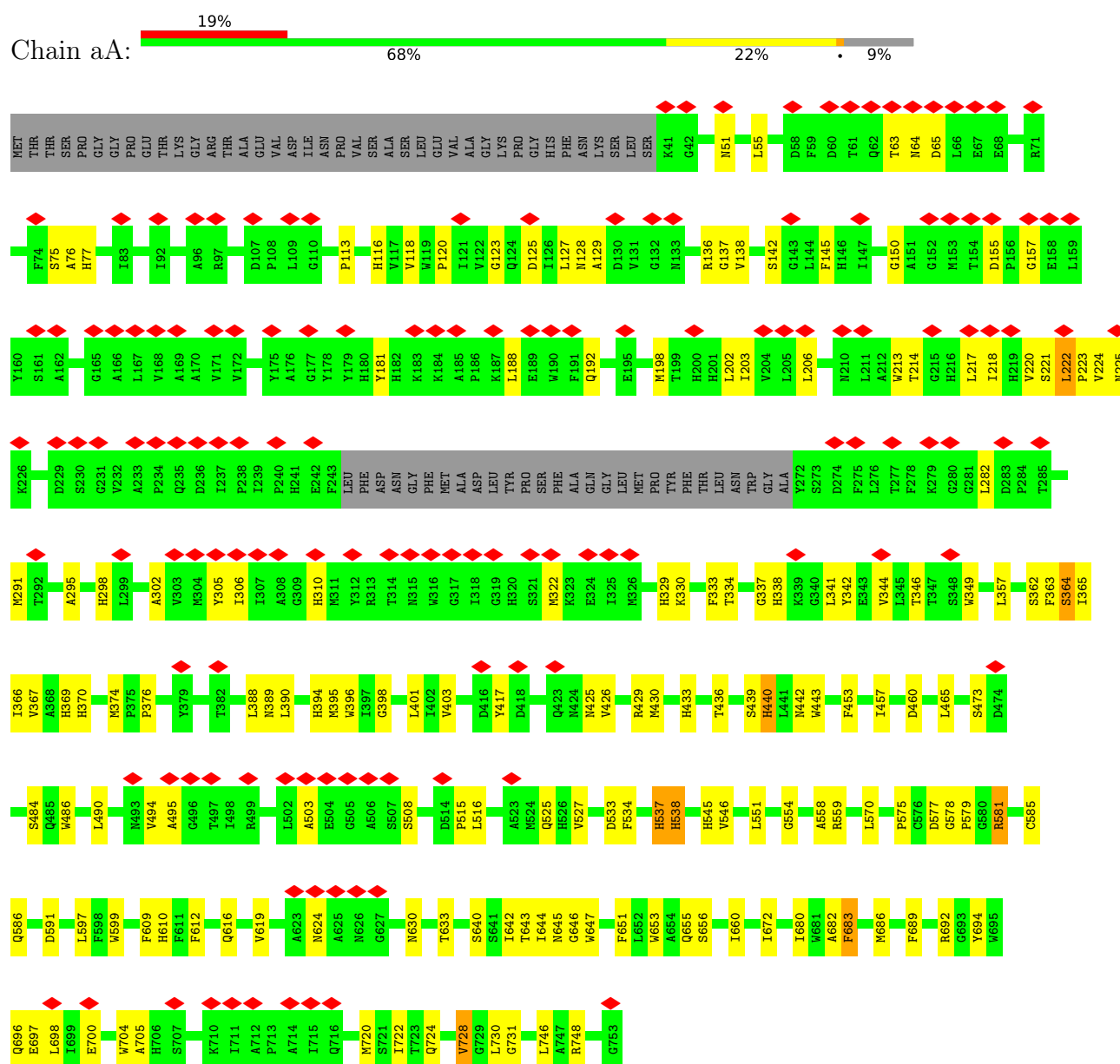
- Molecule 20 is water.

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

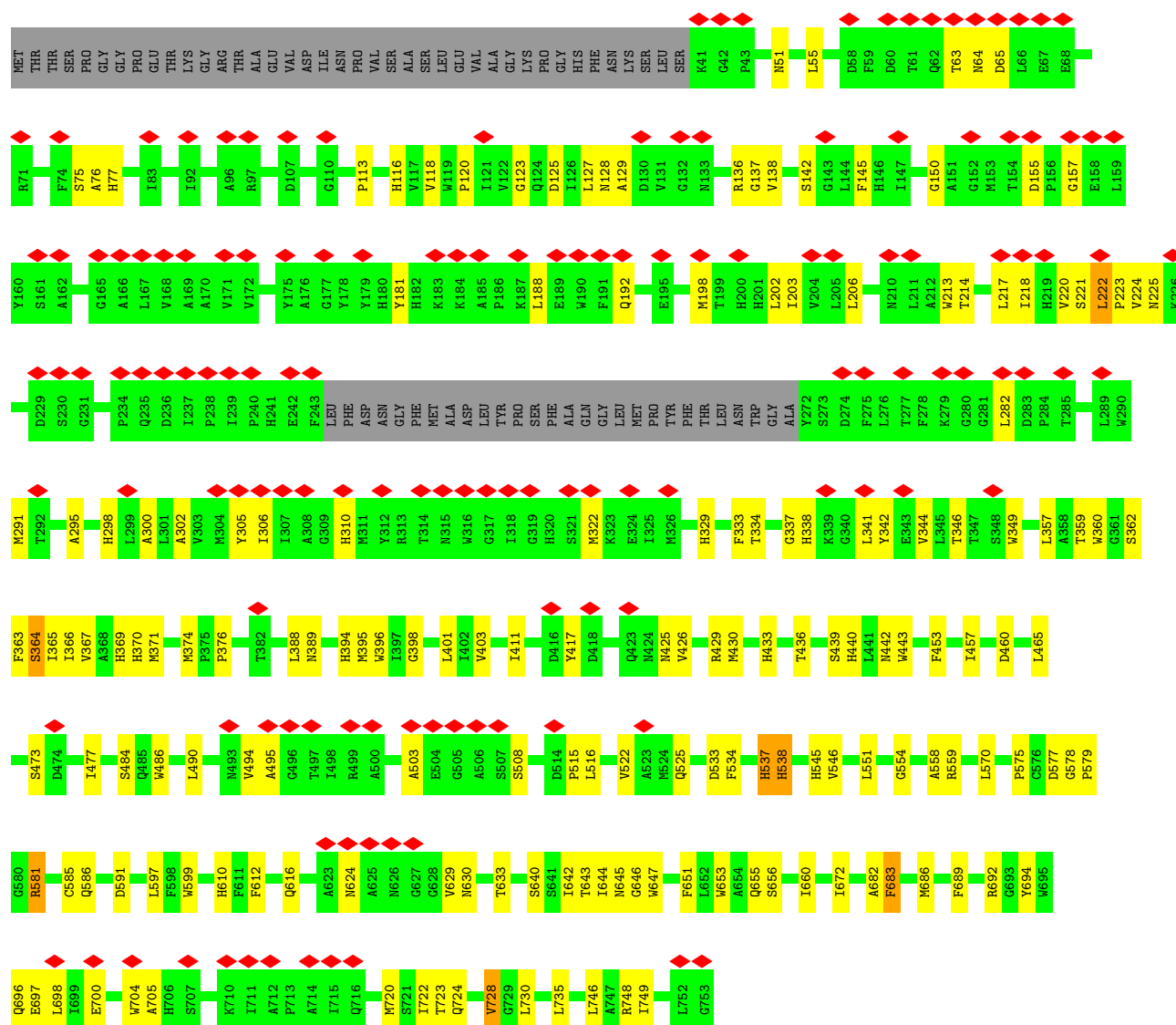
### 3 Residue-property plots

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

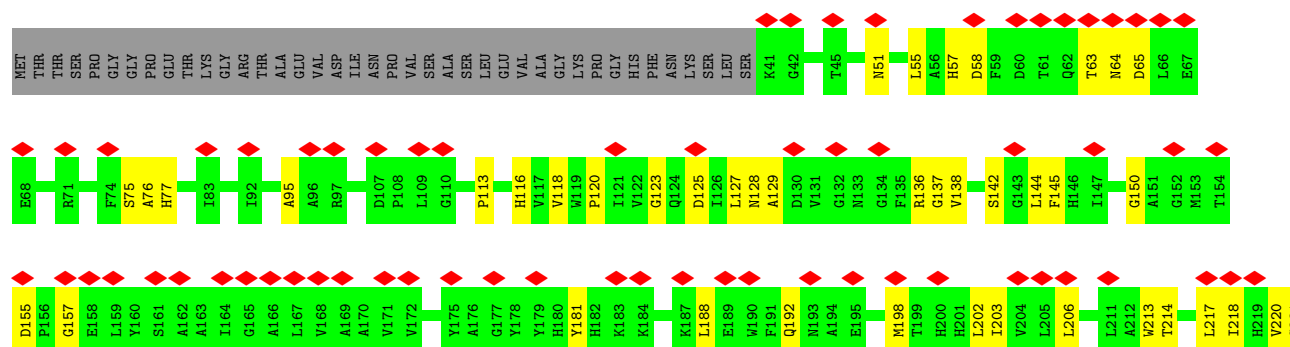
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

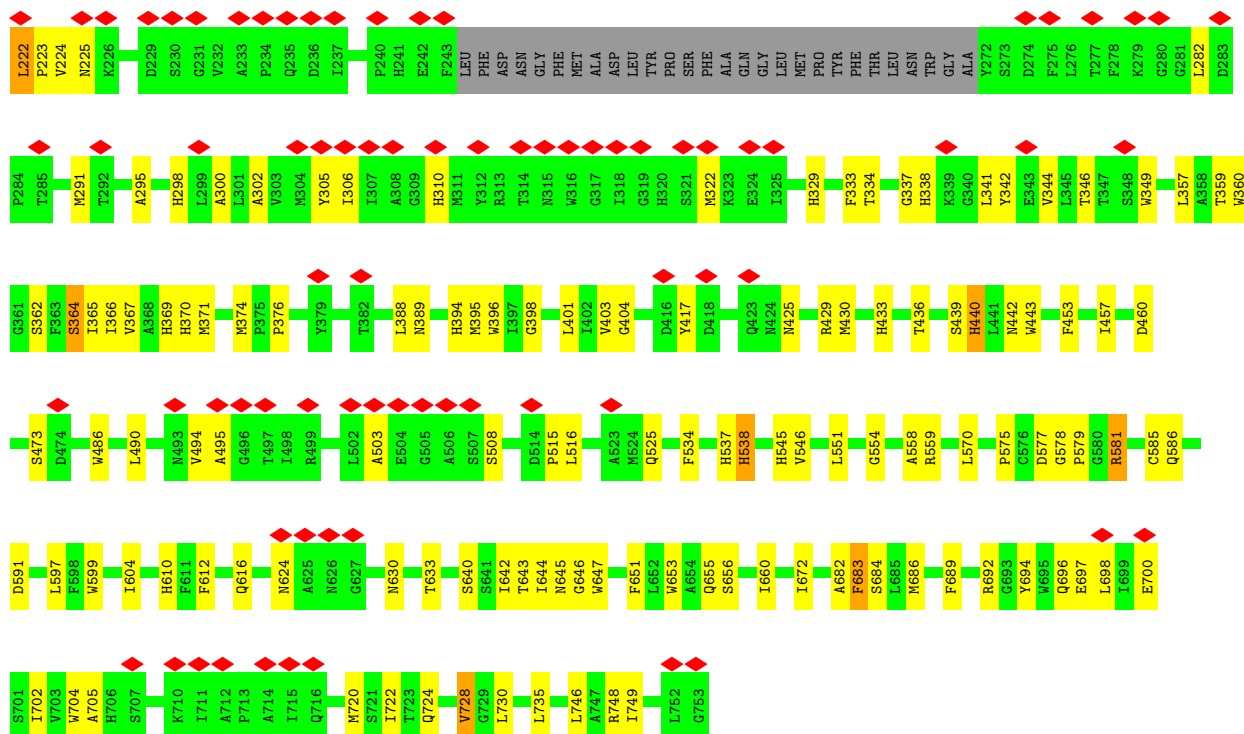


- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



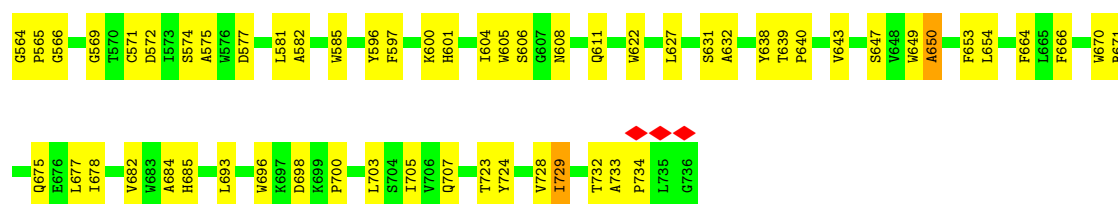
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



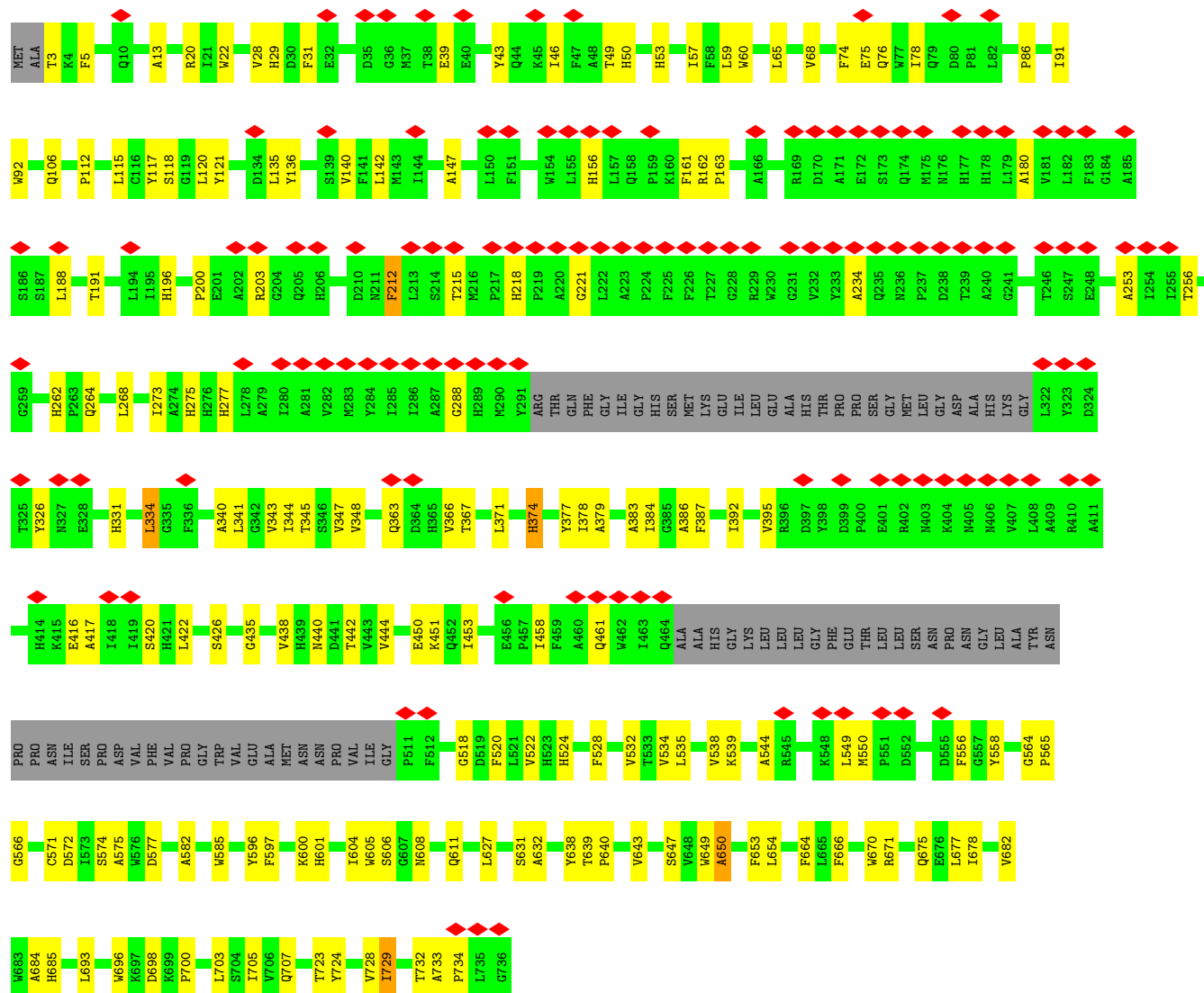


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

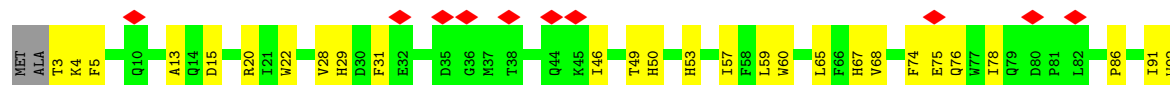


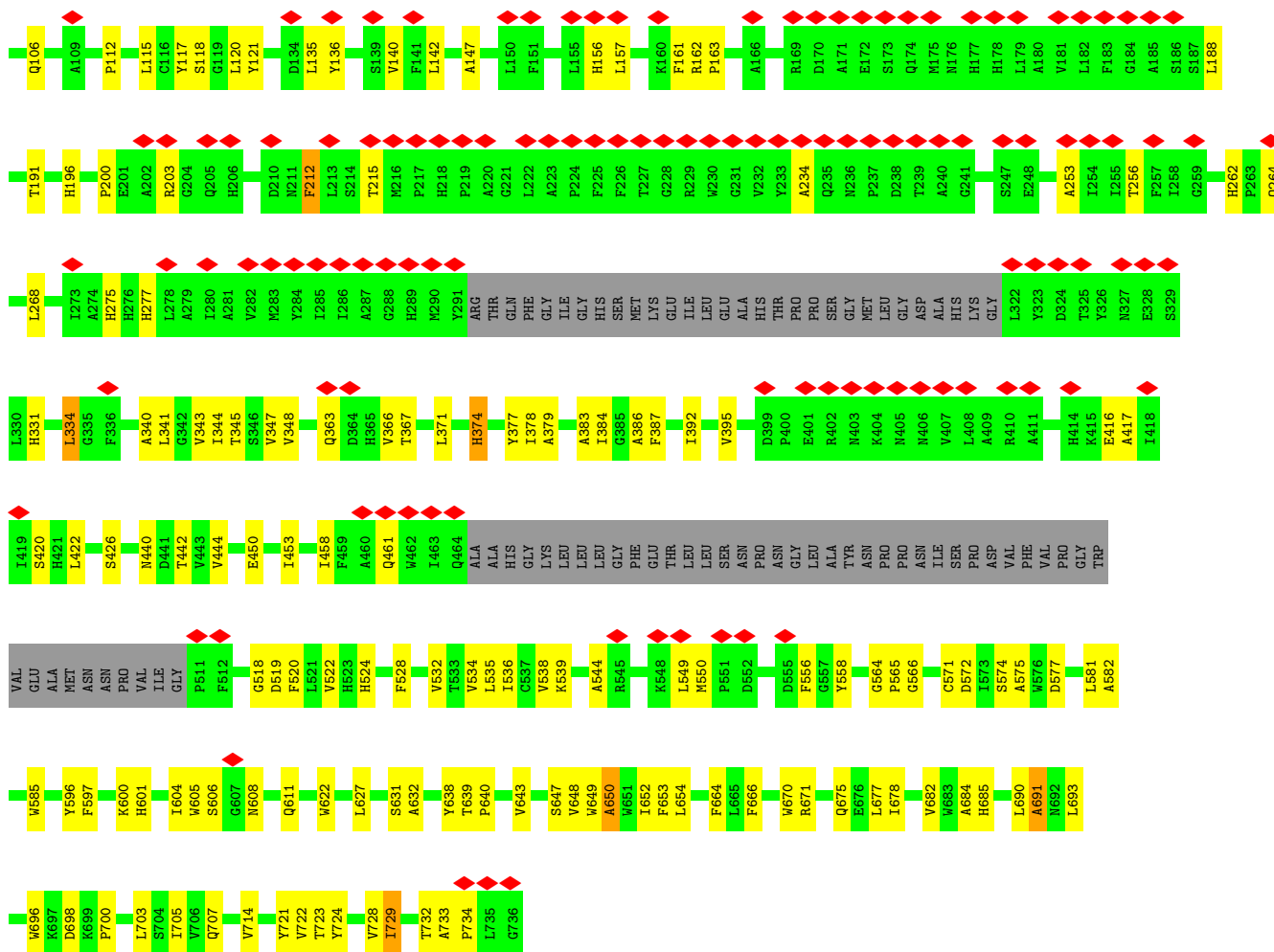


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

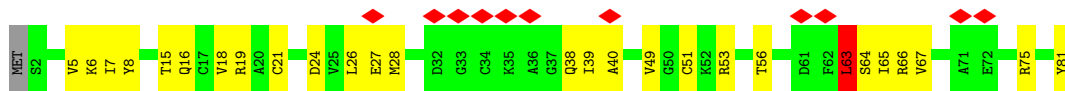


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

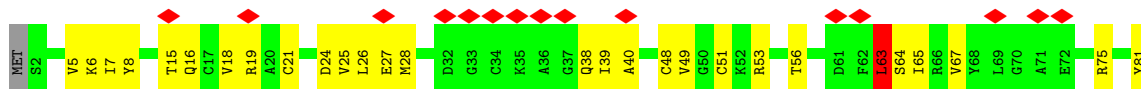




• Molecule 3: Photosystem I iron-sulfur center

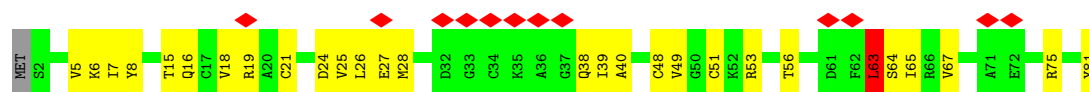


• Molecule 3: Photosystem I iron-sulfur center

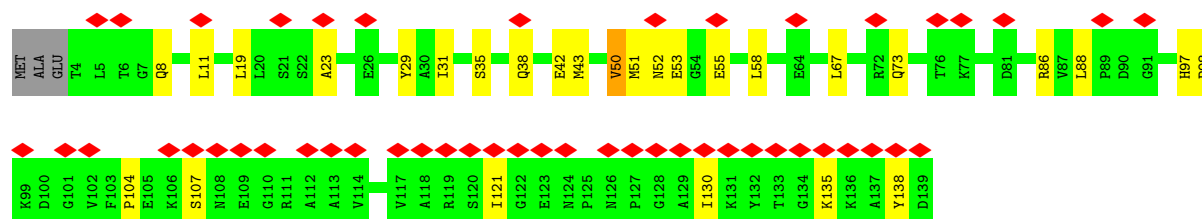
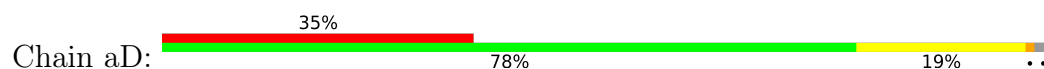


• Molecule 3: Photosystem I iron-sulfur center

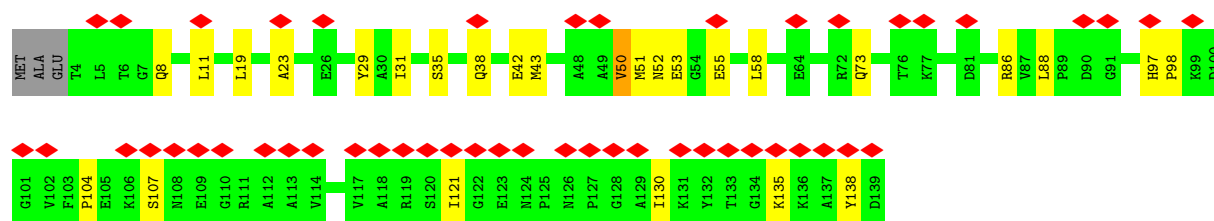
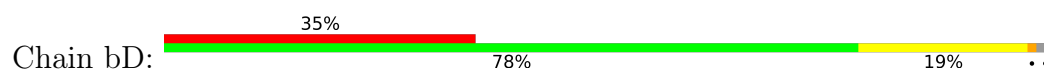




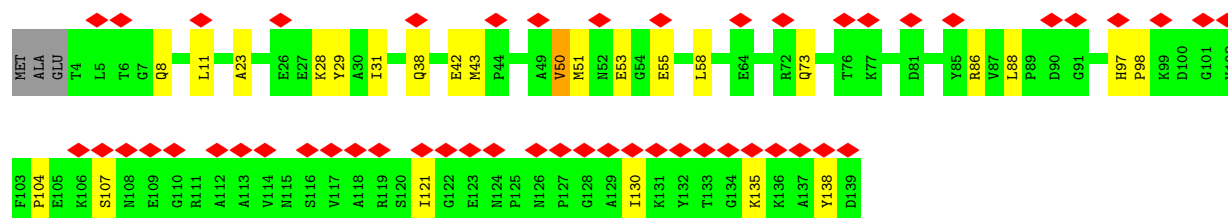
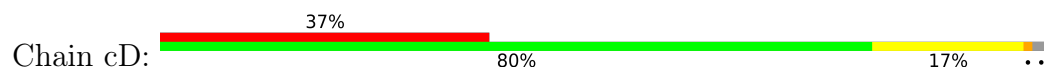
• Molecule 4: Photosystem I protein Psad



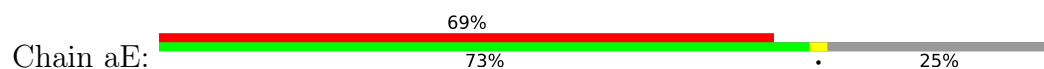
• Molecule 4: Photosystem I protein Psad



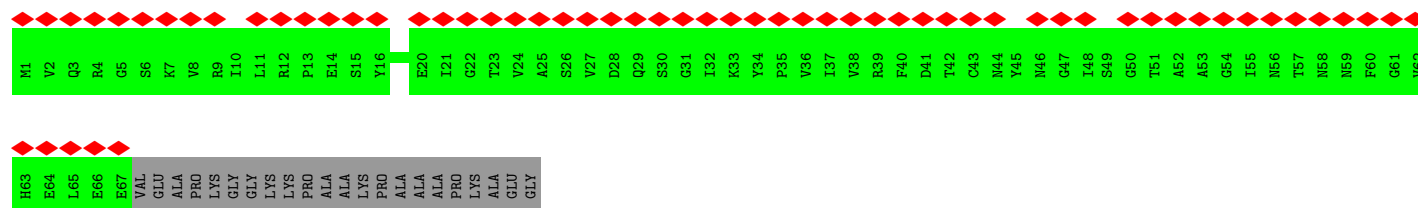
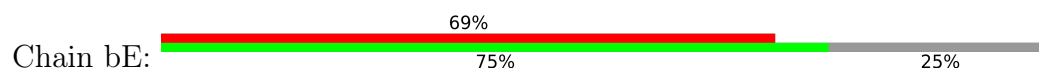
• Molecule 4: Photosystem I protein Psad



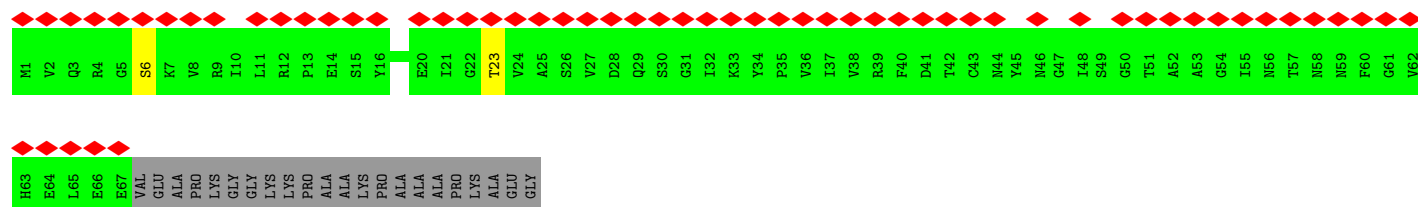
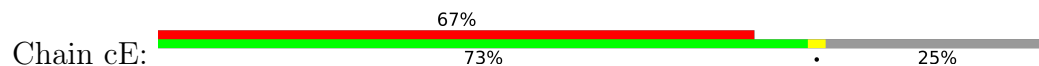
• Molecule 5: Photosystem I reaction center subunit IV



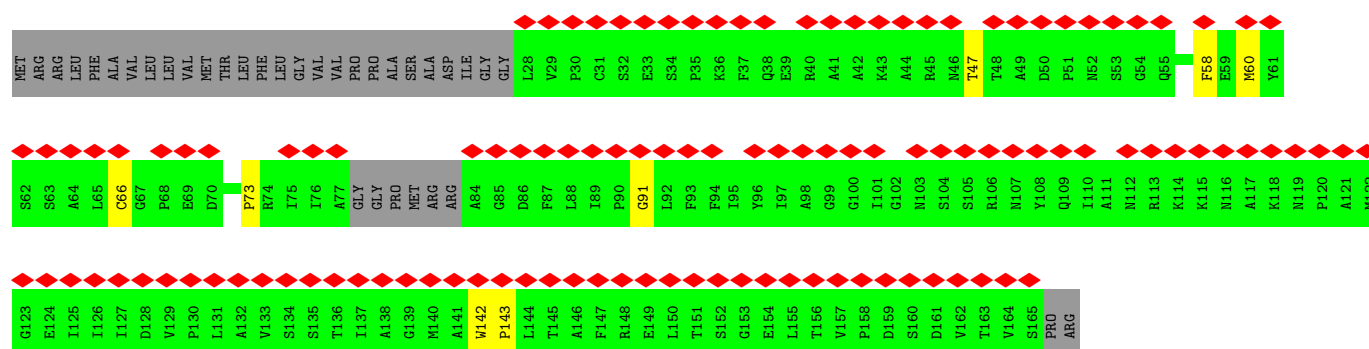
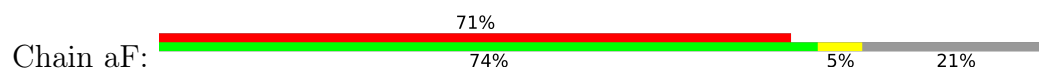
• Molecule 5: Photosystem I reaction center subunit IV



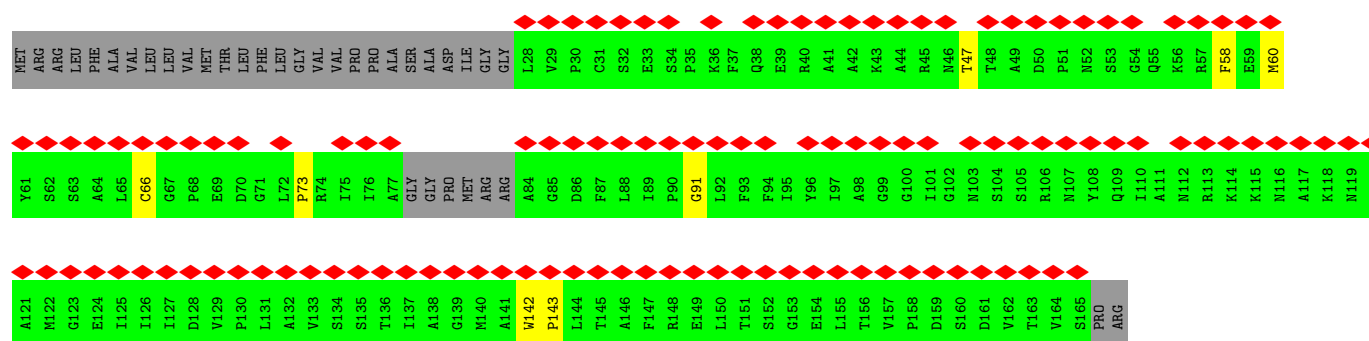
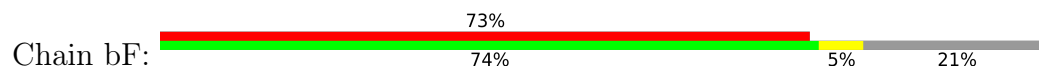
• Molecule 5: Photosystem I reaction center subunit IV



• Molecule 6: Photosystem I protein Psaf



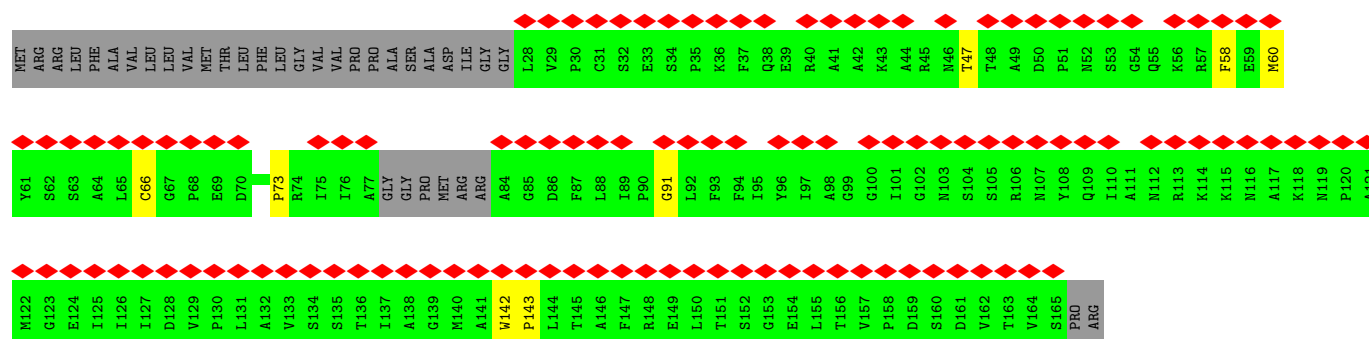
• Molecule 6: Photosystem I protein Psaf



• Molecule 6: Photosystem I protein Psaf



Chain cF: 



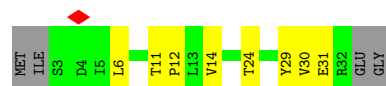
• Molecule 7: Photosystem I protein Psa27

Chain aI: 



• Molecule 7: Photosystem I protein Psa27

Chain bI: 



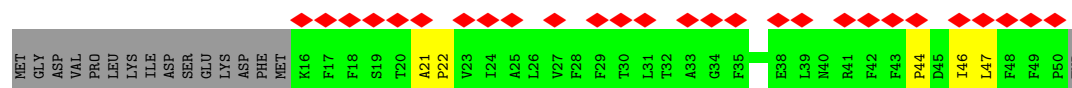
• Molecule 7: Photosystem I protein Psa27

Chain cI: 



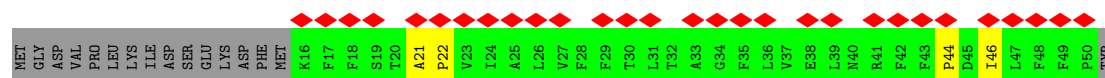
• Molecule 8: Photosystem I reaction center subunit IX

Chain aJ: 

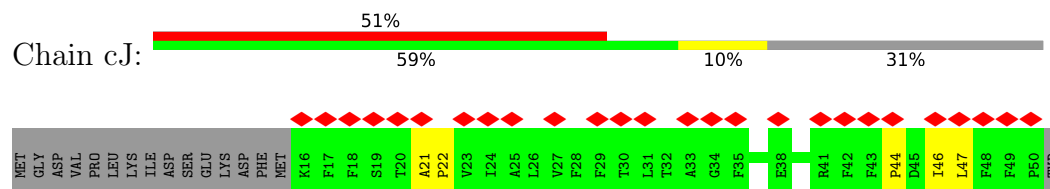


• Molecule 8: Photosystem I reaction center subunit IX

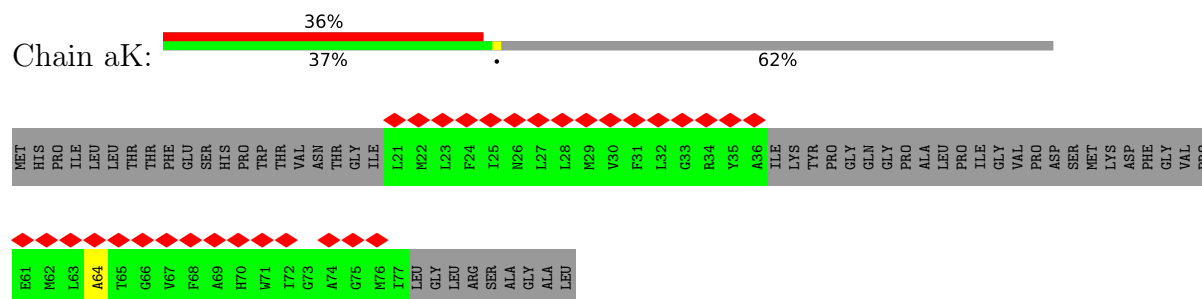
Chain bJ: 



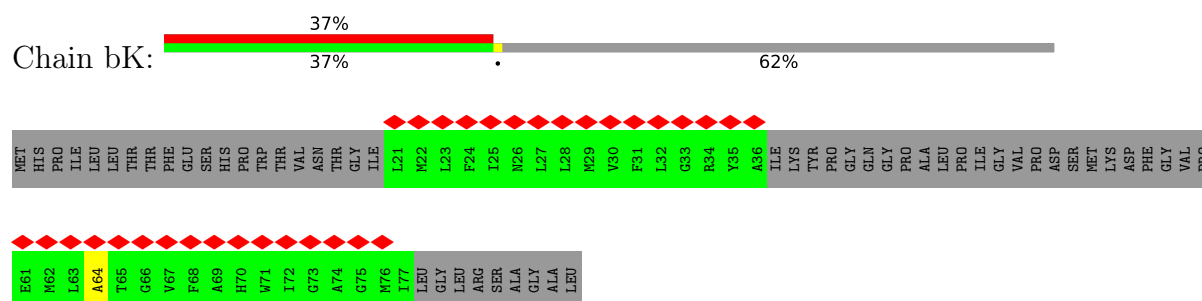
- Molecule 8: Photosystem I reaction center subunit IX



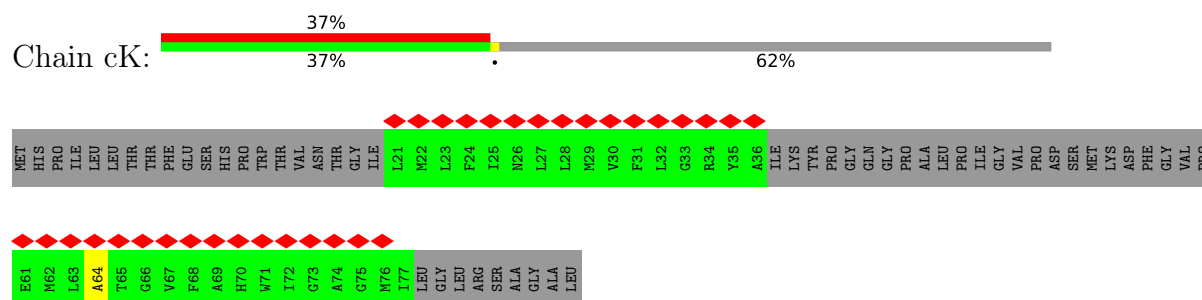
- Molecule 9: Photosystem I reaction center subunit PsaK



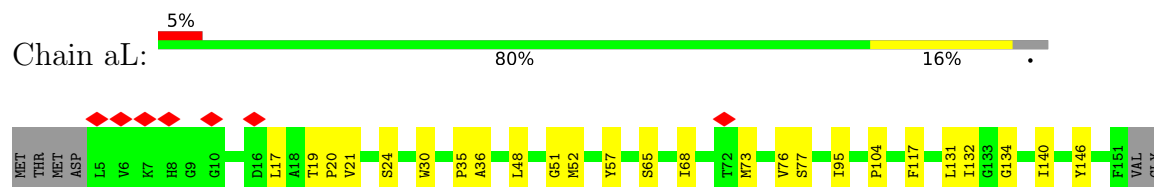
- Molecule 9: Photosystem I reaction center subunit PsaK



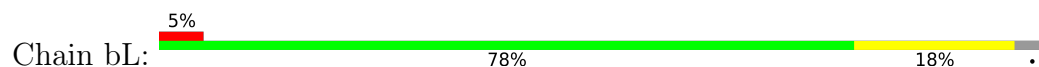
- Molecule 9: Photosystem I reaction center subunit PsaK

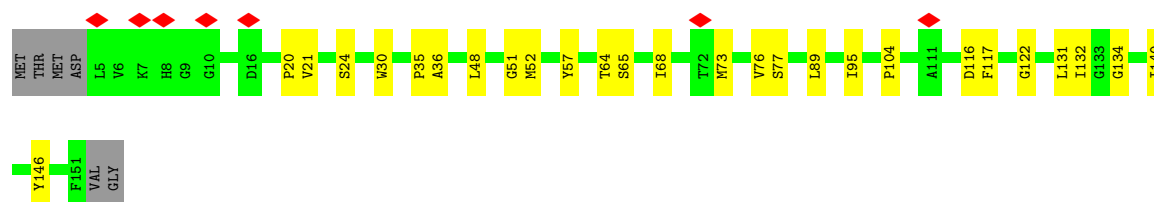


- Molecule 10: Photosystem I protein PsaL

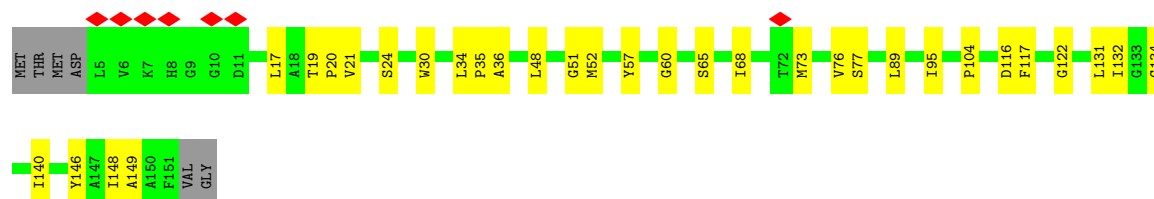
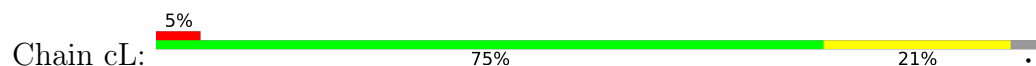


- Molecule 10: Photosystem I protein PsaL





- Molecule 10: Photosystem I protein Psal



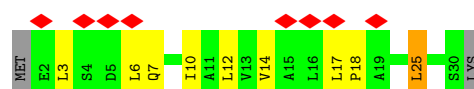
- Molecule 11: Photosystem I protein Psam



- Molecule 11: Photosystem I protein Psam



- Molecule 11: Photosystem I protein Psam



## 4 Experimental information

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: CL7, LHG, LMG, PHO, SF4, G9R, PQN, UNL

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    | 1.11         | 6/5369 (0.1%) | 1.26        | 6/7326 (0.1%) |
| 1   | bA    | 1.11         | 5/5369 (0.1%) | 1.26        | 6/7326 (0.1%) |
| 1   | cA    | 1.11         | 8/5369 (0.1%) | 1.25        | 4/7326 (0.1%) |
| 2   | aB    | 1.07         | 3/5185 (0.1%) | 1.23        | 5/7107 (0.1%) |
| 2   | bB    | 1.07         | 3/5185 (0.1%) | 1.23        | 4/7107 (0.1%) |
| 2   | cB    | 1.07         | 3/5185 (0.1%) | 1.24        | 6/7107 (0.1%) |
| 3   | aC    | 0.96         | 0/582         | 1.18        | 0/792         |
| 3   | bC    | 0.96         | 0/582         | 1.18        | 0/792         |
| 3   | cC    | 0.96         | 0/582         | 1.18        | 0/792         |
| 4   | aD    | 0.89         | 0/1018        | 1.05        | 0/1379        |
| 4   | bD    | 0.90         | 0/1018        | 1.05        | 0/1379        |
| 4   | cD    | 0.90         | 0/1018        | 1.05        | 0/1379        |
| 5   | aE    | 1.14         | 0/379         | 1.24        | 0/524         |
| 5   | bE    | 1.12         | 0/379         | 1.25        | 0/524         |
| 5   | cE    | 1.14         | 0/379         | 1.24        | 0/524         |
| 6   | aF    | 0.99         | 0/863         | 1.30        | 0/1183        |
| 6   | bF    | 0.99         | 0/863         | 1.29        | 0/1183        |
| 6   | cF    | 0.98         | 0/863         | 1.30        | 0/1183        |
| 7   | aI    | 0.96         | 0/230         | 1.31        | 0/313         |
| 7   | bI    | 0.97         | 0/230         | 1.31        | 0/313         |
| 7   | cI    | 0.96         | 0/230         | 1.32        | 0/313         |
| 8   | aJ    | 0.84         | 0/273         | 1.22        | 0/373         |
| 8   | bJ    | 0.84         | 0/273         | 1.22        | 0/373         |
| 8   | cJ    | 0.84         | 0/273         | 1.22        | 0/373         |
| 9   | aK    | 1.14         | 0/159         | 1.71        | 0/217         |
| 9   | bK    | 1.14         | 0/159         | 1.71        | 0/217         |
| 9   | cK    | 1.14         | 0/159         | 1.71        | 0/217         |
| 10  | aL    | 1.11         | 0/1020        | 1.28        | 1/1394 (0.1%) |
| 10  | bL    | 1.11         | 0/1020        | 1.27        | 1/1394 (0.1%) |
| 10  | cL    | 1.11         | 0/1020        | 1.28        | 1/1394 (0.1%) |
| 11  | aM    | 0.97         | 0/205         | 1.37        | 0/281         |
| 11  | bM    | 0.97         | 0/205         | 1.38        | 0/281         |

| Mol | Chain | Bond lengths |                 | Bond angles |                 |
|-----|-------|--------------|-----------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5         |
| 11  | cM    | 0.97         | 0/205           | 1.38        | 0/281           |
| All | All   | 1.07         | 28/45849 (0.1%) | 1.24        | 34/62667 (0.1%) |

All (28) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | cB    | 212 | PHE  | C-N     | 15.21 | 1.52        | 1.33     |
| 2   | bB    | 212 | PHE  | C-N     | 14.97 | 1.52        | 1.33     |
| 2   | aB    | 212 | PHE  | C-N     | 14.84 | 1.52        | 1.33     |
| 1   | cA    | 683 | PHE  | C-N     | -9.32 | 1.21        | 1.34     |
| 1   | aA    | 683 | PHE  | C-N     | -9.00 | 1.22        | 1.34     |
| 1   | bA    | 683 | PHE  | C-N     | -8.95 | 1.22        | 1.34     |
| 2   | cB    | 374 | HIS  | CE1-NE2 | -6.60 | 1.25        | 1.32     |
| 1   | aA    | 369 | HIS  | CE1-NE2 | 6.58  | 1.39        | 1.32     |
| 1   | aA    | 440 | HIS  | CE1-NE2 | 6.25  | 1.38        | 1.32     |
| 1   | aA    | 545 | HIS  | CA-CB   | -6.23 | 1.43        | 1.53     |
| 1   | bA    | 545 | HIS  | CA-CB   | -6.22 | 1.43        | 1.53     |
| 1   | cA    | 369 | HIS  | CE1-NE2 | 6.19  | 1.38        | 1.32     |
| 1   | cA    | 545 | HIS  | CA-CB   | -6.18 | 1.43        | 1.53     |
| 2   | bB    | 374 | HIS  | CE1-NE2 | -6.12 | 1.26        | 1.32     |
| 1   | aA    | 610 | HIS  | CE1-NE2 | 6.06  | 1.38        | 1.32     |
| 1   | bA    | 610 | HIS  | CE1-NE2 | 6.06  | 1.38        | 1.32     |
| 1   | bA    | 369 | HIS  | CE1-NE2 | 6.04  | 1.38        | 1.32     |
| 1   | cA    | 610 | HIS  | CE1-NE2 | 5.63  | 1.38        | 1.32     |
| 2   | aB    | 374 | HIS  | CE1-NE2 | -5.53 | 1.27        | 1.32     |
| 1   | cA    | 537 | HIS  | CE1-NE2 | 5.49  | 1.38        | 1.32     |
| 1   | cA    | 684 | SER  | C-N     | 5.30  | 1.41        | 1.34     |
| 1   | cA    | 364 | SER  | CA-CB   | -5.23 | 1.45        | 1.53     |
| 1   | bA    | 364 | SER  | CA-CB   | -5.19 | 1.45        | 1.53     |
| 1   | aA    | 364 | SER  | CA-CB   | -5.15 | 1.45        | 1.53     |
| 2   | bB    | 654 | LEU  | C-O     | -5.12 | 1.18        | 1.24     |
| 1   | cA    | 440 | HIS  | CE1-NE2 | 5.11  | 1.37        | 1.32     |
| 2   | aB    | 654 | LEU  | C-O     | -5.02 | 1.18        | 1.24     |
| 2   | cB    | 654 | LEU  | C-O     | -5.00 | 1.18        | 1.24     |

All (34) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | aA    | 538 | HIS  | CA-CB-CG | -7.26 | 106.54      | 113.80   |
| 1   | cA    | 538 | HIS  | CA-CB-CG | -7.21 | 106.59      | 113.80   |
| 1   | bA    | 538 | HIS  | CA-CB-CG | -7.17 | 106.64      | 113.80   |
| 2   | cB    | 723 | THR  | N-CA-C   | -6.06 | 104.59      | 111.14   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | bA    | 581 | ARG  | N-CA-C   | -5.99 | 105.55      | 112.86   |
| 2   | aB    | 723 | THR  | N-CA-C   | -5.96 | 104.70      | 111.14   |
| 1   | cA    | 581 | ARG  | N-CA-C   | -5.96 | 105.59      | 112.86   |
| 2   | bB    | 723 | THR  | N-CA-C   | -5.96 | 104.71      | 111.14   |
| 1   | aA    | 581 | ARG  | N-CA-C   | -5.93 | 105.63      | 112.86   |
| 2   | cB    | 691 | ALA  | N-CA-C   | -5.60 | 106.37      | 113.43   |
| 10  | bL    | 132 | ILE  | N-CA-C   | -5.44 | 105.41      | 110.53   |
| 10  | aL    | 132 | ILE  | N-CA-C   | -5.44 | 105.42      | 110.53   |
| 10  | cL    | 132 | ILE  | N-CA-C   | -5.43 | 105.43      | 110.53   |
| 1   | bA    | 394 | HIS  | CA-CB-CG | -5.38 | 108.42      | 113.80   |
| 1   | aA    | 394 | HIS  | CA-CB-CG | -5.35 | 108.45      | 113.80   |
| 2   | aB    | 650 | ALA  | N-CA-C   | -5.32 | 105.49      | 111.28   |
| 2   | cB    | 650 | ALA  | N-CA-C   | -5.30 | 105.50      | 111.28   |
| 1   | aA    | 537 | HIS  | CA-CB-CG | -5.28 | 108.52      | 113.80   |
| 1   | cA    | 394 | HIS  | CA-CB-CG | -5.26 | 108.54      | 113.80   |
| 2   | bB    | 650 | ALA  | N-CA-C   | -5.25 | 105.56      | 111.28   |
| 1   | bA    | 683 | PHE  | CA-C-N   | 5.21  | 127.79      | 120.28   |
| 1   | bA    | 683 | PHE  | C-N-CA   | 5.21  | 127.79      | 120.28   |
| 1   | cA    | 537 | HIS  | CA-CB-CG | -5.21 | 108.58      | 113.80   |
| 2   | aB    | 334 | LEU  | N-CA-CB  | -5.16 | 102.53      | 110.01   |
| 2   | bB    | 334 | LEU  | N-CA-CB  | -5.16 | 102.53      | 110.01   |
| 1   | aA    | 683 | PHE  | CA-C-N   | 5.12  | 127.86      | 120.38   |
| 1   | aA    | 683 | PHE  | C-N-CA   | 5.12  | 127.86      | 120.38   |
| 2   | cB    | 67  | HIS  | CA-CB-CG | -5.12 | 108.68      | 113.80   |
| 2   | aB    | 675 | GLN  | N-CA-C   | -5.09 | 105.81      | 111.36   |
| 2   | cB    | 675 | GLN  | N-CA-C   | -5.09 | 105.81      | 111.36   |
| 2   | bB    | 675 | GLN  | N-CA-C   | -5.08 | 105.82      | 111.36   |
| 1   | bA    | 537 | HIS  | CA-CB-CG | -5.04 | 108.76      | 113.80   |
| 2   | aB    | 67  | HIS  | CA-CB-CG | -5.02 | 108.78      | 113.80   |
| 2   | cB    | 334 | LEU  | N-CA-CB  | -5.00 | 102.76      | 110.01   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | aA    | 5203  | 0        | 4895     | 131     | 0            |
| 1   | bA    | 5203  | 0        | 4895     | 137     | 0            |
| 1   | cA    | 5203  | 0        | 4895     | 132     | 0            |
| 2   | aB    | 5007  | 0        | 4607     | 151     | 0            |
| 2   | bB    | 5007  | 0        | 4607     | 144     | 0            |
| 2   | cB    | 5007  | 0        | 4607     | 152     | 0            |
| 3   | aC    | 573   | 0        | 543      | 26      | 0            |
| 3   | bC    | 573   | 0        | 543      | 25      | 0            |
| 3   | cC    | 573   | 0        | 543      | 25      | 0            |
| 4   | aD    | 999   | 0        | 981      | 23      | 0            |
| 4   | bD    | 999   | 0        | 981      | 20      | 0            |
| 4   | cD    | 999   | 0        | 981      | 19      | 0            |
| 5   | aE    | 375   | 0        | 218      | 1       | 0            |
| 5   | bE    | 375   | 0        | 218      | 0       | 0            |
| 5   | cE    | 375   | 0        | 218      | 1       | 0            |
| 6   | aF    | 847   | 0        | 707      | 7       | 0            |
| 6   | bF    | 847   | 0        | 707      | 7       | 0            |
| 6   | cF    | 847   | 0        | 707      | 7       | 0            |
| 7   | aI    | 225   | 0        | 231      | 11      | 0            |
| 7   | bI    | 225   | 0        | 231      | 12      | 0            |
| 7   | cI    | 225   | 0        | 231      | 13      | 0            |
| 8   | aJ    | 264   | 0        | 237      | 5       | 0            |
| 8   | bJ    | 264   | 0        | 237      | 4       | 0            |
| 8   | cJ    | 264   | 0        | 237      | 5       | 0            |
| 9   | aK    | 161   | 0        | 80       | 1       | 0            |
| 9   | bK    | 161   | 0        | 80       | 1       | 0            |
| 9   | cK    | 161   | 0        | 80       | 1       | 0            |
| 10  | aL    | 999   | 0        | 976      | 20      | 0            |
| 10  | bL    | 999   | 0        | 976      | 23      | 0            |
| 10  | cL    | 999   | 0        | 976      | 28      | 0            |
| 11  | aM    | 205   | 0        | 232      | 11      | 0            |
| 11  | bM    | 205   | 0        | 232      | 10      | 0            |
| 11  | cM    | 205   | 0        | 232      | 10      | 0            |
| 12  | aA    | 65    | 0        | 0        | 0       | 0            |
| 12  | bA    | 65    | 0        | 0        | 0       | 0            |
| 12  | cA    | 65    | 0        | 0        | 0       | 0            |
| 13  | aA    | 64    | 0        | 74       | 7       | 0            |
| 13  | aB    | 64    | 0        | 74       | 9       | 0            |
| 13  | bB    | 128   | 0        | 148      | 17      | 0            |
| 13  | cB    | 128   | 0        | 148      | 19      | 0            |
| 14  | aA    | 1862  | 0        | 1586     | 51      | 0            |
| 14  | aB    | 1410  | 0        | 1250     | 61      | 0            |
| 14  | aF    | 38    | 0        | 24       | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 14  | aJ    | 42    | 0        | 28       | 0       | 0            |
| 14  | aK    | 37    | 0        | 23       | 0       | 0            |
| 14  | aL    | 172   | 0        | 169      | 10      | 0            |
| 14  | bA    | 1862  | 0        | 1586     | 56      | 0            |
| 14  | bB    | 1410  | 0        | 1250     | 59      | 0            |
| 14  | bF    | 38    | 0        | 24       | 1       | 0            |
| 14  | bJ    | 42    | 0        | 28       | 1       | 0            |
| 14  | bK    | 37    | 0        | 23       | 0       | 0            |
| 14  | bL    | 172   | 0        | 169      | 12      | 0            |
| 14  | cA    | 1862  | 0        | 1586     | 54      | 0            |
| 14  | cB    | 1410  | 0        | 1250     | 53      | 0            |
| 14  | cF    | 38    | 0        | 24       | 1       | 0            |
| 14  | cJ    | 42    | 0        | 28       | 0       | 0            |
| 14  | cK    | 37    | 0        | 23       | 0       | 0            |
| 14  | cL    | 172   | 0        | 169      | 13      | 0            |
| 15  | aA    | 150   | 0        | 0        | 0       | 0            |
| 15  | aB    | 120   | 0        | 0        | 0       | 0            |
| 15  | aI    | 80    | 0        | 0        | 0       | 0            |
| 15  | aJ    | 40    | 0        | 0        | 0       | 0            |
| 15  | aL    | 80    | 0        | 0        | 1       | 0            |
| 15  | bA    | 150   | 0        | 0        | 0       | 0            |
| 15  | bB    | 120   | 0        | 0        | 0       | 0            |
| 15  | bI    | 80    | 0        | 0        | 1       | 0            |
| 15  | bJ    | 40    | 0        | 0        | 0       | 0            |
| 15  | bL    | 80    | 0        | 0        | 2       | 0            |
| 15  | cA    | 110   | 0        | 0        | 0       | 0            |
| 15  | cB    | 120   | 0        | 0        | 0       | 0            |
| 15  | cF    | 40    | 0        | 0        | 0       | 0            |
| 15  | cI    | 80    | 0        | 0        | 1       | 0            |
| 15  | cJ    | 40    | 0        | 0        | 0       | 0            |
| 15  | cL    | 80    | 0        | 0        | 2       | 0            |
| 16  | aA    | 70    | 0        | 91       | 3       | 0            |
| 16  | bA    | 70    | 0        | 90       | 4       | 0            |
| 16  | cA    | 70    | 0        | 90       | 3       | 0            |
| 17  | aA    | 33    | 0        | 46       | 1       | 0            |
| 17  | aB    | 33    | 0        | 46       | 1       | 0            |
| 17  | bA    | 33    | 0        | 46       | 3       | 0            |
| 17  | bB    | 33    | 0        | 46       | 3       | 0            |
| 17  | cA    | 33    | 0        | 46       | 2       | 0            |
| 17  | cB    | 33    | 0        | 46       | 1       | 0            |
| 18  | aB    | 8     | 0        | 0        | 0       | 0            |
| 18  | aC    | 16    | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 18  | bB    | 8     | 0        | 0        | 0       | 0            |
| 18  | bC    | 16    | 0        | 0        | 0       | 0            |
| 18  | cB    | 8     | 0        | 0        | 0       | 0            |
| 18  | cC    | 16    | 0        | 0        | 0       | 0            |
| 19  | aB    | 52    | 0        | 77       | 1       | 0            |
| 19  | bB    | 52    | 0        | 77       | 1       | 0            |
| 19  | cB    | 52    | 0        | 77       | 2       | 0            |
| 20  | aA    | 13    | 0        | 0        | 1       | 0            |
| 20  | aB    | 12    | 0        | 0        | 0       | 0            |
| 20  | aL    | 3     | 0        | 0        | 0       | 0            |
| 20  | bA    | 12    | 0        | 0        | 1       | 0            |
| 20  | bB    | 13    | 0        | 0        | 0       | 0            |
| 20  | bL    | 3     | 0        | 0        | 0       | 0            |
| 20  | cA    | 13    | 0        | 0        | 1       | 0            |
| 20  | cB    | 12    | 0        | 0        | 0       | 0            |
| 20  | cL    | 3     | 0        | 0        | 0       | 0            |
| All | All   | 57966 | 0        | 51583    | 1222    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (1222) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 2:aB:53:HIS:HD1     | 14:aB:3031:CL7:H3A | 1.35                     | 0.91              |
| 2:bB:528:PHE:HE1    | 13:bB:801:PHO:HBA2 | 1.39                     | 0.88              |
| 2:bB:53:HIS:HD1     | 14:bB:832:CL7:H3A  | 1.39                     | 0.88              |
| 2:cB:528:PHE:HE1    | 13:cB:801:PHO:HBA2 | 1.39                     | 0.88              |
| 13:aA:3102:PHO:HBA2 | 2:aB:528:PHE:HE1   | 1.38                     | 0.87              |
| 2:cB:53:HIS:HD1     | 14:cB:832:CL7:H3A  | 1.41                     | 0.85              |
| 14:cB:807:CL7:H12C  | 7:cI:14:VAL:HG21   | 1.58                     | 0.84              |
| 14:bB:807:CL7:H12C  | 7:bI:14:VAL:HG21   | 1.59                     | 0.84              |
| 7:aI:6:LEU:HD21     | 11:aM:12:LEU:HD11  | 1.58                     | 0.83              |
| 14:aB:3006:CL7:H12C | 7:aI:14:VAL:HG21   | 1.58                     | 0.82              |
| 7:bI:6:LEU:HD21     | 11:bM:12:LEU:HD11  | 1.60                     | 0.82              |
| 7:cI:6:LEU:HD21     | 11:cM:12:LEU:HD11  | 1.60                     | 0.81              |
| 2:aB:212:PHE:HA     | 2:aB:215:THR:OG1   | 1.83                     | 0.79              |
| 2:cB:212:PHE:HA     | 2:cB:215:THR:OG1   | 1.82                     | 0.79              |
| 2:aB:558:TYR:O      | 2:aB:574:SER:OG    | 2.02                     | 0.78              |
| 2:bB:20:ARG:NH2     | 7:bI:30:VAL:O      | 2.17                     | 0.78              |
| 2:cB:558:TYR:O      | 2:cB:574:SER:OG    | 2.02                     | 0.78              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:cB:20:ARG:NH2     | 7:cI:30:VAL:O       | 2.17                     | 0.78              |
| 2:bB:212:PHE:HA     | 2:bB:215:THR:OG1    | 1.83                     | 0.77              |
| 2:bB:558:TYR:O      | 2:bB:574:SER:OG     | 2.02                     | 0.76              |
| 1:cA:128:ASN:HD22   | 1:cA:137:GLY:HA2    | 1.53                     | 0.74              |
| 1:bA:128:ASN:HD22   | 1:bA:137:GLY:HA2    | 1.53                     | 0.72              |
| 1:aA:128:ASN:HD22   | 1:aA:137:GLY:HA2    | 1.53                     | 0.71              |
| 1:aA:322:MET:HG2    | 14:aA:3117:CL7:HED2 | 1.73                     | 0.71              |
| 1:aA:599:TRP:CH2    | 14:aA:3103:CL7:HAB  | 2.26                     | 0.71              |
| 1:bA:322:MET:HG2    | 14:bA:3116:CL7:HED2 | 1.73                     | 0.71              |
| 13:aA:3102:PHO:HBA2 | 2:aB:528:PHE:CE1    | 2.25                     | 0.70              |
| 1:bA:599:TRP:CH2    | 14:bA:3102:CL7:HAB  | 2.27                     | 0.70              |
| 1:cA:322:MET:HG2    | 14:cA:3116:CL7:HED2 | 1.75                     | 0.69              |
| 14:bA:3142:CL7:C4D  | 14:bA:3142:CL7:H2   | 2.22                     | 0.69              |
| 1:aA:333:PHE:O      | 1:aA:429:ARG:NH2    | 2.25                     | 0.69              |
| 1:cA:333:PHE:O      | 1:cA:429:ARG:NH2    | 2.25                     | 0.69              |
| 2:cB:585:TRP:CH2    | 14:cB:803:CL7:HAB   | 2.28                     | 0.69              |
| 1:bA:333:PHE:O      | 1:bA:429:ARG:NH2    | 2.25                     | 0.69              |
| 2:bB:528:PHE:CE1    | 13:bB:801:PHO:HBA2  | 2.25                     | 0.69              |
| 1:cA:142:SER:HA     | 14:cA:3140:CL7:HMA2 | 1.76                     | 0.68              |
| 14:bB:806:CL7:H51C  | 19:bB:830:LMG:H332  | 1.75                     | 0.68              |
| 14:cA:3102:CL7:H91C | 13:cB:805:PHO:H102  | 1.74                     | 0.68              |
| 2:cB:528:PHE:CE1    | 13:cB:801:PHO:HBA2  | 2.27                     | 0.67              |
| 14:cB:807:CL7:H92C  | 14:cB:807:CL7:HMC2  | 1.75                     | 0.67              |
| 14:bA:3128:CL7:H191 | 14:bL:204:CL7:H72C  | 1.77                     | 0.67              |
| 3:bC:15:THR:HG22    | 3:bC:15:THR:O       | 1.94                     | 0.67              |
| 2:cB:453:ILE:HD11   | 14:cB:822:CL7:HHB   | 1.76                     | 0.67              |
| 3:cC:15:THR:O       | 3:cC:15:THR:HG22    | 1.94                     | 0.67              |
| 3:aC:15:THR:O       | 3:aC:15:THR:HG22    | 1.94                     | 0.67              |
| 14:aB:3019:CL7:HAB  | 14:aB:3031:CL7:HMA3 | 1.77                     | 0.66              |
| 2:bB:268:LEU:HD13   | 14:bB:815:CL7:HMA2  | 1.78                     | 0.66              |
| 2:aB:377:TYR:HD2    | 14:aB:3018:CL7:HAB  | 1.61                     | 0.66              |
| 3:cC:51:CYS:SG      | 3:cC:53:ARG:HG3     | 2.36                     | 0.66              |
| 14:bA:3102:CL7:H91C | 13:bB:805:PHO:H102  | 1.76                     | 0.66              |
| 2:bB:453:ILE:HD11   | 14:bB:822:CL7:HHB   | 1.78                     | 0.66              |
| 3:bC:51:CYS:SG      | 3:bC:53:ARG:HG3     | 2.36                     | 0.65              |
| 2:aB:585:TRP:CH2    | 14:aB:3002:CL7:HAB  | 2.32                     | 0.65              |
| 2:aB:387:PHE:HZ     | 14:aB:3016:CL7:HAB  | 1.61                     | 0.65              |
| 3:aC:51:CYS:SG      | 3:aC:53:ARG:HG3     | 2.36                     | 0.65              |
| 14:aA:3103:CL7:H91C | 13:aB:3004:PHO:H102 | 1.78                     | 0.65              |
| 2:bB:585:TRP:CH2    | 14:bB:803:CL7:HAB   | 2.31                     | 0.65              |
| 2:aB:724:TYR:HB2    | 14:aB:3003:CL7:HED2 | 1.78                     | 0.64              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:bB:234:ALA:HB2    | 14:bB:814:CL7:HMA2  | 1.79                     | 0.64              |
| 14:cA:3123:CL7:H2   | 14:cL:204:CL7:H43C  | 1.79                     | 0.64              |
| 2:aB:120:LEU:HD21   | 14:aB:3032:CL7:HBA2 | 1.77                     | 0.64              |
| 14:aB:3006:CL7:H92C | 14:aB:3006:CL7:HMC2 | 1.78                     | 0.63              |
| 2:aB:86:PRO:HB3     | 2:aB:121:TYR:CD2    | 2.34                     | 0.63              |
| 2:bB:86:PRO:HB3     | 2:bB:121:TYR:CD2    | 2.34                     | 0.62              |
| 1:cA:640:SER:O      | 1:cA:646:GLY:HA3    | 2.00                     | 0.62              |
| 1:aA:396:TRP:CD1    | 14:aA:3141:CL7:HAB  | 2.33                     | 0.62              |
| 2:cB:86:PRO:HB3     | 2:cB:121:TYR:CD2    | 2.34                     | 0.62              |
| 14:aA:3108:CL7:H71C | 14:aA:3142:CL7:H151 | 1.82                     | 0.62              |
| 14:bA:3131:CL7:HAB  | 17:bA:3143:PQN:H172 | 1.80                     | 0.62              |
| 2:cB:585:TRP:HH2    | 14:cB:803:CL7:HAB   | 1.64                     | 0.62              |
| 2:aB:453:ILE:HD11   | 14:aB:3021:CL7:HHB  | 1.82                     | 0.62              |
| 1:bA:640:SER:O      | 1:bA:646:GLY:HA3    | 1.99                     | 0.62              |
| 11:cM:14:VAL:O      | 11:cM:18:PRO:HD2    | 2.00                     | 0.61              |
| 14:cA:3123:CL7:HMD3 | 10:cL:21:VAL:HG21   | 1.82                     | 0.61              |
| 1:aA:640:SER:O      | 1:aA:646:GLY:HA3    | 1.99                     | 0.61              |
| 2:aB:377:TYR:CD2    | 14:aB:3018:CL7:HAB  | 2.35                     | 0.61              |
| 11:aM:14:VAL:O      | 11:aM:18:PRO:HD2    | 2.00                     | 0.61              |
| 1:bA:486:TRP:CH2    | 1:bA:490:LEU:HD13   | 2.36                     | 0.61              |
| 1:aA:142:SER:HA     | 14:aA:3141:CL7:HMA2 | 1.82                     | 0.61              |
| 14:bA:3106:CL7:HMA2 | 14:bA:3106:CL7:H2   | 1.83                     | 0.61              |
| 2:bB:643:VAL:HG13   | 2:bB:647:SER:HB2    | 1.83                     | 0.60              |
| 14:bB:820:CL7:HAB   | 14:bB:832:CL7:HMA3  | 1.81                     | 0.60              |
| 1:aA:486:TRP:CH2    | 1:aA:490:LEU:HD13   | 2.36                     | 0.60              |
| 1:cA:486:TRP:CH2    | 1:cA:490:LEU:HD13   | 2.37                     | 0.60              |
| 2:cB:76:GLN:OE1     | 2:cB:76:GLN:N       | 2.34                     | 0.60              |
| 2:cB:643:VAL:HG13   | 2:cB:647:SER:HB2    | 1.84                     | 0.60              |
| 11:bM:14:VAL:O      | 11:bM:18:PRO:HD2    | 2.00                     | 0.60              |
| 2:bB:724:TYR:HB2    | 14:bB:804:CL7:HED2  | 1.82                     | 0.60              |
| 2:aB:643:VAL:HG13   | 2:aB:647:SER:HB2    | 1.83                     | 0.60              |
| 1:cA:599:TRP:CH2    | 14:cA:3102:CL7:HAB  | 2.36                     | 0.60              |
| 2:cB:268:LEU:HD13   | 14:cB:815:CL7:HMA2  | 1.84                     | 0.59              |
| 2:bB:585:TRP:HH2    | 14:bB:803:CL7:HAB   | 1.68                     | 0.59              |
| 14:aA:3107:CL7:HMA2 | 14:aA:3107:CL7:H2   | 1.83                     | 0.59              |
| 1:bA:689:PHE:HB2    | 13:bB:801:PHO:HBC2  | 1.84                     | 0.59              |
| 4:aD:19:LEU:HB3     | 4:aD:23:ALA:HB2     | 1.84                     | 0.59              |
| 14:cB:827:CL7:OBB   | 14:cB:827:CL7:HHC   | 2.01                     | 0.59              |
| 1:aA:430:MET:HA     | 1:aA:433:HIS:CE1    | 2.38                     | 0.59              |
| 1:cA:689:PHE:HB2    | 13:cB:801:PHO:HBC2  | 1.85                     | 0.59              |
| 14:cB:820:CL7:HAB   | 14:cB:832:CL7:HMA3  | 1.85                     | 0.59              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 14:bB:807:CL7:HMC2  | 14:bB:807:CL7:H92C  | 1.85                     | 0.59              |
| 1:aA:689:PHE:HB2    | 13:aA:3102:PHO:HBC2 | 1.84                     | 0.58              |
| 4:bD:19:LEU:HB3     | 4:bD:23:ALA:HB2     | 1.84                     | 0.58              |
| 1:cA:396:TRP:CD1    | 14:cA:3140:CL7:HAB  | 2.38                     | 0.58              |
| 2:cB:387:PHE:HZ     | 14:cB:817:CL7:HAB   | 1.68                     | 0.58              |
| 4:cD:11:LEU:HB2     | 4:cD:50:VAL:HG13    | 1.85                     | 0.58              |
| 2:bB:218:HIS:HB3    | 2:bB:221:GLY:HA3    | 1.84                     | 0.58              |
| 1:aA:697:GLU:O      | 1:aA:700:GLU:HG2    | 2.03                     | 0.58              |
| 14:aB:3026:CL7:OBB  | 14:aB:3026:CL7:HHC  | 2.02                     | 0.58              |
| 1:bA:616:GLN:HG3    | 1:bA:633:THR:OG1    | 2.04                     | 0.58              |
| 1:bA:697:GLU:O      | 1:bA:700:GLU:HG2    | 2.03                     | 0.58              |
| 3:bC:27:GLU:HA      | 4:bD:104:PRO:HB3    | 1.85                     | 0.58              |
| 1:cA:430:MET:HA     | 1:cA:433:HIS:CE1    | 2.39                     | 0.58              |
| 1:cA:697:GLU:O      | 1:cA:700:GLU:HG2    | 2.03                     | 0.58              |
| 14:cA:3125:CL7:H143 | 14:cA:3128:CL7:H151 | 1.84                     | 0.58              |
| 13:aA:3102:PHO:HMB1 | 13:aA:3102:PHO:HBB1 | 1.85                     | 0.58              |
| 2:aB:53:HIS:ND1     | 14:aB:3031:CL7:H3A  | 2.15                     | 0.58              |
| 1:cA:616:GLN:HG3    | 1:cA:633:THR:OG1    | 2.04                     | 0.58              |
| 2:aB:15:ASP:HB3     | 2:aB:20:ARG:HB2     | 1.86                     | 0.58              |
| 3:aC:27:GLU:HA      | 4:aD:104:PRO:HB3    | 1.85                     | 0.58              |
| 1:aA:616:GLN:HG3    | 1:aA:633:THR:OG1    | 2.04                     | 0.57              |
| 2:aB:585:TRP:HH2    | 14:aB:3002:CL7:HAB  | 1.68                     | 0.57              |
| 2:bB:387:PHE:HZ     | 14:bB:817:CL7:HAB   | 1.67                     | 0.57              |
| 4:cD:29:TYR:OH      | 4:cD:86:ARG:NH1     | 2.38                     | 0.57              |
| 2:bB:203:ARG:NH1    | 2:bB:253:ALA:O      | 2.34                     | 0.57              |
| 3:cC:27:GLU:HA      | 4:cD:104:PRO:HB3    | 1.85                     | 0.57              |
| 2:aB:203:ARG:NH1    | 2:aB:253:ALA:O      | 2.34                     | 0.57              |
| 1:aA:495:ALA:O      | 1:aA:503:ALA:HB3    | 2.05                     | 0.57              |
| 3:bC:75:ARG:HD3     | 4:bD:86:ARG:HH12    | 1.70                     | 0.57              |
| 10:aL:35:PRO:HG3    | 14:aL:203:CL7:HED2  | 1.87                     | 0.57              |
| 3:aC:75:ARG:HD3     | 4:aD:86:ARG:HH12    | 1.69                     | 0.57              |
| 4:aD:11:LEU:HB2     | 4:aD:50:VAL:HG13    | 1.85                     | 0.57              |
| 14:cA:3107:CL7:H121 | 14:cA:3141:CL7:H203 | 1.85                     | 0.57              |
| 4:aD:29:TYR:OH      | 4:aD:86:ARG:NH1     | 2.38                     | 0.57              |
| 2:cB:520:PHE:CE1    | 2:cB:524:HIS:CE1    | 2.93                     | 0.57              |
| 14:bB:827:CL7:HHC   | 14:bB:827:CL7:OBB   | 2.05                     | 0.57              |
| 4:bD:29:TYR:OH      | 4:bD:86:ARG:NH1     | 2.38                     | 0.57              |
| 4:bD:11:LEU:HB2     | 4:bD:50:VAL:HG13    | 1.85                     | 0.57              |
| 2:bB:76:GLN:N       | 2:bB:76:GLN:OE1     | 2.34                     | 0.56              |
| 1:bA:430:MET:HA     | 1:bA:433:HIS:CE1    | 2.41                     | 0.56              |
| 1:bA:495:ALA:O      | 1:bA:503:ALA:HB3    | 2.05                     | 0.56              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 14:bB:806:CL7:H12C  | 14:bB:820:CL7:HBA2  | 1.86                     | 0.56              |
| 1:cA:495:ALA:O      | 1:cA:503:ALA:HB3    | 2.05                     | 0.56              |
| 14:cB:808:CL7:H152  | 14:cB:808:CL7:HBA2  | 1.85                     | 0.56              |
| 7:cI:11:THR:HB      | 7:cI:12:PRO:HD3     | 1.88                     | 0.56              |
| 2:aB:76:GLN:OE1     | 2:aB:76:GLN:N       | 2.34                     | 0.56              |
| 14:cB:819:CL7:H91C  | 14:cB:819:CL7:HBC3  | 1.87                     | 0.56              |
| 14:cB:822:CL7:HED1  | 8:cJ:47:LEU:HA      | 1.87                     | 0.56              |
| 2:aB:520:PHE:CE1    | 2:aB:524:HIS:CE1    | 2.93                     | 0.56              |
| 14:bB:808:CL7:H152  | 14:bB:808:CL7:HBA2  | 1.88                     | 0.56              |
| 2:bB:520:PHE:CE1    | 2:bB:524:HIS:CE1    | 2.93                     | 0.56              |
| 7:bI:11:THR:HB      | 7:bI:12:PRO:HD3     | 1.87                     | 0.56              |
| 4:aD:42:GLU:N       | 4:aD:73:GLN:OE1     | 2.38                     | 0.56              |
| 2:cB:724:TYR:HB2    | 14:cB:804:CL7:HED2  | 1.88                     | 0.56              |
| 3:cC:75:ARG:HD3     | 4:cD:86:ARG:HH12    | 1.69                     | 0.56              |
| 1:aA:155:ASP:OD1    | 1:aA:157:GLY:N      | 2.39                     | 0.55              |
| 2:aB:46:ILE:CG2     | 2:aB:50:HIS:HE1     | 2.20                     | 0.55              |
| 1:aA:453:PHE:CZ     | 1:aA:457:ILE:HD11   | 2.42                     | 0.55              |
| 1:bA:490:LEU:HD23   | 1:bA:490:LEU:O      | 2.06                     | 0.55              |
| 3:aC:28:MET:O       | 4:aD:107:SER:HA     | 2.07                     | 0.55              |
| 14:cA:3141:CL7:H93C | 14:cA:3142:CL7:HAA1 | 1.88                     | 0.55              |
| 1:aA:490:LEU:O      | 1:aA:490:LEU:HD23   | 2.06                     | 0.55              |
| 1:aA:490:LEU:O      | 1:aA:494:VAL:HB     | 2.07                     | 0.55              |
| 1:bA:453:PHE:CZ     | 1:bA:457:ILE:HD11   | 2.42                     | 0.55              |
| 1:cA:359:THR:HG22   | 14:cA:3120:CL7:H41C | 1.87                     | 0.55              |
| 1:cA:453:PHE:CZ     | 1:cA:457:ILE:HD11   | 2.42                     | 0.55              |
| 7:aI:24:THR:HG23    | 10:aL:95:ILE:HG21   | 1.89                     | 0.55              |
| 3:cC:28:MET:O       | 4:cD:107:SER:HA     | 2.07                     | 0.55              |
| 1:bA:142:SER:HA     | 14:bA:3140:CL7:HMA2 | 1.89                     | 0.55              |
| 1:bA:490:LEU:O      | 1:bA:494:VAL:HB     | 2.07                     | 0.55              |
| 1:cA:75:SER:HB3     | 1:cA:181:TYR:HB2    | 1.89                     | 0.55              |
| 1:cA:155:ASP:OD1    | 1:cA:157:GLY:N      | 2.39                     | 0.55              |
| 1:bA:155:ASP:OD1    | 1:bA:157:GLY:N      | 2.39                     | 0.55              |
| 1:cA:490:LEU:HD23   | 1:cA:490:LEU:O      | 2.06                     | 0.55              |
| 1:cA:490:LEU:O      | 1:cA:494:VAL:HB     | 2.07                     | 0.55              |
| 2:cB:46:ILE:CG2     | 2:cB:50:HIS:HE1     | 2.20                     | 0.55              |
| 1:bA:597:LEU:CD1    | 1:bA:730:LEU:HD21   | 2.37                     | 0.55              |
| 7:aI:11:THR:HB      | 7:aI:12:PRO:HD3     | 1.88                     | 0.55              |
| 2:aB:234:ALA:HB2    | 14:aB:3013:CL7:HMA2 | 1.88                     | 0.55              |
| 2:aB:374:HIS:CE1    | 2:aB:378:ILE:HD12   | 2.42                     | 0.55              |
| 14:aB:3005:CL7:H12C | 14:aB:3019:CL7:HBA2 | 1.88                     | 0.55              |
| 2:bB:46:ILE:CG2     | 2:bB:50:HIS:HE1     | 2.20                     | 0.55              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:aB:664:PHE:HB3    | 13:aB:3004:PHO:HMC2 | 1.89                     | 0.54              |
| 2:bB:374:HIS:CE1    | 2:bB:378:ILE:HD12   | 2.42                     | 0.54              |
| 1:aA:597:LEU:CD1    | 1:aA:730:LEU:HD21   | 2.37                     | 0.54              |
| 1:bA:75:SER:HB3     | 1:bA:181:TYR:HB2    | 1.89                     | 0.54              |
| 14:bA:3118:CL7:HMB3 | 14:bA:3139:CL7:H52C | 1.89                     | 0.54              |
| 7:cI:24:THR:HG23    | 10:cL:95:ILE:HG21   | 1.89                     | 0.54              |
| 2:bB:451:LYS:HE3    | 14:bB:822:CL7:O1D   | 2.08                     | 0.54              |
| 2:bB:693:LEU:HD11   | 10:bL:36:ALA:HB1    | 1.89                     | 0.54              |
| 3:bC:28:MET:O       | 4:bD:107:SER:HA     | 2.07                     | 0.54              |
| 7:bI:24:THR:HG23    | 10:bL:95:ILE:HG21   | 1.89                     | 0.54              |
| 14:cA:3120:CL7:HMB2 | 14:cA:3126:CL7:HAA1 | 1.88                     | 0.54              |
| 4:bD:42:GLU:N       | 4:bD:73:GLN:OE1     | 2.38                     | 0.54              |
| 3:cC:16:GLN:HA      | 3:cC:16:GLN:OE1     | 2.08                     | 0.54              |
| 20:aA:3207:HOH:O    | 2:aB:685:HIS:HD2    | 1.89                     | 0.54              |
| 2:cB:341:LEU:O      | 2:cB:345:THR:HG22   | 2.08                     | 0.54              |
| 1:aA:113:PRO:HB3    | 1:aA:145:PHE:CD2    | 2.43                     | 0.54              |
| 2:aB:341:LEU:O      | 2:aB:345:THR:HG22   | 2.08                     | 0.54              |
| 2:aB:451:LYS:HE3    | 14:aB:3021:CL7:O1D  | 2.08                     | 0.54              |
| 1:cA:113:PRO:HB3    | 1:cA:145:PHE:CD2    | 2.43                     | 0.54              |
| 1:cA:401:LEU:HD21   | 14:cA:3106:CL7:H142 | 1.88                     | 0.54              |
| 2:cB:522:VAL:HG11   | 2:cB:596:TYR:HB2    | 1.90                     | 0.54              |
| 1:aA:75:SER:HB3     | 1:aA:181:TYR:HB2    | 1.89                     | 0.54              |
| 1:aA:401:LEU:HD21   | 14:aA:3107:CL7:H142 | 1.89                     | 0.54              |
| 2:aB:693:LEU:HD11   | 10:aL:36:ALA:HB1    | 1.89                     | 0.54              |
| 1:cA:349:TRP:HB3    | 14:cA:3105:CL7:HAC1 | 1.89                     | 0.54              |
| 1:cA:597:LEU:CD1    | 1:cA:730:LEU:HD21   | 2.37                     | 0.54              |
| 10:aL:52:MET:HE1    | 10:cL:131:LEU:HD21  | 1.90                     | 0.54              |
| 1:aA:376:PRO:HG3    | 14:aA:3115:CL7:HBA1 | 1.90                     | 0.54              |
| 2:aB:366:VAL:HG11   | 2:aB:733:ALA:HA     | 1.90                     | 0.54              |
| 1:bA:411:ILE:HG21   | 14:bA:3141:CL7:HED1 | 1.90                     | 0.54              |
| 2:cB:140:VAL:HG13   | 11:cM:14:VAL:HG21   | 1.90                     | 0.54              |
| 10:cL:48:LEU:HG     | 10:cL:52:MET:HE2    | 1.90                     | 0.54              |
| 2:aB:92:TRP:CE3     | 7:aI:11:THR:HB      | 2.44                     | 0.53              |
| 10:aL:131:LEU:HD21  | 10:bL:52:MET:HE1    | 1.90                     | 0.53              |
| 2:bB:377:TYR:CD2    | 14:bB:819:CL7:HAB   | 2.43                     | 0.53              |
| 2:cB:203:ARG:NH1    | 2:cB:253:ALA:O      | 2.34                     | 0.53              |
| 2:cB:693:LEU:HD11   | 10:cL:36:ALA:HB1    | 1.89                     | 0.53              |
| 10:aL:48:LEU:HG     | 10:aL:52:MET:HE2    | 1.90                     | 0.53              |
| 14:bB:810:CL7:H192  | 14:cL:203:CL7:H192  | 1.90                     | 0.53              |
| 20:bA:3207:HOH:O    | 2:bB:685:HIS:HD2    | 1.91                     | 0.53              |
| 10:bL:131:LEU:HD21  | 10:cL:52:MET:HE1    | 1.90                     | 0.53              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:cB:92:TRP:CE3     | 7:cI:11:THR:HB      | 2.44                     | 0.53              |
| 2:cB:690:LEU:HD12   | 14:cL:204:CL7:H11C  | 1.89                     | 0.53              |
| 14:aA:3107:CL7:H3A  | 14:aA:3142:CL7:CAB  | 2.39                     | 0.53              |
| 2:aB:522:VAL:HG11   | 2:aB:596:TYR:HB2    | 1.90                     | 0.53              |
| 3:aC:16:GLN:HA      | 3:aC:16:GLN:OE1     | 2.08                     | 0.53              |
| 2:bB:140:VAL:HG13   | 11:bM:14:VAL:HG21   | 1.90                     | 0.53              |
| 13:bB:801:PHO:HBB1  | 13:bB:801:PHO:HMB1  | 1.90                     | 0.53              |
| 2:cB:374:HIS:CE1    | 2:cB:378:ILE:HD12   | 2.44                     | 0.53              |
| 4:cD:23:ALA:HB1     | 4:cD:28:LYS:HG2     | 1.89                     | 0.53              |
| 1:bA:401:LEU:HD21   | 14:bA:3106:CL7:H142 | 1.89                     | 0.53              |
| 2:cB:366:VAL:HG11   | 2:cB:733:ALA:HA     | 1.90                     | 0.53              |
| 2:cB:535:LEU:HD12   | 2:cB:535:LEU:O      | 2.08                     | 0.53              |
| 2:aB:363:GLN:N      | 2:aB:363:GLN:OE1    | 2.42                     | 0.53              |
| 3:aC:15:THR:HA      | 3:aC:28:MET:HE3     | 1.91                     | 0.53              |
| 1:bA:113:PRO:HB3    | 1:bA:145:PHE:CD2    | 2.43                     | 0.53              |
| 2:bB:438:VAL:HG13   | 14:bB:803:CL7:H61C  | 1.90                     | 0.53              |
| 2:bB:522:VAL:HG11   | 2:bB:596:TYR:HB2    | 1.90                     | 0.53              |
| 1:cA:698:LEU:HD21   | 13:cB:801:PHO:HED2  | 1.90                     | 0.53              |
| 2:bB:341:LEU:O      | 2:bB:345:THR:HG22   | 2.08                     | 0.53              |
| 3:bC:16:GLN:OE1     | 3:bC:16:GLN:HA      | 2.08                     | 0.53              |
| 10:cL:60:GLY:HA2    | 14:cL:205:CL7:HMA1  | 1.91                     | 0.53              |
| 2:aB:535:LEU:HD12   | 2:aB:535:LEU:O      | 2.08                     | 0.53              |
| 3:cC:15:THR:HA      | 3:cC:28:MET:HE3     | 1.91                     | 0.53              |
| 10:cL:17:LEU:O      | 10:cL:19:THR:HG23   | 2.09                     | 0.53              |
| 1:aA:349:TRP:HB3    | 14:aA:3106:CL7:HAC1 | 1.91                     | 0.52              |
| 2:bB:363:GLN:N      | 2:bB:363:GLN:OE1    | 2.42                     | 0.52              |
| 2:bB:535:LEU:O      | 2:bB:535:LEU:HD12   | 2.08                     | 0.52              |
| 2:cB:363:GLN:OE1    | 2:cB:363:GLN:N      | 2.42                     | 0.52              |
| 2:cB:682:VAL:HG13   | 2:cB:696:TRP:CZ2    | 2.44                     | 0.52              |
| 1:cA:724:GLN:O      | 1:cA:728:VAL:HG13   | 2.09                     | 0.52              |
| 1:aA:442:ASN:ND2    | 13:aB:3004:PHO:HED2 | 2.23                     | 0.52              |
| 14:aA:3123:CL7:H42C | 14:aL:203:CL7:H141  | 1.92                     | 0.52              |
| 10:bL:48:LEU:HG     | 10:bL:52:MET:HE2    | 1.90                     | 0.52              |
| 2:cB:714:VAL:HG22   | 19:cB:830:LMG:H372  | 1.90                     | 0.52              |
| 4:cD:42:GLU:N       | 4:cD:73:GLN:OE1     | 2.38                     | 0.52              |
| 3:cC:38:GLN:HG2     | 4:cD:107:SER:HB2    | 1.92                     | 0.52              |
| 14:bA:3123:CL7:H2   | 14:bL:204:CL7:H43C  | 1.90                     | 0.52              |
| 2:bB:682:VAL:HG13   | 2:bB:696:TRP:CZ2    | 2.44                     | 0.52              |
| 20:cA:3207:HOH:O    | 2:cB:685:HIS:HD2    | 1.92                     | 0.52              |
| 13:cB:801:PHO:H13   | 14:cB:803:CL7:H142  | 1.92                     | 0.52              |
| 1:aA:515:PRO:HB3    | 1:aA:525:GLN:OE1    | 2.09                     | 0.52              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:bB:92:TRP:CE3     | 7:bI:11:THR:HB      | 2.44                     | 0.52              |
| 1:cA:515:PRO:HB3    | 1:cA:525:GLN:OE1    | 2.09                     | 0.52              |
| 2:cB:671:ARG:HD2    | 2:cB:703:LEU:O      | 2.10                     | 0.52              |
| 1:aA:389:ASN:OD1    | 1:aA:746:LEU:HD21   | 2.10                     | 0.52              |
| 1:aA:682:ALA:HB3    | 13:aA:3102:PHO:HBB2 | 1.92                     | 0.52              |
| 2:aB:191:THR:HG22   | 2:aB:277:HIS:CB     | 2.40                     | 0.52              |
| 2:aB:664:PHE:CB     | 13:aB:3004:PHO:HMC2 | 2.40                     | 0.52              |
| 2:aB:671:ARG:HD2    | 2:aB:703:LEU:O      | 2.10                     | 0.52              |
| 2:aB:682:VAL:HG13   | 2:aB:696:TRP:CZ2    | 2.44                     | 0.52              |
| 1:bA:515:PRO:HB3    | 1:bA:525:GLN:OE1    | 2.09                     | 0.52              |
| 14:bA:3115:CL7:HMA1 | 9:bK:64:ALA:HB2     | 1.91                     | 0.52              |
| 2:bB:366:VAL:HG11   | 2:bB:733:ALA:HA     | 1.90                     | 0.52              |
| 2:bB:671:ARG:HD2    | 2:bB:703:LEU:O      | 2.10                     | 0.52              |
| 3:bC:38:GLN:HG2     | 4:bD:107:SER:HB2    | 1.92                     | 0.52              |
| 2:cB:191:THR:HG22   | 2:cB:277:HIS:CB     | 2.40                     | 0.52              |
| 1:aA:433:HIS:O      | 1:aA:436:THR:HG22   | 2.10                     | 0.52              |
| 1:aA:724:GLN:O      | 1:aA:728:VAL:HG13   | 2.10                     | 0.52              |
| 1:bA:282:LEU:HB2    | 1:bA:516:LEU:HD13   | 1.92                     | 0.52              |
| 1:bA:433:HIS:O      | 1:bA:436:THR:HG22   | 2.10                     | 0.52              |
| 1:bA:723:THR:HG22   | 16:bA:3137:LHG:HC41 | 1.92                     | 0.52              |
| 2:bB:191:THR:HG22   | 2:bB:277:HIS:CB     | 2.40                     | 0.52              |
| 1:cA:577:ASP:OD2    | 1:cA:581:ARG:NH2    | 2.42                     | 0.52              |
| 1:cA:433:HIS:O      | 1:cA:436:THR:HG22   | 2.10                     | 0.51              |
| 13:cB:801:PHO:HBB1  | 13:cB:801:PHO:HMB1  | 1.92                     | 0.51              |
| 14:aA:3119:CL7:HMB2 | 14:aA:3140:CL7:H61C | 1.93                     | 0.51              |
| 14:bA:3141:CL7:H202 | 14:bA:3142:CL7:HBA1 | 1.93                     | 0.51              |
| 1:aA:282:LEU:HB2    | 1:aA:516:LEU:HD13   | 1.92                     | 0.51              |
| 2:aB:188:LEU:O      | 2:aB:191:THR:OG1    | 2.23                     | 0.51              |
| 1:bA:682:ALA:HB3    | 13:bB:801:PHO:HBB2  | 1.92                     | 0.51              |
| 14:cB:807:CL7:HBC2  | 14:cB:807:CL7:HHH   | 1.92                     | 0.51              |
| 14:aA:3116:CL7:HMA1 | 9:aK:64:ALA:HB2     | 1.92                     | 0.51              |
| 1:aA:330:LYS:O      | 14:aA:3134:CL7:HBC3 | 2.10                     | 0.51              |
| 2:bB:136:TYR:OH     | 11:bM:7:GLN:O       | 2.25                     | 0.51              |
| 2:bB:664:PHE:CB     | 13:bB:805:PHO:HMC2  | 2.41                     | 0.51              |
| 14:cB:816:CL7:H2    | 14:cB:832:CL7:H192  | 1.93                     | 0.51              |
| 1:aA:366:ILE:HG23   | 1:aA:370:HIS:CE1    | 2.46                     | 0.51              |
| 2:aB:140:VAL:HG13   | 11:aM:14:VAL:HG21   | 1.92                     | 0.51              |
| 2:aB:387:PHE:CZ     | 14:aB:3016:CL7:HAB  | 2.43                     | 0.51              |
| 3:aC:38:GLN:HG2     | 4:aD:107:SER:HB2    | 1.92                     | 0.51              |
| 1:cA:282:LEU:HB2    | 1:cA:516:LEU:HD13   | 1.92                     | 0.51              |
| 1:bA:389:ASN:OD1    | 1:bA:746:LEU:HD21   | 2.10                     | 0.51              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 13:bB:805:PHO:CMB   | 13:bB:805:PHO:HBB1  | 2.41                     | 0.51              |
| 14:bB:808:CL7:NC    | 14:bB:808:CL7:H2    | 2.26                     | 0.51              |
| 3:bC:15:THR:HA      | 3:bC:28:MET:HE3     | 1.91                     | 0.51              |
| 1:aA:388:LEU:HD22   | 1:aA:612:PHE:CE1    | 2.46                     | 0.51              |
| 1:bA:203:ILE:HG12   | 1:bA:306:ILE:HA     | 1.93                     | 0.51              |
| 2:cB:627:LEU:O      | 2:cB:631:SER:OG     | 2.26                     | 0.51              |
| 14:cB:808:CL7:NC    | 14:cB:808:CL7:H2    | 2.26                     | 0.51              |
| 2:aB:438:VAL:HG13   | 14:aB:3002:CL7:H61C | 1.93                     | 0.51              |
| 14:aB:3006:CL7:HBC2 | 14:aB:3006:CL7:HHD  | 1.92                     | 0.51              |
| 2:bB:664:PHE:HB3    | 13:bB:805:PHO:HMC2  | 1.92                     | 0.51              |
| 3:bC:7:ILE:HD12     | 3:bC:7:ILE:N        | 2.26                     | 0.51              |
| 14:cB:826:CL7:H161  | 10:cL:89:LEU:HD11   | 1.93                     | 0.51              |
| 1:cA:203:ILE:HG12   | 1:cA:306:ILE:HA     | 1.93                     | 0.51              |
| 2:cB:664:PHE:HB3    | 13:cB:805:PHO:HMC2  | 1.92                     | 0.51              |
| 1:aA:203:ILE:HG12   | 1:aA:306:ILE:HA     | 1.93                     | 0.50              |
| 2:bB:22:TRP:CG      | 2:bB:707:GLN:HE22   | 2.29                     | 0.50              |
| 6:bF:66:CYS:HB3     | 6:bF:73:PRO:HA      | 1.93                     | 0.50              |
| 1:cA:389:ASN:OD1    | 1:cA:746:LEU:HD21   | 2.10                     | 0.50              |
| 2:aB:22:TRP:CG      | 2:aB:707:GLN:HE22   | 2.30                     | 0.50              |
| 1:bA:366:ILE:HG23   | 1:bA:370:HIS:CE1    | 2.46                     | 0.50              |
| 1:cA:388:LEU:HD22   | 1:cA:612:PHE:CE1    | 2.46                     | 0.50              |
| 1:cA:655:GLN:HB3    | 1:cA:748:ARG:HD2    | 1.93                     | 0.50              |
| 1:aA:390:LEU:HD11   | 14:aA:3122:CL7:HED2 | 1.93                     | 0.50              |
| 1:bA:349:TRP:HB3    | 14:bA:3105:CL7:HAC1 | 1.93                     | 0.50              |
| 1:bA:724:GLN:O      | 1:bA:728:VAL:HG13   | 2.10                     | 0.50              |
| 2:bB:435:GLY:HA3    | 14:bB:822:CL7:HAB   | 1.93                     | 0.50              |
| 14:aB:3018:CL7:H91C | 14:aB:3018:CL7:HBC3 | 1.94                     | 0.50              |
| 2:bB:188:LEU:O      | 2:bB:191:THR:OG1    | 2.22                     | 0.50              |
| 2:cB:700:PRO:O      | 3:cC:81:TYR:OH      | 2.29                     | 0.50              |
| 1:bA:376:PRO:HG3    | 14:bA:3114:CL7:HBA1 | 1.93                     | 0.50              |
| 13:bB:801:PHO:H13   | 14:bB:803:CL7:H142  | 1.94                     | 0.50              |
| 1:cA:220:VAL:O      | 1:cA:224:VAL:HG23   | 2.12                     | 0.50              |
| 2:cB:75:GLU:O       | 2:cB:78:ILE:HG12    | 2.12                     | 0.50              |
| 14:bA:3128:CL7:H92C | 14:bA:3128:CL7:H51C | 1.91                     | 0.50              |
| 2:cB:22:TRP:CG      | 2:cB:707:GLN:HE22   | 2.29                     | 0.50              |
| 1:aA:389:ASN:HD21   | 1:aA:746:LEU:CD2    | 2.25                     | 0.50              |
| 1:aA:579:PRO:HD3    | 2:aB:564:GLY:HA2    | 1.94                     | 0.50              |
| 1:bA:579:PRO:HD3    | 2:bB:564:GLY:HA2    | 1.94                     | 0.50              |
| 14:bA:3113:CL7:HED2 | 14:bA:3114:CL7:O1A  | 2.12                     | 0.50              |
| 2:cB:690:LEU:HD11   | 10:cL:34:LEU:HD13   | 1.94                     | 0.50              |
| 1:aA:220:VAL:O      | 1:aA:224:VAL:HG23   | 2.12                     | 0.50              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:aA:484:SER:CB     | 14:aA:3129:CL7:HED2 | 2.41                     | 0.50              |
| 1:aA:704:TRP:CH2    | 2:aB:417:ALA:HB2    | 2.47                     | 0.50              |
| 3:aC:7:ILE:N        | 3:aC:7:ILE:HD12     | 2.26                     | 0.50              |
| 1:cA:366:ILE:HG23   | 1:cA:370:HIS:CE1    | 2.46                     | 0.50              |
| 1:cA:442:ASN:ND2    | 13:cB:805:PHO:HED2  | 2.26                     | 0.50              |
| 1:cA:682:ALA:HB3    | 13:cB:801:PHO:HBB2  | 1.94                     | 0.50              |
| 3:cC:7:ILE:N        | 3:cC:7:ILE:HD12     | 2.26                     | 0.50              |
| 2:aB:136:TYR:OH     | 11:aM:7:GLN:O       | 2.25                     | 0.50              |
| 1:bA:388:LEU:HD22   | 1:bA:612:PHE:CE1    | 2.46                     | 0.50              |
| 2:cB:53:HIS:ND1     | 14:cB:832:CL7:H3A   | 2.20                     | 0.50              |
| 2:cB:120:LEU:HD21   | 14:cB:833:CL7:HBA2  | 1.93                     | 0.50              |
| 2:cB:234:ALA:HB2    | 14:cB:814:CL7:HMA2  | 1.92                     | 0.50              |
| 1:aA:225:ASN:ND2    | 1:aA:291:MET:SD     | 2.85                     | 0.49              |
| 2:bB:75:GLU:O       | 2:bB:78:ILE:HG12    | 2.12                     | 0.49              |
| 14:cA:3118:CL7:HMB3 | 14:cA:3139:CL7:H52C | 1.93                     | 0.49              |
| 2:cB:698:ASP:OD2    | 7:cI:31:GLU:OE2     | 2.30                     | 0.49              |
| 14:aA:3124:CL7:H2   | 14:aL:203:CL7:H43C  | 1.94                     | 0.49              |
| 2:aB:518:GLY:O      | 2:aB:522:VAL:HG23   | 2.12                     | 0.49              |
| 6:aF:66:CYS:HB3     | 6:aF:73:PRO:HA      | 1.93                     | 0.49              |
| 2:bB:518:GLY:O      | 2:bB:522:VAL:HG23   | 2.12                     | 0.49              |
| 14:cA:3131:CL7:HAB  | 17:cA:3143:PQN:H172 | 1.94                     | 0.49              |
| 1:aA:672:ILE:HD11   | 2:aB:442:THR:HA     | 1.93                     | 0.49              |
| 1:bA:220:VAL:O      | 1:bA:224:VAL:HG23   | 2.12                     | 0.49              |
| 1:bA:225:ASN:ND2    | 1:bA:291:MET:SD     | 2.85                     | 0.49              |
| 1:bA:329:HIS:O      | 1:bA:338:HIS:HD2    | 1.95                     | 0.49              |
| 1:bA:655:GLN:HB3    | 1:bA:748:ARG:HD2    | 1.93                     | 0.49              |
| 2:bB:678:ILE:HD11   | 17:bB:828:PQN:H142  | 1.94                     | 0.49              |
| 2:bB:698:ASP:OD2    | 7:bI:31:GLU:OE2     | 2.30                     | 0.49              |
| 14:bB:807:CL7:HBC2  | 14:bB:807:CL7:HHD   | 1.92                     | 0.49              |
| 1:cA:329:HIS:O      | 1:cA:338:HIS:HD2    | 1.95                     | 0.49              |
| 1:cA:579:PRO:HD3    | 2:cB:564:GLY:HA2    | 1.94                     | 0.49              |
| 1:cA:696:GLN:HB3    | 2:cB:549:LEU:HD22   | 1.94                     | 0.49              |
| 14:cB:807:CL7:HBA2  | 14:cB:807:CL7:HBD   | 1.95                     | 0.49              |
| 1:aA:329:HIS:O      | 1:aA:338:HIS:HD2    | 1.95                     | 0.49              |
| 1:aA:655:GLN:HB3    | 1:aA:748:ARG:HD2    | 1.93                     | 0.49              |
| 2:aB:136:TYR:HB2    | 11:aM:3:LEU:HD11    | 1.94                     | 0.49              |
| 14:aB:3019:CL7:H41C | 14:aB:3030:CL7:HBC3 | 1.93                     | 0.49              |
| 1:bA:578:GLY:HA2    | 2:bB:565:PRO:HD3    | 1.95                     | 0.49              |
| 1:cA:217:LEU:HD23   | 1:cA:295:ALA:HA     | 1.94                     | 0.49              |
| 2:aB:75:GLU:O       | 2:aB:78:ILE:HG12    | 2.12                     | 0.49              |
| 2:aB:698:ASP:OD2    | 7:aI:31:GLU:OE2     | 2.30                     | 0.49              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:cA:546:VAL:HG11   | 1:cA:599:TRP:CE2    | 2.48                     | 0.49              |
| 1:aA:578:GLY:HA2    | 2:aB:565:PRO:HD3    | 1.95                     | 0.49              |
| 1:bA:546:VAL:HG11   | 1:bA:599:TRP:CE2    | 2.47                     | 0.49              |
| 1:cA:225:ASN:ND2    | 1:cA:291:MET:SD     | 2.85                     | 0.49              |
| 14:cA:3124:CL7:HMB1 | 15:cL:202:UNL:C35   | 2.42                     | 0.49              |
| 1:aA:577:ASP:OD2    | 1:aA:581:ARG:NH2    | 2.42                     | 0.49              |
| 14:aA:3117:CL7:H2A  | 14:aA:3117:CL7:HED3 | 1.93                     | 0.49              |
| 1:bA:577:ASP:OD2    | 1:bA:581:ARG:NH2    | 2.42                     | 0.49              |
| 1:cA:389:ASN:HD21   | 1:cA:746:LEU:CD2    | 2.25                     | 0.49              |
| 3:cC:5:VAL:HG13     | 3:cC:67:VAL:HG22    | 1.95                     | 0.49              |
| 1:aA:546:VAL:HG11   | 1:aA:599:TRP:CE2    | 2.48                     | 0.49              |
| 14:aA:3107:CL7:HMA3 | 14:aA:3107:CL7:H102 | 1.95                     | 0.49              |
| 2:aB:268:LEU:HD13   | 14:aB:3014:CL7:HMA2 | 1.94                     | 0.49              |
| 1:bA:389:ASN:HD21   | 1:bA:746:LEU:CD2    | 2.25                     | 0.49              |
| 1:bA:442:ASN:ND2    | 13:bB:805:PHO:HED2  | 2.27                     | 0.49              |
| 2:cB:518:GLY:O      | 2:cB:522:VAL:HG23   | 2.12                     | 0.49              |
| 2:bB:136:TYR:HB2    | 11:bM:3:LEU:HD11    | 1.95                     | 0.49              |
| 10:bL:68:ILE:HD12   | 10:bL:73:MET:HB3    | 1.94                     | 0.49              |
| 1:cA:578:GLY:HA2    | 2:cB:565:PRO:HD3    | 1.94                     | 0.49              |
| 2:cB:374:HIS:NE2    | 2:cB:378:ILE:HD12   | 2.28                     | 0.49              |
| 6:cF:66:CYS:HB3     | 6:cF:73:PRO:HA      | 1.93                     | 0.49              |
| 1:aA:696:GLN:HB3    | 2:aB:549:LEU:HD22   | 1.94                     | 0.49              |
| 14:aA:3123:CL7:H42C | 14:aL:203:CL7:C14   | 2.42                     | 0.49              |
| 14:aB:3007:CL7:H71C | 14:aB:3007:CL7:H111 | 1.54                     | 0.49              |
| 14:aB:3007:CL7:NC   | 14:aB:3007:CL7:H2   | 2.27                     | 0.49              |
| 14:bA:3116:CL7:H2A  | 14:bA:3116:CL7:HED3 | 1.94                     | 0.49              |
| 14:bA:3123:CL7:HMD3 | 10:bL:21:VAL:HG21   | 1.95                     | 0.49              |
| 2:bB:639:THR:HB     | 2:bB:640:PRO:HD2    | 1.95                     | 0.49              |
| 13:bB:805:PHO:HBB1  | 13:bB:805:PHO:HMB1  | 1.95                     | 0.49              |
| 2:cB:191:THR:HG22   | 2:cB:277:HIS:HB2    | 1.95                     | 0.49              |
| 2:aB:191:THR:HG22   | 2:aB:277:HIS:HB2    | 1.95                     | 0.48              |
| 2:bB:597:PHE:HA     | 14:bB:823:CL7:HBC3  | 1.94                     | 0.48              |
| 1:cA:704:TRP:CH2    | 2:cB:417:ALA:HB2    | 2.48                     | 0.48              |
| 2:aB:450:GLU:HG2    | 6:aF:58:PHE:CZ      | 2.48                     | 0.48              |
| 2:aB:639:THR:HB     | 2:aB:640:PRO:HD2    | 1.95                     | 0.48              |
| 14:aB:3003:CL7:OBB  | 14:aB:3003:CL7:HHC  | 2.12                     | 0.48              |
| 1:bA:696:GLN:HB3    | 2:bB:549:LEU:HD22   | 1.94                     | 0.48              |
| 2:cB:639:THR:HB     | 2:cB:640:PRO:HD2    | 1.95                     | 0.48              |
| 14:cL:203:CL7:H152  | 14:cL:203:CL7:H18   | 1.62                     | 0.48              |
| 1:aA:217:LEU:HD23   | 1:aA:295:ALA:HA     | 1.94                     | 0.48              |
| 2:cB:450:GLU:HG2    | 6:cF:58:PHE:CZ      | 2.47                     | 0.48              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:aA:597:LEU:HD13   | 1:aA:730:LEU:HD21   | 1.95                     | 0.48              |
| 10:bL:68:ILE:HD11   | 10:bL:77:SER:HB2    | 1.94                     | 0.48              |
| 1:cA:202:LEU:O      | 1:cA:202:LEU:HD23   | 2.14                     | 0.48              |
| 14:cA:3125:CL7:H171 | 14:cL:204:CL7:HMB1  | 1.94                     | 0.48              |
| 2:cB:374:HIS:CE1    | 2:cB:378:ILE:CD1    | 2.97                     | 0.48              |
| 2:cB:664:PHE:CB     | 13:cB:805:PHO:HMC2  | 2.42                     | 0.48              |
| 10:cL:68:ILE:HD12   | 10:cL:73:MET:HB3    | 1.95                     | 0.48              |
| 2:aB:374:HIS:CE1    | 2:aB:378:ILE:CD1    | 2.96                     | 0.48              |
| 2:aB:374:HIS:NE2    | 2:aB:378:ILE:HD12   | 2.28                     | 0.48              |
| 10:aL:68:ILE:HD12   | 10:aL:73:MET:HB3    | 1.94                     | 0.48              |
| 2:bB:374:HIS:CE1    | 2:bB:378:ILE:CD1    | 2.96                     | 0.48              |
| 10:aL:68:ILE:HD11   | 10:aL:77:SER:HB2    | 1.94                     | 0.48              |
| 1:bA:484:SER:CB     | 14:bA:3128:CL7:HED2 | 2.44                     | 0.48              |
| 2:bB:453:ILE:HD11   | 14:bB:822:CL7:CHB   | 2.44                     | 0.48              |
| 14:cB:804:CL7:OBB   | 14:cB:804:CL7:HHC   | 2.13                     | 0.48              |
| 3:aC:5:VAL:HG13     | 3:aC:67:VAL:HG22    | 1.95                     | 0.48              |
| 2:bB:334:LEU:HD21   | 14:bB:820:CL7:C2B   | 2.44                     | 0.48              |
| 2:cB:118:SER:O      | 2:cB:120:LEU:N      | 2.44                     | 0.48              |
| 2:cB:721:TYR:HE2    | 19:cB:830:LMG:H402  | 1.79                     | 0.48              |
| 14:cB:833:CL7:HBA1  | 14:cB:833:CL7:H3A   | 1.63                     | 0.48              |
| 2:aB:60:TRP:HD1     | 14:aB:3007:CL7:H171 | 1.78                     | 0.48              |
| 14:aB:3019:CL7:HMA1 | 14:aB:3031:CL7:HBC2 | 1.96                     | 0.48              |
| 4:bD:19:LEU:HB3     | 4:bD:23:ALA:CB      | 2.43                     | 0.48              |
| 1:cA:597:LEU:HD13   | 1:cA:730:LEU:HD21   | 1.96                     | 0.48              |
| 1:cA:672:ILE:HD11   | 2:cB:442:THR:HA     | 1.94                     | 0.48              |
| 10:cL:68:ILE:HD11   | 10:cL:77:SER:HB2    | 1.95                     | 0.48              |
| 1:bA:217:LEU:HD23   | 1:bA:295:ALA:HA     | 1.95                     | 0.48              |
| 14:bB:826:CL7:H161  | 10:bL:89:LEU:HD11   | 1.96                     | 0.48              |
| 2:cB:59:LEU:HB3     | 14:cB:807:CL7:H91C  | 1.94                     | 0.48              |
| 2:cB:690:LEU:HD11   | 10:cL:34:LEU:CD1    | 2.44                     | 0.48              |
| 1:cA:116:HIS:HB3    | 1:cA:138:VAL:HB     | 1.96                     | 0.48              |
| 14:aA:3126:CL7:H171 | 14:aL:203:CL7:HMB1  | 1.95                     | 0.47              |
| 14:aB:3007:CL7:H152 | 14:aB:3007:CL7:HBA2 | 1.96                     | 0.47              |
| 11:aM:25:LEU:HD12   | 11:aM:25:LEU:O      | 2.14                     | 0.47              |
| 1:bA:443:TRP:CD1    | 14:bA:3124:CL7:HED2 | 2.49                     | 0.47              |
| 2:bB:700:PRO:O      | 3:bC:81:TYR:OH      | 2.29                     | 0.47              |
| 14:cA:3141:CL7:H192 | 14:cA:3141:CL7:H161 | 1.72                     | 0.47              |
| 14:aA:3133:CL7:H13  | 14:aB:3025:CL7:H12C | 1.96                     | 0.47              |
| 2:aB:344:ILE:O      | 2:aB:347:VAL:HG22   | 2.15                     | 0.47              |
| 3:aC:6:LYS:HG3      | 4:aD:138:TYR:HB2    | 1.96                     | 0.47              |
| 14:cA:3140:CL7:H162 | 14:cA:3140:CL7:H141 | 1.64                     | 0.47              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:cB:453:ILE:HD11   | 14:cB:822:CL7:CHB   | 2.44                     | 0.47              |
| 2:aB:46:ILE:CG2     | 2:aB:50:HIS:CE1     | 2.98                     | 0.47              |
| 14:aB:3006:CL7:HBA2 | 14:aB:3006:CL7:HBD  | 1.96                     | 0.47              |
| 4:aD:19:LEU:HB3     | 4:aD:23:ALA:CB      | 2.43                     | 0.47              |
| 1:bA:704:TRP:CH2    | 2:bB:417:ALA:HB2    | 2.48                     | 0.47              |
| 1:cA:586:GLN:HA     | 1:cA:591:ASP:CG     | 2.39                     | 0.47              |
| 2:cB:377:TYR:CD2    | 14:cB:819:CL7:HAB   | 2.49                     | 0.47              |
| 1:aA:116:HIS:HB3    | 1:aA:138:VAL:HB     | 1.96                     | 0.47              |
| 1:aA:586:GLN:HA     | 1:aA:591:ASP:CG     | 2.39                     | 0.47              |
| 2:aB:422:LEU:HD13   | 2:aB:535:LEU:HA     | 1.96                     | 0.47              |
| 2:bB:450:GLU:HG2    | 6:bF:58:PHE:CZ      | 2.48                     | 0.47              |
| 11:bM:25:LEU:O      | 11:bM:25:LEU:HD12   | 2.14                     | 0.47              |
| 2:cB:136:TYR:HB2    | 11:cM:3:LEU:HD11    | 1.96                     | 0.47              |
| 2:cB:334:LEU:HD21   | 14:cB:820:CL7:C2B   | 2.44                     | 0.47              |
| 2:aB:60:TRP:CD1     | 14:aB:3007:CL7:H171 | 2.49                     | 0.47              |
| 3:bC:5:VAL:HG13     | 3:bC:67:VAL:HG22    | 1.95                     | 0.47              |
| 1:cA:376:PRO:HG3    | 14:cA:3114:CL7:HBA1 | 1.97                     | 0.47              |
| 1:bA:116:HIS:HB3    | 1:bA:138:VAL:HB     | 1.95                     | 0.47              |
| 1:bA:417:TYR:CD2    | 1:bA:559:ARG:HD2    | 2.50                     | 0.47              |
| 14:bB:804:CL7:HHC   | 14:bB:804:CL7:OBB   | 2.13                     | 0.47              |
| 1:cA:735:LEU:HD22   | 14:cA:3142:CL7:HMA1 | 1.96                     | 0.47              |
| 1:aA:365:ILE:HG23   | 1:aA:395:MET:HE1    | 1.97                     | 0.47              |
| 1:aA:417:TYR:CD2    | 1:aA:559:ARG:HD2    | 2.50                     | 0.47              |
| 3:aC:65:ILE:HG23    | 3:aC:65:ILE:O       | 2.15                     | 0.47              |
| 1:bA:586:GLN:HA     | 1:bA:591:ASP:CG     | 2.39                     | 0.47              |
| 2:bB:191:THR:HG22   | 2:bB:277:HIS:HB2    | 1.95                     | 0.47              |
| 2:bB:374:HIS:NE2    | 2:bB:378:ILE:HD12   | 2.28                     | 0.47              |
| 1:cA:302:ALA:O      | 1:cA:306:ILE:HG12   | 2.15                     | 0.47              |
| 14:cA:3115:CL7:HMA1 | 9:cK:64:ALA:HB2     | 1.96                     | 0.47              |
| 14:cA:3140:CL7:H18  | 14:cB:803:CL7:H121  | 1.96                     | 0.47              |
| 14:cA:3141:CL7:H162 | 14:cA:3141:CL7:H121 | 1.55                     | 0.47              |
| 3:cC:6:LYS:HG3      | 4:cD:138:TYR:HB2    | 1.96                     | 0.47              |
| 3:cC:65:ILE:O       | 3:cC:65:ILE:HG23    | 2.15                     | 0.47              |
| 1:aA:202:LEU:O      | 1:aA:202:LEU:HD23   | 2.14                     | 0.47              |
| 2:bB:383:ALA:O      | 2:bB:386:ALA:HB3    | 2.15                     | 0.47              |
| 14:bB:826:CL7:HAB   | 17:bB:828:PQN:H172  | 1.97                     | 0.47              |
| 2:cB:581:LEU:HB3    | 13:cB:801:PHO:HMD1  | 1.97                     | 0.47              |
| 1:aA:575:PRO:HB3    | 1:aA:722:ILE:HB     | 1.97                     | 0.47              |
| 2:aB:344:ILE:O      | 2:aB:348:VAL:HG23   | 2.15                     | 0.47              |
| 10:aL:20:PRO:O      | 10:aL:24:SER:HB3    | 2.15                     | 0.47              |
| 10:bL:20:PRO:O      | 10:bL:24:SER:HB3    | 2.15                     | 0.47              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:aA:302:ALA:O      | 1:aA:306:ILE:HG12   | 2.15                     | 0.47              |
| 1:aA:430:MET:HA     | 1:aA:433:HIS:HE1    | 1.80                     | 0.47              |
| 13:aA:3102:PHO:HMD1 | 2:aB:581:LEU:HB3    | 1.96                     | 0.47              |
| 1:bA:202:LEU:HD23   | 1:bA:202:LEU:O      | 2.14                     | 0.47              |
| 1:cA:118:VAL:HG11   | 1:cA:127:LEU:HB2    | 1.97                     | 0.47              |
| 1:cA:334:THR:CB     | 16:cA:3138:LHG:HC2  | 2.45                     | 0.47              |
| 1:cA:365:ILE:HG23   | 1:cA:395:MET:HE1    | 1.97                     | 0.47              |
| 14:aB:3025:CL7:H41C | 14:aB:3025:CL7:H62C | 1.75                     | 0.46              |
| 14:aL:202:CL7:C1B   | 14:aL:203:CL7:HED1  | 2.45                     | 0.46              |
| 1:bA:585:CYS:HB2    | 2:bB:670:TRP:HB3    | 1.97                     | 0.46              |
| 1:bA:597:LEU:HD13   | 1:bA:730:LEU:HD21   | 1.96                     | 0.46              |
| 1:cA:417:TYR:CD2    | 1:cA:559:ARG:HD2    | 2.50                     | 0.46              |
| 14:cA:3142:CL7:H41C | 14:cA:3142:CL7:H62C | 1.40                     | 0.46              |
| 2:aB:383:ALA:O      | 2:aB:386:ALA:HB3    | 2.15                     | 0.46              |
| 3:bC:6:LYS:HG3      | 4:bD:138:TYR:HB2    | 1.96                     | 0.46              |
| 14:aA:3126:CL7:H162 | 14:aA:3129:CL7:H193 | 1.96                     | 0.46              |
| 14:aA:3141:CL7:H91C | 14:aB:3002:CL7:H193 | 1.96                     | 0.46              |
| 1:bA:129:ALA:O      | 1:bA:136:ARG:HA     | 2.16                     | 0.46              |
| 1:bA:334:THR:CB     | 16:bA:3138:LHG:HC2  | 2.45                     | 0.46              |
| 2:bB:46:ILE:CG2     | 2:bB:50:HIS:CE1     | 2.98                     | 0.46              |
| 14:cA:3123:CL7:O1A  | 10:cL:21:VAL:HG12   | 2.14                     | 0.46              |
| 14:cB:810:CL7:H62C  | 14:cB:810:CL7:H93C  | 1.58                     | 0.46              |
| 10:cL:57:TYR:CD1    | 10:cL:57:TYR:C      | 2.93                     | 0.46              |
| 1:aA:442:ASN:HD22   | 2:aB:677:LEU:HD11   | 1.80                     | 0.46              |
| 2:aB:3:THR:N        | 2:aB:13:ALA:O       | 2.49                     | 0.46              |
| 1:bA:302:ALA:O      | 1:bA:306:ILE:HG12   | 2.15                     | 0.46              |
| 2:bB:92:TRP:CZ3     | 7:bI:11:THR:HB      | 2.51                     | 0.46              |
| 2:bB:422:LEU:HD13   | 2:bB:535:LEU:HA     | 1.96                     | 0.46              |
| 1:cA:442:ASN:HD22   | 2:cB:677:LEU:HD11   | 1.79                     | 0.46              |
| 2:cB:666:PHE:CZ     | 14:cB:827:CL7:HBC3  | 2.50                     | 0.46              |
| 1:aA:129:ALA:O      | 1:aA:136:ARG:HA     | 2.15                     | 0.46              |
| 1:bA:698:LEU:HD21   | 13:bB:801:PHO:HED2  | 1.96                     | 0.46              |
| 14:bA:3106:CL7:H3A  | 14:bA:3141:CL7:CAB  | 2.45                     | 0.46              |
| 2:cB:92:TRP:CZ3     | 7:cI:11:THR:HB      | 2.51                     | 0.46              |
| 2:cB:344:ILE:O      | 2:cB:348:VAL:HG23   | 2.16                     | 0.46              |
| 11:cM:25:LEU:HD12   | 11:cM:25:LEU:O      | 2.14                     | 0.46              |
| 1:aA:341:LEU:HA     | 1:aA:344:VAL:HG22   | 1.98                     | 0.46              |
| 1:aA:570:LEU:HD21   | 3:aC:53:ARG:NH1     | 2.31                     | 0.46              |
| 14:aA:3107:CL7:H92C | 16:aA:3138:LHG:H332 | 1.98                     | 0.46              |
| 2:aB:453:ILE:HD11   | 14:aB:3021:CL7:CHB  | 2.46                     | 0.46              |
| 10:aL:17:LEU:O      | 10:aL:19:THR:HG23   | 2.15                     | 0.46              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:bA:430:MET:HA     | 1:bA:433:HIS:HE1    | 1.81                     | 0.46              |
| 14:bA:3122:CL7:H42C | 14:bL:204:CL7:C14   | 2.46                     | 0.46              |
| 14:bB:819:CL7:H3A   | 14:bB:819:CL7:HBA1  | 1.68                     | 0.46              |
| 3:bC:65:ILE:HG23    | 3:bC:65:ILE:O       | 2.15                     | 0.46              |
| 1:cA:129:ALA:O      | 1:cA:136:ARG:HA     | 2.15                     | 0.46              |
| 1:cA:683:PHE:CE1    | 1:cA:686:MET:CE     | 2.98                     | 0.46              |
| 2:cB:384:ILE:HD11   | 2:cB:582:ALA:CB     | 2.46                     | 0.46              |
| 2:aB:92:TRP:CZ3     | 7:aI:11:THR:HB      | 2.51                     | 0.46              |
| 2:aB:682:VAL:HG11   | 3:aC:81:TYR:CG      | 2.51                     | 0.46              |
| 1:bA:575:PRO:HB3    | 1:bA:722:ILE:HB     | 1.97                     | 0.46              |
| 2:bB:344:ILE:O      | 2:bB:347:VAL:HG22   | 2.15                     | 0.46              |
| 1:cA:439:SER:HB2    | 2:cB:684:ALA:HB2    | 1.98                     | 0.46              |
| 13:cB:801:PHO:H93   | 13:cB:801:PHO:H61   | 1.73                     | 0.46              |
| 10:cL:20:PRO:O      | 10:cL:24:SER:HB3    | 2.15                     | 0.46              |
| 1:aA:439:SER:HB2    | 2:aB:684:ALA:HB2    | 1.97                     | 0.46              |
| 1:aA:443:TRP:CD1    | 14:aA:3125:CL7:HED2 | 2.51                     | 0.46              |
| 2:aB:550:MET:HE2    | 2:aB:556:PHE:CD1    | 2.51                     | 0.46              |
| 1:bA:118:VAL:HG11   | 1:bA:127:LEU:HB2    | 1.97                     | 0.46              |
| 1:bA:365:ILE:HG23   | 1:bA:395:MET:HE1    | 1.97                     | 0.46              |
| 2:bB:387:PHE:CZ     | 14:bB:817:CL7:HAB   | 2.51                     | 0.46              |
| 2:bB:650:ALA:O      | 2:bB:653:PHE:HB3    | 2.16                     | 0.46              |
| 1:cA:443:TRP:CD1    | 14:cA:3124:CL7:HED2 | 2.51                     | 0.46              |
| 1:cA:575:PRO:HB3    | 1:cA:722:ILE:HB     | 1.97                     | 0.46              |
| 14:cA:3106:CL7:H3A  | 14:cA:3141:CL7:CAB  | 2.45                     | 0.46              |
| 2:cB:46:ILE:CG2     | 2:cB:50:HIS:CE1     | 2.98                     | 0.46              |
| 2:cB:383:ALA:O      | 2:cB:386:ALA:HB3    | 2.15                     | 0.46              |
| 2:cB:387:PHE:CZ     | 14:cB:817:CL7:HAB   | 2.50                     | 0.46              |
| 4:cD:97:HIS:HB3     | 4:cD:98:PRO:HD3     | 1.98                     | 0.46              |
| 1:aA:683:PHE:CE1    | 1:aA:686:MET:CE     | 2.99                     | 0.46              |
| 2:aB:384:ILE:HD11   | 2:aB:582:ALA:CB     | 2.46                     | 0.46              |
| 2:aB:700:PRO:O      | 3:aC:81:TYR:OH      | 2.28                     | 0.46              |
| 14:aB:3023:CL7:H61C | 14:aB:3023:CL7:H41C | 1.82                     | 0.46              |
| 10:bL:30:TRP:CZ2    | 14:bL:203:CL7:HAB   | 2.51                     | 0.46              |
| 1:cA:570:LEU:HD21   | 3:cC:53:ARG:NH1     | 2.31                     | 0.46              |
| 2:cB:550:MET:HE2    | 2:cB:556:PHE:CD1    | 2.51                     | 0.46              |
| 14:cB:826:CL7:H93C  | 15:cI:101:UNL:C38   | 2.46                     | 0.46              |
| 1:aA:426:VAL:HG23   | 14:aA:3140:CL7:HBC3 | 1.97                     | 0.46              |
| 2:aB:50:HIS:HD2     | 14:aB:3031:CL7:HAA2 | 1.80                     | 0.46              |
| 2:aB:59:LEU:HB3     | 14:aB:3006:CL7:H91C | 1.98                     | 0.46              |
| 2:aB:147:ALA:HB2    | 11:aM:18:PRO:HD3    | 1.98                     | 0.46              |
| 2:aB:334:LEU:HD21   | 14:aB:3019:CL7:C2B  | 2.46                     | 0.46              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:aB:519:ASP:OD1    | 2:aB:596:TYR:OH     | 2.33                     | 0.46              |
| 1:bA:357:LEU:HD22   | 1:bA:401:LEU:HD22   | 1.98                     | 0.46              |
| 1:bA:360:TRP:HZ3    | 14:bA:3114:CL7:H13  | 1.81                     | 0.46              |
| 2:bB:3:THR:N        | 2:bB:13:ALA:O       | 2.49                     | 0.46              |
| 2:bB:550:MET:HE2    | 2:bB:556:PHE:CD1    | 2.51                     | 0.46              |
| 6:bF:91:GLY:HA2     | 14:bF:201:CL7:HMC2  | 1.98                     | 0.46              |
| 1:aA:599:TRP:HE1    | 13:aB:3004:PHO:C1D  | 2.29                     | 0.45              |
| 14:aB:3005:CL7:H122 | 14:aB:3005:CL7:H162 | 1.73                     | 0.45              |
| 4:aD:97:HIS:HB3     | 4:aD:98:PRO:HD3     | 1.98                     | 0.45              |
| 1:bA:439:SER:HB2    | 2:bB:684:ALA:HB2    | 1.98                     | 0.45              |
| 14:bA:3128:CL7:H162 | 14:bA:3128:CL7:H122 | 1.41                     | 0.45              |
| 14:bB:807:CL7:HBA2  | 14:bB:807:CL7:HBD   | 1.98                     | 0.45              |
| 2:cB:422:LEU:HD13   | 2:cB:535:LEU:HA     | 1.97                     | 0.45              |
| 2:cB:650:ALA:O      | 2:cB:653:PHE:HB3    | 2.16                     | 0.45              |
| 13:aB:3004:PHO:CMB  | 13:aB:3004:PHO:HBB1 | 2.45                     | 0.45              |
| 1:bA:722:ILE:HD13   | 2:bB:571:CYS:SG     | 2.57                     | 0.45              |
| 2:bB:344:ILE:O      | 2:bB:348:VAL:HG23   | 2.15                     | 0.45              |
| 2:bB:384:ILE:HD11   | 2:bB:582:ALA:CB     | 2.46                     | 0.45              |
| 1:cA:585:CYS:HB2    | 2:cB:670:TRP:HB3    | 1.97                     | 0.45              |
| 2:cB:188:LEU:O      | 2:cB:191:THR:OG1    | 2.22                     | 0.45              |
| 14:cB:826:CL7:H51C  | 14:cB:826:CL7:H8    | 1.66                     | 0.45              |
| 6:cF:142:TRP:N      | 6:cF:143:PRO:CD     | 2.80                     | 0.45              |
| 14:cL:203:CL7:C1B   | 14:cL:204:CL7:HED1  | 2.46                     | 0.45              |
| 1:aA:365:ILE:HG13   | 1:aA:398:GLY:HA3    | 1.99                     | 0.45              |
| 14:aB:3025:CL7:H51C | 14:aB:3025:CL7:H8   | 1.64                     | 0.45              |
| 10:aL:30:TRP:CZ2    | 14:aL:202:CL7:HAB   | 2.51                     | 0.45              |
| 2:bB:682:VAL:HG11   | 3:bC:81:TYR:CG      | 2.51                     | 0.45              |
| 1:aA:188:LEU:O      | 1:aA:192:GLN:HG2    | 2.17                     | 0.45              |
| 14:aB:3018:CL7:HBA1 | 14:aB:3018:CL7:H3A  | 1.61                     | 0.45              |
| 4:aD:88:LEU:N       | 4:aD:88:LEU:HD22    | 2.32                     | 0.45              |
| 6:aF:142:TRP:N      | 6:aF:143:PRO:CD     | 2.80                     | 0.45              |
| 1:bA:570:LEU:HD21   | 3:bC:53:ARG:NH1     | 2.31                     | 0.45              |
| 4:bD:97:HIS:HB3     | 4:bD:98:PRO:HD3     | 1.98                     | 0.45              |
| 1:cA:643:THR:O      | 1:cA:647:TRP:HD1    | 1.99                     | 0.45              |
| 2:cB:3:THR:N        | 2:cB:13:ALA:O       | 2.49                     | 0.45              |
| 2:cB:682:VAL:HG11   | 3:cC:81:TYR:CG      | 2.51                     | 0.45              |
| 4:cD:88:LEU:N       | 4:cD:88:LEU:HD22    | 2.32                     | 0.45              |
| 10:aL:140:ILE:HG13  | 15:aL:205:UNL:C22   | 2.47                     | 0.45              |
| 1:bA:672:ILE:HG23   | 14:bB:803:CL7:H71C  | 1.99                     | 0.45              |
| 14:bA:3132:CL7:H13  | 14:bB:826:CL7:H12C  | 1.97                     | 0.45              |
| 2:bB:91:ILE:HB      | 2:bB:112:PRO:HB2    | 1.99                     | 0.45              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:cA:341:LEU:HA     | 1:cA:344:VAL:HG22  | 1.98                     | 0.45              |
| 14:cA:3123:CL7:CMD  | 10:cL:21:VAL:HG21  | 2.47                     | 0.45              |
| 2:cB:572:ASP:HA     | 2:cB:577:ASP:CG    | 2.42                     | 0.45              |
| 1:aA:118:VAL:HG11   | 1:aA:127:LEU:HB2   | 1.97                     | 0.45              |
| 1:aA:214:THR:HG23   | 1:aA:298:HIS:HB3   | 1.99                     | 0.45              |
| 2:aB:572:ASP:HA     | 2:aB:577:ASP:CG    | 2.42                     | 0.45              |
| 6:aF:60:MET:HE1     | 8:aJ:46:ILE:HG23   | 1.99                     | 0.45              |
| 1:bA:188:LEU:O      | 1:bA:192:GLN:HG2   | 2.17                     | 0.45              |
| 1:bA:599:TRP:HE1    | 13:bB:805:PHO:C1D  | 2.29                     | 0.45              |
| 10:bL:35:PRO:HG3    | 14:bL:204:CL7:HED2 | 1.98                     | 0.45              |
| 1:cA:430:MET:HA     | 1:cA:433:HIS:HE1   | 1.80                     | 0.45              |
| 14:cB:804:CL7:H142  | 14:cB:804:CL7:H112 | 1.85                     | 0.45              |
| 1:aA:585:CYS:HB2    | 2:aB:670:TRP:HB3   | 1.98                     | 0.45              |
| 2:aB:650:ALA:O      | 2:aB:653:PHE:HB3   | 2.16                     | 0.45              |
| 2:bB:377:TYR:HD2    | 14:bB:819:CL7:HAB  | 1.82                     | 0.45              |
| 1:cA:214:THR:HG23   | 1:cA:298:HIS:HB3   | 1.99                     | 0.45              |
| 2:cB:550:MET:CE     | 2:cB:556:PHE:CD1   | 3.00                     | 0.45              |
| 3:cC:15:THR:O       | 3:cC:15:THR:CG2    | 2.63                     | 0.45              |
| 2:aB:31:PHE:CE2     | 2:aB:49:THR:HG21   | 2.52                     | 0.45              |
| 1:bA:365:ILE:HG13   | 1:bA:398:GLY:HA3   | 1.99                     | 0.45              |
| 1:bA:442:ASN:HD22   | 2:bB:677:LEU:HD11  | 1.81                     | 0.45              |
| 1:bA:533:ASP:O      | 1:bA:537:HIS:ND1   | 2.43                     | 0.45              |
| 1:bA:643:THR:O      | 1:bA:647:TRP:HD1   | 1.99                     | 0.45              |
| 1:bA:683:PHE:CE1    | 1:bA:686:MET:CE    | 2.98                     | 0.45              |
| 14:bA:3122:CL7:H42C | 14:bL:204:CL7:H142 | 1.99                     | 0.45              |
| 2:bB:60:TRP:CD1     | 14:bB:808:CL7:H171 | 2.52                     | 0.45              |
| 13:bB:805:PHO:H201  | 14:bB:827:CL7:H2   | 1.99                     | 0.45              |
| 14:bB:826:CL7:H93C  | 15:bI:101:UNL:C38  | 2.47                     | 0.45              |
| 4:bD:88:LEU:HD22    | 4:bD:88:LEU:N      | 2.32                     | 0.45              |
| 1:cA:599:TRP:HE1    | 13:cB:805:PHO:C1D  | 2.30                     | 0.45              |
| 2:cB:91:ILE:HB      | 2:cB:112:PRO:HB2   | 1.99                     | 0.45              |
| 11:cM:6:LEU:O       | 11:cM:10:ILE:HG12  | 2.17                     | 0.45              |
| 1:aA:533:ASP:O      | 1:aA:537:HIS:ND1   | 2.42                     | 0.45              |
| 2:aB:118:SER:O      | 2:aB:120:LEU:N     | 2.44                     | 0.45              |
| 2:aB:196:HIS:O      | 2:aB:200:PRO:HG2   | 2.17                     | 0.45              |
| 2:aB:366:VAL:HG23   | 2:aB:367:THR:N     | 2.32                     | 0.45              |
| 5:aE:6:SER:O        | 5:aE:23:THR:HA     | 2.16                     | 0.45              |
| 14:bB:816:CL7:H2    | 14:bB:832:CL7:H192 | 1.98                     | 0.45              |
| 10:bL:140:ILE:HG13  | 15:bL:201:UNL:C22  | 2.47                     | 0.45              |
| 14:bL:203:CL7:H18   | 14:bL:203:CL7:H152 | 1.67                     | 0.45              |
| 1:cA:51:ASN:O       | 1:cA:55:LEU:HG     | 2.17                     | 0.45              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:cB:136:TYR:OH     | 11:cM:7:GLN:O       | 2.25                     | 0.45              |
| 14:cB:819:CL7:HBA1  | 14:cB:819:CL7:H3A   | 1.57                     | 0.45              |
| 14:aA:3107:CL7:H41C | 14:aA:3107:CL7:H62C | 1.81                     | 0.45              |
| 2:aB:91:ILE:HB      | 2:aB:112:PRO:HB2    | 1.99                     | 0.45              |
| 19:aB:3029:LMG:H352 | 19:aB:3029:LMG:H381 | 1.67                     | 0.45              |
| 1:bA:341:LEU:HA     | 1:bA:344:VAL:HG22   | 1.98                     | 0.45              |
| 6:bF:142:TRP:N      | 6:bF:143:PRO:CD     | 2.80                     | 0.45              |
| 1:cA:198:MET:HE2    | 1:cA:198:MET:HA     | 1.99                     | 0.45              |
| 2:cB:31:PHE:CE2     | 2:cB:49:THR:HG21    | 2.52                     | 0.45              |
| 2:cB:344:ILE:O      | 2:cB:347:VAL:HG22   | 2.16                     | 0.45              |
| 2:cB:678:ILE:HD11   | 17:cB:828:PQN:H142  | 1.98                     | 0.45              |
| 3:cC:21:CYS:SG      | 3:cC:24:ASP:N       | 2.90                     | 0.45              |
| 10:cL:35:PRO:HG3    | 14:cL:204:CL7:HED2  | 1.98                     | 0.45              |
| 1:aA:585:CYS:SG     | 2:aB:705:ILE:CD1    | 3.05                     | 0.44              |
| 1:bA:76:ALA:O       | 1:bA:77:HIS:C       | 2.60                     | 0.44              |
| 1:bA:214:THR:HG23   | 1:bA:298:HIS:HB3    | 1.99                     | 0.44              |
| 14:bA:3124:CL7:HAA2 | 15:bL:202:UNL:C17   | 2.47                     | 0.44              |
| 2:bB:31:PHE:CE2     | 2:bB:49:THR:HG21    | 2.52                     | 0.44              |
| 2:bB:733:ALA:N      | 2:bB:734:PRO:HD2    | 2.32                     | 0.44              |
| 11:bM:6:LEU:O       | 11:bM:10:ILE:HG12   | 2.17                     | 0.44              |
| 1:cA:585:CYS:SG     | 2:cB:705:ILE:CD1    | 3.05                     | 0.44              |
| 2:cB:196:HIS:O      | 2:cB:200:PRO:HG2    | 2.17                     | 0.44              |
| 14:cB:827:CL7:H93C  | 14:cB:827:CL7:H112  | 1.77                     | 0.44              |
| 1:aA:643:THR:O      | 1:aA:647:TRP:HD1    | 1.99                     | 0.44              |
| 2:aB:395:VAL:HG13   | 2:aB:544:ALA:HB1    | 1.99                     | 0.44              |
| 2:aB:597:PHE:HA     | 14:aB:3022:CL7:HBC3 | 1.99                     | 0.44              |
| 3:aC:15:THR:O       | 3:aC:15:THR:CG2     | 2.63                     | 0.44              |
| 1:bA:51:ASN:O       | 1:bA:55:LEU:HG      | 2.17                     | 0.44              |
| 2:bB:196:HIS:O      | 2:bB:200:PRO:HG2    | 2.17                     | 0.44              |
| 3:bC:21:CYS:SG      | 3:bC:24:ASP:N       | 2.90                     | 0.44              |
| 10:bL:104:PRO:HD2   | 10:bL:117:PHE:O     | 2.18                     | 0.44              |
| 17:cA:3143:PQN:H141 | 17:cA:3143:PQN:H161 | 1.65                     | 0.44              |
| 2:cB:395:VAL:HG13   | 2:cB:544:ALA:HB1    | 1.99                     | 0.44              |
| 2:cB:649:TRP:CE2    | 2:cB:729:ILE:HG21   | 2.52                     | 0.44              |
| 1:aA:624:ASN:HB3    | 1:aA:630:ASN:HD21   | 1.82                     | 0.44              |
| 1:aA:731:GLY:HA2    | 16:aA:3138:LHG:H352 | 1.99                     | 0.44              |
| 2:aB:550:MET:CE     | 2:aB:556:PHE:CD1    | 3.00                     | 0.44              |
| 2:aB:733:ALA:N      | 2:aB:734:PRO:HD2    | 2.32                     | 0.44              |
| 1:bA:585:CYS:SG     | 2:bB:705:ILE:CD1    | 3.06                     | 0.44              |
| 2:bB:120:LEU:HD21   | 14:bB:833:CL7:HBA2  | 1.98                     | 0.44              |
| 2:bB:395:VAL:HG13   | 2:bB:544:ALA:HB1    | 1.99                     | 0.44              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:cA:581:ARG:HG2    | 3:cC:49:VAL:HB      | 2.00                     | 0.44              |
| 2:cB:733:ALA:N      | 2:cB:734:PRO:HD2    | 2.32                     | 0.44              |
| 1:aA:76:ALA:O       | 1:aA:77:HIS:C       | 2.60                     | 0.44              |
| 8:aJ:21:ALA:N       | 8:aJ:22:PRO:HD2     | 2.33                     | 0.44              |
| 11:aM:6:LEU:O       | 11:aM:10:ILE:HG12   | 2.17                     | 0.44              |
| 2:bB:426:SER:HB3    | 2:bB:532:VAL:HG22   | 1.99                     | 0.44              |
| 1:cA:365:ILE:HG13   | 1:cA:398:GLY:HA3    | 1.98                     | 0.44              |
| 1:cA:624:ASN:HB3    | 1:cA:630:ASN:HD21   | 1.83                     | 0.44              |
| 14:cA:3103:CL7:C4C  | 8:cJ:22:PRO:HG3     | 2.48                     | 0.44              |
| 10:cL:140:ILE:HG13  | 15:cL:201:UNL:C22   | 2.47                     | 0.44              |
| 1:aA:51:ASN:O       | 1:aA:55:LEU:HG      | 2.17                     | 0.44              |
| 1:aA:198:MET:HE2    | 1:aA:198:MET:HA     | 2.00                     | 0.44              |
| 2:aB:649:TRP:CE2    | 2:aB:729:ILE:HG21   | 2.52                     | 0.44              |
| 13:aB:3004:PHO:H143 | 13:aB:3004:PHO:H161 | 1.78                     | 0.44              |
| 3:aC:21:CYS:SG      | 3:aC:24:ASP:N       | 2.90                     | 0.44              |
| 1:bA:581:ARG:HG2    | 3:bC:49:VAL:HB      | 2.00                     | 0.44              |
| 2:bB:65:LEU:CD1     | 2:bB:142:LEU:HD12   | 2.47                     | 0.44              |
| 10:bL:30:TRP:CH2    | 14:bL:203:CL7:HAB   | 2.53                     | 0.44              |
| 1:cA:76:ALA:O       | 1:cA:77:HIS:C       | 2.59                     | 0.44              |
| 2:cB:65:LEU:CD1     | 2:cB:142:LEU:HD12   | 2.48                     | 0.44              |
| 2:cB:106:GLN:HG3    | 2:cB:115:LEU:HD21   | 2.00                     | 0.44              |
| 14:aB:3009:CL7:H192 | 14:bL:203:CL7:H192  | 1.99                     | 0.44              |
| 3:aC:7:ILE:HG12     | 3:aC:40:ALA:HB3     | 2.00                     | 0.44              |
| 10:aL:104:PRO:HD2   | 10:aL:117:PHE:O     | 2.18                     | 0.44              |
| 1:bA:359:THR:HG22   | 14:bA:3120:CL7:H41C | 2.00                     | 0.44              |
| 14:bA:3141:CL7:H62C | 14:bA:3141:CL7:H93C | 1.67                     | 0.44              |
| 2:bB:59:LEU:HB3     | 14:bB:807:CL7:H91C  | 1.99                     | 0.44              |
| 2:cB:60:TRP:CD1     | 14:cB:808:CL7:H171  | 2.52                     | 0.44              |
| 2:cB:558:TYR:CD1    | 2:cB:575:ALA:HB3    | 2.53                     | 0.44              |
| 1:aA:357:LEU:HD22   | 1:aA:401:LEU:HD22   | 1.99                     | 0.44              |
| 1:aA:534:PHE:CE1    | 1:aA:538:HIS:CE1    | 3.06                     | 0.44              |
| 13:aB:3004:PHO:HBB1 | 13:aB:3004:PHO:HMB1 | 1.99                     | 0.44              |
| 10:aL:57:TYR:CD1    | 10:aL:57:TYR:C      | 2.93                     | 0.44              |
| 2:bB:550:MET:CE     | 2:bB:556:PHE:CD1    | 3.00                     | 0.44              |
| 14:bB:832:CL7:H143  | 14:bB:832:CL7:H112  | 1.88                     | 0.44              |
| 1:cA:357:LEU:HD22   | 1:cA:401:LEU:HD22   | 1.98                     | 0.44              |
| 8:cJ:21:ALA:N       | 8:cJ:22:PRO:HD2     | 2.33                     | 0.44              |
| 2:aB:92:TRP:CH2     | 7:aI:12:PRO:CG      | 3.01                     | 0.44              |
| 2:aB:426:SER:HB3    | 2:aB:532:VAL:HG22   | 1.99                     | 0.44              |
| 14:bA:3142:CL7:H8   | 13:bB:801:PHO:H151  | 2.00                     | 0.44              |
| 14:bA:3142:CL7:H92C | 17:bA:3143:PQN:H191 | 2.00                     | 0.44              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:bB:649:TRP:CE2    | 2:bB:729:ILE:HG21   | 2.52                     | 0.44              |
| 10:cL:104:PRO:HD2   | 10:cL:117:PHE:O     | 2.18                     | 0.44              |
| 14:aA:3121:CL7:HMB2 | 14:aA:3127:CL7:HAA1 | 2.00                     | 0.44              |
| 2:aB:678:ILE:HD11   | 17:aB:3027:PQN:H142 | 2.00                     | 0.44              |
| 14:aB:3032:CL7:H3A  | 14:aB:3032:CL7:HBA1 | 1.76                     | 0.44              |
| 4:aD:130:ILE:HG21   | 4:aD:135:LYS:O      | 2.18                     | 0.44              |
| 2:bB:92:TRP:CZ3     | 7:bI:12:PRO:HD3     | 2.53                     | 0.44              |
| 2:bB:147:ALA:HB2    | 11:bM:18:PRO:HD3    | 1.99                     | 0.44              |
| 6:bF:60:MET:HE1     | 8:bJ:46:ILE:HG23    | 1.99                     | 0.44              |
| 1:cA:749:ILE:HD12   | 1:cA:749:ILE:HA     | 1.88                     | 0.44              |
| 14:cB:820:CL7:HMA1  | 14:cB:832:CL7:HBC2  | 1.99                     | 0.44              |
| 4:cD:8:GLN:NE2      | 4:cD:53:GLU:O       | 2.51                     | 0.44              |
| 4:cD:130:ILE:O      | 4:cD:130:ILE:CG2    | 2.66                     | 0.44              |
| 1:aA:651:PHE:O      | 1:aA:655:GLN:HB2    | 2.18                     | 0.43              |
| 14:aA:3141:CL7:H91C | 14:aA:3141:CL7:H112 | 1.65                     | 0.43              |
| 2:bB:53:HIS:ND1     | 14:bB:832:CL7:H3A   | 2.19                     | 0.43              |
| 2:bB:558:TYR:CD1    | 2:bB:575:ALA:HB3    | 2.53                     | 0.43              |
| 14:bB:806:CL7:H3A   | 14:bB:820:CL7:CAB   | 2.48                     | 0.43              |
| 4:bD:35:SER:OG      | 4:bD:52:ASN:O       | 2.36                     | 0.43              |
| 4:bD:130:ILE:O      | 4:bD:130:ILE:CG2    | 2.66                     | 0.43              |
| 8:bJ:21:ALA:N       | 8:bJ:22:PRO:HD2     | 2.33                     | 0.43              |
| 1:cA:63:THR:HG22    | 1:cA:64:ASN:N       | 2.33                     | 0.43              |
| 2:cB:147:ALA:HB2    | 11:cM:18:PRO:HD3    | 1.99                     | 0.43              |
| 1:aA:63:THR:HG22    | 1:aA:64:ASN:N       | 2.33                     | 0.43              |
| 1:aA:581:ARG:HG2    | 3:aC:49:VAL:HB      | 2.00                     | 0.43              |
| 1:aA:585:CYS:SG     | 2:aB:705:ILE:HD13   | 2.58                     | 0.43              |
| 14:aA:3111:CL7:HED3 | 14:aA:3111:CL7:HBD  | 1.84                     | 0.43              |
| 2:aB:566:GLY:HA2    | 3:aC:56:THR:HG23    | 2.00                     | 0.43              |
| 14:bA:3106:CL7:H161 | 14:bA:3106:CL7:H193 | 1.54                     | 0.43              |
| 16:bA:3137:LHG:H252 | 16:bA:3137:LHG:H281 | 1.75                     | 0.43              |
| 17:bA:3143:PQN:H161 | 17:bA:3143:PQN:H141 | 1.65                     | 0.43              |
| 2:bB:572:ASP:HA     | 2:bB:577:ASP:CG     | 2.42                     | 0.43              |
| 4:bD:8:GLN:HG2      | 4:bD:55:GLU:O       | 2.18                     | 0.43              |
| 1:cA:188:LEU:O      | 1:cA:192:GLN:HG2    | 2.17                     | 0.43              |
| 2:cB:426:SER:HB3    | 2:cB:532:VAL:HG22   | 1.99                     | 0.43              |
| 14:cB:832:CL7:H122  | 14:cB:833:CL7:C3D   | 2.49                     | 0.43              |
| 1:aA:645:ASN:HB2    | 2:aB:638:TYR:OH     | 2.18                     | 0.43              |
| 14:aA:3108:CL7:H3A  | 14:aA:3108:CL7:HBA1 | 1.87                     | 0.43              |
| 2:aB:558:TYR:CD1    | 2:aB:575:ALA:HB3    | 2.53                     | 0.43              |
| 1:bA:534:PHE:CE1    | 1:bA:538:HIS:CE1    | 3.06                     | 0.43              |
| 14:bA:3129:CL7:OBB  | 14:bA:3129:CL7:HMB1 | 2.17                     | 0.43              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:bB:366:VAL:HG23   | 2:bB:367:THR:N      | 2.32                     | 0.43              |
| 2:bB:367:THR:HG22   | 2:bB:371:LEU:HD12   | 2.00                     | 0.43              |
| 14:bB:820:CL7:HMA1  | 14:bB:832:CL7:HBC2  | 2.00                     | 0.43              |
| 1:cA:123:GLY:HA2    | 6:cF:47:THR:HA      | 2.00                     | 0.43              |
| 1:cA:310:HIS:NE2    | 14:cA:3115:CL7:NB   | 2.66                     | 0.43              |
| 1:cA:460:ASP:OD2    | 1:cA:644:ILE:HB     | 2.19                     | 0.43              |
| 4:cD:8:GLN:HG2      | 4:cD:55:GLU:O       | 2.18                     | 0.43              |
| 5:cE:6:SER:O        | 5:cE:23:THR:HA      | 2.19                     | 0.43              |
| 14:aA:3124:CL7:O1A  | 10:aL:21:VAL:HG12   | 2.18                     | 0.43              |
| 14:aA:3142:CL7:H193 | 14:aA:3143:CL7:HHB  | 2.01                     | 0.43              |
| 2:aB:92:TRP:CH2     | 7:aI:12:PRO:HG3     | 2.53                     | 0.43              |
| 1:bA:198:MET:HA     | 1:bA:198:MET:HE2    | 1.99                     | 0.43              |
| 1:bA:651:PHE:O      | 1:bA:655:GLN:HB2    | 2.18                     | 0.43              |
| 1:cA:95:ALA:HB2     | 1:cA:144:LEU:HD21   | 1.99                     | 0.43              |
| 2:cB:92:TRP:CH2     | 7:cI:12:PRO:CG      | 3.01                     | 0.43              |
| 2:cB:522:VAL:HG13   | 14:cB:804:CL7:H141  | 2.01                     | 0.43              |
| 14:cB:804:CL7:H61C  | 14:cB:804:CL7:H102  | 1.73                     | 0.43              |
| 14:aA:3107:CL7:H193 | 14:aA:3107:CL7:H161 | 1.71                     | 0.43              |
| 2:aB:65:LEU:CD1     | 2:aB:142:LEU:HD12   | 2.47                     | 0.43              |
| 14:aB:3031:CL7:H121 | 14:aB:3031:CL7:H162 | 1.93                     | 0.43              |
| 1:bA:624:ASN:HB3    | 1:bA:630:ASN:HD21   | 1.82                     | 0.43              |
| 1:cA:585:CYS:SG     | 2:cB:705:ILE:HD13   | 2.58                     | 0.43              |
| 14:cA:3106:CL7:H192 | 14:cA:3106:CL7:H161 | 1.68                     | 0.43              |
| 2:cB:191:THR:CG2    | 2:cB:277:HIS:HB3    | 2.49                     | 0.43              |
| 1:aA:310:HIS:NE2    | 14:aA:3116:CL7:NB   | 2.66                     | 0.43              |
| 2:aB:106:GLN:HG3    | 2:aB:115:LEU:HD21   | 2.00                     | 0.43              |
| 4:aD:130:ILE:CG2    | 4:aD:130:ILE:O      | 2.66                     | 0.43              |
| 1:bA:396:TRP:CD1    | 14:bA:3140:CL7:HAB  | 2.54                     | 0.43              |
| 3:bC:63:LEU:O       | 4:bD:121:ILE:HG13   | 2.19                     | 0.43              |
| 1:cA:57:HIS:HD1     | 14:cA:3105:CL7:CAB  | 2.31                     | 0.43              |
| 1:cA:360:TRP:HZ3    | 14:cA:3114:CL7:H13  | 1.83                     | 0.43              |
| 1:cA:473:SER:HB3    | 1:cA:642:ILE:HD13   | 2.01                     | 0.43              |
| 1:cA:651:PHE:O      | 1:cA:655:GLN:HB2    | 2.18                     | 0.43              |
| 2:cB:366:VAL:HG23   | 2:cB:367:THR:N      | 2.32                     | 0.43              |
| 1:aA:367:VAL:HG21   | 14:aA:3122:CL7:HHD  | 2.00                     | 0.43              |
| 2:aB:92:TRP:CZ3     | 7:aI:12:PRO:HD3     | 2.53                     | 0.43              |
| 2:aB:627:LEU:O      | 2:aB:631:SER:OG     | 2.26                     | 0.43              |
| 1:bA:310:HIS:NE2    | 14:bA:3115:CL7:NB   | 2.66                     | 0.43              |
| 2:bB:671:ARG:CD     | 2:bB:703:LEU:O      | 2.66                     | 0.43              |
| 1:cA:300:ALA:HA     | 14:cA:3112:CL7:HMC2 | 2.00                     | 0.43              |
| 1:cA:746:LEU:HD23   | 1:cA:746:LEU:HA     | 1.74                     | 0.43              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:cB:92:TRP:CH2     | 7:cI:12:PRO:HG3     | 2.53                     | 0.43              |
| 2:cB:366:VAL:CG1    | 2:cB:733:ALA:HA     | 2.49                     | 0.43              |
| 1:aA:465:LEU:HG     | 14:aB:3008:CL7:HMC2 | 2.01                     | 0.43              |
| 1:aA:722:ILE:HD13   | 2:aB:571:CYS:SG     | 2.59                     | 0.43              |
| 2:aB:331:HIS:CD2    | 2:aB:392:ILE:HG22   | 2.54                     | 0.43              |
| 2:aB:366:VAL:CG1    | 2:aB:733:ALA:HA     | 2.49                     | 0.43              |
| 1:bA:460:ASP:OD2    | 1:bA:644:ILE:HB     | 2.19                     | 0.43              |
| 1:bA:585:CYS:SG     | 2:bB:705:ILE:HD13   | 2.58                     | 0.43              |
| 2:bB:92:TRP:CH2     | 7:bI:12:PRO:CG      | 3.02                     | 0.43              |
| 2:bB:106:GLN:HG3    | 2:bB:115:LEU:HD21   | 2.00                     | 0.43              |
| 2:bB:608:ASN:O      | 2:bB:611:GLN:HB3    | 2.19                     | 0.43              |
| 3:bC:7:ILE:HG12     | 3:bC:40:ALA:HB3     | 2.00                     | 0.43              |
| 1:cA:389:ASN:HD21   | 1:cA:746:LEU:HD21   | 1.84                     | 0.43              |
| 14:cA:3113:CL7:HAC1 | 14:cA:3126:CL7:H12C | 2.01                     | 0.43              |
| 16:cA:3137:LHG:H252 | 16:cA:3137:LHG:H281 | 1.79                     | 0.43              |
| 2:cB:367:THR:HG22   | 2:cB:371:LEU:HD12   | 2.00                     | 0.43              |
| 2:cB:519:ASP:OD1    | 2:cB:596:TYR:OH     | 2.33                     | 0.43              |
| 13:cB:805:PHO:CMB   | 13:cB:805:PHO:HBB1  | 2.48                     | 0.43              |
| 2:aB:671:ARG:CD     | 2:aB:703:LEU:O      | 2.66                     | 0.43              |
| 1:bA:645:ASN:HB2    | 2:bB:638:TYR:OH     | 2.18                     | 0.43              |
| 14:bA:3103:CL7:C4C  | 8:bJ:22:PRO:HG3     | 2.48                     | 0.43              |
| 14:bA:3114:CL7:H92C | 14:bA:3114:CL7:H61C | 1.52                     | 0.43              |
| 2:bB:92:TRP:CH2     | 7:bI:12:PRO:HG3     | 2.54                     | 0.43              |
| 2:bB:191:THR:CG2    | 2:bB:277:HIS:HB3    | 2.49                     | 0.43              |
| 2:bB:340:ALA:O      | 2:bB:343:VAL:HG22   | 2.19                     | 0.43              |
| 14:bB:832:CL7:H122  | 14:bB:833:CL7:C2D   | 2.48                     | 0.43              |
| 14:bL:203:CL7:C1B   | 14:bL:204:CL7:HED1  | 2.48                     | 0.43              |
| 2:cB:340:ALA:O      | 2:cB:343:VAL:HG22   | 2.19                     | 0.43              |
| 2:cB:671:ARG:CD     | 2:cB:703:LEU:O      | 2.66                     | 0.43              |
| 3:cC:7:ILE:HG12     | 3:cC:40:ALA:HB3     | 2.00                     | 0.43              |
| 14:aA:3104:CL7:C4C  | 8:aJ:22:PRO:HG3     | 2.49                     | 0.43              |
| 2:aB:68:VAL:HG13    | 2:aB:121:TYR:CE1    | 2.54                     | 0.43              |
| 2:aB:191:THR:CG2    | 2:aB:277:HIS:HB3    | 2.48                     | 0.43              |
| 2:aB:521:LEU:HD23   | 2:aB:521:LEU:HA     | 1.90                     | 0.43              |
| 10:aL:76:VAL:HG21   | 10:bL:146:TYR:HE2   | 1.84                     | 0.43              |
| 1:bA:123:GLY:HA2    | 6:bF:47:THR:HA      | 2.01                     | 0.43              |
| 1:bA:546:VAL:HG11   | 1:bA:599:TRP:CZ2    | 2.54                     | 0.43              |
| 14:bA:3106:CL7:HMA3 | 14:bA:3106:CL7:H102 | 2.00                     | 0.43              |
| 14:bA:3115:CL7:HBC2 | 14:bA:3115:CL7:HMC3 | 2.01                     | 0.43              |
| 2:bB:161:PHE:O      | 2:bB:163:PRO:HD3    | 2.19                     | 0.43              |
| 4:bD:8:GLN:NE2      | 4:bD:53:GLU:O       | 2.51                     | 0.43              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:cB:461:GLN:OE1    | 2:cB:461:GLN:HA     | 2.19                     | 0.43              |
| 2:cB:608:ASN:O      | 2:cB:611:GLN:HB3    | 2.19                     | 0.43              |
| 2:aB:74:PHE:CD2     | 2:aB:135:LEU:HD11   | 2.54                     | 0.42              |
| 1:bA:362:SER:O      | 1:bA:366:ILE:HD12   | 2.19                     | 0.42              |
| 1:bA:389:ASN:HD21   | 1:bA:746:LEU:HD21   | 1.84                     | 0.42              |
| 2:bB:331:HIS:CD2    | 2:bB:392:ILE:HG22   | 2.54                     | 0.42              |
| 1:cA:203:ILE:HG23   | 1:cA:306:ILE:HD13   | 2.01                     | 0.42              |
| 14:cA:3116:CL7:HED3 | 14:cA:3116:CL7:H2A  | 2.00                     | 0.42              |
| 2:cB:68:VAL:HG13    | 2:cB:121:TYR:CE1    | 2.54                     | 0.42              |
| 2:cB:157:LEU:HD12   | 2:cB:157:LEU:HA     | 1.93                     | 0.42              |
| 2:cB:566:GLY:HA2    | 3:cC:56:THR:HG23    | 2.01                     | 0.42              |
| 13:cB:805:PHO:HBB1  | 13:cB:805:PHO:HMB1  | 2.00                     | 0.42              |
| 1:aA:123:GLY:HA2    | 6:aF:47:THR:HA      | 2.01                     | 0.42              |
| 1:aA:430:MET:HE2    | 14:aA:3140:CL7:H172 | 2.00                     | 0.42              |
| 1:aA:460:ASP:OD2    | 1:aA:644:ILE:HB     | 2.19                     | 0.42              |
| 17:aA:3144:PQN:H141 | 17:aA:3144:PQN:H161 | 1.55                     | 0.42              |
| 14:aB:3007:CL7:O1A  | 14:aB:3018:CL7:HBD  | 2.19                     | 0.42              |
| 3:aC:15:THR:HG22    | 3:aC:19:ARG:NE      | 2.35                     | 0.42              |
| 1:bA:692:ARG:HG3    | 1:bA:720:MET:O      | 2.19                     | 0.42              |
| 1:bA:746:LEU:HD23   | 1:bA:746:LEU:HA     | 1.74                     | 0.42              |
| 14:bJ:101:CL7:HBA1  | 14:bJ:101:CL7:H3A   | 1.77                     | 0.42              |
| 10:bL:57:TYR:CD1    | 10:bL:57:TYR:C      | 2.93                     | 0.42              |
| 10:bL:76:VAL:HG21   | 10:cL:146:TYR:HE2   | 1.83                     | 0.42              |
| 1:cA:362:SER:O      | 1:cA:366:ILE:HD12   | 2.19                     | 0.42              |
| 1:cA:534:PHE:CE1    | 1:cA:538:HIS:CE1    | 3.07                     | 0.42              |
| 2:cB:597:PHE:HA     | 14:cB:823:CL7:HBC3  | 2.00                     | 0.42              |
| 1:aA:365:ILE:HG21   | 14:aA:3120:CL7:C3D  | 2.49                     | 0.42              |
| 2:aB:340:ALA:O      | 2:aB:343:VAL:HG22   | 2.19                     | 0.42              |
| 4:aD:8:GLN:HG2      | 4:aD:55:GLU:O       | 2.18                     | 0.42              |
| 4:aD:8:GLN:NE2      | 4:aD:53:GLU:O       | 2.51                     | 0.42              |
| 4:aD:35:SER:OG      | 4:aD:52:ASN:O       | 2.36                     | 0.42              |
| 1:bA:357:LEU:HD21   | 14:bA:3141:CL7:OBB  | 2.19                     | 0.42              |
| 14:bA:3124:CL7:HAB  | 14:bA:3125:CL7:CHB  | 2.49                     | 0.42              |
| 2:bB:5:PHE:CD2      | 7:bI:29:TYR:CE2     | 3.08                     | 0.42              |
| 2:bB:68:VAL:HG13    | 2:bB:121:TYR:CE1    | 2.54                     | 0.42              |
| 14:bB:806:CL7:H62C  | 14:bB:806:CL7:H93C  | 1.81                     | 0.42              |
| 14:bB:819:CL7:H62C  | 14:bB:819:CL7:H92C  | 1.77                     | 0.42              |
| 14:bB:832:CL7:H122  | 14:bB:833:CL7:C1D   | 2.50                     | 0.42              |
| 1:cA:365:ILE:HG21   | 14:cA:3119:CL7:C3D  | 2.49                     | 0.42              |
| 1:cA:645:ASN:HB2    | 2:cB:638:TYR:OH     | 2.19                     | 0.42              |
| 4:cD:130:ILE:HG21   | 4:cD:135:LYS:O      | 2.18                     | 0.42              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:aA:357:LEU:HD23   | 1:aA:357:LEU:HA     | 1.81                     | 0.42              |
| 2:aB:367:THR:HG22   | 2:aB:371:LEU:HD12   | 2.00                     | 0.42              |
| 2:aB:461:GLN:OE1    | 2:aB:461:GLN:HA     | 2.19                     | 0.42              |
| 1:bA:63:THR:HG22    | 1:bA:64:ASN:N       | 2.33                     | 0.42              |
| 1:bA:150:GLY:O      | 1:bA:221:SER:HB3    | 2.19                     | 0.42              |
| 1:bA:403:VAL:HG11   | 1:bA:597:LEU:HG     | 2.01                     | 0.42              |
| 1:bA:653:TRP:CZ2    | 2:bB:632:ALA:HB2    | 2.55                     | 0.42              |
| 14:bA:3119:CL7:HBA1 | 14:bA:3119:CL7:H3A  | 1.87                     | 0.42              |
| 6:bF:142:TRP:CD1    | 6:bF:143:PRO:HD3    | 2.55                     | 0.42              |
| 1:cA:198:MET:HE3    | 14:cA:3116:CL7:HMA2 | 2.01                     | 0.42              |
| 1:cA:403:VAL:HG11   | 1:cA:597:LEU:HG     | 2.01                     | 0.42              |
| 1:cA:722:ILE:HD13   | 2:cB:571:CYS:SG     | 2.59                     | 0.42              |
| 2:cB:50:HIS:HD2     | 14:cB:832:CL7:HAA2  | 1.83                     | 0.42              |
| 2:cB:161:PHE:O      | 2:cB:163:PRO:HD3    | 2.19                     | 0.42              |
| 4:cD:38:GLN:HA      | 4:cD:51:MET:O       | 2.19                     | 0.42              |
| 2:aB:522:VAL:HG13   | 14:aB:3003:CL7:H141 | 2.01                     | 0.42              |
| 14:bA:3125:CL7:HED2 | 10:bL:65:SER:O      | 2.20                     | 0.42              |
| 2:bB:566:GLY:HA2    | 3:bC:56:THR:HG23    | 2.01                     | 0.42              |
| 4:bD:130:ILE:HG21   | 4:bD:135:LYS:O      | 2.18                     | 0.42              |
| 1:cA:367:VAL:HG21   | 14:cA:3121:CL7:HHD  | 2.01                     | 0.42              |
| 2:cB:648:VAL:HG21   | 14:cB:809:CL7:HMD1  | 2.01                     | 0.42              |
| 1:aA:473:SER:HB3    | 1:aA:642:ILE:HD13   | 2.01                     | 0.42              |
| 2:aB:161:PHE:O      | 2:aB:163:PRO:HD3    | 2.19                     | 0.42              |
| 2:aB:384:ILE:HD11   | 2:aB:582:ALA:HB3    | 2.02                     | 0.42              |
| 10:aL:51:GLY:O      | 10:aL:134:GLY:HA2   | 2.20                     | 0.42              |
| 1:bA:213:TRP:HD1    | 1:bA:298:HIS:CD2    | 2.38                     | 0.42              |
| 1:bA:367:VAL:HG21   | 14:bA:3121:CL7:HHD  | 2.01                     | 0.42              |
| 14:bA:3106:CL7:H201 | 16:bA:3137:LHG:H223 | 2.00                     | 0.42              |
| 14:bA:3125:CL7:H8   | 10:bL:57:TYR:OH     | 2.19                     | 0.42              |
| 2:bB:74:PHE:CD2     | 2:bB:135:LEU:HD11   | 2.54                     | 0.42              |
| 3:bC:18:VAL:HG22    | 3:bC:26:LEU:CB      | 2.50                     | 0.42              |
| 1:cA:546:VAL:HG11   | 1:cA:599:TRP:CZ2    | 2.55                     | 0.42              |
| 2:cB:331:HIS:CD2    | 2:cB:392:ILE:HG22   | 2.54                     | 0.42              |
| 3:cC:63:LEU:O       | 4:cD:121:ILE:HG13   | 2.19                     | 0.42              |
| 1:aA:120:PRO:HB3    | 1:aA:125:ASP:HB3    | 2.02                     | 0.42              |
| 1:aA:334:THR:CB     | 16:aA:3139:LHG:HC2  | 2.49                     | 0.42              |
| 2:aB:5:PHE:CD2      | 7:aI:29:TYR:CE2     | 3.08                     | 0.42              |
| 2:aB:117:TYR:CE1    | 2:aB:366:VAL:HG21   | 2.55                     | 0.42              |
| 2:aB:366:VAL:HG12   | 2:aB:732:THR:HG22   | 2.02                     | 0.42              |
| 2:aB:534:VAL:O      | 2:aB:538:VAL:HG13   | 2.20                     | 0.42              |
| 4:aD:38:GLN:HA      | 4:aD:51:MET:O       | 2.19                     | 0.42              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:bA:735:LEU:HD22   | 14:bA:3142:CL7:HMA1 | 2.01                     | 0.42              |
| 14:bA:3142:CL7:H41C | 14:bA:3142:CL7:H62C | 1.57                     | 0.42              |
| 2:cB:74:PHE:CD2     | 2:cB:135:LEU:HD11   | 2.54                     | 0.42              |
| 2:cB:384:ILE:HD11   | 2:cB:582:ALA:HB3    | 2.02                     | 0.42              |
| 6:cF:142:TRP:CD1    | 6:cF:143:PRO:HD3    | 2.55                     | 0.42              |
| 1:aA:653:TRP:CZ2    | 2:aB:632:ALA:HB2    | 2.55                     | 0.42              |
| 14:aA:3109:CL7:CHC  | 14:aA:3141:CL7:H172 | 2.50                     | 0.42              |
| 2:aB:608:ASN:O      | 2:aB:611:GLN:HB3    | 2.19                     | 0.42              |
| 1:bA:120:PRO:HB3    | 1:bA:125:ASP:HB3    | 2.02                     | 0.42              |
| 1:bA:554:GLY:O      | 1:bA:558:ALA:HB2    | 2.20                     | 0.42              |
| 2:bB:366:VAL:CG1    | 2:bB:733:ALA:HA     | 2.49                     | 0.42              |
| 3:bC:15:THR:O       | 3:bC:15:THR:CG2     | 2.63                     | 0.42              |
| 10:bL:51:GLY:O      | 10:bL:134:GLY:HA2   | 2.20                     | 0.42              |
| 1:cA:403:VAL:HG22   | 1:cA:551:LEU:HD11   | 2.02                     | 0.42              |
| 2:cB:28:VAL:HG13    | 2:cB:29:HIS:CD2     | 2.55                     | 0.42              |
| 2:cB:92:TRP:CZ3     | 7:cI:12:PRO:HD3     | 2.54                     | 0.42              |
| 1:aA:203:ILE:HG23   | 1:aA:306:ILE:HD13   | 2.01                     | 0.42              |
| 3:aC:18:VAL:HG22    | 3:aC:26:LEU:CB      | 2.50                     | 0.42              |
| 3:aC:63:LEU:O       | 4:aD:121:ILE:HG13   | 2.19                     | 0.42              |
| 10:aL:146:TYR:HE2   | 10:cL:76:VAL:HG21   | 1.84                     | 0.42              |
| 1:bA:63:THR:HG22    | 1:bA:65:ASP:H       | 1.85                     | 0.42              |
| 1:bA:374:MET:HG2    | 1:bA:508:SER:HB2    | 2.02                     | 0.42              |
| 1:bA:694:TYR:CE2    | 2:bB:539:LYS:HE3    | 2.55                     | 0.42              |
| 1:cA:150:GLY:O      | 1:cA:221:SER:HB3    | 2.19                     | 0.42              |
| 2:cB:256:THR:O      | 2:cB:275:HIS:ND1    | 2.53                     | 0.42              |
| 2:cB:422:LEU:HD23   | 2:cB:422:LEU:HA     | 1.94                     | 0.42              |
| 6:cF:60:MET:HE1     | 8:cJ:46:ILE:HG23    | 2.02                     | 0.42              |
| 1:aA:342:TYR:CE1    | 1:aA:346:THR:HG21   | 2.55                     | 0.42              |
| 1:aA:389:ASN:HD21   | 1:aA:746:LEU:HD21   | 1.84                     | 0.42              |
| 1:aA:403:VAL:HG11   | 1:aA:597:LEU:HG     | 2.01                     | 0.42              |
| 1:aA:680:ILE:HD13   | 1:aA:680:ILE:HA     | 1.84                     | 0.42              |
| 4:aD:43:MET:SD      | 4:aD:58:LEU:HD21    | 2.60                     | 0.42              |
| 1:bA:473:SER:HB3    | 1:bA:642:ILE:HD13   | 2.00                     | 0.42              |
| 2:bB:156:HIS:O      | 2:bB:162:ARG:HA     | 2.20                     | 0.42              |
| 14:cA:3115:CL7:HBC2 | 14:cA:3115:CL7:HMC3 | 2.01                     | 0.42              |
| 14:cA:3119:CL7:HBA1 | 14:cA:3119:CL7:H3A  | 1.85                     | 0.42              |
| 14:cA:3128:CL7:H122 | 14:cA:3128:CL7:H162 | 1.34                     | 0.42              |
| 2:cB:262:HIS:NE2    | 2:cB:264:GLN:HB3    | 2.35                     | 0.42              |
| 1:aA:374:MET:HG2    | 1:aA:508:SER:HB2    | 2.02                     | 0.41              |
| 1:aA:692:ARG:HG3    | 1:aA:720:MET:O      | 2.19                     | 0.41              |
| 1:aA:694:TYR:CE2    | 2:aB:539:LYS:HE3    | 2.55                     | 0.41              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:aB:256:THR:O      | 2:aB:275:HIS:ND1    | 2.53                     | 0.41              |
| 6:aF:142:TRP:CD1    | 6:aF:143:PRO:HD3    | 2.55                     | 0.41              |
| 1:bA:365:ILE:HG21   | 14:bA:3119:CL7:C3D  | 2.50                     | 0.41              |
| 2:bB:384:ILE:HD11   | 2:bB:582:ALA:HB3    | 2.02                     | 0.41              |
| 11:bM:17:LEU:HB3    | 11:bM:18:PRO:CD     | 2.50                     | 0.41              |
| 1:cA:120:PRO:HB3    | 1:cA:125:ASP:HB3    | 2.02                     | 0.41              |
| 1:cA:554:GLY:O      | 1:cA:558:ALA:HB2    | 2.20                     | 0.41              |
| 1:cA:692:ARG:HG3    | 1:cA:720:MET:O      | 2.19                     | 0.41              |
| 14:cA:3125:CL7:H8   | 10:cL:57:TYR:OH     | 2.20                     | 0.41              |
| 2:cB:5:PHE:CD2      | 7:cI:29:TYR:CE2     | 3.08                     | 0.41              |
| 2:cB:136:TYR:CZ     | 11:cM:7:GLN:HB3     | 2.55                     | 0.41              |
| 2:cB:534:VAL:O      | 2:cB:538:VAL:HG13   | 2.20                     | 0.41              |
| 13:cB:801:PHO:HBA1  | 13:cB:801:PHO:H11   | 1.65                     | 0.41              |
| 14:cB:806:CL7:H3A   | 14:cB:820:CL7:CAB   | 2.50                     | 0.41              |
| 3:cC:8:TYR:HD1      | 3:cC:64:SER:O       | 2.03                     | 0.41              |
| 14:aA:3129:CL7:OBB  | 14:aA:3129:CL7:HHC  | 2.20                     | 0.41              |
| 2:aB:156:HIS:O      | 2:aB:162:ARG:HA     | 2.20                     | 0.41              |
| 13:aB:3004:PHO:H201 | 14:aB:3026:CL7:H2   | 2.01                     | 0.41              |
| 3:aC:8:TYR:HD1      | 3:aC:64:SER:O       | 2.03                     | 0.41              |
| 1:bA:371:MET:HE2    | 1:bA:371:MET:HB3    | 1.81                     | 0.41              |
| 2:bB:118:SER:O      | 2:bB:120:LEU:N      | 2.44                     | 0.41              |
| 2:bB:262:HIS:NE2    | 2:bB:264:GLN:HB3    | 2.35                     | 0.41              |
| 2:bB:461:GLN:HA     | 2:bB:461:GLN:OE1    | 2.19                     | 0.41              |
| 3:bC:15:THR:HG22    | 3:bC:19:ARG:NE      | 2.35                     | 0.41              |
| 4:bD:43:MET:SD      | 4:bD:58:LEU:HD21    | 2.60                     | 0.41              |
| 8:bJ:44:PRO:O       | 8:bJ:46:ILE:HG13    | 2.20                     | 0.41              |
| 10:bL:64:THR:HG21   | 14:bL:205:CL7:HMB1  | 2.00                     | 0.41              |
| 1:cA:374:MET:HG2    | 1:cA:508:SER:HB2    | 2.02                     | 0.41              |
| 1:cA:404:GLY:HA3    | 14:cA:3141:CL7:C2C  | 2.50                     | 0.41              |
| 14:cA:3140:CL7:H192 | 14:cA:3140:CL7:H161 | 1.77                     | 0.41              |
| 2:cB:156:HIS:O      | 2:cB:162:ARG:HA     | 2.21                     | 0.41              |
| 2:cB:600:LYS:O      | 2:cB:604:ILE:HG23   | 2.21                     | 0.41              |
| 1:aA:362:SER:O      | 1:aA:366:ILE:HD12   | 2.19                     | 0.41              |
| 1:aA:546:VAL:HG11   | 1:aA:599:TRP:CZ2    | 2.54                     | 0.41              |
| 1:aA:746:LEU:HD23   | 1:aA:746:LEU:HA     | 1.74                     | 0.41              |
| 14:aA:3125:CL7:H161 | 14:aA:3125:CL7:H143 | 1.78                     | 0.41              |
| 14:aA:3126:CL7:H8   | 10:aL:57:TYR:OH     | 2.19                     | 0.41              |
| 14:aB:3007:CL7:H93C | 14:aB:3007:CL7:H61C | 1.79                     | 0.41              |
| 14:aB:3019:CL7:HBA1 | 14:aB:3019:CL7:HBD  | 2.02                     | 0.41              |
| 4:aD:42:GLU:O       | 4:aD:73:GLN:NE2     | 2.49                     | 0.41              |
| 1:bA:337:GLY:O      | 1:bA:425:ASN:HB2    | 2.21                     | 0.41              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:bB:60:TRP:HD1     | 14:bB:808:CL7:H171  | 1.84                     | 0.41              |
| 1:cA:65:ASP:OD1     | 1:cA:65:ASP:N       | 2.54                     | 0.41              |
| 14:cB:808:CL7:O1A   | 14:cB:819:CL7:HBD   | 2.19                     | 0.41              |
| 3:cC:15:THR:HG22    | 3:cC:19:ARG:NE      | 2.35                     | 0.41              |
| 8:cJ:44:PRO:O       | 8:cJ:46:ILE:HG13    | 2.21                     | 0.41              |
| 1:aA:63:THR:HG22    | 1:aA:65:ASP:H       | 1.85                     | 0.41              |
| 1:aA:150:GLY:O      | 1:aA:221:SER:HB3    | 2.19                     | 0.41              |
| 1:aA:554:GLY:O      | 1:aA:558:ALA:HB2    | 2.20                     | 0.41              |
| 1:aA:704:TRP:CD2    | 2:aB:416:GLU:CB     | 3.03                     | 0.41              |
| 2:aB:666:PHE:CZ     | 14:aB:3026:CL7:HBC3 | 2.55                     | 0.41              |
| 3:aC:24:ASP:HB2     | 4:aD:67:LEU:HD11    | 2.02                     | 0.41              |
| 1:bA:198:MET:O      | 1:bA:202:LEU:HB2    | 2.21                     | 0.41              |
| 1:bA:403:VAL:HG22   | 1:bA:551:LEU:HD11   | 2.02                     | 0.41              |
| 2:bB:256:THR:O      | 2:bB:275:HIS:ND1    | 2.53                     | 0.41              |
| 2:bB:724:TYR:CE2    | 2:bB:728:VAL:CG2    | 3.04                     | 0.41              |
| 4:bD:38:GLN:HA      | 4:bD:51:MET:O       | 2.19                     | 0.41              |
| 1:cA:653:TRP:CZ2    | 2:cB:632:ALA:HB2    | 2.55                     | 0.41              |
| 14:cB:808:CL7:H43C  | 14:cB:819:CL7:H11C  | 2.03                     | 0.41              |
| 10:cL:51:GLY:O      | 10:cL:134:GLY:HA2   | 2.20                     | 0.41              |
| 1:aA:213:TRP:HD1    | 1:aA:298:HIS:CD2    | 2.38                     | 0.41              |
| 2:aB:262:HIS:NE2    | 2:aB:264:GLN:HB3    | 2.35                     | 0.41              |
| 2:aB:600:LYS:O      | 2:aB:604:ILE:HG23   | 2.21                     | 0.41              |
| 2:bB:666:PHE:CZ     | 14:bB:827:CL7:HBC3  | 2.55                     | 0.41              |
| 14:bB:826:CL7:H18   | 14:bL:204:CL7:CHC   | 2.50                     | 0.41              |
| 1:cA:218:ILE:O      | 1:cA:223:PRO:HD3    | 2.21                     | 0.41              |
| 1:cA:683:PHE:CE1    | 1:cA:686:MET:HE1    | 2.56                     | 0.41              |
| 2:cB:596:TYR:HA     | 2:cB:622:TRP:HH2    | 1.86                     | 0.41              |
| 14:aA:3116:CL7:HBC2 | 14:aA:3116:CL7:HMC3 | 2.01                     | 0.41              |
| 2:aB:136:TYR:CZ     | 11:aM:7:GLN:HB3     | 2.55                     | 0.41              |
| 2:aB:724:TYR:CE2    | 2:aB:728:VAL:CG2    | 3.04                     | 0.41              |
| 14:aB:3019:CL7:H92C | 14:aB:3019:CL7:H62C | 1.88                     | 0.41              |
| 1:bA:342:TYR:CE1    | 1:bA:346:THR:HG21   | 2.55                     | 0.41              |
| 2:bB:366:VAL:HG12   | 2:bB:732:THR:HG22   | 2.01                     | 0.41              |
| 1:cA:213:TRP:HD1    | 1:cA:298:HIS:CD2    | 2.38                     | 0.41              |
| 1:cA:705:ALA:HB2    | 2:cB:420:SER:OG     | 2.20                     | 0.41              |
| 2:cB:15:ASP:HB3     | 2:cB:20:ARG:HB2     | 2.03                     | 0.41              |
| 2:cB:652:ILE:HG23   | 2:cB:722:VAL:HG13   | 2.02                     | 0.41              |
| 3:cC:18:VAL:HG22    | 3:cC:26:LEU:CB      | 2.50                     | 0.41              |
| 6:cF:91:GLY:HA2     | 14:cF:201:CL7:HMC2  | 2.03                     | 0.41              |
| 1:aA:337:GLY:O      | 1:aA:425:ASN:HB2    | 2.21                     | 0.41              |
| 1:aA:390:LEU:CD1    | 14:aA:3122:CL7:HED2 | 2.51                     | 0.41              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:aA:527:VAL:HG22   | 1:aA:619:VAL:HG21   | 2.03                     | 0.41              |
| 2:aB:39:GLU:O       | 2:aB:43:TYR:HD1     | 2.04                     | 0.41              |
| 2:aB:392:ILE:HG12   | 2:aB:558:TYR:CD2    | 2.56                     | 0.41              |
| 1:bA:218:ILE:O      | 1:bA:223:PRO:HD3    | 2.21                     | 0.41              |
| 1:bA:465:LEU:HD21   | 14:bB:809:CL7:C1C   | 2.51                     | 0.41              |
| 14:bA:3132:CL7:H2   | 14:bA:3132:CL7:ND   | 2.36                     | 0.41              |
| 2:bB:440:ASN:O      | 2:bB:444:VAL:HG23   | 2.21                     | 0.41              |
| 3:bC:8:TYR:HD1      | 3:bC:64:SER:O       | 2.03                     | 0.41              |
| 1:cA:58:ASP:OD1     | 14:cA:3141:CL7:HED3 | 2.21                     | 0.41              |
| 1:cA:704:TRP:CD2    | 2:cB:416:GLU:CB     | 3.04                     | 0.41              |
| 14:cB:826:CL7:H18   | 14:cL:204:CL7:CHC   | 2.50                     | 0.41              |
| 1:aA:656:SER:O      | 1:aA:660:ILE:HG12   | 2.21                     | 0.41              |
| 1:aA:698:LEU:HD21   | 13:aA:3102:PHO:HED2 | 2.01                     | 0.41              |
| 1:aA:705:ALA:HB2    | 2:aB:420:SER:OG     | 2.21                     | 0.41              |
| 2:aB:28:VAL:HG13    | 2:aB:29:HIS:CD2     | 2.55                     | 0.41              |
| 2:aB:136:TYR:CD1    | 11:aM:3:LEU:HD21    | 2.56                     | 0.41              |
| 14:aB:3005:CL7:H3A  | 14:aB:3019:CL7:CAB  | 2.50                     | 0.41              |
| 14:aB:3019:CL7:H151 | 14:aB:3026:CL7:HAA1 | 2.02                     | 0.41              |
| 14:aL:202:CL7:H192  | 14:cB:810:CL7:H192  | 2.03                     | 0.41              |
| 1:cA:63:THR:HG22    | 1:cA:65:ASP:H       | 1.85                     | 0.41              |
| 1:cA:694:TYR:CE2    | 2:cB:539:LYS:HE3    | 2.55                     | 0.41              |
| 16:cA:3137:LHG:H182 | 14:cA:3141:CL7:H101 | 2.01                     | 0.41              |
| 2:cB:28:VAL:HG21    | 14:cB:831:CL7:C3D   | 2.50                     | 0.41              |
| 2:cB:691:ALA:C      | 2:cB:693:LEU:N      | 2.79                     | 0.41              |
| 1:aA:218:ILE:O      | 1:aA:223:PRO:HD3    | 2.21                     | 0.41              |
| 1:aA:403:VAL:HG22   | 1:aA:551:LEU:HD11   | 2.02                     | 0.41              |
| 2:aB:440:ASN:O      | 2:aB:444:VAL:HG23   | 2.21                     | 0.41              |
| 2:aB:596:TYR:HA     | 2:aB:622:TRP:HH2    | 1.86                     | 0.41              |
| 14:aB:3018:CL7:H93C | 14:aB:3018:CL7:H61C | 1.75                     | 0.41              |
| 3:aC:63:LEU:HD21    | 3:aC:66:ARG:NH2     | 2.35                     | 0.41              |
| 8:aJ:44:PRO:O       | 8:aJ:46:ILE:HG13    | 2.21                     | 0.41              |
| 14:aL:202:CL7:H141  | 7:cI:24:THR:HG21    | 2.03                     | 0.41              |
| 14:aL:203:CL7:H111  | 14:aL:203:CL7:H152  | 1.68                     | 0.41              |
| 11:aM:17:LEU:HB3    | 11:aM:18:PRO:CD     | 2.51                     | 0.41              |
| 1:bA:203:ILE:HG23   | 1:bA:306:ILE:HD13   | 2.01                     | 0.41              |
| 1:bA:206:LEU:HB3    | 1:bA:305:TYR:CD2    | 2.56                     | 0.41              |
| 1:bA:300:ALA:HA     | 14:bA:3112:CL7:HMC2 | 2.02                     | 0.41              |
| 1:bA:363:PHE:O      | 1:bA:367:VAL:HG23   | 2.21                     | 0.41              |
| 1:bA:749:ILE:HD12   | 1:bA:749:ILE:HA     | 1.88                     | 0.41              |
| 14:bA:3120:CL7:H43C | 14:bA:3120:CL7:H12C | 1.91                     | 0.41              |
| 2:bB:28:VAL:HG13    | 2:bB:29:HIS:CD2     | 2.55                     | 0.41              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:bB:117:TYR:CE1    | 2:bB:366:VAL:HG21   | 2.55                     | 0.41              |
| 2:bB:136:TYR:CZ     | 11:bM:7:GLN:HB3     | 2.55                     | 0.41              |
| 2:bB:345:THR:CG2    | 2:bB:379:ALA:HA     | 2.51                     | 0.41              |
| 2:bB:534:VAL:O      | 2:bB:538:VAL:HG13   | 2.20                     | 0.41              |
| 2:bB:600:LYS:O      | 2:bB:604:ILE:HG23   | 2.21                     | 0.41              |
| 14:bB:833:CL7:H3A   | 14:bB:833:CL7:HBA1  | 1.77                     | 0.41              |
| 1:cA:198:MET:O      | 1:cA:202:LEU:HB2    | 2.21                     | 0.41              |
| 14:cA:3114:CL7:H92C | 14:cA:3114:CL7:H61C | 1.50                     | 0.41              |
| 14:cA:3116:CL7:H61C | 14:cA:3116:CL7:H41C | 1.59                     | 0.41              |
| 2:cB:120:LEU:HD23   | 2:cB:120:LEU:HA     | 1.93                     | 0.41              |
| 2:cB:392:ILE:HG12   | 2:cB:558:TYR:CD2    | 2.56                     | 0.41              |
| 13:cB:805:PHO:H161  | 13:cB:805:PHO:H143  | 1.81                     | 0.41              |
| 3:cC:25:VAL:HG21    | 3:cC:48:CYS:HA      | 2.03                     | 0.41              |
| 4:cD:43:MET:SD      | 4:cD:58:LEU:HD21    | 2.60                     | 0.41              |
| 10:cL:30:TRP:HH2    | 14:cL:203:CL7:H71C  | 1.85                     | 0.41              |
| 14:cL:203:CL7:H12C  | 14:cL:203:CL7:HBA1  | 1.89                     | 0.41              |
| 2:aB:601:HIS:HB3    | 2:aB:605:TRP:CZ2    | 2.56                     | 0.41              |
| 14:aB:3021:CL7:HED1 | 8:aJ:47:LEU:HA      | 2.03                     | 0.41              |
| 1:bA:65:ASP:OD1     | 1:bA:65:ASP:N       | 2.54                     | 0.41              |
| 1:bA:436:THR:O      | 1:bA:440:HIS:ND1    | 2.53                     | 0.41              |
| 2:bB:28:VAL:HG21    | 14:bB:831:CL7:C3D   | 2.51                     | 0.41              |
| 2:bB:273:ILE:HG23   | 14:bB:816:CL7:HMA3  | 2.03                     | 0.41              |
| 1:cA:357:LEU:HA     | 1:cA:357:LEU:HD23   | 1.82                     | 0.41              |
| 1:cA:473:SER:HB3    | 1:cA:642:ILE:CD1    | 2.51                     | 0.41              |
| 2:cB:3:THR:O        | 2:cB:4:LYS:C        | 2.64                     | 0.41              |
| 2:cB:440:ASN:O      | 2:cB:444:VAL:HG23   | 2.21                     | 0.41              |
| 2:cB:601:HIS:HB3    | 2:cB:605:TRP:CZ2    | 2.56                     | 0.41              |
| 10:cL:148:ILE:HD12  | 10:cL:149:ALA:N     | 2.36                     | 0.41              |
| 1:aA:363:PHE:O      | 1:aA:367:VAL:HG23   | 2.21                     | 0.40              |
| 1:aA:465:LEU:HD21   | 14:aB:3008:CL7:C1C  | 2.51                     | 0.40              |
| 14:aA:3114:CL7:HED2 | 14:aA:3115:CL7:O1A  | 2.21                     | 0.40              |
| 2:aB:345:THR:CG2    | 2:aB:379:ALA:HA     | 2.51                     | 0.40              |
| 6:aF:91:GLY:HA2     | 14:aF:201:CL7:HMC2  | 2.03                     | 0.40              |
| 1:bA:656:SER:O      | 1:bA:660:ILE:HG12   | 2.21                     | 0.40              |
| 14:bA:3128:CL7:HHC  | 14:bA:3128:CL7:OBB  | 2.21                     | 0.40              |
| 2:bB:601:HIS:HB3    | 2:bB:605:TRP:CZ2    | 2.56                     | 0.40              |
| 10:bL:116:ASP:O     | 10:bL:122:GLY:HA3   | 2.21                     | 0.40              |
| 2:cB:366:VAL:HG12   | 2:cB:732:THR:HG22   | 2.02                     | 0.40              |
| 1:aA:609:PHE:HB3    | 1:aA:647:TRP:HZ3    | 1.86                     | 0.40              |
| 1:bA:683:PHE:CE1    | 1:bA:686:MET:HE1    | 2.56                     | 0.40              |
| 2:bB:39:GLU:O       | 2:bB:43:TYR:HD1     | 2.04                     | 0.40              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 13:bB:805:PHO:H143  | 13:bB:805:PHO:H161  | 1.84                     | 0.40              |
| 14:bB:833:CL7:H62C  | 14:bB:833:CL7:H41C  | 1.70                     | 0.40              |
| 1:cA:337:GLY:O      | 1:cA:425:ASN:HB2    | 2.21                     | 0.40              |
| 1:cA:371:MET:HE2    | 1:cA:371:MET:HB3    | 1.81                     | 0.40              |
| 2:cB:345:THR:CG2    | 2:cB:379:ALA:HA     | 2.51                     | 0.40              |
| 2:cB:536:ILE:HG12   | 13:cB:801:PHO:HMD3  | 2.03                     | 0.40              |
| 14:cB:832:CL7:H143  | 14:cB:832:CL7:H112  | 1.83                     | 0.40              |
| 1:aA:222:LEU:N      | 1:aA:223:PRO:HD2    | 2.37                     | 0.40              |
| 1:aA:436:THR:O      | 1:aA:440:HIS:ND1    | 2.53                     | 0.40              |
| 14:aA:3133:CL7:H112 | 14:aA:3133:CL7:H91C | 1.78                     | 0.40              |
| 14:aA:3141:CL7:H141 | 14:aA:3141:CL7:H162 | 1.84                     | 0.40              |
| 2:aB:28:VAL:HG21    | 14:aB:3030:CL7:C3D  | 2.52                     | 0.40              |
| 1:bA:426:VAL:O      | 1:bA:430:MET:HG2    | 2.21                     | 0.40              |
| 1:bA:522:VAL:HG21   | 1:bA:629:VAL:HG11   | 2.03                     | 0.40              |
| 1:bA:694:TYR:CD1    | 1:bA:694:TYR:C      | 2.99                     | 0.40              |
| 2:bB:535:LEU:HD12   | 2:bB:535:LEU:C      | 2.47                     | 0.40              |
| 14:bB:820:CL7:H141  | 14:bB:820:CL7:H161  | 1.84                     | 0.40              |
| 1:cA:222:LEU:N      | 1:cA:223:PRO:HD2    | 2.37                     | 0.40              |
| 1:cA:656:SER:O      | 1:cA:660:ILE:HG12   | 2.21                     | 0.40              |
| 14:cA:3142:CL7:H3A  | 14:cA:3142:CL7:HBA1 | 1.88                     | 0.40              |
| 4:cD:42:GLU:O       | 4:cD:73:GLN:NE2     | 2.49                     | 0.40              |
| 1:aA:198:MET:O      | 1:aA:202:LEU:HB2    | 2.21                     | 0.40              |
| 14:aA:3126:CL7:HED2 | 10:aL:65:SER:O      | 2.21                     | 0.40              |
| 2:aB:326:TYR:CD1    | 2:aB:326:TYR:C      | 2.99                     | 0.40              |
| 2:aB:565:PRO:HA     | 2:aB:569:GLY:HA2    | 2.04                     | 0.40              |
| 4:aD:130:ILE:O      | 4:aD:130:ILE:HG22   | 2.22                     | 0.40              |
| 1:bA:704:TRP:CD2    | 2:bB:416:GLU:CB     | 3.03                     | 0.40              |
| 1:bA:705:ALA:HB2    | 2:bB:420:SER:OG     | 2.22                     | 0.40              |
| 2:bB:180:ALA:HB2    | 2:bB:288:GLY:HA3    | 2.04                     | 0.40              |
| 2:bB:326:TYR:CD1    | 2:bB:326:TYR:C      | 3.00                     | 0.40              |
| 1:cA:342:TYR:CE1    | 1:cA:346:THR:HG21   | 2.55                     | 0.40              |
| 14:cA:3125:CL7:HED2 | 10:cL:65:SER:O      | 2.22                     | 0.40              |
| 2:cB:724:TYR:CE2    | 2:cB:728:VAL:CG2    | 3.04                     | 0.40              |
| 14:cL:204:CL7:H192  | 14:cL:204:CL7:H161  | 1.77                     | 0.40              |
| 11:cM:17:LEU:HB3    | 11:cM:18:PRO:CD     | 2.51                     | 0.40              |
| 1:aA:206:LEU:HB3    | 1:aA:305:TYR:CD2    | 2.56                     | 0.40              |
| 2:aB:141:PHE:O      | 2:aB:145:VAL:HG23   | 2.22                     | 0.40              |
| 2:aB:180:ALA:HB2    | 2:aB:288:GLY:HA3    | 2.04                     | 0.40              |
| 2:aB:535:LEU:HD12   | 2:aB:535:LEU:C      | 2.47                     | 0.40              |
| 2:aB:561:PRO:HB3    | 2:aB:705:ILE:HB     | 2.03                     | 0.40              |
| 14:aB:3009:CL7:H93C | 14:aB:3009:CL7:H62C | 1.60                     | 0.40              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:bA:222:LEU:N      | 1:bA:223:PRO:HD2    | 2.37                     | 0.40              |
| 1:bA:477:ILE:HD11   | 14:bA:3125:CL7:HED1 | 2.04                     | 0.40              |
| 1:bA:672:ILE:HD11   | 2:bB:442:THR:HA     | 2.03                     | 0.40              |
| 1:bA:683:PHE:CE1    | 1:bA:686:MET:HE2    | 2.57                     | 0.40              |
| 2:bB:392:ILE:HG12   | 2:bB:558:TYR:CD2    | 2.56                     | 0.40              |
| 2:bB:627:LEU:O      | 2:bB:631:SER:OG     | 2.26                     | 0.40              |
| 14:bB:826:CL7:H43C  | 14:bB:826:CL7:H62C  | 1.93                     | 0.40              |
| 17:bB:828:PQN:H172  | 17:bB:828:PQN:H211  | 1.61                     | 0.40              |
| 3:bC:25:VAL:HG21    | 3:bC:48:CYS:HA      | 2.03                     | 0.40              |
| 1:cA:206:LEU:HB3    | 1:cA:305:TYR:CD2    | 2.56                     | 0.40              |
| 1:cA:395:MET:HB3    | 1:cA:604:ILE:HG23   | 2.04                     | 0.40              |
| 1:cA:436:THR:O      | 1:cA:440:HIS:ND1    | 2.53                     | 0.40              |
| 14:cA:3139:CL7:H161 | 14:cA:3139:CL7:H193 | 1.73                     | 0.40              |
| 2:cB:117:TYR:CE1    | 2:cB:366:VAL:HG21   | 2.55                     | 0.40              |
| 10:cL:116:ASP:O     | 10:cL:122:GLY:HA3   | 2.21                     | 0.40              |
| 14:cL:203:CL7:C2B   | 14:cL:204:CL7:HED1  | 2.52                     | 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    | 681/753 (90%) | 637 (94%) | 44 (6%) | 0        | 100         | 100 |
| 1   | bA    | 681/753 (90%) | 635 (93%) | 46 (7%) | 0        | 100         | 100 |
| 1   | cA    | 681/753 (90%) | 637 (94%) | 44 (6%) | 0        | 100         | 100 |
| 2   | aB    | 652/736 (89%) | 616 (94%) | 36 (6%) | 0        | 100         | 100 |
| 2   | bB    | 652/736 (89%) | 616 (94%) | 36 (6%) | 0        | 100         | 100 |
| 2   | cB    | 652/736 (89%) | 616 (94%) | 36 (6%) | 0        | 100         | 100 |
| 3   | aC    | 78/81 (96%)   | 72 (92%)  | 5 (6%)  | 1 (1%)   | 9           | 18  |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 3   | bC    | 78/81 (96%)     | 72 (92%)   | 5 (6%)   | 1 (1%)   | 9           | 18  |
| 3   | cC    | 78/81 (96%)     | 72 (92%)   | 5 (6%)   | 1 (1%)   | 9           | 18  |
| 4   | aD    | 134/139 (96%)   | 126 (94%)  | 8 (6%)   | 0        | 100         | 100 |
| 4   | bD    | 134/139 (96%)   | 126 (94%)  | 8 (6%)   | 0        | 100         | 100 |
| 4   | cD    | 134/139 (96%)   | 126 (94%)  | 8 (6%)   | 0        | 100         | 100 |
| 5   | aE    | 65/89 (73%)     | 61 (94%)   | 4 (6%)   | 0        | 100         | 100 |
| 5   | bE    | 65/89 (73%)     | 61 (94%)   | 4 (6%)   | 0        | 100         | 100 |
| 5   | cE    | 65/89 (73%)     | 61 (94%)   | 4 (6%)   | 0        | 100         | 100 |
| 6   | aF    | 128/167 (77%)   | 120 (94%)  | 8 (6%)   | 0        | 100         | 100 |
| 6   | bF    | 128/167 (77%)   | 120 (94%)  | 8 (6%)   | 0        | 100         | 100 |
| 6   | cF    | 128/167 (77%)   | 119 (93%)  | 9 (7%)   | 0        | 100         | 100 |
| 7   | aI    | 28/34 (82%)     | 27 (96%)   | 1 (4%)   | 0        | 100         | 100 |
| 7   | bI    | 28/34 (82%)     | 27 (96%)   | 1 (4%)   | 0        | 100         | 100 |
| 7   | cI    | 28/34 (82%)     | 27 (96%)   | 1 (4%)   | 0        | 100         | 100 |
| 8   | aJ    | 33/51 (65%)     | 31 (94%)   | 2 (6%)   | 0        | 100         | 100 |
| 8   | bJ    | 33/51 (65%)     | 31 (94%)   | 2 (6%)   | 0        | 100         | 100 |
| 8   | cJ    | 33/51 (65%)     | 31 (94%)   | 2 (6%)   | 0        | 100         | 100 |
| 9   | aK    | 29/86 (34%)     | 29 (100%)  | 0        | 0        | 100         | 100 |
| 9   | bK    | 29/86 (34%)     | 29 (100%)  | 0        | 0        | 100         | 100 |
| 9   | cK    | 29/86 (34%)     | 29 (100%)  | 0        | 0        | 100         | 100 |
| 10  | aL    | 145/153 (95%)   | 142 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 10  | bL    | 145/153 (95%)   | 142 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 10  | cL    | 145/153 (95%)   | 142 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 11  | aM    | 27/31 (87%)     | 27 (100%)  | 0        | 0        | 100         | 100 |
| 11  | bM    | 27/31 (87%)     | 27 (100%)  | 0        | 0        | 100         | 100 |
| 11  | cM    | 27/31 (87%)     | 27 (100%)  | 0        | 0        | 100         | 100 |
| All | All   | 6000/6960 (86%) | 5661 (94%) | 336 (6%) | 3 (0%)   | 49          | 68  |

All (3) Ramachandran outliers are listed below:

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

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

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|-------------|-----|
| 1   | aA    | 500/606 (82%) | 497 (99%) | 3 (1%)   | 78          | 91  |
| 1   | bA    | 500/606 (82%) | 497 (99%) | 3 (1%)   | 78          | 91  |
| 1   | cA    | 500/606 (82%) | 496 (99%) | 4 (1%)   | 73          | 88  |
| 2   | aB    | 471/594 (79%) | 467 (99%) | 4 (1%)   | 73          | 88  |
| 2   | bB    | 471/594 (79%) | 467 (99%) | 4 (1%)   | 73          | 88  |
| 2   | cB    | 471/594 (79%) | 467 (99%) | 4 (1%)   | 73          | 88  |
| 3   | aC    | 60/69 (87%)   | 58 (97%)  | 2 (3%)   | 33          | 61  |
| 3   | bC    | 60/69 (87%)   | 58 (97%)  | 2 (3%)   | 33          | 61  |
| 3   | cC    | 60/69 (87%)   | 58 (97%)  | 2 (3%)   | 33          | 61  |
| 4   | aD    | 99/112 (88%)  | 97 (98%)  | 2 (2%)   | 48          | 75  |
| 4   | bD    | 99/112 (88%)  | 97 (98%)  | 2 (2%)   | 48          | 75  |
| 4   | cD    | 99/112 (88%)  | 97 (98%)  | 2 (2%)   | 48          | 75  |
| 5   | aE    | 11/69 (16%)   | 11 (100%) | 0        | 100         | 100 |
| 5   | bE    | 11/69 (16%)   | 11 (100%) | 0        | 100         | 100 |
| 5   | cE    | 11/69 (16%)   | 11 (100%) | 0        | 100         | 100 |
| 6   | aF    | 62/133 (47%)  | 62 (100%) | 0        | 100         | 100 |
| 6   | bF    | 62/133 (47%)  | 62 (100%) | 0        | 100         | 100 |
| 6   | cF    | 62/133 (47%)  | 62 (100%) | 0        | 100         | 100 |
| 7   | aI    | 23/26 (88%)   | 23 (100%) | 0        | 100         | 100 |
| 7   | bI    | 23/26 (88%)   | 23 (100%) | 0        | 100         | 100 |
| 7   | cI    | 23/26 (88%)   | 23 (100%) | 0        | 100         | 100 |
| 8   | aJ    | 23/46 (50%)   | 23 (100%) | 0        | 100         | 100 |
| 8   | bJ    | 23/46 (50%)   | 23 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 8   | cJ    | 23/46 (50%)     | 23 (100%)  | 0        | 100         | 100 |
| 10  | aL    | 96/112 (86%)    | 96 (100%)  | 0        | 100         | 100 |
| 10  | bL    | 96/112 (86%)    | 96 (100%)  | 0        | 100         | 100 |
| 10  | cL    | 96/112 (86%)    | 96 (100%)  | 0        | 100         | 100 |
| 11  | aM    | 23/25 (92%)     | 22 (96%)   | 1 (4%)   | 26          | 51  |
| 11  | bM    | 23/25 (92%)     | 22 (96%)   | 1 (4%)   | 26          | 51  |
| 11  | cM    | 23/25 (92%)     | 22 (96%)   | 1 (4%)   | 26          | 51  |
| All | All   | 4104/5376 (76%) | 4067 (99%) | 37 (1%)  | 68          | 87  |

All (37) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | aA    | 222 | LEU  |
| 1   | aA    | 364 | SER  |
| 1   | aA    | 728 | VAL  |
| 2   | aB    | 57  | ILE  |
| 2   | aB    | 458 | ILE  |
| 2   | aB    | 606 | SER  |
| 2   | aB    | 729 | ILE  |
| 3   | aC    | 39  | ILE  |
| 3   | aC    | 63  | LEU  |
| 4   | aD    | 31  | ILE  |
| 4   | aD    | 50  | VAL  |
| 11  | aM    | 25  | LEU  |
| 1   | bA    | 222 | LEU  |
| 1   | bA    | 364 | SER  |
| 1   | bA    | 728 | VAL  |
| 2   | bB    | 57  | ILE  |
| 2   | bB    | 458 | ILE  |
| 2   | bB    | 606 | SER  |
| 2   | bB    | 729 | ILE  |
| 3   | bC    | 39  | ILE  |
| 3   | bC    | 63  | LEU  |
| 4   | bD    | 31  | ILE  |
| 4   | bD    | 50  | VAL  |
| 11  | bM    | 25  | LEU  |
| 1   | cA    | 222 | LEU  |
| 1   | cA    | 364 | SER  |
| 1   | cA    | 702 | ILE  |
| 1   | cA    | 728 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | cB    | 57  | ILE  |
| 2   | cB    | 458 | ILE  |
| 2   | cB    | 606 | SER  |
| 2   | cB    | 729 | ILE  |
| 3   | cC    | 39  | ILE  |
| 3   | cC    | 63  | LEU  |
| 4   | cD    | 31  | ILE  |
| 4   | cD    | 50  | VAL  |
| 11  | cM    | 25  | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | aA    | 80  | HIS  |
| 1   | aA    | 128 | ASN  |
| 1   | aA    | 356 | ASN  |
| 1   | aA    | 442 | ASN  |
| 1   | aA    | 491 | GLN  |
| 1   | aA    | 608 | ASN  |
| 2   | aB    | 34  | HIS  |
| 2   | aB    | 337 | HIS  |
| 2   | aB    | 685 | HIS  |
| 3   | aC    | 38  | GLN  |
| 4   | aD    | 38  | GLN  |
| 4   | aD    | 52  | ASN  |
| 1   | bA    | 80  | HIS  |
| 1   | bA    | 128 | ASN  |
| 1   | bA    | 442 | ASN  |
| 1   | bA    | 491 | GLN  |
| 1   | bA    | 608 | ASN  |
| 2   | bB    | 34  | HIS  |
| 2   | bB    | 337 | HIS  |
| 2   | bB    | 365 | HIS  |
| 2   | bB    | 685 | HIS  |
| 4   | bD    | 38  | GLN  |
| 4   | bD    | 52  | ASN  |
| 1   | cA    | 80  | HIS  |
| 1   | cA    | 128 | ASN  |
| 1   | cA    | 356 | ASN  |
| 1   | cA    | 442 | ASN  |
| 1   | cA    | 608 | ASN  |
| 2   | cB    | 34  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | cB    | 102 | GLN  |
| 2   | cB    | 337 | HIS  |
| 2   | cB    | 365 | HIS  |
| 2   | cB    | 685 | HIS  |
| 3   | cC    | 38  | GLN  |
| 4   | cD    | 38  | GLN  |
| 4   | cD    | 52  | ASN  |

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

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 12  | G9R  | cA    | 3101 | 1    | 69,73,73     | 2.21 | 19 (27%) | 83,113,113  | 3.42 | 37 (44%) |
| 14  | CL7  | bA    | 3126 | 1    | 58,61,73     | 2.36 | 19 (32%) | 66,97,113   | 1.51 | 12 (18%) |
| 14  | CL7  | aA    | 3142 | 1    | 71,73,73     | 2.21 | 24 (33%) | 80,113,113  | 1.57 | 16 (20%) |
| 14  | CL7  | cA    | 3113 | 1    | 47,49,73     | 2.59 | 20 (42%) | 51,84,113   | 1.80 | 13 (25%) |
| 14  | CL7  | cL    | 205  | 20   | 48,50,73     | 2.91 | 23 (47%) | 51,85,113   | 1.74 | 12 (23%) |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | CL7  | cB    | 808  | 2    | 71,73,73     | 2.27 | 25 (35%) | 80,113,113  | 1.97 | 17 (21%) |
| 14  | CL7  | cA    | 3130 | 1    | 47,49,73     | 2.67 | 20 (42%) | 51,84,113   | 1.65 | 12 (23%) |
| 14  | CL7  | bL    | 203  | 10   | 71,73,73     | 2.33 | 20 (28%) | 80,113,113  | 1.87 | 22 (27%) |
| 14  | CL7  | aA    | 3120 | 20   | 52,54,73     | 2.65 | 20 (38%) | 57,90,113   | 2.05 | 14 (24%) |
| 13  | PHO  | cB    | 805  | -    | 58,69,69     | 3.19 | 23 (39%) | 56,99,99    | 2.71 | 17 (30%) |
| 14  | CL7  | aF    | 201  | 2    | 43,46,73     | 2.69 | 20 (46%) | 46,80,113   | 1.74 | 8 (17%)  |
| 14  | CL7  | cA    | 3129 | 1    | 47,49,73     | 3.21 | 24 (51%) | 51,84,113   | 2.43 | 22 (43%) |
| 14  | CL7  | bB    | 827  | 2    | 71,73,73     | 2.50 | 27 (38%) | 80,113,113  | 1.97 | 28 (35%) |
| 14  | CL7  | bA    | 3103 | 1    | 47,49,73     | 2.60 | 20 (42%) | 51,84,113   | 1.79 | 14 (27%) |
| 14  | CL7  | bA    | 3129 | 1    | 47,49,73     | 3.23 | 27 (57%) | 51,84,113   | 2.45 | 22 (43%) |
| 14  | CL7  | aK    | 101  | -    | 45,45,73     | 2.49 | 18 (40%) | 49,78,113   | 1.69 | 12 (24%) |
| 14  | CL7  | cB    | 816  | 2    | 56,58,73     | 2.69 | 22 (39%) | 62,95,113   | 1.98 | 21 (33%) |
| 14  | CL7  | aA    | 3140 | -    | 71,73,73     | 2.14 | 17 (23%) | 80,113,113  | 1.53 | 13 (16%) |
| 14  | CL7  | aB    | 3009 | 2    | 71,73,73     | 2.39 | 27 (38%) | 80,113,113  | 1.82 | 23 (28%) |
| 14  | CL7  | bB    | 825  | 2    | 43,46,73     | 2.77 | 21 (48%) | 46,80,113   | 1.55 | 8 (17%)  |
| 14  | CL7  | cA    | 3139 | -    | 71,73,73     | 2.20 | 20 (28%) | 80,113,113  | 1.65 | 16 (20%) |
| 14  | CL7  | bA    | 3118 | -    | 43,46,73     | 2.65 | 20 (46%) | 46,80,113   | 1.64 | 8 (17%)  |
| 14  | CL7  | aA    | 3122 | 1    | 47,49,73     | 2.67 | 22 (46%) | 51,84,113   | 1.95 | 12 (23%) |
| 14  | CL7  | cB    | 823  | 2    | 47,49,73     | 2.57 | 20 (42%) | 51,84,113   | 2.08 | 18 (35%) |
| 18  | SF4  | bB    | 802  | 2,1  | 0,12,12      | -    | -        | -           | -    | -        |
| 14  | CL7  | bB    | 814  | 2    | 47,49,73     | 2.47 | 19 (40%) | 51,84,113   | 1.79 | 14 (27%) |
| 14  | CL7  | aA    | 3130 | 1    | 47,49,73     | 3.13 | 27 (57%) | 51,84,113   | 2.43 | 20 (39%) |
| 14  | CL7  | aB    | 3024 | 2    | 43,46,73     | 2.76 | 20 (46%) | 46,80,113   | 1.64 | 11 (23%) |
| 14  | CL7  | bB    | 817  | -    | 47,49,73     | 2.57 | 21 (44%) | 51,84,113   | 1.92 | 13 (25%) |
| 14  | CL7  | aB    | 3006 | 2    | 71,73,73     | 2.24 | 25 (35%) | 80,113,113  | 1.81 | 25 (31%) |
| 14  | CL7  | bB    | 832  | 2    | 71,73,73     | 2.32 | 23 (32%) | 80,113,113  | 1.83 | 20 (25%) |
| 14  | CL7  | cA    | 3124 | 1    | 71,73,73     | 2.46 | 27 (38%) | 80,113,113  | 2.22 | 21 (26%) |
| 14  | CL7  | cA    | 3106 | 1    | 71,73,73     | 2.43 | 26 (36%) | 80,113,113  | 1.75 | 20 (25%) |
| 14  | CL7  | cB    | 810  | 2    | 71,73,73     | 2.44 | 27 (38%) | 80,113,113  | 1.79 | 23 (28%) |
| 14  | CL7  | cB    | 821  | 2    | 43,46,73     | 2.59 | 20 (46%) | 46,80,113   | 1.58 | 9 (19%)  |
| 14  | CL7  | aA    | 3114 | 1    | 47,49,73     | 2.54 | 20 (42%) | 51,84,113   | 1.72 | 13 (25%) |
| 14  | CL7  | aA    | 3108 | 1    | 71,73,73     | 2.23 | 20 (28%) | 80,113,113  | 1.63 | 16 (20%) |
| 14  | CL7  | cA    | 3110 | 1    | 47,49,73     | 2.57 | 21 (44%) | 51,84,113   | 1.80 | 12 (23%) |
| 14  | CL7  | bA    | 3139 | -    | 71,73,73     | 2.25 | 18 (25%) | 80,113,113  | 1.62 | 14 (17%) |
| 14  | CL7  | cB    | 833  | 2    | 61,63,73     | 2.57 | 25 (40%) | 68,101,113  | 1.72 | 16 (23%) |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | CL7  | aA    | 3110 | 1    | 47,49,73     | 2.52 | 17 (36%) | 51,84,113   | 1.87 | 16 (31%) |
| 14  | CL7  | cA    | 3122 | 1    | 56,58,73     | 2.51 | 23 (41%) | 62,95,113   | 2.10 | 17 (27%) |
| 14  | CL7  | bA    | 3105 | 1    | 47,49,73     | 2.87 | 22 (46%) | 51,84,113   | 2.08 | 21 (41%) |
| 16  | LHG  | cA    | 3137 | -    | 48,48,48     | 0.97 | 5 (10%)  | 51,54,54    | 1.02 | 3 (5%)   |
| 17  | PQN  | bB    | 828  | -    | 34,34,34     | 2.48 | 13 (38%) | 42,45,45    | 1.55 | 6 (14%)  |
| 14  | CL7  | bL    | 204  | 10   | 71,73,73     | 2.37 | 21 (29%) | 80,113,113  | 1.99 | 23 (28%) |
| 14  | CL7  | cA    | 3125 | 1    | 71,73,73     | 2.37 | 24 (33%) | 80,113,113  | 2.00 | 23 (28%) |
| 14  | CL7  | aA    | 3109 | 1    | 48,50,73     | 2.60 | 18 (37%) | 51,85,113   | 1.87 | 17 (33%) |
| 18  | SF4  | bC    | 102  | 3    | 0,12,12      | -    | -        | -           | -    | -        |
| 14  | CL7  | aA    | 3117 | -    | 59,61,73     | 2.31 | 19 (32%) | 65,98,113   | 1.90 | 18 (27%) |
| 14  | CL7  | aB    | 3021 | 2    | 47,49,73     | 2.67 | 19 (40%) | 51,84,113   | 2.02 | 13 (25%) |
| 14  | CL7  | cB    | 826  | 20   | 71,73,73     | 2.43 | 25 (35%) | 80,113,113  | 1.75 | 22 (27%) |
| 14  | CL7  | aB    | 3011 | 2    | 43,46,73     | 2.70 | 21 (48%) | 46,80,113   | 1.60 | 10 (21%) |
| 17  | PQN  | cB    | 828  | -    | 34,34,34     | 2.55 | 13 (38%) | 42,45,45    | 1.51 | 6 (14%)  |
| 14  | CL7  | bB    | 824  | 2    | 62,64,73     | 2.43 | 20 (32%) | 69,102,113  | 1.72 | 19 (27%) |
| 14  | CL7  | cA    | 3131 | -    | 47,49,73     | 2.64 | 19 (40%) | 51,84,113   | 1.82 | 16 (31%) |
| 14  | CL7  | aA    | 3106 | 1    | 47,49,73     | 2.73 | 21 (44%) | 51,84,113   | 1.96 | 20 (39%) |
| 14  | CL7  | cA    | 3108 | 1    | 48,50,73     | 2.62 | 20 (41%) | 51,85,113   | 2.04 | 17 (33%) |
| 13  | PHO  | aA    | 3102 | -    | 58,69,69     | 3.52 | 18 (31%) | 56,99,99    | 2.32 | 15 (26%) |
| 14  | CL7  | cB    | 815  | 2    | 47,49,73     | 2.63 | 20 (42%) | 51,84,113   | 1.63 | 13 (25%) |
| 14  | CL7  | cB    | 819  | 2    | 62,64,73     | 2.83 | 25 (40%) | 69,102,113  | 1.82 | 15 (21%) |
| 19  | LMG  | cB    | 830  | -    | 52,52,55     | 0.92 | 3 (5%)   | 60,60,63    | 1.35 | 7 (11%)  |
| 14  | CL7  | cB    | 820  | 2    | 71,73,73     | 2.41 | 26 (36%) | 80,113,113  | 1.67 | 14 (17%) |
| 14  | CL7  | bA    | 3123 | 1    | 57,59,73     | 2.60 | 22 (38%) | 63,96,113   | 2.20 | 21 (33%) |
| 14  | CL7  | bA    | 3116 | -    | 59,61,73     | 2.38 | 20 (33%) | 65,98,113   | 1.91 | 18 (27%) |
| 13  | PHO  | bB    | 805  | -    | 58,69,69     | 3.14 | 23 (39%) | 56,99,99    | 2.59 | 16 (28%) |
| 14  | CL7  | cA    | 3117 | 1    | 43,46,73     | 2.63 | 19 (44%) | 46,80,113   | 1.67 | 12 (26%) |
| 14  | CL7  | aB    | 3013 | 2    | 47,49,73     | 2.47 | 20 (42%) | 51,84,113   | 1.79 | 14 (27%) |
| 14  | CL7  | bA    | 3131 | -    | 47,49,73     | 2.64 | 20 (42%) | 51,84,113   | 1.81 | 15 (29%) |
| 14  | CL7  | cB    | 807  | 2    | 71,73,73     | 2.25 | 24 (33%) | 80,113,113  | 1.77 | 24 (30%) |
| 16  | LHG  | bA    | 3137 | -    | 48,48,48     | 1.08 | 5 (10%)  | 51,54,54    | 0.97 | 3 (5%)   |
| 14  | CL7  | aA    | 3111 | 1    | 47,49,73     | 2.51 | 20 (42%) | 51,84,113   | 1.79 | 12 (23%) |
| 14  | CL7  | cA    | 3115 | 1    | 43,46,73     | 2.52 | 17 (39%) | 46,80,113   | 1.65 | 12 (26%) |
| 14  | CL7  | aB    | 3019 | 2    | 71,73,73     | 2.39 | 26 (36%) | 80,113,113  | 1.77 | 19 (23%) |
| 14  | CL7  | aJ    | 101  | 8    | 47,50,73     | 2.56 | 18 (38%) | 51,85,113   | 1.52 | 10 (19%) |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 17  | PQN  | aA    | 3144 | -    | 34,34,34     | 2.03 | 11 (32%) | 42,45,45    | 1.34 | 5 (11%)  |
| 14  | CL7  | bA    | 3107 | 1    | 71,73,73     | 2.30 | 21 (29%) | 80,113,113  | 1.67 | 16 (20%) |
| 13  | PHO  | bB    | 801  | -    | 58,69,69     | 3.59 | 18 (31%) | 56,99,99    | 2.25 | 15 (26%) |
| 14  | CL7  | cA    | 3114 | 1    | 71,73,73     | 2.20 | 23 (32%) | 80,113,113  | 1.92 | 26 (32%) |
| 14  | CL7  | cF    | 201  | 2    | 43,46,73     | 2.69 | 21 (48%) | 46,80,113   | 1.72 | 7 (15%)  |
| 14  | CL7  | aA    | 3127 | 1    | 58,61,73     | 2.36 | 20 (34%) | 66,97,113   | 1.47 | 12 (18%) |
| 14  | CL7  | bA    | 3111 | 1    | 43,46,73     | 2.66 | 18 (41%) | 46,80,113   | 1.69 | 9 (19%)  |
| 14  | CL7  | cA    | 3103 | 1    | 47,49,73     | 2.62 | 20 (42%) | 51,84,113   | 1.74 | 16 (31%) |
| 14  | CL7  | cA    | 3119 | 20   | 52,54,73     | 2.77 | 23 (44%) | 57,90,113   | 2.18 | 15 (26%) |
| 14  | CL7  | bA    | 3109 | 1    | 47,49,73     | 2.59 | 17 (36%) | 51,84,113   | 1.88 | 17 (33%) |
| 18  | SF4  | cB    | 802  | 2,1  | 0,12,12      | -    | -        | -           | -    | -        |
| 14  | CL7  | aB    | 3022 | 2    | 47,49,73     | 2.56 | 20 (42%) | 51,84,113   | 2.07 | 18 (35%) |
| 14  | CL7  | cB    | 804  | 2    | 71,73,73     | 2.61 | 31 (43%) | 80,113,113  | 1.94 | 20 (25%) |
| 14  | CL7  | aB    | 3031 | 2    | 71,73,73     | 2.36 | 24 (33%) | 80,113,113  | 1.93 | 20 (25%) |
| 18  | SF4  | bC    | 101  | 3    | 0,12,12      | -    | -        | -           | -    | -        |
| 14  | CL7  | bB    | 808  | 2    | 71,73,73     | 2.30 | 23 (32%) | 80,113,113  | 1.91 | 19 (23%) |
| 14  | CL7  | bJ    | 101  | 8    | 47,50,73     | 2.56 | 17 (36%) | 51,85,113   | 1.55 | 8 (15%)  |
| 14  | CL7  | bK    | 101  | -    | 45,45,73     | 2.59 | 19 (42%) | 49,78,113   | 1.76 | 12 (24%) |
| 14  | CL7  | aB    | 3012 | 2    | 43,46,73     | 2.68 | 18 (41%) | 46,80,113   | 1.61 | 11 (23%) |
| 14  | CL7  | cA    | 3111 | 1    | 43,46,73     | 2.66 | 18 (41%) | 46,80,113   | 1.72 | 10 (21%) |
| 16  | LHG  | cA    | 3138 | 14   | 20,20,48     | 1.60 | 4 (20%)  | 22,25,54    | 1.17 | 2 (9%)   |
| 16  | LHG  | bA    | 3138 | 14   | 20,20,48     | 1.64 | 4 (20%)  | 22,25,54    | 1.25 | 2 (9%)   |
| 14  | CL7  | aA    | 3129 | 1    | 71,73,73     | 2.27 | 20 (28%) | 80,113,113  | 1.85 | 24 (30%) |
| 14  | CL7  | aA    | 3105 | 1    | 47,49,73     | 2.58 | 20 (42%) | 51,84,113   | 1.81 | 12 (23%) |
| 14  | CL7  | aA    | 3116 | 1    | 43,46,73     | 2.51 | 16 (37%) | 46,80,113   | 1.66 | 12 (26%) |
| 14  | CL7  | aL    | 204  | 20   | 48,50,73     | 2.89 | 23 (47%) | 51,85,113   | 1.70 | 15 (29%) |
| 14  | CL7  | cK    | 101  | -    | 45,45,73     | 2.55 | 20 (44%) | 49,78,113   | 1.61 | 10 (20%) |
| 14  | CL7  | bB    | 809  | 2    | 56,58,73     | 2.63 | 26 (46%) | 62,95,113   | 1.95 | 19 (30%) |
| 14  | CL7  | bA    | 3119 | 20   | 52,54,73     | 2.77 | 22 (42%) | 57,90,113   | 2.14 | 16 (28%) |
| 14  | CL7  | aB    | 3015 | 2    | 56,58,73     | 2.70 | 25 (44%) | 62,95,113   | 1.90 | 13 (20%) |
| 14  | CL7  | bB    | 821  | 2    | 43,46,73     | 2.58 | 19 (44%) | 46,80,113   | 1.55 | 9 (19%)  |
| 12  | G9R  | aA    | 3101 | 1    | 69,73,73     | 2.12 | 21 (30%) | 83,113,113  | 3.44 | 34 (40%) |
| 14  | CL7  | cB    | 831  | 2    | 60,62,73     | 2.31 | 23 (38%) | 66,99,113   | 1.67 | 16 (24%) |
| 14  | CL7  | aB    | 3020 | 2    | 43,46,73     | 2.59 | 19 (44%) | 46,80,113   | 1.56 | 9 (19%)  |
| 14  | CL7  | aL    | 202  | 10   | 71,73,73     | 2.29 | 20 (28%) | 80,113,113  | 1.80 | 19 (23%) |



| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | CL7  | bA    | 3113 | 1    | 47,49,73     | 2.60 | 20 (42%) | 51,84,113   | 1.75 | 13 (25%) |
| 14  | CL7  | aL    | 203  | 10   | 71,73,73     | 2.33 | 24 (33%) | 80,113,113  | 1.92 | 25 (31%) |
| 14  | CL7  | cA    | 3104 | 1    | 47,49,73     | 2.62 | 20 (42%) | 51,84,113   | 1.83 | 13 (25%) |
| 14  | CL7  | bB    | 826  | 20   | 71,73,73     | 2.41 | 24 (33%) | 80,113,113  | 1.73 | 20 (25%) |
| 14  | CL7  | cB    | 818  | 2    | 47,49,73     | 2.55 | 19 (40%) | 51,84,113   | 1.70 | 14 (27%) |
| 14  | CL7  | cA    | 3121 | 1    | 47,49,73     | 2.79 | 24 (51%) | 51,84,113   | 1.97 | 14 (27%) |
| 14  | CL7  | bA    | 3125 | 1    | 71,73,73     | 2.43 | 25 (35%) | 80,113,113  | 2.03 | 18 (22%) |
| 14  | CL7  | bB    | 818  | 2    | 47,49,73     | 2.57 | 20 (42%) | 51,84,113   | 1.82 | 14 (27%) |
| 14  | CL7  | cA    | 3116 | -    | 59,61,73     | 2.40 | 20 (33%) | 65,98,113   | 1.99 | 20 (30%) |
| 14  | CL7  | cB    | 822  | 2    | 47,49,73     | 2.66 | 20 (42%) | 51,84,113   | 2.09 | 12 (23%) |
| 14  | CL7  | bB    | 811  | 2    | 47,49,73     | 2.68 | 19 (40%) | 51,84,113   | 1.85 | 14 (27%) |
| 14  | CL7  | aA    | 3143 | 1    | 71,73,73     | 2.33 | 22 (30%) | 80,113,113  | 1.65 | 16 (20%) |
| 14  | CL7  | cA    | 3102 | 20   | 71,73,73     | 2.49 | 23 (32%) | 80,113,113  | 2.18 | 28 (35%) |
| 14  | CL7  | cB    | 811  | 2    | 47,49,73     | 2.66 | 17 (36%) | 51,84,113   | 1.76 | 13 (25%) |
| 14  | CL7  | bB    | 815  | 2    | 47,49,73     | 2.63 | 21 (44%) | 51,84,113   | 1.63 | 14 (27%) |
| 14  | CL7  | cA    | 3142 | 1    | 71,73,73     | 2.39 | 21 (29%) | 80,113,113  | 1.70 | 17 (21%) |
| 14  | CL7  | cA    | 3105 | 1    | 47,49,73     | 2.88 | 21 (44%) | 51,84,113   | 2.08 | 20 (39%) |
| 14  | CL7  | bB    | 804  | 2    | 71,73,73     | 2.66 | 30 (42%) | 80,113,113  | 1.99 | 23 (28%) |
| 14  | CL7  | aB    | 3016 | -    | 47,49,73     | 2.58 | 20 (42%) | 51,84,113   | 1.92 | 13 (25%) |
| 13  | PHO  | aB    | 3004 | -    | 58,69,69     | 3.19 | 22 (37%) | 56,99,99    | 2.65 | 17 (30%) |
| 14  | CL7  | bB    | 803  | 20   | 71,73,73     | 2.35 | 26 (36%) | 80,113,113  | 2.02 | 18 (22%) |
| 14  | CL7  | cA    | 3112 | 1    | 47,49,73     | 2.59 | 20 (42%) | 51,84,113   | 1.78 | 13 (25%) |
| 14  | CL7  | bA    | 3124 | 1    | 71,73,73     | 2.45 | 28 (39%) | 80,113,113  | 2.19 | 20 (25%) |
| 14  | CL7  | bA    | 3121 | 1    | 47,49,73     | 2.81 | 25 (53%) | 51,84,113   | 1.98 | 16 (31%) |
| 14  | CL7  | cA    | 3144 | -    | 47,49,73     | 2.50 | 19 (40%) | 51,84,113   | 1.77 | 14 (27%) |
| 14  | CL7  | bA    | 3106 | 1    | 71,73,73     | 2.38 | 25 (35%) | 80,113,113  | 1.76 | 22 (27%) |
| 14  | CL7  | cL    | 204  | 10   | 71,73,73     | 2.43 | 23 (32%) | 80,113,113  | 1.91 | 23 (28%) |
| 14  | CL7  | bB    | 819  | 2    | 62,64,73     | 2.82 | 25 (40%) | 69,102,113  | 1.81 | 17 (24%) |
| 14  | CL7  | cA    | 3140 | 1    | 71,73,73     | 2.30 | 21 (29%) | 80,113,113  | 1.80 | 21 (26%) |
| 18  | SF4  | aC    | 102  | 3    | 0,12,12      | -    | -        | -           | -    | -        |
| 14  | CL7  | bA    | 3141 | 1    | 71,73,73     | 2.26 | 25 (35%) | 80,113,113  | 1.59 | 13 (16%) |
| 14  | CL7  | bA    | 3145 | -    | 47,49,73     | 2.51 | 19 (40%) | 51,84,113   | 1.79 | 13 (25%) |
| 14  | CL7  | cL    | 203  | 10   | 71,73,73     | 2.30 | 21 (29%) | 80,113,113  | 1.76 | 18 (22%) |
| 14  | CL7  | aB    | 3030 | 2    | 60,62,73     | 2.34 | 23 (38%) | 66,99,113   | 1.71 | 15 (22%) |
| 14  | CL7  | cB    | 809  | 2    | 56,58,73     | 2.56 | 24 (42%) | 62,95,113   | 1.87 | 15 (24%) |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | CL7  | aA    | 3107 | 1    | 71,73,73     | 2.27 | 27 (38%) | 80,113,113  | 1.71 | 20 (25%) |
| 14  | CL7  | cB    | 814  | 2    | 47,49,73     | 2.47 | 19 (40%) | 51,84,113   | 1.77 | 14 (27%) |
| 14  | CL7  | bA    | 3104 | 1    | 47,49,73     | 2.61 | 20 (42%) | 51,84,113   | 1.80 | 14 (27%) |
| 18  | SF4  | aB    | 3001 | 2,1  | 0,12,12      | -    | -        | -           |      |          |
| 14  | CL7  | aA    | 3103 | 20   | 71,73,73     | 2.40 | 24 (33%) | 80,113,113  | 1.98 | 23 (28%) |
| 14  | CL7  | bL    | 205  | 20   | 48,50,73     | 2.89 | 25 (52%) | 51,85,113   | 1.75 | 14 (27%) |
| 14  | CL7  | cA    | 3123 | 1    | 57,59,73     | 2.71 | 28 (49%) | 63,96,113   | 2.22 | 18 (28%) |
| 14  | CL7  | bF    | 201  | 2    | 43,46,73     | 2.68 | 21 (48%) | 46,80,113   | 1.69 | 8 (17%)  |
| 17  | PQN  | bA    | 3143 | -    | 34,34,34     | 2.06 | 12 (35%) | 42,45,45    | 1.67 | 6 (14%)  |
| 14  | CL7  | aA    | 3104 | 1    | 47,49,73     | 2.55 | 20 (42%) | 51,84,113   | 1.73 | 16 (31%) |
| 14  | CL7  | aB    | 3010 | 2    | 47,49,73     | 2.62 | 18 (38%) | 51,84,113   | 1.84 | 14 (27%) |
| 14  | CL7  | cB    | 827  | 2    | 71,73,73     | 2.51 | 28 (39%) | 80,113,113  | 1.91 | 21 (26%) |
| 14  | CL7  | cB    | 832  | 2    | 71,73,73     | 2.36 | 24 (33%) | 80,113,113  | 1.83 | 20 (25%) |
| 16  | LHG  | aA    | 3138 | -    | 48,48,48     | 0.97 | 4 (8%)   | 51,54,54    | 0.95 | 3 (5%)   |
| 14  | CL7  | bA    | 3132 | 20   | 71,73,73     | 2.62 | 31 (43%) | 80,113,113  | 1.86 | 22 (27%) |
| 14  | CL7  | aB    | 3005 | 2    | 71,73,73     | 2.52 | 24 (33%) | 80,113,113  | 1.63 | 18 (22%) |
| 14  | CL7  | cB    | 813  | 2    | 43,46,73     | 2.68 | 18 (41%) | 46,80,113   | 1.62 | 9 (19%)  |
| 12  | G9R  | bA    | 3101 | 1    | 69,73,73     | 2.18 | 22 (31%) | 83,113,113  | 3.70 | 38 (45%) |
| 14  | CL7  | bB    | 820  | 2    | 71,73,73     | 2.39 | 28 (39%) | 80,113,113  | 1.74 | 17 (21%) |
| 14  | CL7  | aA    | 3113 | 1    | 47,49,73     | 2.52 | 20 (42%) | 51,84,113   | 1.77 | 14 (27%) |
| 14  | CL7  | bB    | 810  | 2    | 71,73,73     | 2.41 | 25 (35%) | 80,113,113  | 1.76 | 20 (25%) |
| 14  | CL7  | cA    | 3107 | 1    | 71,73,73     | 2.28 | 21 (29%) | 80,113,113  | 1.63 | 16 (20%) |
| 14  | CL7  | cA    | 3118 | -    | 43,46,73     | 2.60 | 19 (44%) | 46,80,113   | 1.77 | 10 (21%) |
| 14  | CL7  | aA    | 3128 | 1    | 57,59,73     | 2.60 | 22 (38%) | 63,96,113   | 1.83 | 19 (30%) |
| 14  | CL7  | cA    | 3109 | 1    | 47,49,73     | 2.58 | 17 (36%) | 51,84,113   | 1.87 | 16 (31%) |
| 14  | CL7  | bA    | 3108 | 1    | 48,50,73     | 2.72 | 22 (45%) | 51,85,113   | 1.89 | 18 (35%) |
| 17  | PQN  | aB    | 3027 | -    | 34,34,34     | 2.53 | 14 (41%) | 42,45,45    | 1.47 | 6 (14%)  |
| 14  | CL7  | aA    | 3125 | 1    | 71,73,73     | 2.33 | 27 (38%) | 80,113,113  | 2.05 | 21 (26%) |
| 14  | CL7  | cA    | 3127 | 1    | 57,59,73     | 2.67 | 25 (43%) | 63,96,113   | 1.91 | 20 (31%) |
| 14  | CL7  | cB    | 817  | -    | 47,49,73     | 2.59 | 21 (44%) | 51,84,113   | 1.92 | 14 (27%) |
| 14  | CL7  | aA    | 3131 | 1    | 47,49,73     | 2.62 | 20 (42%) | 51,84,113   | 1.65 | 12 (23%) |
| 14  | CL7  | bA    | 3128 | 1    | 71,73,73     | 2.51 | 27 (38%) | 80,113,113  | 2.01 | 28 (35%) |
| 14  | CL7  | bA    | 3130 | 1    | 47,49,73     | 2.66 | 21 (44%) | 51,84,113   | 1.65 | 12 (23%) |
| 14  | CL7  | aA    | 3146 | -    | 47,49,73     | 2.48 | 19 (40%) | 51,84,113   | 1.87 | 14 (27%) |
| 14  | CL7  | bB    | 816  | 2    | 56,58,73     | 2.69 | 23 (41%) | 62,95,113   | 2.06 | 19 (30%) |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 19  | LMG  | aB    | 3029 | -    | 52,52,55     | 0.86 | 1 (1%)   | 60,60,63    | 1.22 | 7 (11%)  |
| 19  | LMG  | bB    | 830  | -    | 52,52,55     | 0.97 | 3 (5%)   | 60,60,63    | 1.28 | 6 (10%)  |
| 14  | CL7  | aB    | 3018 | 2    | 62,64,73     | 2.82 | 25 (40%) | 69,102,113  | 1.92 | 17 (24%) |
| 14  | CL7  | aB    | 3017 | 2    | 47,49,73     | 2.56 | 18 (38%) | 51,84,113   | 1.81 | 14 (27%) |
| 14  | CL7  | cA    | 3126 | 1    | 58,61,73     | 2.36 | 20 (34%) | 66,97,113   | 1.78 | 16 (24%) |
| 14  | CL7  | aA    | 3123 | 1    | 56,58,73     | 2.44 | 20 (35%) | 62,95,113   | 2.08 | 20 (32%) |
| 14  | CL7  | bA    | 3115 | 1    | 43,46,73     | 2.53 | 17 (39%) | 46,80,113   | 1.64 | 13 (28%) |
| 14  | CL7  | bB    | 822  | 2    | 47,49,73     | 2.66 | 19 (40%) | 51,84,113   | 1.96 | 10 (19%) |
| 14  | CL7  | aA    | 3119 | -    | 43,46,73     | 2.58 | 18 (41%) | 46,80,113   | 1.77 | 10 (21%) |
| 14  | CL7  | aA    | 3121 | 1    | 57,59,73     | 2.46 | 20 (35%) | 63,96,113   | 1.99 | 16 (25%) |
| 14  | CL7  | aB    | 3008 | 2    | 56,58,73     | 2.53 | 26 (46%) | 62,95,113   | 1.83 | 19 (30%) |
| 14  | CL7  | bA    | 3117 | 1    | 43,46,73     | 2.64 | 19 (44%) | 46,80,113   | 1.68 | 12 (26%) |
| 18  | SF4  | cC    | 101  | 3    | 0,12,12      | -    | -        | -           | -    | -        |
| 14  | CL7  | aB    | 3032 | 2    | 61,63,73     | 2.54 | 27 (44%) | 68,101,113  | 1.74 | 17 (25%) |
| 14  | CL7  | bB    | 831  | 2    | 60,62,73     | 2.35 | 23 (38%) | 66,99,113   | 1.68 | 16 (24%) |
| 14  | CL7  | aA    | 3141 | 1    | 71,73,73     | 2.18 | 21 (29%) | 80,113,113  | 1.63 | 19 (23%) |
| 14  | CL7  | bB    | 823  | 2    | 47,49,73     | 2.56 | 19 (40%) | 51,84,113   | 2.11 | 18 (35%) |
| 14  | CL7  | aA    | 3134 | 16   | 47,49,73     | 2.52 | 19 (40%) | 51,84,113   | 1.83 | 13 (25%) |
| 14  | CL7  | cB    | 825  | 2    | 43,46,73     | 2.75 | 20 (46%) | 46,80,113   | 1.68 | 11 (23%) |
| 14  | CL7  | cB    | 812  | 2    | 43,46,73     | 2.68 | 21 (48%) | 46,80,113   | 1.63 | 10 (21%) |
| 14  | CL7  | cB    | 824  | 2    | 62,64,73     | 2.42 | 20 (32%) | 69,102,113  | 1.75 | 16 (23%) |
| 16  | LHG  | aA    | 3139 | 14   | 20,20,48     | 1.51 | 3 (15%)  | 22,25,54    | 1.28 | 3 (13%)  |
| 14  | CL7  | aB    | 3002 | 20   | 71,73,73     | 2.33 | 25 (35%) | 80,113,113  | 1.84 | 16 (20%) |
| 14  | CL7  | aB    | 3014 | 2    | 47,49,73     | 2.56 | 19 (40%) | 51,84,113   | 1.59 | 11 (21%) |
| 14  | CL7  | bA    | 3140 | 1    | 71,73,73     | 2.31 | 21 (29%) | 80,113,113  | 1.79 | 18 (22%) |
| 14  | CL7  | bB    | 812  | 2    | 43,46,73     | 2.68 | 21 (48%) | 46,80,113   | 1.62 | 10 (21%) |
| 14  | CL7  | bB    | 833  | 2    | 61,63,73     | 2.55 | 25 (40%) | 68,101,113  | 1.69 | 17 (25%) |
| 14  | CL7  | cA    | 3128 | 1    | 71,73,73     | 2.47 | 25 (35%) | 80,113,113  | 1.91 | 25 (31%) |
| 14  | CL7  | bB    | 807  | 2    | 71,73,73     | 2.24 | 25 (35%) | 80,113,113  | 1.78 | 22 (27%) |
| 14  | CL7  | aA    | 3124 | 1    | 57,59,73     | 2.60 | 24 (42%) | 63,96,113   | 2.03 | 20 (31%) |
| 14  | CL7  | aA    | 3132 | -    | 47,49,73     | 2.58 | 19 (40%) | 51,84,113   | 1.86 | 16 (31%) |
| 14  | CL7  | bA    | 3122 | 1    | 56,58,73     | 2.51 | 21 (37%) | 62,95,113   | 2.10 | 20 (32%) |
| 14  | CL7  | cA    | 3133 | 16   | 47,49,73     | 2.57 | 20 (42%) | 51,84,113   | 1.86 | 14 (27%) |
| 14  | CL7  | bA    | 3102 | 20   | 71,73,73     | 2.52 | 26 (36%) | 80,113,113  | 2.09 | 26 (32%) |
| 14  | CL7  | cB    | 803  | 20   | 71,73,73     | 2.38 | 26 (36%) | 80,113,113  | 2.04 | 22 (27%) |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | CL7  | cJ    | 101  | 8    | 47,50,73     | 2.54 | 19 (40%) | 51,85,113   | 1.51 | 8 (15%)  |
| 14  | CL7  | bA    | 3133 | 16   | 47,49,73     | 2.56 | 21 (44%) | 51,84,113   | 1.90 | 13 (25%) |
| 14  | CL7  | aB    | 3003 | 2    | 71,73,73     | 2.55 | 30 (42%) | 80,113,113  | 1.89 | 20 (25%) |
| 18  | SF4  | aC    | 101  | 3    | 0,12,12      | -    | -        | -           |      |          |
| 14  | CL7  | aB    | 3025 | 20   | 71,73,73     | 2.43 | 24 (33%) | 80,113,113  | 1.85 | 23 (28%) |
| 14  | CL7  | cA    | 3141 | 1    | 71,73,73     | 2.25 | 22 (30%) | 80,113,113  | 1.66 | 15 (18%) |
| 14  | CL7  | aB    | 3007 | 2    | 71,73,73     | 2.30 | 27 (38%) | 80,113,113  | 1.94 | 20 (25%) |
| 14  | CL7  | bA    | 3127 | 1    | 57,59,73     | 2.61 | 23 (40%) | 63,96,113   | 1.92 | 19 (30%) |
| 14  | CL7  | bA    | 3142 | 1    | 71,73,73     | 2.39 | 21 (29%) | 80,113,113  | 1.70 | 18 (22%) |
| 14  | CL7  | bA    | 3114 | 1    | 71,73,73     | 2.20 | 23 (32%) | 80,113,113  | 1.93 | 24 (30%) |
| 14  | CL7  | cA    | 3120 | 1    | 57,59,73     | 2.50 | 23 (40%) | 63,96,113   | 1.83 | 17 (26%) |
| 14  | CL7  | aA    | 3112 | 1    | 43,46,73     | 2.64 | 17 (39%) | 46,80,113   | 1.64 | 10 (21%) |
| 14  | CL7  | aB    | 3026 | 2    | 71,73,73     | 2.60 | 28 (39%) | 80,113,113  | 1.91 | 24 (30%) |
| 14  | CL7  | bB    | 806  | 2    | 71,73,73     | 2.53 | 23 (32%) | 80,113,113  | 1.61 | 15 (18%) |
| 14  | CL7  | cB    | 806  | 2    | 71,73,73     | 2.50 | 24 (33%) | 80,113,113  | 1.67 | 17 (21%) |
| 14  | CL7  | bB    | 813  | 2    | 43,46,73     | 2.68 | 18 (41%) | 46,80,113   | 1.62 | 10 (21%) |
| 17  | PQN  | cA    | 3143 | -    | 34,34,34     | 2.07 | 10 (29%) | 42,45,45    | 1.62 | 6 (14%)  |
| 14  | CL7  | aB    | 3023 | 2    | 62,64,73     | 2.46 | 21 (33%) | 69,102,113  | 1.70 | 16 (23%) |
| 14  | CL7  | aA    | 3118 | 1    | 43,46,73     | 2.59 | 19 (44%) | 46,80,113   | 1.63 | 11 (23%) |
| 14  | CL7  | bA    | 3112 | 1    | 47,49,73     | 2.60 | 21 (44%) | 51,84,113   | 1.78 | 13 (25%) |
| 14  | CL7  | bA    | 3110 | 1    | 47,49,73     | 2.59 | 20 (42%) | 51,84,113   | 1.78 | 12 (23%) |
| 13  | PHO  | cB    | 801  | -    | 58,69,69     | 3.57 | 18 (31%) | 56,99,99    | 2.32 | 15 (26%) |
| 14  | CL7  | cA    | 3132 | 20   | 71,73,73     | 2.58 | 31 (43%) | 80,113,113  | 1.94 | 26 (32%) |
| 14  | CL7  | aA    | 3126 | 1    | 71,73,73     | 2.32 | 23 (32%) | 80,113,113  | 1.74 | 21 (26%) |
| 14  | CL7  | aA    | 3115 | 1    | 71,73,73     | 2.11 | 20 (28%) | 80,113,113  | 1.83 | 24 (30%) |
| 14  | CL7  | aA    | 3133 | 20   | 71,73,73     | 2.54 | 30 (42%) | 80,113,113  | 1.89 | 23 (28%) |
| 14  | CL7  | bA    | 3120 | 1    | 57,59,73     | 2.48 | 23 (40%) | 63,96,113   | 1.88 | 16 (25%) |
| 18  | SF4  | cC    | 102  | 3    | 0,12,12      | -    | -        | -           |      |          |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res  | Link | Chirals   | Torsions     | Rings |
|-----|------|-------|------|------|-----------|--------------|-------|
| 12  | G9R  | cA    | 3101 | 1    | 1/1/15/20 | 5/39/115/115 | -     |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14  | CL7  | bA    | 3126 | 1    | 1/1/11/20 | 12/26/98/115  | -       |
| 14  | CL7  | aA    | 3142 | 1    | 2/2/15/20 | 16/39/115/115 | -       |
| 14  | CL7  | cA    | 3113 | 1    | 1/1/10/20 | 0/10/86/115   | -       |
| 14  | CL7  | cL    | 205  | 20   | 2/2/10/20 | 2/12/88/115   | -       |
| 14  | CL7  | cB    | 808  | 2    | 2/2/15/20 | 16/39/115/115 | -       |
| 14  | CL7  | cA    | 3130 | 1    | 2/2/10/20 | 4/10/86/115   | -       |
| 14  | CL7  | bL    | 203  | 10   | 2/2/15/20 | 23/39/115/115 | -       |
| 14  | CL7  | aA    | 3120 | 20   | 2/2/11/20 | 3/17/93/115   | -       |
| 14  | CL7  | aF    | 201  | 2    | 2/2/9/20  | 0/4/80/115    | -       |
| 13  | PHO  | cB    | 805  | -    | -         | 19/37/103/103 | 0/5/6/6 |
| 14  | CL7  | cA    | 3129 | 1    | 1/1/10/20 | 2/10/86/115   | -       |
| 14  | CL7  | bB    | 827  | 2    | 2/2/15/20 | 16/39/115/115 | -       |
| 14  | CL7  | bA    | 3103 | 1    | 2/2/10/20 | 4/10/86/115   | -       |
| 14  | CL7  | bA    | 3129 | 1    | 1/1/10/20 | 2/10/86/115   | -       |
| 14  | CL7  | aK    | 101  | -    | 2/2/8/20  | 2/4/76/115    | -       |
| 14  | CL7  | cB    | 816  | 2    | 2/2/12/20 | 6/21/97/115   | -       |
| 14  | CL7  | aA    | 3140 | -    | 2/2/15/20 | 20/39/115/115 | -       |
| 14  | CL7  | aB    | 3009 | 2    | 2/2/15/20 | 19/39/115/115 | -       |
| 14  | CL7  | bB    | 825  | 2    | 2/2/9/20  | 0/4/80/115    | -       |
| 14  | CL7  | cA    | 3139 | -    | 2/2/15/20 | 18/39/115/115 | -       |
| 14  | CL7  | bA    | 3118 | -    | 2/2/9/20  | 0/4/80/115    | -       |
| 14  | CL7  | aA    | 3122 | 1    | 1/1/10/20 | 2/10/86/115   | -       |
| 14  | CL7  | cB    | 823  | 2    | 2/2/10/20 | 7/10/86/115   | -       |
| 18  | SF4  | bB    | 802  | 2,1  | -         | -             | 0/6/5/5 |
| 14  | CL7  | bB    | 814  | 2    | 1/1/10/20 | 3/10/86/115   | -       |
| 14  | CL7  | aA    | 3130 | 1    | 1/1/10/20 | 3/10/86/115   | -       |
| 14  | CL7  | aB    | 3024 | 2    | 2/2/9/20  | 0/4/80/115    | -       |
| 14  | CL7  | bB    | 817  | -    | 2/2/10/20 | 6/10/86/115   | -       |
| 14  | CL7  | aB    | 3006 | 2    | 1/1/15/20 | 15/39/115/115 | -       |
| 14  | CL7  | bB    | 832  | 2    | 2/2/15/20 | 18/39/115/115 | -       |
| 14  | CL7  | cA    | 3124 | 1    | 2/2/15/20 | 11/39/115/115 | -       |
| 14  | CL7  | cA    | 3106 | 1    | 2/2/15/20 | 18/39/115/115 | -       |
| 14  | CL7  | cB    | 810  | 2    | 2/2/15/20 | 18/39/115/115 | -       |
| 14  | CL7  | cB    | 821  | 2    | 1/1/9/20  | 2/4/80/115    | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14  | CL7  | aA    | 3114 | 1    | 2/2/10/20 | 2/10/86/115   | -       |
| 14  | CL7  | aA    | 3108 | 1    | 1/1/15/20 | 16/39/115/115 | -       |
| 14  | CL7  | cA    | 3110 | 1    | 1/1/10/20 | 2/10/86/115   | -       |
| 14  | CL7  | bA    | 3139 | -    | 2/2/15/20 | 19/39/115/115 | -       |
| 14  | CL7  | cB    | 833  | 2    | 2/2/13/20 | 11/27/103/115 | -       |
| 14  | CL7  | aA    | 3110 | 1    | 2/2/10/20 | 2/10/86/115   | -       |
| 14  | CL7  | cA    | 3122 | 1    | 2/2/12/20 | 10/21/97/115  | -       |
| 14  | CL7  | bA    | 3105 | 1    | 2/2/10/20 | 4/10/86/115   | -       |
| 16  | LHG  | cA    | 3137 | -    | -         | 15/53/53/53   | -       |
| 17  | PQN  | bB    | 828  | -    | -         | 7/23/43/43    | 0/2/2/2 |
| 14  | CL7  | bL    | 204  | 10   | 2/2/15/20 | 12/39/115/115 | -       |
| 14  | CL7  | cA    | 3125 | 1    | 2/2/15/20 | 11/39/115/115 | -       |
| 14  | CL7  | aA    | 3109 | 1    | 1/1/10/20 | 5/12/88/115   | -       |
| 18  | SF4  | bC    | 102  | 3    | -         | -             | 0/6/5/5 |
| 14  | CL7  | aA    | 3117 | -    | 2/2/12/20 | 10/25/101/115 | -       |
| 14  | CL7  | aB    | 3021 | 2    | 1/1/10/20 | 5/10/86/115   | -       |
| 14  | CL7  | cB    | 826  | 20   | 2/2/15/20 | 18/39/115/115 | -       |
| 14  | CL7  | aB    | 3011 | 2    | 2/2/9/20  | 2/4/80/115    | -       |
| 17  | PQN  | cB    | 828  | -    | -         | 8/23/43/43    | 0/2/2/2 |
| 14  | CL7  | bB    | 824  | 2    | 2/2/13/20 | 12/29/105/115 | -       |
| 14  | CL7  | cA    | 3131 | -    | 2/2/10/20 | 7/10/86/115   | -       |
| 14  | CL7  | aA    | 3106 | 1    | 2/2/10/20 | 5/10/86/115   | -       |
| 14  | CL7  | cA    | 3108 | 1    | 1/1/10/20 | 6/12/88/115   | -       |
| 14  | CL7  | cB    | 819  | 2    | 2/2/13/20 | 11/29/105/115 | -       |
| 14  | CL7  | cB    | 815  | 2    | 2/2/10/20 | 1/10/86/115   | -       |
| 13  | PHO  | aA    | 3102 | -    | -         | 9/37/103/103  | 0/5/6/6 |
| 19  | LMG  | cB    | 830  | -    | -         | 18/47/67/70   | 0/1/1/1 |
| 14  | CL7  | cB    | 820  | 2    | 2/2/15/20 | 15/39/115/115 | -       |
| 14  | CL7  | bA    | 3123 | 1    | 2/2/12/20 | 6/23/99/115   | -       |
| 14  | CL7  | bA    | 3116 | -    | 2/2/12/20 | 11/25/101/115 | -       |
| 13  | PHO  | bB    | 805  | -    | -         | 19/37/103/103 | 0/5/6/6 |
| 14  | CL7  | cA    | 3117 | 1    | 2/2/9/20  | 2/4/80/115    | -       |
| 14  | CL7  | aB    | 3013 | 2    | 1/1/10/20 | 3/10/86/115   | -       |
| 14  | CL7  | bA    | 3131 | -    | 2/2/10/20 | 6/10/86/115   | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14  | CL7  | cB    | 807  | 2    | 1/1/15/20 | 16/39/115/115 | -       |
| 16  | LHG  | bA    | 3137 | -    | -         | 17/53/53/53   | -       |
| 14  | CL7  | aA    | 3111 | 1    | 1/1/10/20 | 2/10/86/115   | -       |
| 14  | CL7  | cA    | 3115 | 1    | 1/1/9/20  | 4/4/80/115    | -       |
| 14  | CL7  | aB    | 3019 | 2    | 2/2/15/20 | 18/39/115/115 | -       |
| 14  | CL7  | aJ    | 101  | 8    | 1/1/10/20 | 2/9/85/115    | -       |
| 17  | PQN  | aA    | 3144 | -    | -         | 14/23/43/43   | 0/2/2/2 |
| 14  | CL7  | bA    | 3107 | 1    | 1/1/15/20 | 14/39/115/115 | -       |
| 14  | CL7  | cA    | 3114 | 1    | 1/1/15/20 | 19/39/115/115 | -       |
| 14  | CL7  | cF    | 201  | 2    | 2/2/9/20  | 0/4/80/115    | -       |
| 13  | PHO  | bB    | 801  | -    | -         | 12/37/103/103 | 0/5/6/6 |
| 14  | CL7  | aA    | 3127 | 1    | 1/1/11/20 | 13/26/98/115  | -       |
| 14  | CL7  | bA    | 3111 | 1    | 2/2/9/20  | 1/4/80/115    | -       |
| 14  | CL7  | cA    | 3103 | 1    | 2/2/10/20 | 5/10/86/115   | -       |
| 14  | CL7  | cA    | 3119 | 20   | 2/2/11/20 | 3/17/93/115   | -       |
| 14  | CL7  | bA    | 3109 | 1    | 2/2/10/20 | 4/10/86/115   | -       |
| 18  | SF4  | cB    | 802  | 2,1  | -         | -             | 0/6/5/5 |
| 14  | CL7  | aB    | 3022 | 2    | 2/2/10/20 | 6/10/86/115   | -       |
| 14  | CL7  | cB    | 804  | 2    | 1/1/15/20 | 6/39/115/115  | -       |
| 14  | CL7  | aB    | 3031 | 2    | 2/2/15/20 | 17/39/115/115 | -       |
| 18  | SF4  | bC    | 101  | 3    | -         | -             | 0/6/5/5 |
| 14  | CL7  | bB    | 808  | 2    | 2/2/15/20 | 13/39/115/115 | -       |
| 14  | CL7  | bJ    | 101  | 8    | 1/1/10/20 | 6/9/85/115    | -       |
| 14  | CL7  | bK    | 101  | -    | 2/2/8/20  | 2/4/76/115    | -       |
| 14  | CL7  | aB    | 3012 | 2    | 2/2/9/20  | 0/4/80/115    | -       |
| 14  | CL7  | cA    | 3111 | 1    | 2/2/9/20  | 2/4/80/115    | -       |
| 16  | LHG  | cA    | 3138 | 14   | -         | 12/23/23/53   | -       |
| 16  | LHG  | bA    | 3138 | 14   | -         | 11/23/23/53   | -       |
| 14  | CL7  | aA    | 3129 | 1    | 2/2/15/20 | 18/39/115/115 | -       |
| 14  | CL7  | aA    | 3116 | 1    | 1/1/9/20  | 4/4/80/115    | -       |
| 14  | CL7  | aA    | 3105 | 1    | 2/2/10/20 | 5/10/86/115   | -       |
| 14  | CL7  | aL    | 204  | 20   | 2/2/10/20 | 2/12/88/115   | -       |
| 14  | CL7  | cK    | 101  | -    | 2/2/8/20  | 2/4/76/115    | -       |
| 14  | CL7  | bB    | 809  | 2    | 2/2/12/20 | 7/21/97/115   | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14  | CL7  | bA    | 3119 | 20   | 2/2/11/20 | 3/17/93/115   | -       |
| 14  | CL7  | aB    | 3015 | 2    | 2/2/12/20 | 6/21/97/115   | -       |
| 14  | CL7  | bB    | 821  | 2    | 1/1/9/20  | 2/4/80/115    | -       |
| 12  | G9R  | aA    | 3101 | 1    | 1/1/15/20 | 5/39/115/115  | -       |
| 14  | CL7  | cB    | 831  | 2    | 2/2/12/20 | 9/26/102/115  | -       |
| 14  | CL7  | aB    | 3020 | 2    | 1/1/9/20  | 2/4/80/115    | -       |
| 14  | CL7  | aL    | 202  | 10   | 2/2/15/20 | 19/39/115/115 | -       |
| 14  | CL7  | bA    | 3113 | 1    | 1/1/10/20 | 2/10/86/115   | -       |
| 14  | CL7  | aL    | 203  | 10   | 2/2/15/20 | 16/39/115/115 | -       |
| 14  | CL7  | cA    | 3104 | 1    | 2/2/10/20 | 6/10/86/115   | -       |
| 14  | CL7  | bB    | 826  | 20   | 2/2/15/20 | 17/39/115/115 | -       |
| 14  | CL7  | cB    | 818  | 2    | 2/2/10/20 | 5/10/86/115   | -       |
| 14  | CL7  | cA    | 3121 | 1    | 2/2/10/20 | 1/10/86/115   | -       |
| 14  | CL7  | bA    | 3125 | 1    | 2/2/15/20 | 9/39/115/115  | -       |
| 14  | CL7  | bB    | 818  | 2    | 2/2/10/20 | 8/10/86/115   | -       |
| 14  | CL7  | cA    | 3116 | -    | 2/2/12/20 | 10/25/101/115 | -       |
| 14  | CL7  | cB    | 822  | 2    | 1/1/10/20 | 5/10/86/115   | -       |
| 14  | CL7  | bB    | 811  | 2    | 2/2/10/20 | 1/10/86/115   | -       |
| 14  | CL7  | aA    | 3143 | 1    | 1/1/15/20 | 20/39/115/115 | -       |
| 14  | CL7  | cA    | 3102 | 20   | 1/1/15/20 | 9/39/115/115  | -       |
| 14  | CL7  | cB    | 811  | 2    | 2/2/10/20 | 4/10/86/115   | -       |
| 14  | CL7  | bB    | 815  | 2    | 2/2/10/20 | 1/10/86/115   | -       |
| 14  | CL7  | cA    | 3142 | 1    | 2/2/15/20 | 17/39/115/115 | -       |
| 14  | CL7  | cA    | 3105 | 1    | 2/2/10/20 | 5/10/86/115   | -       |
| 14  | CL7  | bB    | 804  | 2    | 2/2/15/20 | 7/39/115/115  | -       |
| 14  | CL7  | aB    | 3016 | -    | 2/2/10/20 | 6/10/86/115   | -       |
| 13  | PHO  | aB    | 3004 | -    | -         | 20/37/103/103 | 0/5/6/6 |
| 14  | CL7  | bB    | 803  | 20   | 2/2/15/20 | 13/39/115/115 | -       |
| 14  | CL7  | cA    | 3112 | 1    | 2/2/10/20 | 6/10/86/115   | -       |
| 14  | CL7  | bA    | 3124 | 1    | 2/2/15/20 | 11/39/115/115 | -       |
| 14  | CL7  | bA    | 3121 | 1    | 2/2/10/20 | 3/10/86/115   | -       |
| 14  | CL7  | cA    | 3144 | -    | 2/2/10/20 | 5/10/86/115   | -       |
| 14  | CL7  | bA    | 3106 | 1    | 2/2/15/20 | 22/39/115/115 | -       |
| 14  | CL7  | cL    | 204  | 10   | 2/2/15/20 | 19/39/115/115 | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14  | CL7  | bB    | 819  | 2    | 2/2/13/20 | 11/29/105/115 | -       |
| 14  | CL7  | cA    | 3140 | 1    | 2/2/15/20 | 17/39/115/115 | -       |
| 18  | SF4  | aC    | 102  | 3    | -         | -             | 0/6/5/5 |
| 14  | CL7  | bA    | 3141 | 1    | 2/2/15/20 | 13/39/115/115 | -       |
| 14  | CL7  | bA    | 3145 | -    | 2/2/10/20 | 5/10/86/115   | -       |
| 14  | CL7  | cL    | 203  | 10   | 2/2/15/20 | 21/39/115/115 | -       |
| 14  | CL7  | aB    | 3030 | 2    | 2/2/12/20 | 9/26/102/115  | -       |
| 14  | CL7  | cB    | 809  | 2    | 2/2/12/20 | 6/21/97/115   | -       |
| 14  | CL7  | aA    | 3107 | 1    | 2/2/15/20 | 21/39/115/115 | -       |
| 14  | CL7  | cB    | 814  | 2    | 1/1/10/20 | 2/10/86/115   | -       |
| 14  | CL7  | bA    | 3104 | 1    | 2/2/10/20 | 6/10/86/115   | -       |
| 18  | SF4  | aB    | 3001 | 2,1  | -         | -             | 0/6/5/5 |
| 14  | CL7  | aA    | 3103 | 20   | 1/1/15/20 | 10/39/115/115 | -       |
| 14  | CL7  | bL    | 205  | 20   | 2/2/10/20 | 3/12/88/115   | -       |
| 14  | CL7  | cA    | 3123 | 1    | 2/2/12/20 | 5/23/99/115   | -       |
| 14  | CL7  | bF    | 201  | 2    | 2/2/9/20  | 0/4/80/115    | -       |
| 17  | PQN  | bA    | 3143 | -    | -         | 15/23/43/43   | 0/2/2/2 |
| 14  | CL7  | aA    | 3104 | 1    | 2/2/10/20 | 4/10/86/115   | -       |
| 14  | CL7  | aB    | 3010 | 2    | 2/2/10/20 | 3/10/86/115   | -       |
| 14  | CL7  | cB    | 827  | 2    | 1/1/15/20 | 18/39/115/115 | -       |
| 14  | CL7  | cB    | 832  | 2    | 2/2/15/20 | 20/39/115/115 | -       |
| 16  | LHG  | aA    | 3138 | -    | -         | 16/53/53/53   | -       |
| 14  | CL7  | bA    | 3132 | 20   | 2/2/15/20 | 17/39/115/115 | -       |
| 14  | CL7  | aB    | 3005 | 2    | 2/2/15/20 | 8/39/115/115  | -       |
| 14  | CL7  | cB    | 813  | 2    | 2/2/9/20  | 2/4/80/115    | -       |
| 12  | G9R  | bA    | 3101 | 1    | -         | 9/39/115/115  | -       |
| 14  | CL7  | bB    | 820  | 2    | 2/2/15/20 | 12/39/115/115 | -       |
| 14  | CL7  | aA    | 3113 | 1    | 2/2/10/20 | 5/10/86/115   | -       |
| 14  | CL7  | bB    | 810  | 2    | 2/2/15/20 | 22/39/115/115 | -       |
| 14  | CL7  | cA    | 3107 | 1    | 1/1/15/20 | 15/39/115/115 | -       |
| 14  | CL7  | cA    | 3118 | -    | 1/1/9/20  | 0/4/80/115    | -       |
| 14  | CL7  | aA    | 3128 | 1    | 2/2/12/20 | 10/23/99/115  | -       |
| 14  | CL7  | cA    | 3109 | 1    | 2/2/10/20 | 3/10/86/115   | -       |
| 14  | CL7  | bA    | 3108 | 1    | 1/1/10/20 | 6/12/88/115   | -       |
| 17  | PQN  | aB    | 3027 | -    | -         | 8/23/43/43    | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14  | CL7  | aA    | 3125 | 1    | 2/2/15/20 | 9/39/115/115  | -       |
| 14  | CL7  | cA    | 3127 | 1    | 2/2/12/20 | 9/23/99/115   | -       |
| 14  | CL7  | cB    | 817  | -    | 2/2/10/20 | 6/10/86/115   | -       |
| 14  | CL7  | aA    | 3131 | 1    | 1/1/10/20 | 5/10/86/115   | -       |
| 14  | CL7  | bA    | 3128 | 1    | 2/2/15/20 | 17/39/115/115 | -       |
| 14  | CL7  | bA    | 3130 | 1    | 2/2/10/20 | 6/10/86/115   | -       |
| 14  | CL7  | aA    | 3146 | -    | 2/2/10/20 | 7/10/86/115   | -       |
| 14  | CL7  | bB    | 816  | 2    | 1/1/12/20 | 3/21/97/115   | -       |
| 19  | LMG  | aB    | 3029 | -    | -         | 20/47/67/70   | 0/1/1/1 |
| 19  | LMG  | bB    | 830  | -    | -         | 18/47/67/70   | 0/1/1/1 |
| 14  | CL7  | aB    | 3018 | 2    | 2/2/13/20 | 11/29/105/115 | -       |
| 14  | CL7  | aB    | 3017 | 2    | 2/2/10/20 | 8/10/86/115   | -       |
| 14  | CL7  | cA    | 3126 | 1    | 2/2/11/20 | 12/26/98/115  | -       |
| 14  | CL7  | aA    | 3123 | 1    | 2/2/12/20 | 9/21/97/115   | -       |
| 14  | CL7  | bA    | 3115 | 1    | 1/1/9/20  | 4/4/80/115    | -       |
| 14  | CL7  | bB    | 822  | 2    | 1/1/10/20 | 4/10/86/115   | -       |
| 14  | CL7  | aA    | 3119 | -    | 1/1/9/20  | 0/4/80/115    | -       |
| 14  | CL7  | aA    | 3121 | 1    | 2/2/12/20 | 6/23/99/115   | -       |
| 14  | CL7  | aB    | 3008 | 2    | 2/2/12/20 | 6/21/97/115   | -       |
| 14  | CL7  | bA    | 3117 | 1    | 2/2/9/20  | 2/4/80/115    | -       |
| 18  | SF4  | cC    | 101  | 3    | -         | -             | 0/6/5/5 |
| 14  | CL7  | aB    | 3032 | 2    | 2/2/13/20 | 10/27/103/115 | -       |
| 14  | CL7  | bB    | 831  | 2    | 2/2/12/20 | 8/26/102/115  | -       |
| 14  | CL7  | aA    | 3141 | 1    | 2/2/15/20 | 18/39/115/115 | -       |
| 14  | CL7  | bB    | 823  | 2    | 2/2/10/20 | 7/10/86/115   | -       |
| 14  | CL7  | aA    | 3134 | 16   | 2/2/10/20 | 8/10/86/115   | -       |
| 14  | CL7  | cB    | 825  | 2    | 2/2/9/20  | 0/4/80/115    | -       |
| 14  | CL7  | cB    | 812  | 2    | 2/2/9/20  | 2/4/80/115    | -       |
| 14  | CL7  | cB    | 824  | 2    | 2/2/13/20 | 15/29/105/115 | -       |
| 16  | LHG  | aA    | 3139 | 14   | -         | 9/23/23/53    | -       |
| 14  | CL7  | aB    | 3002 | 20   | 2/2/15/20 | 21/39/115/115 | -       |
| 14  | CL7  | aB    | 3014 | 2    | 1/1/10/20 | 1/10/86/115   | -       |
| 14  | CL7  | bA    | 3140 | 1    | 2/2/15/20 | 17/39/115/115 | -       |
| 14  | CL7  | bB    | 812  | 2    | 2/2/9/20  | 2/4/80/115    | -       |
| 14  | CL7  | bB    | 833  | 2    | 2/2/13/20 | 11/27/103/115 | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14  | CL7  | cA    | 3128 | 1    | 2/2/15/20 | 19/39/115/115 | -       |
| 14  | CL7  | bB    | 807  | 2    | 1/1/15/20 | 15/39/115/115 | -       |
| 14  | CL7  | aA    | 3124 | 1    | 2/2/12/20 | 6/23/99/115   | -       |
| 14  | CL7  | aA    | 3132 | -    | 2/2/10/20 | 7/10/86/115   | -       |
| 14  | CL7  | bA    | 3122 | 1    | 2/2/12/20 | 9/21/97/115   | -       |
| 14  | CL7  | cA    | 3133 | 16   | 2/2/10/20 | 4/10/86/115   | -       |
| 14  | CL7  | bA    | 3102 | 20   | 1/1/15/20 | 8/39/115/115  | -       |
| 14  | CL7  | cB    | 803  | 20   | 2/2/15/20 | 15/39/115/115 | -       |
| 14  | CL7  | cJ    | 101  | 8    | 1/1/10/20 | 3/9/85/115    | -       |
| 14  | CL7  | bA    | 3133 | 16   | 2/2/10/20 | 5/10/86/115   | -       |
| 14  | CL7  | aB    | 3003 | 2    | 2/2/15/20 | 4/39/115/115  | -       |
| 18  | SF4  | aC    | 101  | 3    | -         | -             | 0/6/5/5 |
| 14  | CL7  | aB    | 3025 | 20   | 2/2/15/20 | 16/39/115/115 | -       |
| 14  | CL7  | cA    | 3141 | 1    | 2/2/15/20 | 16/39/115/115 | -       |
| 14  | CL7  | aB    | 3007 | 2    | 2/2/15/20 | 13/39/115/115 | -       |
| 14  | CL7  | bA    | 3127 | 1    | 2/2/12/20 | 9/23/99/115   | -       |
| 14  | CL7  | bA    | 3142 | 1    | 2/2/15/20 | 16/39/115/115 | -       |
| 14  | CL7  | bA    | 3114 | 1    | 2/2/15/20 | 19/39/115/115 | -       |
| 14  | CL7  | cA    | 3120 | 1    | 2/2/12/20 | 7/23/99/115   | -       |
| 14  | CL7  | aA    | 3112 | 1    | 2/2/9/20  | 2/4/80/115    | -       |
| 14  | CL7  | aB    | 3026 | 2    | 2/2/15/20 | 18/39/115/115 | -       |
| 14  | CL7  | bB    | 806  | 2    | 2/2/15/20 | 15/39/115/115 | -       |
| 14  | CL7  | cB    | 806  | 2    | 2/2/15/20 | 13/39/115/115 | -       |
| 14  | CL7  | bB    | 813  | 2    | 2/2/9/20  | 0/4/80/115    | -       |
| 17  | PQN  | cA    | 3143 | -    | -         | 13/23/43/43   | 0/2/2/2 |
| 14  | CL7  | aB    | 3023 | 2    | 2/2/13/20 | 16/29/105/115 | -       |
| 14  | CL7  | aA    | 3118 | 1    | 2/2/9/20  | 2/4/80/115    | -       |
| 14  | CL7  | bA    | 3112 | 1    | 2/2/10/20 | 5/10/86/115   | -       |
| 14  | CL7  | bA    | 3110 | 1    | 2/2/10/20 | 3/10/86/115   | -       |
| 13  | PHO  | cB    | 801  | -    | -         | 10/37/103/103 | 0/5/6/6 |
| 14  | CL7  | cA    | 3132 | 20   | 2/2/15/20 | 19/39/115/115 | -       |
| 14  | CL7  | aA    | 3126 | 1    | 2/2/15/20 | 13/39/115/115 | -       |
| 14  | CL7  | aA    | 3115 | 1    | 2/2/15/20 | 17/39/115/115 | -       |
| 14  | CL7  | aA    | 3133 | 20   | 2/2/15/20 | 17/39/115/115 | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions    | Rings   |
|-----|------|-------|------|------|-----------|-------------|---------|
| 14  | CL7  | bA    | 3120 | 1    | 2/2/12/20 | 7/23/99/115 | -       |
| 18  | SF4  | cC    | 102  | 3    | -         | -           | 0/6/5/5 |

All (4894) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 13  | cB    | 801  | PHO  | C3A-C2A | -14.42 | 1.41        | 1.54     |
| 13  | bB    | 801  | PHO  | C3A-C2A | -14.37 | 1.41        | 1.54     |
| 13  | aA    | 3102 | PHO  | C3A-C2A | -13.81 | 1.42        | 1.54     |
| 13  | aA    | 3102 | PHO  | OBD-CAD | 11.47  | 1.38        | 1.22     |
| 13  | cB    | 801  | PHO  | OBD-CAD | 11.30  | 1.38        | 1.22     |
| 13  | bB    | 801  | PHO  | OBD-CAD | 11.15  | 1.37        | 1.22     |
| 13  | aB    | 3004 | PHO  | C2-C3   | 9.08   | 1.54        | 1.33     |
| 13  | aA    | 3102 | PHO  | C2-C3   | 8.88   | 1.54        | 1.33     |
| 13  | bB    | 801  | PHO  | C2-C3   | 8.87   | 1.54        | 1.33     |
| 13  | cB    | 805  | PHO  | C2-C3   | 8.82   | 1.54        | 1.33     |
| 13  | cB    | 801  | PHO  | C2-C3   | 8.76   | 1.54        | 1.33     |
| 13  | bB    | 801  | PHO  | CHA-CBD | -8.63  | 1.41        | 1.51     |
| 13  | cB    | 801  | PHO  | CHA-CBD | -8.60  | 1.41        | 1.51     |
| 14  | cA    | 3102 | CL7  | C4B-NB  | -8.57  | 1.27        | 1.37     |
| 13  | bB    | 805  | PHO  | C2-C3   | 8.52   | 1.53        | 1.33     |
| 13  | bB    | 805  | PHO  | OBD-CAD | 8.48   | 1.34        | 1.22     |
| 14  | bA    | 3102 | CL7  | C4B-NB  | -8.15  | 1.27        | 1.37     |
| 13  | cB    | 805  | PHO  | OBD-CAD | 8.13   | 1.33        | 1.22     |
| 13  | aA    | 3102 | PHO  | CHA-CBD | -8.12  | 1.42        | 1.51     |
| 14  | bA    | 3125 | CL7  | C4C-C3C | -8.12  | 1.30        | 1.45     |
| 13  | aB    | 3004 | PHO  | OBD-CAD | 8.11   | 1.33        | 1.22     |
| 14  | cB    | 806  | CL7  | MG-NB   | -8.04  | 1.89        | 2.05     |
| 14  | cA    | 3125 | CL7  | C4C-C3C | -8.04  | 1.30        | 1.45     |
| 13  | cB    | 801  | PHO  | C1A-C2A | -8.00  | 1.39        | 1.51     |
| 14  | bB    | 806  | CL7  | MG-NB   | -7.96  | 1.90        | 2.05     |
| 14  | bA    | 3129 | CL7  | MG-ND   | -7.94  | 1.90        | 2.05     |
| 13  | bB    | 801  | PHO  | C1A-C2A | -7.88  | 1.40        | 1.51     |
| 14  | cB    | 804  | CL7  | C4C-C3C | -7.82  | 1.31        | 1.45     |
| 14  | bB    | 804  | CL7  | C4B-NB  | -7.81  | 1.28        | 1.37     |
| 14  | aB    | 3005 | CL7  | MG-NB   | -7.80  | 1.90        | 2.05     |
| 14  | cA    | 3132 | CL7  | C1B-C2B | -7.77  | 1.25        | 1.43     |
| 14  | aA    | 3126 | CL7  | C4C-C3C | -7.76  | 1.31        | 1.45     |
| 14  | cA    | 3129 | CL7  | MG-ND   | -7.72  | 1.90        | 2.05     |
| 14  | cA    | 3127 | CL7  | C4C-C3C | -7.69  | 1.31        | 1.45     |
| 14  | aA    | 3133 | CL7  | C1B-C2B | -7.68  | 1.25        | 1.43     |
| 14  | bA    | 3132 | CL7  | C1B-C2B | -7.65  | 1.25        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | bB    | 809  | CL7  | C4C-C3C | -7.62 | 1.31        | 1.45     |
| 14  | cB    | 819  | CL7  | C4B-NB  | -7.58 | 1.28        | 1.37     |
| 14  | cB    | 809  | CL7  | C4C-C3C | -7.56 | 1.31        | 1.45     |
| 14  | bA    | 3127 | CL7  | C4C-C3C | -7.55 | 1.31        | 1.45     |
| 13  | aA    | 3102 | PHO  | C1A-C2A | -7.52 | 1.40        | 1.51     |
| 14  | bB    | 804  | CL7  | C4C-C3C | -7.51 | 1.31        | 1.45     |
| 14  | aA    | 3128 | CL7  | C4C-C3C | -7.50 | 1.31        | 1.45     |
| 14  | bA    | 3123 | CL7  | C4C-C3C | -7.50 | 1.31        | 1.45     |
| 14  | aA    | 3130 | CL7  | MG-ND   | -7.49 | 1.90        | 2.05     |
| 14  | cA    | 3123 | CL7  | C4C-C3C | -7.42 | 1.32        | 1.45     |
| 14  | aB    | 3025 | CL7  | C1B-C2B | -7.38 | 1.25        | 1.43     |
| 14  | aB    | 3003 | CL7  | C4C-C3C | -7.38 | 1.32        | 1.45     |
| 14  | bB    | 833  | CL7  | C4C-C3C | -7.36 | 1.32        | 1.45     |
| 14  | bA    | 3121 | CL7  | MG-NB   | -7.32 | 1.91        | 2.05     |
| 14  | bB    | 826  | CL7  | C1B-C2B | -7.31 | 1.26        | 1.43     |
| 14  | cL    | 203  | CL7  | C4B-NB  | -7.30 | 1.28        | 1.37     |
| 14  | cB    | 826  | CL7  | C1B-C2B | -7.29 | 1.26        | 1.43     |
| 14  | cB    | 808  | CL7  | C4C-C3C | -7.28 | 1.32        | 1.45     |
| 14  | cA    | 3121 | CL7  | MG-NB   | -7.27 | 1.91        | 2.05     |
| 14  | aB    | 3008 | CL7  | C4C-C3C | -7.27 | 1.32        | 1.45     |
| 13  | aB    | 3004 | PHO  | CHA-CBD | -7.26 | 1.43        | 1.51     |
| 14  | bB    | 819  | CL7  | C4C-C3C | -7.26 | 1.32        | 1.45     |
| 14  | cA    | 3123 | CL7  | C4B-NB  | -7.25 | 1.28        | 1.37     |
| 14  | bA    | 3128 | CL7  | MG-NB   | -7.24 | 1.91        | 2.05     |
| 14  | aB    | 3032 | CL7  | C4C-C3C | -7.23 | 1.32        | 1.45     |
| 14  | aB    | 3019 | CL7  | C4C-C3C | -7.20 | 1.32        | 1.45     |
| 14  | cB    | 833  | CL7  | C4C-C3C | -7.20 | 1.32        | 1.45     |
| 14  | cA    | 3140 | CL7  | C4C-C3C | -7.18 | 1.32        | 1.45     |
| 14  | bA    | 3129 | CL7  | MG-NB   | -7.18 | 1.91        | 2.05     |
| 14  | bA    | 3123 | CL7  | C4B-NB  | -7.16 | 1.29        | 1.37     |
| 14  | cA    | 3125 | CL7  | C1B-C2B | -7.13 | 1.26        | 1.43     |
| 14  | bB    | 820  | CL7  | C4C-C3C | -7.13 | 1.32        | 1.45     |
| 14  | aA    | 3103 | CL7  | C4B-NB  | -7.12 | 1.29        | 1.37     |
| 14  | aB    | 3007 | CL7  | C4C-C3C | -7.12 | 1.32        | 1.45     |
| 14  | cB    | 804  | CL7  | C4B-NB  | -7.11 | 1.29        | 1.37     |
| 14  | aA    | 3130 | CL7  | MG-NB   | -7.09 | 1.91        | 2.05     |
| 14  | cA    | 3129 | CL7  | MG-NB   | -7.09 | 1.91        | 2.05     |
| 14  | cB    | 820  | CL7  | C4C-C3C | -7.09 | 1.32        | 1.45     |
| 14  | aA    | 3124 | CL7  | C4C-C3C | -7.09 | 1.32        | 1.45     |
| 13  | cB    | 805  | PHO  | CHA-CBD | -7.08 | 1.43        | 1.51     |
| 14  | bA    | 3123 | CL7  | C1B-C2B | -7.06 | 1.26        | 1.43     |
| 14  | bA    | 3125 | CL7  | C1B-C2B | -7.05 | 1.26        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 13  | bB    | 805  | PHO  | CHA-CBD | -7.01 | 1.43        | 1.51     |
| 14  | aA    | 3126 | CL7  | C1B-C2B | -7.01 | 1.26        | 1.43     |
| 14  | bB    | 803  | CL7  | C4C-C3C | -6.94 | 1.32        | 1.45     |
| 14  | aB    | 3031 | CL7  | C4C-C3C | -6.93 | 1.32        | 1.45     |
| 14  | aB    | 3003 | CL7  | C4B-NB  | -6.93 | 1.29        | 1.37     |
| 14  | aL    | 202  | CL7  | C4B-NB  | -6.92 | 1.29        | 1.37     |
| 14  | aB    | 3018 | CL7  | C4C-C3C | -6.92 | 1.32        | 1.45     |
| 14  | bA    | 3140 | CL7  | C4C-C3C | -6.92 | 1.32        | 1.45     |
| 14  | aA    | 3122 | CL7  | MG-NB   | -6.90 | 1.92        | 2.05     |
| 14  | cB    | 803  | CL7  | C4C-C3C | -6.89 | 1.33        | 1.45     |
| 14  | cB    | 832  | CL7  | C4C-C3C | -6.89 | 1.33        | 1.45     |
| 14  | aB    | 3018 | CL7  | MG-NB   | -6.87 | 1.92        | 2.05     |
| 14  | bB    | 819  | CL7  | C4B-NB  | -6.85 | 1.29        | 1.37     |
| 14  | cA    | 3126 | CL7  | C4C-C3C | -6.84 | 1.33        | 1.45     |
| 14  | cB    | 824  | CL7  | MG-NA   | -6.82 | 1.92        | 2.05     |
| 14  | cB    | 816  | CL7  | MG-NB   | -6.82 | 1.92        | 2.05     |
| 14  | bA    | 3104 | CL7  | C4C-C3C | -6.81 | 1.33        | 1.45     |
| 14  | bB    | 819  | CL7  | MG-NB   | -6.81 | 1.92        | 2.05     |
| 14  | aB    | 3030 | CL7  | C4C-C3C | -6.80 | 1.33        | 1.45     |
| 14  | aB    | 3023 | CL7  | MG-NA   | -6.79 | 1.92        | 2.05     |
| 14  | cA    | 3128 | CL7  | MG-NB   | -6.78 | 1.92        | 2.05     |
| 14  | cA    | 3122 | CL7  | C4C-C3C | -6.78 | 1.33        | 1.45     |
| 14  | cB    | 819  | CL7  | C4C-C3C | -6.76 | 1.33        | 1.45     |
| 14  | aB    | 3015 | CL7  | MG-NB   | -6.74 | 1.92        | 2.05     |
| 14  | cA    | 3103 | CL7  | C4C-C3C | -6.74 | 1.33        | 1.45     |
| 14  | bB    | 807  | CL7  | C4C-C3C | -6.73 | 1.33        | 1.45     |
| 14  | aA    | 3123 | CL7  | C4C-C3C | -6.72 | 1.33        | 1.45     |
| 14  | bA    | 3113 | CL7  | C4C-C3C | -6.72 | 1.33        | 1.45     |
| 14  | cA    | 3104 | CL7  | C4C-C3C | -6.72 | 1.33        | 1.45     |
| 14  | cA    | 3106 | CL7  | MG-NB   | -6.71 | 1.92        | 2.05     |
| 14  | cA    | 3116 | CL7  | C1B-C2B | -6.71 | 1.27        | 1.43     |
| 14  | bB    | 832  | CL7  | C4C-C3C | -6.71 | 1.33        | 1.45     |
| 14  | aA    | 3105 | CL7  | C4C-C3C | -6.70 | 1.33        | 1.45     |
| 14  | bB    | 832  | CL7  | MG-ND   | -6.70 | 1.92        | 2.05     |
| 14  | bA    | 3102 | CL7  | C1C-C2C | -6.70 | 1.32        | 1.45     |
| 14  | aA    | 3129 | CL7  | MG-NB   | -6.69 | 1.92        | 2.05     |
| 14  | aB    | 3002 | CL7  | C4C-C3C | -6.69 | 1.33        | 1.45     |
| 14  | bA    | 3103 | CL7  | C4C-C3C | -6.68 | 1.33        | 1.45     |
| 14  | cB    | 819  | CL7  | MG-NB   | -6.68 | 1.92        | 2.05     |
| 14  | aA    | 3121 | CL7  | C4C-C3C | -6.68 | 1.33        | 1.45     |
| 14  | cB    | 832  | CL7  | MG-ND   | -6.67 | 1.92        | 2.05     |
| 14  | cB    | 807  | CL7  | C4C-C3C | -6.67 | 1.33        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | aB    | 3023 | CL7  | C4C-C3C | -6.67 | 1.33        | 1.45     |
| 14  | bB    | 808  | CL7  | C4C-C3C | -6.66 | 1.33        | 1.45     |
| 14  | bA    | 3122 | CL7  | C4C-C3C | -6.66 | 1.33        | 1.45     |
| 14  | bA    | 3120 | CL7  | C4C-C3C | -6.66 | 1.33        | 1.45     |
| 14  | bA    | 3116 | CL7  | C1B-C2B | -6.65 | 1.27        | 1.43     |
| 13  | bB    | 805  | PHO  | C1A-C2A | -6.65 | 1.41        | 1.51     |
| 14  | cA    | 3113 | CL7  | C4C-C3C | -6.65 | 1.33        | 1.45     |
| 14  | cB    | 809  | CL7  | C1B-C2B | -6.64 | 1.27        | 1.43     |
| 14  | cA    | 3139 | CL7  | C4C-C3C | -6.63 | 1.33        | 1.45     |
| 14  | bB    | 824  | CL7  | MG-NA   | -6.63 | 1.92        | 2.05     |
| 14  | bB    | 831  | CL7  | C4C-C3C | -6.62 | 1.33        | 1.45     |
| 14  | bB    | 816  | CL7  | MG-NB   | -6.62 | 1.92        | 2.05     |
| 14  | cA    | 3120 | CL7  | C4C-C3C | -6.62 | 1.33        | 1.45     |
| 14  | bA    | 3126 | CL7  | C4C-C3C | -6.61 | 1.33        | 1.45     |
| 14  | aA    | 3124 | CL7  | C1B-C2B | -6.61 | 1.27        | 1.43     |
| 14  | aB    | 3006 | CL7  | C4C-C3C | -6.60 | 1.33        | 1.45     |
| 14  | bL    | 203  | CL7  | C4B-NB  | -6.58 | 1.29        | 1.37     |
| 14  | aA    | 3127 | CL7  | C4C-C3C | -6.58 | 1.33        | 1.45     |
| 14  | aA    | 3114 | CL7  | C4C-C3C | -6.58 | 1.33        | 1.45     |
| 14  | aB    | 3031 | CL7  | MG-ND   | -6.57 | 1.92        | 2.05     |
| 14  | cA    | 3130 | CL7  | C4C-C3C | -6.55 | 1.33        | 1.45     |
| 14  | bA    | 3139 | CL7  | C4C-C3C | -6.55 | 1.33        | 1.45     |
| 14  | aA    | 3124 | CL7  | C4B-NB  | -6.55 | 1.29        | 1.37     |
| 14  | bB    | 813  | CL7  | C4C-C3C | -6.54 | 1.33        | 1.45     |
| 14  | aB    | 3011 | CL7  | C4C-C3C | -6.54 | 1.33        | 1.45     |
| 14  | cB    | 813  | CL7  | C4C-C3C | -6.53 | 1.33        | 1.45     |
| 14  | cA    | 3128 | CL7  | C4C-C3C | -6.52 | 1.33        | 1.45     |
| 14  | aB    | 3018 | CL7  | C4B-NB  | -6.51 | 1.29        | 1.37     |
| 14  | bA    | 3142 | CL7  | C4C-C3C | -6.51 | 1.33        | 1.45     |
| 14  | bA    | 3131 | CL7  | C4C-C3C | -6.51 | 1.33        | 1.45     |
| 14  | cB    | 831  | CL7  | C4C-C3C | -6.51 | 1.33        | 1.45     |
| 14  | cF    | 201  | CL7  | C4C-C3C | -6.50 | 1.33        | 1.45     |
| 14  | cA    | 3105 | CL7  | MG-ND   | -6.50 | 1.92        | 2.05     |
| 14  | aB    | 3017 | CL7  | C4C-C3C | -6.49 | 1.33        | 1.45     |
| 14  | aB    | 3008 | CL7  | C1B-C2B | -6.49 | 1.28        | 1.43     |
| 14  | cB    | 812  | CL7  | C4C-C3C | -6.48 | 1.33        | 1.45     |
| 14  | cA    | 3123 | CL7  | C1B-C2B | -6.48 | 1.28        | 1.43     |
| 14  | bA    | 3130 | CL7  | C4C-C3C | -6.48 | 1.33        | 1.45     |
| 14  | aA    | 3104 | CL7  | C4C-C3C | -6.47 | 1.33        | 1.45     |
| 14  | bB    | 812  | CL7  | C4C-C3C | -6.47 | 1.33        | 1.45     |
| 14  | aA    | 3142 | CL7  | C4C-C3C | -6.47 | 1.33        | 1.45     |
| 14  | cA    | 3131 | CL7  | C4C-C3C | -6.46 | 1.33        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | aB    | 3012 | CL7  | C4C-C3C | -6.46 | 1.33        | 1.45     |
| 14  | aB    | 3018 | CL7  | MG-NA   | -6.45 | 1.93        | 2.05     |
| 14  | aA    | 3141 | CL7  | C4C-C3C | -6.45 | 1.33        | 1.45     |
| 14  | bA    | 3106 | CL7  | MG-NB   | -6.45 | 1.93        | 2.05     |
| 13  | cB    | 805  | PHO  | C1A-C2A | -6.45 | 1.42        | 1.51     |
| 14  | cB    | 808  | CL7  | C1B-C2B | -6.44 | 1.28        | 1.43     |
| 14  | bB    | 824  | CL7  | C4C-C3C | -6.44 | 1.33        | 1.45     |
| 14  | bB    | 809  | CL7  | C1B-C2B | -6.43 | 1.28        | 1.43     |
| 14  | bA    | 3108 | CL7  | C4C-C3C | -6.42 | 1.33        | 1.45     |
| 14  | aA    | 3119 | CL7  | C4C-C3C | -6.41 | 1.33        | 1.45     |
| 14  | bB    | 823  | CL7  | C4C-C3C | -6.41 | 1.33        | 1.45     |
| 14  | cL    | 205  | CL7  | C4B-NB  | -6.40 | 1.29        | 1.37     |
| 14  | cA    | 3117 | CL7  | C4C-C3C | -6.40 | 1.33        | 1.45     |
| 14  | bA    | 3105 | CL7  | MG-ND   | -6.40 | 1.93        | 2.05     |
| 14  | cL    | 204  | CL7  | C4B-NB  | -6.39 | 1.29        | 1.37     |
| 14  | bB    | 826  | CL7  | C4C-C3C | -6.39 | 1.33        | 1.45     |
| 14  | bA    | 3111 | CL7  | C4C-C3C | -6.39 | 1.33        | 1.45     |
| 14  | bA    | 3107 | CL7  | C4C-C3C | -6.39 | 1.33        | 1.45     |
| 14  | cB    | 815  | CL7  | C4C-C3C | -6.39 | 1.33        | 1.45     |
| 14  | cA    | 3121 | CL7  | C4C-C3C | -6.39 | 1.33        | 1.45     |
| 14  | bA    | 3121 | CL7  | C4C-C3C | -6.38 | 1.33        | 1.45     |
| 14  | bA    | 3117 | CL7  | C4C-C3C | -6.38 | 1.33        | 1.45     |
| 14  | cA    | 3142 | CL7  | C4C-C3C | -6.38 | 1.33        | 1.45     |
| 14  | bB    | 815  | CL7  | C4C-C3C | -6.38 | 1.33        | 1.45     |
| 14  | bA    | 3132 | CL7  | C4C-C3C | -6.38 | 1.33        | 1.45     |
| 14  | cA    | 3124 | CL7  | C4C-C3C | -6.37 | 1.33        | 1.45     |
| 14  | cA    | 3111 | CL7  | C4C-C3C | -6.37 | 1.33        | 1.45     |
| 14  | aA    | 3132 | CL7  | C4C-C3C | -6.37 | 1.33        | 1.45     |
| 14  | cA    | 3116 | CL7  | C4C-C3C | -6.37 | 1.33        | 1.45     |
| 14  | cB    | 806  | CL7  | C4C-C3C | -6.37 | 1.33        | 1.45     |
| 14  | cA    | 3119 | CL7  | CAA-C2A | -6.37 | 1.42        | 1.54     |
| 14  | bF    | 201  | CL7  | C4C-C3C | -6.37 | 1.33        | 1.45     |
| 14  | cA    | 3128 | CL7  | C2A-C1A | -6.36 | 1.41        | 1.50     |
| 14  | aA    | 3112 | CL7  | C4C-C3C | -6.36 | 1.33        | 1.45     |
| 14  | bB    | 818  | CL7  | C4C-C3C | -6.36 | 1.33        | 1.45     |
| 14  | cB    | 824  | CL7  | C4C-C3C | -6.36 | 1.33        | 1.45     |
| 14  | bB    | 806  | CL7  | C4C-C3C | -6.36 | 1.33        | 1.45     |
| 14  | cB    | 818  | CL7  | C4C-C3C | -6.36 | 1.33        | 1.45     |
| 14  | cA    | 3102 | CL7  | C1C-C2C | -6.36 | 1.32        | 1.45     |
| 14  | cB    | 817  | CL7  | C4C-C3C | -6.36 | 1.33        | 1.45     |
| 14  | bA    | 3109 | CL7  | C4C-C3C | -6.35 | 1.33        | 1.45     |
| 14  | cA    | 3118 | CL7  | C4C-C3C | -6.35 | 1.33        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | cA    | 3109 | CL7  | C4C-C3C | -6.35 | 1.33        | 1.45     |
| 17  | cB    | 828  | PQN  | C11-C12 | -6.35 | 1.41        | 1.50     |
| 14  | bB    | 817  | CL7  | C4C-C3C | -6.35 | 1.33        | 1.45     |
| 14  | bA    | 3141 | CL7  | C4C-C3C | -6.35 | 1.33        | 1.45     |
| 14  | bA    | 3128 | CL7  | C4C-C3C | -6.35 | 1.33        | 1.45     |
| 14  | aF    | 201  | CL7  | C4C-C3C | -6.34 | 1.33        | 1.45     |
| 14  | cB    | 823  | CL7  | C4C-C3C | -6.34 | 1.33        | 1.45     |
| 14  | aA    | 3110 | CL7  | C4C-C3C | -6.34 | 1.33        | 1.45     |
| 14  | cA    | 3105 | CL7  | MG-NC   | -6.34 | 1.93        | 2.05     |
| 14  | cA    | 3132 | CL7  | C4C-C3C | -6.33 | 1.33        | 1.45     |
| 14  | cA    | 3107 | CL7  | C1B-C2B | -6.33 | 1.28        | 1.43     |
| 14  | bA    | 3118 | CL7  | C4C-C3C | -6.33 | 1.34        | 1.45     |
| 14  | aB    | 3022 | CL7  | C4C-C3C | -6.33 | 1.34        | 1.45     |
| 14  | bA    | 3116 | CL7  | C4C-C3C | -6.33 | 1.34        | 1.45     |
| 14  | cB    | 827  | CL7  | MG-NB   | -6.32 | 1.93        | 2.05     |
| 14  | cA    | 3107 | CL7  | C4C-C3C | -6.32 | 1.34        | 1.45     |
| 14  | aA    | 3131 | CL7  | C4C-C3C | -6.32 | 1.34        | 1.45     |
| 14  | bL    | 205  | CL7  | C4C-C3C | -6.32 | 1.34        | 1.45     |
| 14  | bA    | 3105 | CL7  | MG-NC   | -6.31 | 1.93        | 2.05     |
| 14  | bK    | 101  | CL7  | C4C-C3C | -6.31 | 1.34        | 1.45     |
| 13  | aB    | 3004 | PHO  | C1A-C2A | -6.31 | 1.42        | 1.51     |
| 14  | cA    | 3127 | CL7  | C4B-NB  | -6.31 | 1.30        | 1.37     |
| 17  | bB    | 828  | PQN  | C11-C12 | -6.30 | 1.41        | 1.50     |
| 14  | cA    | 3141 | CL7  | C4C-C3C | -6.30 | 1.34        | 1.45     |
| 14  | bB    | 827  | CL7  | MG-NB   | -6.30 | 1.93        | 2.05     |
| 14  | aA    | 3118 | CL7  | C4C-C3C | -6.29 | 1.34        | 1.45     |
| 14  | cA    | 3141 | CL7  | C1B-C2B | -6.28 | 1.28        | 1.43     |
| 14  | aA    | 3117 | CL7  | C1B-C2B | -6.28 | 1.28        | 1.43     |
| 14  | bA    | 3119 | CL7  | CAA-C2A | -6.28 | 1.42        | 1.54     |
| 14  | aA    | 3121 | CL7  | C1B-C2B | -6.28 | 1.28        | 1.43     |
| 14  | cL    | 205  | CL7  | C4C-C3C | -6.27 | 1.34        | 1.45     |
| 14  | aB    | 3016 | CL7  | C4C-C3C | -6.26 | 1.34        | 1.45     |
| 14  | aB    | 3031 | CL7  | C4B-NB  | -6.26 | 1.30        | 1.37     |
| 14  | bA    | 3107 | CL7  | C1B-C2B | -6.26 | 1.28        | 1.43     |
| 14  | bA    | 3127 | CL7  | C4B-NB  | -6.25 | 1.30        | 1.37     |
| 14  | bB    | 819  | CL7  | MG-NA   | -6.25 | 1.93        | 2.05     |
| 14  | aL    | 204  | CL7  | C4C-C3C | -6.24 | 1.34        | 1.45     |
| 14  | bB    | 825  | CL7  | C4C-C3C | -6.23 | 1.34        | 1.45     |
| 14  | cB    | 810  | CL7  | C1B-C2B | -6.23 | 1.28        | 1.43     |
| 14  | aA    | 3107 | CL7  | MG-NB   | -6.22 | 1.93        | 2.05     |
| 14  | bB    | 821  | CL7  | C4C-C3C | -6.22 | 1.34        | 1.45     |
| 14  | cB    | 821  | CL7  | C4C-C3C | -6.22 | 1.34        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | aB    | 3021 | CL7  | C4C-C3C | -6.21 | 1.34        | 1.45     |
| 14  | aA    | 3103 | CL7  | C1C-C2C | -6.21 | 1.33        | 1.45     |
| 14  | bA    | 3126 | CL7  | C1B-C2B | -6.21 | 1.28        | 1.43     |
| 14  | bA    | 3141 | CL7  | C1B-C2B | -6.21 | 1.28        | 1.43     |
| 14  | cB    | 803  | CL7  | C4B-NB  | -6.20 | 1.30        | 1.37     |
| 14  | cA    | 3133 | CL7  | C4C-C3C | -6.20 | 1.34        | 1.45     |
| 14  | bJ    | 101  | CL7  | C4C-C3C | -6.20 | 1.34        | 1.45     |
| 14  | aA    | 3106 | CL7  | MG-ND   | -6.19 | 1.93        | 2.05     |
| 14  | aB    | 3009 | CL7  | C4C-C3C | -6.19 | 1.34        | 1.45     |
| 14  | aA    | 3143 | CL7  | C4C-C3C | -6.19 | 1.34        | 1.45     |
| 14  | aA    | 3120 | CL7  | CAA-C2A | -6.19 | 1.42        | 1.54     |
| 14  | cB    | 826  | CL7  | C4C-C3C | -6.18 | 1.34        | 1.45     |
| 17  | aB    | 3027 | PQN  | C11-C12 | -6.18 | 1.41        | 1.50     |
| 14  | aB    | 3020 | CL7  | C4C-C3C | -6.17 | 1.34        | 1.45     |
| 14  | cL    | 204  | CL7  | MG-NB   | -6.17 | 1.93        | 2.05     |
| 14  | bB    | 808  | CL7  | C1B-C2B | -6.17 | 1.28        | 1.43     |
| 14  | aB    | 3014 | CL7  | C4C-C3C | -6.17 | 1.34        | 1.45     |
| 14  | cL    | 204  | CL7  | C4C-C3C | -6.17 | 1.34        | 1.45     |
| 14  | bA    | 3129 | CL7  | MG-NC   | -6.16 | 1.93        | 2.05     |
| 14  | bA    | 3119 | CL7  | C1B-C2B | -6.16 | 1.28        | 1.43     |
| 14  | cJ    | 101  | CL7  | C4C-C3C | -6.16 | 1.34        | 1.45     |
| 14  | aA    | 3117 | CL7  | C4C-C3C | -6.16 | 1.34        | 1.45     |
| 14  | aB    | 3005 | CL7  | C4C-C3C | -6.16 | 1.34        | 1.45     |
| 14  | bA    | 3133 | CL7  | C4C-C3C | -6.15 | 1.34        | 1.45     |
| 14  | cA    | 3119 | CL7  | C4C-C3C | -6.15 | 1.34        | 1.45     |
| 14  | cA    | 3106 | CL7  | MG-ND   | -6.15 | 1.93        | 2.05     |
| 14  | cA    | 3126 | CL7  | C1B-C2B | -6.15 | 1.28        | 1.43     |
| 14  | cB    | 810  | CL7  | C4C-C3C | -6.14 | 1.34        | 1.45     |
| 14  | aL    | 204  | CL7  | MG-NB   | -6.14 | 1.93        | 2.05     |
| 14  | aA    | 3127 | CL7  | C1B-C2B | -6.14 | 1.28        | 1.43     |
| 14  | aA    | 3140 | CL7  | C4C-C3C | -6.12 | 1.34        | 1.45     |
| 14  | bA    | 3127 | CL7  | MG-NB   | -6.12 | 1.93        | 2.05     |
| 14  | bL    | 205  | CL7  | MG-NB   | -6.12 | 1.93        | 2.05     |
| 14  | aB    | 3007 | CL7  | C1B-C2B | -6.12 | 1.28        | 1.43     |
| 14  | bA    | 3119 | CL7  | C4C-C3C | -6.12 | 1.34        | 1.45     |
| 14  | aA    | 3120 | CL7  | C4C-C3C | -6.12 | 1.34        | 1.45     |
| 14  | bB    | 814  | CL7  | C4C-C3C | -6.12 | 1.34        | 1.45     |
| 14  | aB    | 3018 | CL7  | C1B-C2B | -6.12 | 1.28        | 1.43     |
| 14  | aA    | 3108 | CL7  | C4C-C3C | -6.11 | 1.34        | 1.45     |
| 14  | bB    | 811  | CL7  | C4C-C3C | -6.11 | 1.34        | 1.45     |
| 14  | cB    | 814  | CL7  | C4C-C3C | -6.11 | 1.34        | 1.45     |
| 14  | aJ    | 101  | CL7  | C4C-C3C | -6.11 | 1.34        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | cA    | 3133 | CL7  | C1B-C2B | -6.11 | 1.28        | 1.43     |
| 14  | cL    | 203  | CL7  | C4C-C3C | -6.10 | 1.34        | 1.45     |
| 14  | cB    | 832  | CL7  | C4B-NB  | -6.10 | 1.30        | 1.37     |
| 14  | bB    | 810  | CL7  | C1B-C2B | -6.10 | 1.28        | 1.43     |
| 14  | aA    | 3133 | CL7  | C4C-C3C | -6.09 | 1.34        | 1.45     |
| 14  | bA    | 3108 | CL7  | C4B-NB  | -6.09 | 1.30        | 1.37     |
| 14  | aB    | 3013 | CL7  | C4C-C3C | -6.09 | 1.34        | 1.45     |
| 14  | cA    | 3119 | CL7  | C1B-C2B | -6.08 | 1.28        | 1.43     |
| 14  | cA    | 3127 | CL7  | MG-NB   | -6.08 | 1.93        | 2.05     |
| 14  | cK    | 101  | CL7  | C4C-C3C | -6.08 | 1.34        | 1.45     |
| 14  | aB    | 3026 | CL7  | MG-NB   | -6.08 | 1.93        | 2.05     |
| 14  | cA    | 3129 | CL7  | C3A-C2A | -6.07 | 1.48        | 1.54     |
| 14  | bB    | 822  | CL7  | C4C-C3C | -6.06 | 1.34        | 1.45     |
| 14  | cB    | 819  | CL7  | MG-NA   | -6.06 | 1.93        | 2.05     |
| 14  | aA    | 3142 | CL7  | C1B-C2B | -6.04 | 1.29        | 1.43     |
| 14  | cA    | 3142 | CL7  | MG-NC   | -6.04 | 1.93        | 2.05     |
| 14  | bA    | 3110 | CL7  | C4C-C3C | -6.04 | 1.34        | 1.45     |
| 14  | cA    | 3106 | CL7  | C4C-C3C | -6.04 | 1.34        | 1.45     |
| 14  | aA    | 3122 | CL7  | C4C-C3C | -6.03 | 1.34        | 1.45     |
| 14  | bL    | 204  | CL7  | C1B-C2B | -6.03 | 1.29        | 1.43     |
| 14  | cB    | 833  | CL7  | C1B-C2B | -6.03 | 1.29        | 1.43     |
| 14  | bA    | 3133 | CL7  | C1B-C2B | -6.03 | 1.29        | 1.43     |
| 14  | bB    | 832  | CL7  | C4B-NB  | -6.03 | 1.30        | 1.37     |
| 14  | cA    | 3110 | CL7  | C4C-C3C | -6.03 | 1.34        | 1.45     |
| 14  | aB    | 3009 | CL7  | C1B-C2B | -6.02 | 1.29        | 1.43     |
| 14  | cB    | 822  | CL7  | C4C-C3C | -6.02 | 1.34        | 1.45     |
| 14  | aA    | 3109 | CL7  | C4C-C3C | -6.02 | 1.34        | 1.45     |
| 14  | bA    | 3145 | CL7  | C4C-C3C | -6.02 | 1.34        | 1.45     |
| 14  | aA    | 3108 | CL7  | C1B-C2B | -6.01 | 1.29        | 1.43     |
| 14  | aB    | 3010 | CL7  | C4C-C3C | -6.01 | 1.34        | 1.45     |
| 14  | cB    | 825  | CL7  | C4C-C3C | -6.01 | 1.34        | 1.45     |
| 14  | bB    | 806  | CL7  | MG-NC   | -6.00 | 1.93        | 2.05     |
| 14  | aB    | 3024 | CL7  | C4C-C3C | -6.00 | 1.34        | 1.45     |
| 14  | bA    | 3131 | CL7  | C4B-NB  | -6.00 | 1.30        | 1.37     |
| 14  | aA    | 3111 | CL7  | C4C-C3C | -6.00 | 1.34        | 1.45     |
| 14  | aA    | 3106 | CL7  | MG-NC   | -6.00 | 1.93        | 2.05     |
| 14  | cA    | 3144 | CL7  | C4C-C3C | -5.99 | 1.34        | 1.45     |
| 14  | cA    | 3131 | CL7  | C4B-NB  | -5.99 | 1.30        | 1.37     |
| 14  | cB    | 811  | CL7  | C4C-C3C | -5.99 | 1.34        | 1.45     |
| 14  | cA    | 3142 | CL7  | C1B-C2B | -5.99 | 1.29        | 1.43     |
| 14  | bA    | 3120 | CL7  | C1B-C2B | -5.99 | 1.29        | 1.43     |
| 14  | aA    | 3146 | CL7  | C4C-C3C | -5.99 | 1.34        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | aA    | 3128 | CL7  | MG-NB   | -5.99 | 1.93        | 2.05     |
| 14  | bA    | 3105 | CL7  | MG-NB   | -5.98 | 1.93        | 2.05     |
| 14  | aA    | 3119 | CL7  | C1B-C2B | -5.98 | 1.29        | 1.43     |
| 14  | bA    | 3106 | CL7  | MG-ND   | -5.97 | 1.93        | 2.05     |
| 14  | bB    | 810  | CL7  | C4C-C3C | -5.97 | 1.34        | 1.45     |
| 13  | bB    | 805  | PHO  | C1D-ND  | -5.97 | 1.27        | 1.38     |
| 14  | aA    | 3134 | CL7  | C4C-C3C | -5.97 | 1.34        | 1.45     |
| 14  | aA    | 3128 | CL7  | C4B-NB  | -5.96 | 1.30        | 1.37     |
| 14  | cB    | 806  | CL7  | MG-NC   | -5.96 | 1.94        | 2.05     |
| 14  | bA    | 3142 | CL7  | MG-NC   | -5.95 | 1.94        | 2.05     |
| 14  | cA    | 3120 | CL7  | C1B-C2B | -5.95 | 1.29        | 1.43     |
| 12  | bA    | 3101 | G9R  | O2D-CGD | 5.94  | 1.47        | 1.33     |
| 14  | bA    | 3118 | CL7  | C1B-C2B | -5.93 | 1.29        | 1.43     |
| 14  | bL    | 204  | CL7  | C4C-C3C | -5.93 | 1.34        | 1.45     |
| 14  | aA    | 3106 | CL7  | MG-NB   | -5.93 | 1.94        | 2.05     |
| 14  | bA    | 3128 | CL7  | C2A-C1A | -5.93 | 1.41        | 1.50     |
| 14  | bB    | 804  | CL7  | C1B-C2B | -5.93 | 1.29        | 1.43     |
| 14  | cL    | 205  | CL7  | MG-NB   | -5.92 | 1.94        | 2.05     |
| 14  | bA    | 3112 | CL7  | C4C-C3C | -5.92 | 1.34        | 1.45     |
| 14  | cA    | 3108 | CL7  | C1C-C2C | -5.92 | 1.33        | 1.45     |
| 14  | aB    | 3003 | CL7  | C1B-C2B | -5.92 | 1.29        | 1.43     |
| 14  | cA    | 3105 | CL7  | MG-NB   | -5.92 | 1.94        | 2.05     |
| 14  | aA    | 3120 | CL7  | C1B-C2B | -5.90 | 1.29        | 1.43     |
| 14  | aA    | 3107 | CL7  | MG-ND   | -5.90 | 1.94        | 2.05     |
| 14  | cA    | 3112 | CL7  | C4C-C3C | -5.90 | 1.34        | 1.45     |
| 14  | bA    | 3122 | CL7  | C1B-C2B | -5.89 | 1.29        | 1.43     |
| 14  | cA    | 3118 | CL7  | C1B-C2B | -5.89 | 1.29        | 1.43     |
| 14  | bA    | 3106 | CL7  | C4C-C3C | -5.89 | 1.34        | 1.45     |
| 14  | cA    | 3139 | CL7  | C1B-C2B | -5.89 | 1.29        | 1.43     |
| 14  | cA    | 3129 | CL7  | MG-NC   | -5.89 | 1.94        | 2.05     |
| 14  | cB    | 811  | CL7  | C1B-C2B | -5.88 | 1.29        | 1.43     |
| 14  | aB    | 3005 | CL7  | MG-NC   | -5.88 | 1.94        | 2.05     |
| 14  | cA    | 3102 | CL7  | C4C-C3C | -5.88 | 1.34        | 1.45     |
| 14  | aB    | 3002 | CL7  | C4B-NB  | -5.88 | 1.30        | 1.37     |
| 14  | aA    | 3143 | CL7  | MG-NC   | -5.87 | 1.94        | 2.05     |
| 14  | cA    | 3141 | CL7  | MG-NA   | -5.87 | 1.94        | 2.05     |
| 14  | aA    | 3129 | CL7  | C4C-C3C | -5.86 | 1.34        | 1.45     |
| 14  | bA    | 3124 | CL7  | OBD-CAD | -5.86 | 1.12        | 1.22     |
| 14  | aL    | 204  | CL7  | C4B-NB  | -5.86 | 1.30        | 1.37     |
| 14  | aA    | 3142 | CL7  | MG-NA   | -5.85 | 1.94        | 2.05     |
| 14  | bA    | 3108 | CL7  | C1C-C2C | -5.85 | 1.33        | 1.45     |
| 14  | aA    | 3129 | CL7  | C2A-C1A | -5.85 | 1.42        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | bA    | 3142 | CL7  | C1B-C2B | -5.84 | 1.29        | 1.43     |
| 14  | bA    | 3112 | CL7  | C1B-C2B | -5.84 | 1.29        | 1.43     |
| 14  | cB    | 811  | CL7  | C4B-NB  | -5.84 | 1.30        | 1.37     |
| 14  | bB    | 811  | CL7  | C4B-NB  | -5.84 | 1.30        | 1.37     |
| 14  | bA    | 3119 | CL7  | MG-NA   | -5.84 | 1.94        | 2.05     |
| 14  | bA    | 3119 | CL7  | OBD-CAD | -5.83 | 1.12        | 1.22     |
| 14  | aB    | 3015 | CL7  | MG-NC   | -5.83 | 1.94        | 2.05     |
| 14  | aK    | 101  | CL7  | C4C-C3C | -5.83 | 1.34        | 1.45     |
| 14  | cL    | 204  | CL7  | C1B-C2B | -5.82 | 1.29        | 1.43     |
| 14  | bB    | 833  | CL7  | C1B-C2B | -5.82 | 1.29        | 1.43     |
| 14  | cA    | 3112 | CL7  | C1B-C2B | -5.82 | 1.29        | 1.43     |
| 14  | bB    | 820  | CL7  | C1B-C2B | -5.82 | 1.29        | 1.43     |
| 14  | cB    | 816  | CL7  | MG-NC   | -5.82 | 1.94        | 2.05     |
| 14  | cA    | 3122 | CL7  | C1B-C2B | -5.82 | 1.29        | 1.43     |
| 12  | cA    | 3101 | G9R  | C4B-NB  | -5.81 | 1.30        | 1.37     |
| 14  | cB    | 827  | CL7  | C1C-C2C | -5.80 | 1.33        | 1.45     |
| 14  | bA    | 3125 | CL7  | C2A-C1A | -5.80 | 1.42        | 1.50     |
| 14  | bB    | 822  | CL7  | C1C-C2C | -5.79 | 1.33        | 1.45     |
| 14  | aB    | 3025 | CL7  | C4C-C3C | -5.79 | 1.34        | 1.45     |
| 14  | bL    | 204  | CL7  | C4B-NB  | -5.78 | 1.30        | 1.37     |
| 14  | cB    | 820  | CL7  | C1B-C2B | -5.78 | 1.29        | 1.43     |
| 14  | bA    | 3114 | CL7  | C4C-C3C | -5.78 | 1.34        | 1.45     |
| 14  | aA    | 3134 | CL7  | C1B-C2B | -5.78 | 1.29        | 1.43     |
| 14  | bA    | 3139 | CL7  | C1B-C2B | -5.78 | 1.29        | 1.43     |
| 14  | bB    | 816  | CL7  | MG-NC   | -5.78 | 1.94        | 2.05     |
| 14  | bA    | 3124 | CL7  | C4C-C3C | -5.78 | 1.34        | 1.45     |
| 14  | aA    | 3109 | CL7  | C1C-C2C | -5.77 | 1.33        | 1.45     |
| 14  | aB    | 3019 | CL7  | C1B-C2B | -5.77 | 1.29        | 1.43     |
| 14  | aA    | 3113 | CL7  | C1B-C2B | -5.77 | 1.29        | 1.43     |
| 14  | cA    | 3119 | CL7  | MG-NA   | -5.77 | 1.94        | 2.05     |
| 14  | bA    | 3140 | CL7  | C1B-C2B | -5.77 | 1.29        | 1.43     |
| 14  | cB    | 822  | CL7  | C1C-C2C | -5.77 | 1.33        | 1.45     |
| 14  | aB    | 3031 | CL7  | C1B-C2B | -5.77 | 1.29        | 1.43     |
| 14  | aB    | 3021 | CL7  | C1C-C2C | -5.77 | 1.33        | 1.45     |
| 14  | cB    | 804  | CL7  | C1B-C2B | -5.76 | 1.29        | 1.43     |
| 14  | aB    | 3023 | CL7  | MG-NB   | -5.76 | 1.94        | 2.05     |
| 14  | aA    | 3120 | CL7  | MG-NA   | -5.76 | 1.94        | 2.05     |
| 14  | cB    | 807  | CL7  | C1B-C2B | -5.76 | 1.29        | 1.43     |
| 14  | bL    | 204  | CL7  | MG-NB   | -5.75 | 1.94        | 2.05     |
| 14  | bB    | 807  | CL7  | C1B-C2B | -5.75 | 1.29        | 1.43     |
| 14  | cB    | 815  | CL7  | C1B-C2B | -5.75 | 1.29        | 1.43     |
| 14  | bB    | 815  | CL7  | C1B-C2B | -5.75 | 1.29        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | bA    | 3141 | CL7  | MG-NA   | -5.75 | 1.94        | 2.05     |
| 13  | cB    | 805  | PHO  | C1D-ND  | -5.74 | 1.27        | 1.38     |
| 14  | aA    | 3115 | CL7  | C4C-C3C | -5.74 | 1.35        | 1.45     |
| 14  | bB    | 803  | CL7  | C4B-NB  | -5.73 | 1.30        | 1.37     |
| 13  | aB    | 3004 | PHO  | C1D-ND  | -5.73 | 1.27        | 1.38     |
| 14  | bB    | 811  | CL7  | C1B-C2B | -5.72 | 1.29        | 1.43     |
| 14  | cA    | 3108 | CL7  | C4B-NB  | -5.72 | 1.30        | 1.37     |
| 14  | cA    | 3127 | CL7  | C1C-C2C | -5.72 | 1.34        | 1.45     |
| 14  | aA    | 3141 | CL7  | C1B-C2B | -5.72 | 1.29        | 1.43     |
| 14  | aA    | 3128 | CL7  | C1C-C2C | -5.72 | 1.34        | 1.45     |
| 14  | bL    | 205  | CL7  | C4B-NB  | -5.72 | 1.30        | 1.37     |
| 14  | aA    | 3143 | CL7  | C1B-C2B | -5.72 | 1.29        | 1.43     |
| 14  | bA    | 3139 | CL7  | C4B-NB  | -5.72 | 1.30        | 1.37     |
| 14  | bB    | 812  | CL7  | C1B-C2B | -5.71 | 1.29        | 1.43     |
| 14  | aA    | 3130 | CL7  | MG-NC   | -5.71 | 1.94        | 2.05     |
| 14  | aA    | 3132 | CL7  | C4B-NB  | -5.71 | 1.30        | 1.37     |
| 14  | aB    | 3011 | CL7  | C1B-C2B | -5.70 | 1.29        | 1.43     |
| 14  | aB    | 3026 | CL7  | C1B-C2B | -5.69 | 1.29        | 1.43     |
| 14  | aL    | 203  | CL7  | MG-NB   | -5.69 | 1.94        | 2.05     |
| 14  | aA    | 3113 | CL7  | C4C-C3C | -5.69 | 1.35        | 1.45     |
| 14  | cB    | 832  | CL7  | C1B-C2B | -5.68 | 1.29        | 1.43     |
| 14  | bL    | 203  | CL7  | MG-NB   | -5.68 | 1.94        | 2.05     |
| 14  | aF    | 201  | CL7  | MG-NA   | -5.68 | 1.94        | 2.05     |
| 14  | cA    | 3124 | CL7  | OBD-CAD | -5.68 | 1.12        | 1.22     |
| 14  | aB    | 3032 | CL7  | C1B-C2B | -5.68 | 1.29        | 1.43     |
| 14  | bB    | 819  | CL7  | C1B-C2B | -5.67 | 1.29        | 1.43     |
| 14  | aB    | 3010 | CL7  | C1B-C2B | -5.67 | 1.29        | 1.43     |
| 14  | cA    | 3114 | CL7  | C4C-C3C | -5.67 | 1.35        | 1.45     |
| 14  | aL    | 203  | CL7  | C1B-C2B | -5.67 | 1.29        | 1.43     |
| 14  | cB    | 812  | CL7  | C1B-C2B | -5.66 | 1.29        | 1.43     |
| 14  | cB    | 820  | CL7  | C4B-NB  | -5.66 | 1.30        | 1.37     |
| 14  | aB    | 3006 | CL7  | C1B-C2B | -5.66 | 1.29        | 1.43     |
| 17  | cB    | 828  | PQN  | O4-C4   | -5.66 | 1.11        | 1.23     |
| 12  | aA    | 3101 | G9R  | O2D-CGD | 5.66  | 1.47        | 1.33     |
| 14  | cA    | 3106 | CL7  | C4B-NB  | -5.65 | 1.30        | 1.37     |
| 14  | bA    | 3132 | CL7  | C4B-NB  | -5.65 | 1.30        | 1.37     |
| 13  | cB    | 805  | PHO  | C1B-NB  | -5.65 | 1.28        | 1.38     |
| 14  | bA    | 3142 | CL7  | MG-ND   | -5.64 | 1.94        | 2.05     |
| 14  | cA    | 3122 | CL7  | C1C-C2C | -5.64 | 1.34        | 1.45     |
| 14  | aB    | 3016 | CL7  | C1B-C2B | -5.64 | 1.30        | 1.43     |
| 14  | cA    | 3125 | CL7  | C2A-C1A | -5.64 | 1.42        | 1.50     |
| 14  | aL    | 202  | CL7  | C4C-C3C | -5.64 | 1.35        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 17  | aB    | 3027 | PQN  | O4-C4   | -5.64 | 1.11        | 1.23     |
| 14  | cA    | 3140 | CL7  | C1B-C2B | -5.64 | 1.30        | 1.43     |
| 14  | bA    | 3116 | CL7  | MG-ND   | -5.64 | 1.94        | 2.05     |
| 14  | aA    | 3123 | CL7  | C1B-C2B | -5.64 | 1.30        | 1.43     |
| 14  | cA    | 3110 | CL7  | C1B-C2B | -5.63 | 1.30        | 1.43     |
| 14  | cB    | 818  | CL7  | C1B-C2B | -5.63 | 1.30        | 1.43     |
| 14  | cA    | 3102 | CL7  | OBD-CAD | -5.63 | 1.12        | 1.22     |
| 14  | cB    | 820  | CL7  | MG-NB   | -5.63 | 1.94        | 2.05     |
| 14  | bB    | 818  | CL7  | C1B-C2B | -5.62 | 1.30        | 1.43     |
| 14  | aA    | 3125 | CL7  | C4C-C3C | -5.62 | 1.35        | 1.45     |
| 14  | cA    | 3141 | CL7  | C1C-C2C | -5.62 | 1.34        | 1.45     |
| 14  | bB    | 832  | CL7  | C1B-C2B | -5.62 | 1.30        | 1.43     |
| 14  | aB    | 3019 | CL7  | C4B-NB  | -5.62 | 1.30        | 1.37     |
| 14  | aB    | 3003 | CL7  | MG-ND   | -5.62 | 1.94        | 2.05     |
| 14  | bL    | 204  | CL7  | C1C-C2C | -5.61 | 1.34        | 1.45     |
| 14  | bA    | 3122 | CL7  | C1C-C2C | -5.61 | 1.34        | 1.45     |
| 14  | cB    | 816  | CL7  | MG-ND   | -5.61 | 1.94        | 2.05     |
| 14  | cA    | 3132 | CL7  | C4B-NB  | -5.61 | 1.30        | 1.37     |
| 14  | aB    | 3017 | CL7  | C1B-C2B | -5.61 | 1.30        | 1.43     |
| 14  | bL    | 205  | CL7  | C1B-C2B | -5.61 | 1.30        | 1.43     |
| 14  | bB    | 827  | CL7  | C1C-C2C | -5.61 | 1.34        | 1.45     |
| 14  | bA    | 3102 | CL7  | OBD-CAD | -5.61 | 1.12        | 1.22     |
| 14  | cA    | 3116 | CL7  | MG-ND   | -5.60 | 1.94        | 2.05     |
| 14  | bA    | 3117 | CL7  | C1B-C2B | -5.60 | 1.30        | 1.43     |
| 14  | cA    | 3127 | CL7  | C1B-C2B | -5.60 | 1.30        | 1.43     |
| 14  | bA    | 3106 | CL7  | C4B-NB  | -5.60 | 1.30        | 1.37     |
| 14  | cA    | 3119 | CL7  | OBD-CAD | -5.60 | 1.12        | 1.22     |
| 14  | bB    | 820  | CL7  | C1C-C2C | -5.59 | 1.34        | 1.45     |
| 14  | aA    | 3107 | CL7  | C4C-C3C | -5.58 | 1.35        | 1.45     |
| 14  | aB    | 3024 | CL7  | C1B-C2B | -5.58 | 1.30        | 1.43     |
| 12  | cA    | 3101 | G9R  | O2D-CGD | 5.58  | 1.46        | 1.33     |
| 17  | bB    | 828  | PQN  | O4-C4   | -5.57 | 1.11        | 1.23     |
| 14  | bA    | 3141 | CL7  | C1C-C2C | -5.57 | 1.34        | 1.45     |
| 14  | aA    | 3109 | CL7  | C4B-NB  | -5.57 | 1.30        | 1.37     |
| 14  | bB    | 827  | CL7  | C1B-C2B | -5.57 | 1.30        | 1.43     |
| 14  | bA    | 3129 | CL7  | C3C-C2C | -5.57 | 1.24        | 1.36     |
| 14  | bA    | 3132 | CL7  | OBD-CAD | -5.56 | 1.12        | 1.22     |
| 14  | aL    | 202  | CL7  | MG-NB   | -5.56 | 1.94        | 2.05     |
| 14  | bJ    | 101  | CL7  | C1B-C2B | -5.55 | 1.30        | 1.43     |
| 14  | bA    | 3139 | CL7  | MG-ND   | -5.55 | 1.94        | 2.05     |
| 14  | bB    | 816  | CL7  | MG-ND   | -5.55 | 1.94        | 2.05     |
| 14  | aB    | 3022 | CL7  | C1B-C2B | -5.55 | 1.30        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | bA    | 3124 | CL7  | C1B-C2B | -5.55 | 1.30        | 1.43     |
| 14  | aB    | 3026 | CL7  | C1C-C2C | -5.55 | 1.34        | 1.45     |
| 14  | cA    | 3124 | CL7  | C1B-C2B | -5.55 | 1.30        | 1.43     |
| 14  | aL    | 203  | CL7  | C4B-NB  | -5.54 | 1.31        | 1.37     |
| 14  | cA    | 3114 | CL7  | MG-ND   | -5.54 | 1.94        | 2.05     |
| 14  | bA    | 3106 | CL7  | C1C-C2C | -5.54 | 1.34        | 1.45     |
| 14  | cA    | 3117 | CL7  | C1B-C2B | -5.54 | 1.30        | 1.43     |
| 14  | bB    | 833  | CL7  | MG-NA   | -5.54 | 1.94        | 2.05     |
| 14  | aB    | 3015 | CL7  | MG-ND   | -5.54 | 1.94        | 2.05     |
| 14  | cA    | 3142 | CL7  | MG-ND   | -5.54 | 1.94        | 2.05     |
| 14  | cB    | 823  | CL7  | C1B-C2B | -5.54 | 1.30        | 1.43     |
| 14  | cF    | 201  | CL7  | MG-NA   | -5.53 | 1.94        | 2.05     |
| 14  | cB    | 827  | CL7  | C1B-C2B | -5.53 | 1.30        | 1.43     |
| 14  | aJ    | 101  | CL7  | C1B-C2B | -5.53 | 1.30        | 1.43     |
| 14  | bA    | 3110 | CL7  | C1B-C2B | -5.52 | 1.30        | 1.43     |
| 14  | aA    | 3123 | CL7  | C1C-C2C | -5.52 | 1.34        | 1.45     |
| 12  | aA    | 3101 | G9R  | C3C-C2C | 5.52  | 1.48        | 1.36     |
| 14  | aB    | 3030 | CL7  | C1B-C2B | -5.52 | 1.30        | 1.43     |
| 14  | cB    | 820  | CL7  | C1C-C2C | -5.52 | 1.34        | 1.45     |
| 14  | bA    | 3115 | CL7  | C4C-C3C | -5.52 | 1.35        | 1.45     |
| 14  | bF    | 201  | CL7  | MG-NA   | -5.52 | 1.94        | 2.05     |
| 14  | cB    | 816  | CL7  | MG-NA   | -5.52 | 1.94        | 2.05     |
| 14  | aL    | 204  | CL7  | MG-NC   | -5.52 | 1.94        | 2.05     |
| 14  | cB    | 824  | CL7  | MG-NB   | -5.52 | 1.94        | 2.05     |
| 14  | bL    | 203  | CL7  | C1B-C2B | -5.52 | 1.30        | 1.43     |
| 14  | aB    | 3015 | CL7  | C1B-C2B | -5.51 | 1.30        | 1.43     |
| 14  | cB    | 817  | CL7  | C1B-C2B | -5.51 | 1.30        | 1.43     |
| 14  | aA    | 3105 | CL7  | C1B-C2B | -5.51 | 1.30        | 1.43     |
| 14  | cB    | 819  | CL7  | C1B-C2B | -5.51 | 1.30        | 1.43     |
| 14  | bB    | 823  | CL7  | C1B-C2B | -5.51 | 1.30        | 1.43     |
| 14  | cJ    | 101  | CL7  | C1B-C2B | -5.50 | 1.30        | 1.43     |
| 14  | bB    | 817  | CL7  | C1B-C2B | -5.50 | 1.30        | 1.43     |
| 14  | cA    | 3108 | CL7  | C4C-C3C | -5.50 | 1.35        | 1.45     |
| 14  | cB    | 808  | CL7  | C4B-NB  | -5.50 | 1.31        | 1.37     |
| 14  | aL    | 204  | CL7  | C1B-C2B | -5.50 | 1.30        | 1.43     |
| 14  | cA    | 3124 | CL7  | MG-NC   | -5.50 | 1.94        | 2.05     |
| 14  | aA    | 3125 | CL7  | OBD-CAD | -5.50 | 1.13        | 1.22     |
| 14  | bA    | 3127 | CL7  | C1B-C2B | -5.48 | 1.30        | 1.43     |
| 14  | aA    | 3133 | CL7  | C4B-NB  | -5.48 | 1.31        | 1.37     |
| 17  | aA    | 3144 | PQN  | C11-C12 | -5.48 | 1.42        | 1.50     |
| 14  | cA    | 3115 | CL7  | C4C-C3C | -5.48 | 1.35        | 1.45     |
| 14  | aA    | 3116 | CL7  | C4C-C3C | -5.48 | 1.35        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | cA    | 3128 | CL7  | OBD-CAD | -5.47 | 1.13        | 1.22     |
| 14  | aB    | 3014 | CL7  | C1B-C2B | -5.47 | 1.30        | 1.43     |
| 14  | bA    | 3104 | CL7  | C1B-C2B | -5.47 | 1.30        | 1.43     |
| 14  | aB    | 3015 | CL7  | MG-NA   | -5.46 | 1.95        | 2.05     |
| 14  | bB    | 804  | CL7  | MG-ND   | -5.46 | 1.95        | 2.05     |
| 14  | cB    | 803  | CL7  | C1B-C2B | -5.46 | 1.30        | 1.43     |
| 14  | bL    | 203  | CL7  | C4C-C3C | -5.46 | 1.35        | 1.45     |
| 14  | bA    | 3142 | CL7  | C4B-NB  | -5.45 | 1.31        | 1.37     |
| 14  | cL    | 205  | CL7  | C1B-C2B | -5.45 | 1.30        | 1.43     |
| 14  | aB    | 3019 | CL7  | C1C-C2C | -5.45 | 1.34        | 1.45     |
| 14  | cL    | 205  | CL7  | MG-ND   | -5.45 | 1.95        | 2.05     |
| 14  | bB    | 824  | CL7  | MG-NB   | -5.44 | 1.95        | 2.05     |
| 14  | aA    | 3118 | CL7  | C1B-C2B | -5.44 | 1.30        | 1.43     |
| 14  | bL    | 205  | CL7  | MG-NC   | -5.44 | 1.95        | 2.05     |
| 14  | aL    | 202  | CL7  | C1B-C2B | -5.44 | 1.30        | 1.43     |
| 14  | cB    | 825  | CL7  | C1B-C2B | -5.44 | 1.30        | 1.43     |
| 14  | aL    | 204  | CL7  | MG-ND   | -5.44 | 1.95        | 2.05     |
| 14  | cL    | 203  | CL7  | MG-NB   | -5.44 | 1.95        | 2.05     |
| 14  | aA    | 3142 | CL7  | C1C-C2C | -5.44 | 1.34        | 1.45     |
| 14  | aB    | 3007 | CL7  | C4B-NB  | -5.44 | 1.31        | 1.37     |
| 14  | bB    | 820  | CL7  | C4B-NB  | -5.44 | 1.31        | 1.37     |
| 14  | cA    | 3122 | CL7  | C4B-NB  | -5.43 | 1.31        | 1.37     |
| 14  | aB    | 3010 | CL7  | C4B-NB  | -5.43 | 1.31        | 1.37     |
| 14  | bA    | 3142 | CL7  | MG-NB   | -5.43 | 1.95        | 2.05     |
| 14  | cA    | 3106 | CL7  | C1C-C2C | -5.43 | 1.34        | 1.45     |
| 14  | bB    | 824  | CL7  | C1C-C2C | -5.43 | 1.34        | 1.45     |
| 14  | cL    | 205  | CL7  | MG-NC   | -5.43 | 1.95        | 2.05     |
| 14  | bA    | 3128 | CL7  | OBD-CAD | -5.43 | 1.13        | 1.22     |
| 14  | cA    | 3104 | CL7  | C1B-C2B | -5.43 | 1.30        | 1.43     |
| 14  | aA    | 3123 | CL7  | C4B-NB  | -5.43 | 1.31        | 1.37     |
| 14  | bA    | 3103 | CL7  | C1B-C2B | -5.42 | 1.30        | 1.43     |
| 14  | aA    | 3140 | CL7  | C1B-C2B | -5.42 | 1.30        | 1.43     |
| 14  | bL    | 205  | CL7  | MG-ND   | -5.42 | 1.95        | 2.05     |
| 14  | cL    | 204  | CL7  | MG-ND   | -5.42 | 1.95        | 2.05     |
| 14  | cA    | 3104 | CL7  | MG-ND   | -5.42 | 1.95        | 2.05     |
| 14  | bB    | 825  | CL7  | C1B-C2B | -5.42 | 1.30        | 1.43     |
| 14  | bA    | 3102 | CL7  | C4C-C3C | -5.41 | 1.35        | 1.45     |
| 14  | cA    | 3130 | CL7  | C1B-C2B | -5.41 | 1.30        | 1.43     |
| 14  | cA    | 3109 | CL7  | C1B-C2B | -5.41 | 1.30        | 1.43     |
| 14  | aB    | 3019 | CL7  | MG-NB   | -5.41 | 1.95        | 2.05     |
| 14  | bA    | 3105 | CL7  | C1B-C2B | -5.40 | 1.30        | 1.43     |
| 14  | bA    | 3111 | CL7  | C1B-C2B | -5.40 | 1.30        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | cA    | 3129 | CL7  | C4C-C3C | -5.40 | 1.35        | 1.45     |
| 14  | cA    | 3129 | CL7  | CAB-C3B | -5.40 | 1.33        | 1.45     |
| 14  | bA    | 3130 | CL7  | C1B-C2B | -5.40 | 1.30        | 1.43     |
| 14  | bB    | 816  | CL7  | MG-NA   | -5.40 | 1.95        | 2.05     |
| 14  | aA    | 3112 | CL7  | C1B-C2B | -5.40 | 1.30        | 1.43     |
| 14  | cB    | 816  | CL7  | C1B-C2B | -5.40 | 1.30        | 1.43     |
| 14  | bA    | 3109 | CL7  | C1B-C2B | -5.40 | 1.30        | 1.43     |
| 14  | aA    | 3111 | CL7  | C1B-C2B | -5.40 | 1.30        | 1.43     |
| 14  | cL    | 203  | CL7  | C1B-C2B | -5.39 | 1.30        | 1.43     |
| 14  | bA    | 3127 | CL7  | C1C-C2C | -5.39 | 1.34        | 1.45     |
| 14  | cA    | 3131 | CL7  | C1B-C2B | -5.39 | 1.30        | 1.43     |
| 14  | cA    | 3129 | CL7  | C3C-C2C | -5.39 | 1.25        | 1.36     |
| 14  | bA    | 3104 | CL7  | MG-ND   | -5.39 | 1.95        | 2.05     |
| 14  | cA    | 3111 | CL7  | C1B-C2B | -5.39 | 1.30        | 1.43     |
| 14  | aA    | 3103 | CL7  | C3A-C4A | -5.39 | 1.42        | 1.52     |
| 14  | cB    | 803  | CL7  | MG-NB   | -5.38 | 1.95        | 2.05     |
| 14  | cB    | 831  | CL7  | C1B-C2B | -5.38 | 1.30        | 1.43     |
| 14  | aB    | 3023 | CL7  | C1C-C2C | -5.38 | 1.34        | 1.45     |
| 14  | cA    | 3102 | CL7  | MG-ND   | -5.38 | 1.95        | 2.05     |
| 14  | aL    | 203  | CL7  | C4C-C3C | -5.38 | 1.35        | 1.45     |
| 14  | bL    | 203  | CL7  | C1C-C2C | -5.38 | 1.34        | 1.45     |
| 13  | cB    | 805  | PHO  | C4D-ND  | -5.37 | 1.31        | 1.38     |
| 14  | aA    | 3105 | CL7  | MG-ND   | -5.37 | 1.95        | 2.05     |
| 14  | bB    | 820  | CL7  | MG-NB   | -5.37 | 1.95        | 2.05     |
| 14  | bA    | 3107 | CL7  | MG-ND   | -5.36 | 1.95        | 2.05     |
| 14  | bB    | 803  | CL7  | MG-NB   | -5.35 | 1.95        | 2.05     |
| 14  | bB    | 826  | CL7  | MG-NC   | -5.35 | 1.95        | 2.05     |
| 14  | bA    | 3113 | CL7  | C1B-C2B | -5.35 | 1.30        | 1.43     |
| 14  | aA    | 3143 | CL7  | MG-ND   | -5.35 | 1.95        | 2.05     |
| 14  | cB    | 810  | CL7  | MG-ND   | -5.35 | 1.95        | 2.05     |
| 14  | bA    | 3125 | CL7  | C1C-C2C | -5.35 | 1.34        | 1.45     |
| 14  | bB    | 814  | CL7  | C1B-C2B | -5.35 | 1.30        | 1.43     |
| 14  | bK    | 101  | CL7  | C1B-C2B | -5.35 | 1.30        | 1.43     |
| 13  | aB    | 3004 | PHO  | C4B-NB  | -5.35 | 1.28        | 1.38     |
| 14  | cK    | 101  | CL7  | C1B-C2B | -5.35 | 1.30        | 1.43     |
| 14  | aA    | 3146 | CL7  | C1B-C2B | -5.34 | 1.30        | 1.43     |
| 14  | cL    | 204  | CL7  | C1C-C2C | -5.34 | 1.34        | 1.45     |
| 14  | aL    | 202  | CL7  | C1C-C2C | -5.34 | 1.34        | 1.45     |
| 14  | cA    | 3139 | CL7  | MG-ND   | -5.34 | 1.95        | 2.05     |
| 14  | cB    | 816  | CL7  | C4C-C3C | -5.34 | 1.35        | 1.45     |
| 14  | cB    | 824  | CL7  | C1C-C2C | -5.34 | 1.34        | 1.45     |
| 14  | cA    | 3113 | CL7  | C1B-C2B | -5.34 | 1.30        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | bB    | 831  | CL7  | C1B-C2B | -5.34 | 1.30        | 1.43     |
| 14  | bB    | 808  | CL7  | C4B-NB  | -5.34 | 1.31        | 1.37     |
| 12  | cA    | 3101 | G9R  | C3C-C2C | 5.34  | 1.48        | 1.36     |
| 14  | aB    | 3024 | CL7  | C1C-C2C | -5.34 | 1.34        | 1.45     |
| 14  | bA    | 3102 | CL7  | MG-ND   | -5.34 | 1.95        | 2.05     |
| 14  | cA    | 3105 | CL7  | C1B-C2B | -5.33 | 1.30        | 1.43     |
| 14  | cB    | 827  | CL7  | OBB-CAB | 5.33  | 1.34        | 1.22     |
| 14  | aB    | 3013 | CL7  | C1B-C2B | -5.33 | 1.30        | 1.43     |
| 13  | aA    | 3102 | PHO  | C4A-C3A | -5.33 | 1.41        | 1.51     |
| 14  | aB    | 3026 | CL7  | C4C-C3C | -5.33 | 1.35        | 1.45     |
| 14  | cB    | 814  | CL7  | C1B-C2B | -5.33 | 1.30        | 1.43     |
| 13  | cB    | 801  | PHO  | C4A-C3A | -5.33 | 1.41        | 1.51     |
| 14  | cA    | 3144 | CL7  | C1B-C2B | -5.33 | 1.30        | 1.43     |
| 13  | bB    | 801  | PHO  | C4A-C3A | -5.33 | 1.41        | 1.51     |
| 14  | cB    | 822  | CL7  | C4B-NB  | -5.32 | 1.31        | 1.37     |
| 14  | cA    | 3103 | CL7  | C1B-C2B | -5.32 | 1.30        | 1.43     |
| 14  | bA    | 3114 | CL7  | MG-ND   | -5.31 | 1.95        | 2.05     |
| 14  | aA    | 3130 | CL7  | C3A-C2A | -5.31 | 1.49        | 1.54     |
| 13  | bB    | 805  | PHO  | C1B-NB  | -5.31 | 1.28        | 1.38     |
| 14  | bA    | 3131 | CL7  | C1B-C2B | -5.31 | 1.30        | 1.43     |
| 14  | bB    | 813  | CL7  | C1B-C2B | -5.31 | 1.30        | 1.43     |
| 14  | bA    | 3133 | CL7  | C1C-C2C | -5.31 | 1.34        | 1.45     |
| 14  | cA    | 3121 | CL7  | C1B-C2B | -5.31 | 1.30        | 1.43     |
| 14  | cA    | 3139 | CL7  | MG-NA   | -5.31 | 1.95        | 2.05     |
| 14  | cA    | 3142 | CL7  | MG-NB   | -5.30 | 1.95        | 2.05     |
| 14  | cB    | 813  | CL7  | C1B-C2B | -5.30 | 1.30        | 1.43     |
| 14  | bB    | 816  | CL7  | C1B-C2B | -5.30 | 1.30        | 1.43     |
| 14  | aB    | 3012 | CL7  | C1B-C2B | -5.30 | 1.30        | 1.43     |
| 14  | aA    | 3129 | CL7  | MG-NA   | -5.29 | 1.95        | 2.05     |
| 14  | cB    | 833  | CL7  | MG-NA   | -5.29 | 1.95        | 2.05     |
| 14  | bB    | 816  | CL7  | C4C-C3C | -5.29 | 1.35        | 1.45     |
| 14  | cA    | 3140 | CL7  | C1C-C2C | -5.29 | 1.34        | 1.45     |
| 14  | cB    | 804  | CL7  | MG-ND   | -5.29 | 1.95        | 2.05     |
| 14  | cA    | 3133 | CL7  | C1C-C2C | -5.29 | 1.34        | 1.45     |
| 14  | bB    | 803  | CL7  | C1B-C2B | -5.29 | 1.30        | 1.43     |
| 14  | bA    | 3122 | CL7  | C4B-NB  | -5.28 | 1.31        | 1.37     |
| 14  | bA    | 3145 | CL7  | C1B-C2B | -5.28 | 1.30        | 1.43     |
| 14  | cB    | 833  | CL7  | C1C-C2C | -5.28 | 1.34        | 1.45     |
| 14  | aA    | 3117 | CL7  | MG-ND   | -5.28 | 1.95        | 2.05     |
| 14  | aA    | 3104 | CL7  | C1B-C2B | -5.28 | 1.30        | 1.43     |
| 14  | bB    | 825  | CL7  | C1C-C2C | -5.28 | 1.34        | 1.45     |
| 14  | aA    | 3133 | CL7  | OBD-CAD | -5.28 | 1.13        | 1.22     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | bA    | 3129 | CL7  | C4C-C3C | -5.28 | 1.35        | 1.45     |
| 14  | aA    | 3116 | CL7  | C1B-C2B | -5.27 | 1.30        | 1.43     |
| 14  | bA    | 3115 | CL7  | C1B-C2B | -5.27 | 1.30        | 1.43     |
| 14  | aA    | 3110 | CL7  | C1B-C2B | -5.27 | 1.30        | 1.43     |
| 14  | aB    | 3026 | CL7  | C4B-NB  | -5.27 | 1.31        | 1.37     |
| 14  | aA    | 3128 | CL7  | C1B-C2B | -5.27 | 1.30        | 1.43     |
| 14  | bF    | 201  | CL7  | C1B-C2B | -5.27 | 1.30        | 1.43     |
| 14  | bB    | 827  | CL7  | OBb-CAB | 5.26  | 1.34        | 1.22     |
| 14  | aA    | 3114 | CL7  | C1B-C2B | -5.26 | 1.30        | 1.43     |
| 14  | cA    | 3115 | CL7  | C1B-C2B | -5.26 | 1.30        | 1.43     |
| 14  | cB    | 818  | CL7  | MG-NA   | -5.25 | 1.95        | 2.05     |
| 14  | bA    | 3124 | CL7  | MG-NC   | -5.25 | 1.95        | 2.05     |
| 14  | bA    | 3126 | CL7  | C2A-C1A | -5.25 | 1.46        | 1.52     |
| 14  | bA    | 3139 | CL7  | MG-NA   | -5.25 | 1.95        | 2.05     |
| 14  | cB    | 822  | CL7  | MG-ND   | -5.24 | 1.95        | 2.05     |
| 14  | aB    | 3026 | CL7  | MG-NA   | -5.24 | 1.95        | 2.05     |
| 14  | cA    | 3102 | CL7  | C3A-C4A | -5.24 | 1.42        | 1.52     |
| 14  | aA    | 3103 | CL7  | C4C-C3C | -5.24 | 1.35        | 1.45     |
| 17  | bA    | 3143 | PQN  | C11-C12 | -5.24 | 1.43        | 1.50     |
| 14  | bB    | 818  | CL7  | MG-NA   | -5.23 | 1.95        | 2.05     |
| 14  | cA    | 3132 | CL7  | CAA-C2A | -5.23 | 1.44        | 1.54     |
| 14  | bL    | 204  | CL7  | MG-ND   | -5.23 | 1.95        | 2.05     |
| 14  | bB    | 822  | CL7  | MG-ND   | -5.23 | 1.95        | 2.05     |
| 14  | aA    | 3131 | CL7  | C1B-C2B | -5.23 | 1.30        | 1.43     |
| 14  | aA    | 3132 | CL7  | C1B-C2B | -5.23 | 1.30        | 1.43     |
| 14  | aB    | 3024 | CL7  | MG-NB   | -5.23 | 1.95        | 2.05     |
| 14  | aB    | 3020 | CL7  | C1B-C2B | -5.23 | 1.31        | 1.43     |
| 14  | aA    | 3140 | CL7  | MG-NA   | -5.22 | 1.95        | 2.05     |
| 14  | bA    | 3105 | CL7  | CAB-C3B | -5.22 | 1.34        | 1.45     |
| 14  | bA    | 3141 | CL7  | MG-ND   | -5.22 | 1.95        | 2.05     |
| 14  | cA    | 3113 | CL7  | MG-NA   | -5.22 | 1.95        | 2.05     |
| 14  | bB    | 821  | CL7  | C1B-C2B | -5.22 | 1.31        | 1.43     |
| 14  | cA    | 3107 | CL7  | MG-NC   | -5.22 | 1.95        | 2.05     |
| 14  | cA    | 3112 | CL7  | MG-NC   | -5.22 | 1.95        | 2.05     |
| 14  | aA    | 3107 | CL7  | C1C-C2C | -5.22 | 1.35        | 1.45     |
| 14  | bA    | 3107 | CL7  | C4B-NB  | -5.21 | 1.31        | 1.37     |
| 14  | aA    | 3134 | CL7  | C1C-C2C | -5.21 | 1.35        | 1.45     |
| 14  | bB    | 825  | CL7  | MG-NB   | -5.21 | 1.95        | 2.05     |
| 14  | bA    | 3107 | CL7  | MG-NC   | -5.21 | 1.95        | 2.05     |
| 14  | cA    | 3105 | CL7  | CAB-C3B | -5.21 | 1.34        | 1.45     |
| 14  | bA    | 3108 | CL7  | C1B-C2B | -5.21 | 1.31        | 1.43     |
| 14  | aA    | 3124 | CL7  | MG-NA   | -5.21 | 1.95        | 2.05     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | cB    | 825  | CL7  | C1C-C2C | -5.20 | 1.35        | 1.45     |
| 14  | aB    | 3025 | CL7  | C1D-ND  | -5.20 | 1.31        | 1.37     |
| 12  | bA    | 3101 | G9R  | C3C-C2C | 5.20  | 1.47        | 1.36     |
| 14  | bA    | 3140 | CL7  | C4B-NB  | -5.20 | 1.31        | 1.37     |
| 14  | aB    | 3011 | CL7  | MG-NA   | -5.20 | 1.95        | 2.05     |
| 14  | bB    | 822  | CL7  | C4B-NB  | -5.20 | 1.31        | 1.37     |
| 12  | cA    | 3101 | G9R  | CHD-C1D | 5.19  | 1.48        | 1.38     |
| 14  | bB    | 806  | CL7  | C1B-C2B | -5.19 | 1.31        | 1.43     |
| 14  | bA    | 3129 | CL7  | C3A-C2A | -5.19 | 1.49        | 1.54     |
| 14  | aA    | 3121 | CL7  | C4B-NB  | -5.19 | 1.31        | 1.37     |
| 14  | cA    | 3140 | CL7  | C4B-NB  | -5.19 | 1.31        | 1.37     |
| 14  | cA    | 3128 | CL7  | C1B-C2B | -5.19 | 1.31        | 1.43     |
| 14  | cB    | 827  | CL7  | C4C-C3C | -5.18 | 1.36        | 1.45     |
| 14  | bA    | 3112 | CL7  | MG-NC   | -5.18 | 1.95        | 2.05     |
| 14  | aB    | 3021 | CL7  | MG-ND   | -5.18 | 1.95        | 2.05     |
| 14  | cB    | 826  | CL7  | MG-NC   | -5.18 | 1.95        | 2.05     |
| 14  | cA    | 3125 | CL7  | C1C-C2C | -5.18 | 1.35        | 1.45     |
| 14  | aB    | 3015 | CL7  | C4B-NB  | -5.18 | 1.31        | 1.37     |
| 14  | aA    | 3140 | CL7  | MG-ND   | -5.18 | 1.95        | 2.05     |
| 13  | cB    | 805  | PHO  | C3D-CAD | -5.18 | 1.36        | 1.47     |
| 14  | bA    | 3114 | CL7  | C4B-NB  | -5.17 | 1.31        | 1.37     |
| 14  | aA    | 3126 | CL7  | C2A-C1A | -5.17 | 1.43        | 1.50     |
| 14  | cB    | 809  | CL7  | MG-NA   | -5.17 | 1.95        | 2.05     |
| 14  | aB    | 3018 | CL7  | C4C-NC  | 5.17  | 1.44        | 1.37     |
| 14  | aB    | 3026 | CL7  | OBB-CAB | 5.17  | 1.34        | 1.22     |
| 14  | cA    | 3114 | CL7  | C1B-C2B | -5.16 | 1.31        | 1.43     |
| 14  | aB    | 3032 | CL7  | MG-NA   | -5.16 | 1.95        | 2.05     |
| 14  | bA    | 3113 | CL7  | MG-NA   | -5.16 | 1.95        | 2.05     |
| 14  | bA    | 3140 | CL7  | C1C-C2C | -5.16 | 1.35        | 1.45     |
| 14  | aA    | 3141 | CL7  | C1C-C2C | -5.16 | 1.35        | 1.45     |
| 14  | bB    | 812  | CL7  | MG-NA   | -5.16 | 1.95        | 2.05     |
| 14  | aB    | 3025 | CL7  | MG-NC   | -5.16 | 1.95        | 2.05     |
| 14  | cA    | 3107 | CL7  | MG-ND   | -5.16 | 1.95        | 2.05     |
| 14  | bB    | 803  | CL7  | C1C-C2C | -5.16 | 1.35        | 1.45     |
| 14  | aB    | 3021 | CL7  | C4B-NB  | -5.15 | 1.31        | 1.37     |
| 12  | aA    | 3101 | G9R  | CHD-C1D | 5.15  | 1.48        | 1.38     |
| 14  | cB    | 821  | CL7  | C1B-C2B | -5.15 | 1.31        | 1.43     |
| 14  | aA    | 3140 | CL7  | C4B-NB  | -5.15 | 1.31        | 1.37     |
| 14  | aB    | 3021 | CL7  | C1B-C2B | -5.15 | 1.31        | 1.43     |
| 14  | bB    | 822  | CL7  | MG-NB   | -5.15 | 1.95        | 2.05     |
| 14  | aF    | 201  | CL7  | C1B-C2B | -5.15 | 1.31        | 1.43     |
| 14  | aL    | 203  | CL7  | MG-ND   | -5.14 | 1.95        | 2.05     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | cA    | 3142 | CL7  | C4B-NB  | -5.14 | 1.31        | 1.37     |
| 14  | aA    | 3103 | CL7  | MG-ND   | -5.14 | 1.95        | 2.05     |
| 14  | aK    | 101  | CL7  | C1B-C2B | -5.14 | 1.31        | 1.43     |
| 14  | aB    | 3017 | CL7  | MG-NA   | -5.14 | 1.95        | 2.05     |
| 14  | aA    | 3124 | CL7  | C1C-C2C | -5.14 | 1.35        | 1.45     |
| 14  | aA    | 3106 | CL7  | CAB-C3B | -5.14 | 1.34        | 1.45     |
| 14  | bB    | 816  | CL7  | C4B-NB  | -5.13 | 1.31        | 1.37     |
| 14  | aB    | 3002 | CL7  | MG-NB   | -5.13 | 1.95        | 2.05     |
| 14  | cB    | 812  | CL7  | MG-NA   | -5.13 | 1.95        | 2.05     |
| 14  | cA    | 3108 | CL7  | MG-ND   | -5.13 | 1.95        | 2.05     |
| 14  | aA    | 3143 | CL7  | C4C-NC  | 5.13  | 1.44        | 1.37     |
| 14  | bF    | 201  | CL7  | C1C-C2C | -5.13 | 1.35        | 1.45     |
| 14  | aB    | 3015 | CL7  | C4C-C3C | -5.13 | 1.36        | 1.45     |
| 14  | bA    | 3124 | CL7  | MG-NA   | -5.13 | 1.95        | 2.05     |
| 14  | cF    | 201  | CL7  | C1B-C2B | -5.13 | 1.31        | 1.43     |
| 17  | cA    | 3143 | PQN  | C11-C12 | -5.13 | 1.43        | 1.50     |
| 14  | aA    | 3125 | CL7  | MG-NA   | -5.12 | 1.95        | 2.05     |
| 14  | cB    | 825  | CL7  | MG-NB   | -5.12 | 1.95        | 2.05     |
| 14  | bB    | 809  | CL7  | MG-NA   | -5.12 | 1.95        | 2.05     |
| 14  | cA    | 3141 | CL7  | MG-ND   | -5.12 | 1.95        | 2.05     |
| 14  | cB    | 803  | CL7  | C1C-C2C | -5.12 | 1.35        | 1.45     |
| 14  | aA    | 3130 | CL7  | C3C-C2C | -5.11 | 1.25        | 1.36     |
| 14  | aA    | 3133 | CL7  | CBA-CGA | -5.11 | 1.35        | 1.50     |
| 14  | bA    | 3128 | CL7  | MG-NA   | -5.11 | 1.95        | 2.05     |
| 14  | bB    | 824  | CL7  | C4B-NB  | -5.11 | 1.31        | 1.37     |
| 14  | aA    | 3103 | CL7  | C2A-C1A | -5.11 | 1.43        | 1.50     |
| 14  | bB    | 815  | CL7  | C1C-C2C | -5.11 | 1.35        | 1.45     |
| 14  | bB    | 819  | CL7  | MG-ND   | -5.11 | 1.95        | 2.05     |
| 14  | bA    | 3121 | CL7  | C1B-C2B | -5.10 | 1.31        | 1.43     |
| 14  | bB    | 822  | CL7  | C1B-C2B | -5.10 | 1.31        | 1.43     |
| 14  | cB    | 810  | CL7  | MG-NC   | -5.10 | 1.95        | 2.05     |
| 14  | bB    | 833  | CL7  | C1C-C2C | -5.10 | 1.35        | 1.45     |
| 14  | cA    | 3106 | CL7  | MG-NC   | -5.10 | 1.95        | 2.05     |
| 14  | cA    | 3128 | CL7  | MG-NA   | -5.10 | 1.95        | 2.05     |
| 14  | bA    | 3103 | CL7  | MG-NA   | -5.10 | 1.95        | 2.05     |
| 14  | bA    | 3110 | CL7  | MG-ND   | -5.10 | 1.95        | 2.05     |
| 14  | cB    | 822  | CL7  | C1B-C2B | -5.10 | 1.31        | 1.43     |
| 14  | aA    | 3126 | CL7  | C1C-C2C | -5.10 | 1.35        | 1.45     |
| 14  | cA    | 3108 | CL7  | MG-NC   | -5.09 | 1.95        | 2.05     |
| 14  | bJ    | 101  | CL7  | MG-NA   | -5.09 | 1.95        | 2.05     |
| 14  | aB    | 3012 | CL7  | C4B-NB  | -5.09 | 1.31        | 1.37     |
| 14  | cB    | 825  | CL7  | MG-NA   | -5.09 | 1.95        | 2.05     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | aB    | 3021 | CL7  | MG-NB   | -5.09 | 1.95        | 2.05     |
| 13  | aB    | 3004 | PHO  | C1B-NB  | -5.09 | 1.29        | 1.38     |
| 14  | cB    | 815  | CL7  | C1C-C2C | -5.08 | 1.35        | 1.45     |
| 13  | aB    | 3004 | PHO  | C4D-ND  | -5.08 | 1.31        | 1.38     |
| 14  | cA    | 3112 | CL7  | MG-ND   | -5.08 | 1.95        | 2.05     |
| 13  | cB    | 805  | PHO  | C1B-C2B | 5.08  | 1.45        | 1.39     |
| 14  | cB    | 807  | CL7  | C4B-NB  | -5.08 | 1.31        | 1.37     |
| 14  | bA    | 3109 | CL7  | MG-ND   | -5.08 | 1.95        | 2.05     |
| 14  | aB    | 3023 | CL7  | C4B-NB  | -5.08 | 1.31        | 1.37     |
| 14  | bA    | 3128 | CL7  | MG-NC   | -5.08 | 1.95        | 2.05     |
| 14  | aB    | 3009 | CL7  | MG-ND   | -5.08 | 1.95        | 2.05     |
| 14  | aB    | 3018 | CL7  | MG-NC   | -5.08 | 1.95        | 2.05     |
| 14  | bA    | 3112 | CL7  | MG-ND   | -5.07 | 1.95        | 2.05     |
| 14  | bB    | 807  | CL7  | C1C-C2C | -5.07 | 1.35        | 1.45     |
| 14  | bB    | 813  | CL7  | C4B-NB  | -5.07 | 1.31        | 1.37     |
| 14  | aB    | 3002 | CL7  | C1C-C2C | -5.07 | 1.35        | 1.45     |
| 14  | aB    | 3011 | CL7  | C1C-C2C | -5.07 | 1.35        | 1.45     |
| 14  | aA    | 3106 | CL7  | C1B-C2B | -5.07 | 1.31        | 1.43     |
| 14  | cB    | 832  | CL7  | C1C-C2C | -5.07 | 1.35        | 1.45     |
| 14  | bA    | 3129 | CL7  | CAB-C3B | -5.07 | 1.34        | 1.45     |
| 14  | cA    | 3124 | CL7  | MG-NA   | -5.07 | 1.95        | 2.05     |
| 14  | cA    | 3132 | CL7  | OBD-CAD | -5.07 | 1.13        | 1.22     |
| 14  | cB    | 813  | CL7  | MG-NA   | -5.07 | 1.95        | 2.05     |
| 14  | bA    | 3128 | CL7  | C1B-C2B | -5.07 | 1.31        | 1.43     |
| 14  | bB    | 813  | CL7  | MG-NA   | -5.07 | 1.95        | 2.05     |
| 14  | bB    | 825  | CL7  | MG-ND   | -5.07 | 1.95        | 2.05     |
| 14  | cB    | 810  | CL7  | CAA-C2A | -5.06 | 1.44        | 1.54     |
| 14  | aB    | 3006 | CL7  | C4B-NB  | -5.06 | 1.31        | 1.37     |
| 14  | aJ    | 101  | CL7  | MG-NA   | -5.06 | 1.95        | 2.05     |
| 14  | bA    | 3105 | CL7  | C4C-C3C | -5.06 | 1.36        | 1.45     |
| 14  | aA    | 3143 | CL7  | MG-NA   | -5.05 | 1.95        | 2.05     |
| 14  | aB    | 3012 | CL7  | MG-NA   | -5.05 | 1.95        | 2.05     |
| 14  | aA    | 3107 | CL7  | C4B-NB  | -5.05 | 1.31        | 1.37     |
| 14  | aA    | 3115 | CL7  | MG-ND   | -5.05 | 1.95        | 2.05     |
| 14  | aA    | 3104 | CL7  | MG-NA   | -5.05 | 1.95        | 2.05     |
| 14  | aA    | 3143 | CL7  | MG-NB   | -5.04 | 1.95        | 2.05     |
| 14  | cA    | 3123 | CL7  | C1C-C2C | -5.03 | 1.35        | 1.45     |
| 14  | cB    | 827  | CL7  | MG-ND   | -5.03 | 1.95        | 2.05     |
| 14  | bA    | 3106 | CL7  | MG-NC   | -5.03 | 1.95        | 2.05     |
| 14  | bA    | 3113 | CL7  | C1C-C2C | -5.03 | 1.35        | 1.45     |
| 14  | bA    | 3115 | CL7  | MG-NA   | -5.03 | 1.95        | 2.05     |
| 14  | bB    | 811  | CL7  | MG-NB   | -5.03 | 1.95        | 2.05     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | cA    | 3114 | CL7  | C1C-C2C | -5.03 | 1.35        | 1.45     |
| 14  | aB    | 3022 | CL7  | C4B-NB  | -5.03 | 1.31        | 1.37     |
| 14  | bA    | 3130 | CL7  | C4B-NB  | -5.02 | 1.31        | 1.37     |
| 14  | aA    | 3116 | CL7  | MG-NA   | -5.02 | 1.95        | 2.05     |
| 14  | cB    | 822  | CL7  | MG-NB   | -5.02 | 1.95        | 2.05     |
| 14  | aB    | 3005 | CL7  | C1B-C2B | -5.02 | 1.31        | 1.43     |
| 14  | cA    | 3103 | CL7  | MG-NA   | -5.02 | 1.95        | 2.05     |
| 14  | cL    | 203  | CL7  | C1C-C2C | -5.02 | 1.35        | 1.45     |
| 14  | bB    | 811  | CL7  | MG-ND   | -5.02 | 1.95        | 2.05     |
| 14  | aB    | 3009 | CL7  | MG-NC   | -5.02 | 1.95        | 2.05     |
| 14  | aL    | 203  | CL7  | C1C-C2C | -5.01 | 1.35        | 1.45     |
| 14  | bB    | 810  | CL7  | MG-ND   | -5.01 | 1.95        | 2.05     |
| 14  | bA    | 3140 | CL7  | MG-ND   | -5.01 | 1.95        | 2.05     |
| 14  | bA    | 3108 | CL7  | MG-ND   | -5.01 | 1.95        | 2.05     |
| 14  | aB    | 3007 | CL7  | MG-ND   | -5.01 | 1.95        | 2.05     |
| 14  | bB    | 823  | CL7  | C4B-NB  | -5.00 | 1.31        | 1.37     |
| 14  | cB    | 819  | CL7  | MG-NC   | -5.00 | 1.95        | 2.05     |
| 14  | aA    | 3109 | CL7  | C1B-C2B | -5.00 | 1.31        | 1.43     |
| 14  | cB    | 813  | CL7  | C4B-NB  | -5.00 | 1.31        | 1.37     |
| 14  | aB    | 3006 | CL7  | C1C-C2C | -5.00 | 1.35        | 1.45     |
| 14  | aA    | 3112 | CL7  | MG-NA   | -5.00 | 1.95        | 2.05     |
| 14  | bA    | 3142 | CL7  | MG-NA   | -5.00 | 1.95        | 2.05     |
| 14  | cA    | 3115 | CL7  | MG-NA   | -5.00 | 1.95        | 2.05     |
| 14  | bB    | 824  | CL7  | C1B-C2B | -5.00 | 1.31        | 1.43     |
| 14  | cA    | 3109 | CL7  | MG-ND   | -4.99 | 1.95        | 2.05     |
| 14  | cB    | 812  | CL7  | C1C-C2C | -4.99 | 1.35        | 1.45     |
| 14  | aA    | 3108 | CL7  | MG-ND   | -4.99 | 1.95        | 2.05     |
| 14  | bA    | 3110 | CL7  | MG-NA   | -4.99 | 1.95        | 2.05     |
| 14  | cB    | 806  | CL7  | C1B-C2B | -4.99 | 1.31        | 1.43     |
| 14  | cB    | 824  | CL7  | C4B-NB  | -4.99 | 1.31        | 1.37     |
| 14  | cA    | 3120 | CL7  | C1C-C2C | -4.99 | 1.35        | 1.45     |
| 14  | aF    | 201  | CL7  | C1C-C2C | -4.99 | 1.35        | 1.45     |
| 14  | bB    | 826  | CL7  | C4B-NB  | -4.99 | 1.31        | 1.37     |
| 14  | cA    | 3114 | CL7  | C4B-NB  | -4.98 | 1.31        | 1.37     |
| 14  | bB    | 832  | CL7  | C1C-C2C | -4.98 | 1.35        | 1.45     |
| 14  | aB    | 3024 | CL7  | MG-NA   | -4.98 | 1.95        | 2.05     |
| 14  | aA    | 3109 | CL7  | MG-NC   | -4.98 | 1.95        | 2.05     |
| 14  | aA    | 3113 | CL7  | MG-NC   | -4.98 | 1.95        | 2.05     |
| 14  | aA    | 3108 | CL7  | MG-NC   | -4.98 | 1.95        | 2.05     |
| 14  | bA    | 3132 | CL7  | MG-NB   | -4.98 | 1.95        | 2.05     |
| 14  | cA    | 3108 | CL7  | C1B-C2B | -4.98 | 1.31        | 1.43     |
| 14  | aA    | 3115 | CL7  | C1B-C2B | -4.98 | 1.31        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | cA    | 3142 | CL7  | MG-NA   | -4.97 | 1.95        | 2.05     |
| 14  | cA    | 3129 | CL7  | OBD-CAD | -4.97 | 1.13        | 1.22     |
| 14  | bB    | 819  | CL7  | MG-NC   | -4.97 | 1.95        | 2.05     |
| 14  | bB    | 815  | CL7  | MG-ND   | -4.97 | 1.95        | 2.05     |
| 14  | bA    | 3108 | CL7  | MG-NB   | -4.97 | 1.95        | 2.05     |
| 14  | cB    | 820  | CL7  | MG-ND   | -4.97 | 1.95        | 2.05     |
| 14  | cA    | 3110 | CL7  | MG-NA   | -4.97 | 1.95        | 2.05     |
| 14  | cF    | 201  | CL7  | C1C-C2C | -4.97 | 1.35        | 1.45     |
| 14  | aB    | 3018 | CL7  | MG-ND   | -4.97 | 1.95        | 2.05     |
| 17  | bB    | 828  | PQN  | C10-C1  | -4.96 | 1.38        | 1.48     |
| 14  | bB    | 806  | CL7  | MG-NA   | -4.96 | 1.95        | 2.05     |
| 14  | aB    | 3014 | CL7  | MG-NA   | -4.96 | 1.95        | 2.05     |
| 14  | bA    | 3131 | CL7  | MG-ND   | -4.96 | 1.96        | 2.05     |
| 14  | bB    | 809  | CL7  | C1C-C2C | -4.96 | 1.35        | 1.45     |
| 14  | bB    | 812  | CL7  | C1C-C2C | -4.96 | 1.35        | 1.45     |
| 14  | cA    | 3140 | CL7  | MG-ND   | -4.95 | 1.96        | 2.05     |
| 14  | bB    | 831  | CL7  | C1C-C2C | -4.95 | 1.35        | 1.45     |
| 14  | aB    | 3031 | CL7  | C1C-C2C | -4.95 | 1.35        | 1.45     |
| 14  | aB    | 3024 | CL7  | MG-ND   | -4.95 | 1.96        | 2.05     |
| 14  | cB    | 827  | CL7  | C4B-NB  | -4.95 | 1.31        | 1.37     |
| 14  | cB    | 807  | CL7  | C1C-C2C | -4.95 | 1.35        | 1.45     |
| 14  | cA    | 3120 | CL7  | C4B-NB  | -4.95 | 1.31        | 1.37     |
| 14  | cB    | 808  | CL7  | MG-ND   | -4.95 | 1.96        | 2.05     |
| 13  | aB    | 3004 | PHO  | C1B-C2B | 4.94  | 1.45        | 1.39     |
| 14  | bB    | 807  | CL7  | C4B-NB  | -4.94 | 1.31        | 1.37     |
| 13  | bB    | 805  | PHO  | C4D-ND  | -4.94 | 1.31        | 1.38     |
| 14  | aB    | 3026 | CL7  | MG-NC   | -4.94 | 1.96        | 2.05     |
| 14  | aA    | 3133 | CL7  | CAA-C2A | -4.93 | 1.44        | 1.54     |
| 14  | bB    | 804  | CL7  | OBD-CAD | -4.93 | 1.14        | 1.22     |
| 13  | bB    | 805  | PHO  | C3D-CAD | -4.93 | 1.37        | 1.47     |
| 14  | bA    | 3108 | CL7  | MG-NC   | -4.93 | 1.96        | 2.05     |
| 14  | aA    | 3108 | CL7  | C4B-NB  | -4.93 | 1.31        | 1.37     |
| 14  | cA    | 3113 | CL7  | C1C-C2C | -4.92 | 1.35        | 1.45     |
| 14  | bB    | 810  | CL7  | C4B-NB  | -4.92 | 1.31        | 1.37     |
| 14  | cA    | 3130 | CL7  | C4B-NB  | -4.92 | 1.31        | 1.37     |
| 14  | aA    | 3142 | CL7  | MG-ND   | -4.92 | 1.96        | 2.05     |
| 14  | aB    | 3032 | CL7  | C1C-C2C | -4.92 | 1.35        | 1.45     |
| 14  | bA    | 3114 | CL7  | C1B-C2B | -4.92 | 1.31        | 1.43     |
| 14  | aA    | 3114 | CL7  | C1C-C2C | -4.92 | 1.35        | 1.45     |
| 14  | bA    | 3109 | CL7  | C4B-NB  | -4.92 | 1.31        | 1.37     |
| 14  | aA    | 3125 | CL7  | C1B-C2B | -4.92 | 1.31        | 1.43     |
| 14  | bA    | 3130 | CL7  | C1C-C2C | -4.92 | 1.35        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | bJ    | 101  | CL7  | C4B-NB  | -4.92 | 1.31        | 1.37     |
| 14  | cB    | 809  | CL7  | C1C-C2C | -4.91 | 1.35        | 1.45     |
| 14  | bB    | 808  | CL7  | MG-ND   | -4.91 | 1.96        | 2.05     |
| 14  | aB    | 3014 | CL7  | C1C-C2C | -4.91 | 1.35        | 1.45     |
| 14  | bB    | 825  | CL7  | MG-NA   | -4.91 | 1.96        | 2.05     |
| 14  | cA    | 3110 | CL7  | MG-ND   | -4.91 | 1.96        | 2.05     |
| 14  | cA    | 3107 | CL7  | MG-NA   | -4.90 | 1.96        | 2.05     |
| 14  | cB    | 811  | CL7  | MG-ND   | -4.90 | 1.96        | 2.05     |
| 14  | bB    | 811  | CL7  | MG-NC   | -4.90 | 1.96        | 2.05     |
| 12  | bA    | 3101 | G9R  | CHD-C1D | 4.90  | 1.47        | 1.38     |
| 14  | cB    | 813  | CL7  | C1C-C2C | -4.90 | 1.35        | 1.45     |
| 14  | cB    | 810  | CL7  | C4B-NB  | -4.90 | 1.31        | 1.37     |
| 14  | aA    | 3125 | CL7  | C4B-NB  | -4.90 | 1.31        | 1.37     |
| 14  | cB    | 831  | CL7  | C1C-C2C | -4.90 | 1.35        | 1.45     |
| 14  | cB    | 820  | CL7  | MG-NA   | -4.89 | 1.96        | 2.05     |
| 14  | bA    | 3111 | CL7  | MG-NA   | -4.89 | 1.96        | 2.05     |
| 14  | aA    | 3118 | CL7  | MG-NA   | -4.89 | 1.96        | 2.05     |
| 14  | cA    | 3104 | CL7  | C4B-NB  | -4.89 | 1.31        | 1.37     |
| 14  | aL    | 203  | CL7  | OBD-CAD | -4.89 | 1.14        | 1.22     |
| 14  | aL    | 203  | CL7  | MG-NC   | -4.89 | 1.96        | 2.05     |
| 14  | cB    | 815  | CL7  | MG-NA   | -4.89 | 1.96        | 2.05     |
| 14  | cA    | 3131 | CL7  | MG-ND   | -4.88 | 1.96        | 2.05     |
| 14  | cB    | 819  | CL7  | MG-ND   | -4.88 | 1.96        | 2.05     |
| 14  | aB    | 3030 | CL7  | C1C-C2C | -4.88 | 1.35        | 1.45     |
| 14  | bA    | 3120 | CL7  | C1C-C2C | -4.88 | 1.35        | 1.45     |
| 14  | bA    | 3121 | CL7  | C2A-C1A | -4.88 | 1.43        | 1.52     |
| 14  | cA    | 3109 | CL7  | C4B-NB  | -4.88 | 1.31        | 1.37     |
| 14  | bA    | 3118 | CL7  | C1C-C2C | -4.87 | 1.35        | 1.45     |
| 14  | aB    | 3021 | CL7  | MG-NA   | -4.87 | 1.96        | 2.05     |
| 14  | cA    | 3130 | CL7  | C1C-C2C | -4.87 | 1.35        | 1.45     |
| 14  | cA    | 3105 | CL7  | C4C-C3C | -4.87 | 1.36        | 1.45     |
| 14  | bB    | 804  | CL7  | C1C-C2C | -4.87 | 1.35        | 1.45     |
| 14  | bB    | 815  | CL7  | MG-NA   | -4.87 | 1.96        | 2.05     |
| 14  | cB    | 811  | CL7  | MG-NA   | -4.86 | 1.96        | 2.05     |
| 14  | bA    | 3145 | CL7  | C4B-NB  | -4.86 | 1.31        | 1.37     |
| 14  | cA    | 3117 | CL7  | C1C-C2C | -4.86 | 1.35        | 1.45     |
| 14  | aB    | 3011 | CL7  | MG-ND   | -4.86 | 1.96        | 2.05     |
| 14  | bB    | 822  | CL7  | MG-NA   | -4.86 | 1.96        | 2.05     |
| 14  | cJ    | 101  | CL7  | MG-NA   | -4.86 | 1.96        | 2.05     |
| 14  | cA    | 3126 | CL7  | C1C-C2C | -4.86 | 1.35        | 1.45     |
| 14  | bB    | 817  | CL7  | C4B-NB  | -4.86 | 1.31        | 1.37     |
| 14  | cB    | 810  | CL7  | MG-NB   | -4.86 | 1.96        | 2.05     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | bB    | 806  | CL7  | OBD-CAD | -4.86 | 1.14        | 1.22     |
| 14  | bB    | 819  | CL7  | C4C-NC  | 4.85  | 1.43        | 1.37     |
| 14  | aA    | 3132 | CL7  | MG-ND   | -4.85 | 1.96        | 2.05     |
| 14  | cA    | 3144 | CL7  | C4B-NB  | -4.85 | 1.31        | 1.37     |
| 14  | cB    | 816  | CL7  | C4B-NB  | -4.85 | 1.31        | 1.37     |
| 17  | cB    | 828  | PQN  | C10-C1  | -4.85 | 1.38        | 1.48     |
| 14  | cA    | 3122 | CL7  | MG-NA   | -4.85 | 1.96        | 2.05     |
| 14  | bA    | 3117 | CL7  | C1C-C2C | -4.85 | 1.35        | 1.45     |
| 14  | aA    | 3108 | CL7  | MG-NA   | -4.85 | 1.96        | 2.05     |
| 14  | bA    | 3112 | CL7  | C1C-C2C | -4.85 | 1.35        | 1.45     |
| 14  | aB    | 3012 | CL7  | C1C-C2C | -4.85 | 1.35        | 1.45     |
| 14  | bL    | 204  | CL7  | OBD-CAD | -4.85 | 1.14        | 1.22     |
| 14  | cB    | 824  | CL7  | C1B-C2B | -4.85 | 1.31        | 1.43     |
| 14  | bA    | 3110 | CL7  | C1C-C2C | -4.84 | 1.35        | 1.45     |
| 14  | aA    | 3110 | CL7  | MG-ND   | -4.84 | 1.96        | 2.05     |
| 14  | aB    | 3023 | CL7  | C1B-C2B | -4.84 | 1.31        | 1.43     |
| 14  | cB    | 811  | CL7  | MG-NC   | -4.84 | 1.96        | 2.05     |
| 14  | cB    | 812  | CL7  | MG-ND   | -4.84 | 1.96        | 2.05     |
| 14  | cA    | 3141 | CL7  | C4B-NB  | -4.84 | 1.31        | 1.37     |
| 14  | bB    | 813  | CL7  | C1C-C2C | -4.84 | 1.35        | 1.45     |
| 14  | bB    | 810  | CL7  | MG-NB   | -4.84 | 1.96        | 2.05     |
| 14  | cB    | 806  | CL7  | MG-NA   | -4.84 | 1.96        | 2.05     |
| 14  | cB    | 815  | CL7  | MG-ND   | -4.84 | 1.96        | 2.05     |
| 14  | aA    | 3120 | CL7  | OBD-CAD | -4.83 | 1.14        | 1.22     |
| 14  | cB    | 825  | CL7  | MG-NC   | -4.83 | 1.96        | 2.05     |
| 14  | bB    | 823  | CL7  | C1C-C2C | -4.83 | 1.35        | 1.45     |
| 14  | cB    | 822  | CL7  | MG-NA   | -4.83 | 1.96        | 2.05     |
| 14  | aA    | 3143 | CL7  | C4B-NB  | -4.83 | 1.31        | 1.37     |
| 14  | bB    | 818  | CL7  | MG-ND   | -4.83 | 1.96        | 2.05     |
| 14  | cA    | 3111 | CL7  | MG-NA   | -4.83 | 1.96        | 2.05     |
| 14  | cB    | 826  | CL7  | C1D-ND  | -4.83 | 1.31        | 1.37     |
| 14  | aA    | 3114 | CL7  | MG-NA   | -4.82 | 1.96        | 2.05     |
| 14  | cA    | 3123 | CL7  | MG-NC   | -4.82 | 1.96        | 2.05     |
| 14  | bB    | 812  | CL7  | MG-ND   | -4.82 | 1.96        | 2.05     |
| 14  | cA    | 3133 | CL7  | MG-ND   | -4.82 | 1.96        | 2.05     |
| 14  | aB    | 3017 | CL7  | MG-ND   | -4.82 | 1.96        | 2.05     |
| 14  | aA    | 3131 | CL7  | C4B-NB  | -4.82 | 1.31        | 1.37     |
| 14  | cB    | 823  | CL7  | C4B-NB  | -4.82 | 1.31        | 1.37     |
| 14  | aB    | 3008 | CL7  | C1C-C2C | -4.82 | 1.35        | 1.45     |
| 14  | cA    | 3112 | CL7  | C1C-C2C | -4.81 | 1.35        | 1.45     |
| 14  | bB    | 808  | CL7  | C2A-C1A | -4.81 | 1.43        | 1.50     |
| 14  | cB    | 817  | CL7  | C4B-NB  | -4.81 | 1.31        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | cA    | 3103 | CL7  | MG-ND   | -4.81 | 1.96        | 2.05     |
| 14  | aA    | 3111 | CL7  | C1C-C2C | -4.81 | 1.35        | 1.45     |
| 14  | bA    | 3107 | CL7  | MG-NA   | -4.81 | 1.96        | 2.05     |
| 14  | bB    | 827  | CL7  | C4B-NB  | -4.81 | 1.31        | 1.37     |
| 14  | aJ    | 101  | CL7  | C1C-C2C | -4.81 | 1.35        | 1.45     |
| 14  | aA    | 3127 | CL7  | C2A-C1A | -4.81 | 1.46        | 1.52     |
| 14  | aA    | 3130 | CL7  | CAB-C3B | -4.81 | 1.35        | 1.45     |
| 14  | cB    | 811  | CL7  | MG-NB   | -4.80 | 1.96        | 2.05     |
| 14  | aB    | 3022 | CL7  | C1C-C2C | -4.80 | 1.35        | 1.45     |
| 14  | cK    | 101  | CL7  | C1C-C2C | -4.80 | 1.35        | 1.45     |
| 14  | bB    | 827  | CL7  | MG-NC   | -4.80 | 1.96        | 2.05     |
| 14  | aB    | 3016 | CL7  | C4B-NB  | -4.80 | 1.31        | 1.37     |
| 14  | bB    | 810  | CL7  | MG-NC   | -4.80 | 1.96        | 2.05     |
| 14  | cL    | 204  | CL7  | OBD-CAD | -4.80 | 1.14        | 1.22     |
| 14  | cB    | 818  | CL7  | C1C-C2C | -4.80 | 1.35        | 1.45     |
| 14  | cJ    | 101  | CL7  | C1C-C2C | -4.80 | 1.35        | 1.45     |
| 12  | bA    | 3101 | G9R  | O2A-CGA | 4.80  | 1.47        | 1.33     |
| 14  | aA    | 3113 | CL7  | MG-ND   | -4.80 | 1.96        | 2.05     |
| 14  | aA    | 3122 | CL7  | C1B-C2B | -4.80 | 1.32        | 1.43     |
| 14  | aA    | 3127 | CL7  | C1C-C2C | -4.80 | 1.35        | 1.45     |
| 14  | cB    | 819  | CL7  | C1C-C2C | -4.80 | 1.35        | 1.45     |
| 14  | aB    | 3016 | CL7  | MG-ND   | -4.80 | 1.96        | 2.05     |
| 14  | cA    | 3132 | CL7  | MG-NB   | -4.80 | 1.96        | 2.05     |
| 14  | aA    | 3129 | CL7  | C1B-C2B | -4.79 | 1.32        | 1.43     |
| 14  | aB    | 3019 | CL7  | MG-ND   | -4.79 | 1.96        | 2.05     |
| 14  | aA    | 3109 | CL7  | MG-ND   | -4.79 | 1.96        | 2.05     |
| 14  | aB    | 3008 | CL7  | MG-NA   | -4.79 | 1.96        | 2.05     |
| 14  | cB    | 825  | CL7  | MG-ND   | -4.79 | 1.96        | 2.05     |
| 14  | cA    | 3109 | CL7  | C1C-C2C | -4.79 | 1.35        | 1.45     |
| 14  | cA    | 3117 | CL7  | MG-NA   | -4.78 | 1.96        | 2.05     |
| 14  | aJ    | 101  | CL7  | C4B-NB  | -4.78 | 1.31        | 1.37     |
| 14  | aA    | 3131 | CL7  | C1C-C2C | -4.78 | 1.35        | 1.45     |
| 14  | aA    | 3112 | CL7  | C4B-NB  | -4.78 | 1.31        | 1.37     |
| 14  | bA    | 3111 | CL7  | MG-NC   | -4.78 | 1.96        | 2.05     |
| 14  | aB    | 3002 | CL7  | C1B-C2B | -4.78 | 1.32        | 1.43     |
| 14  | aA    | 3142 | CL7  | C4B-NB  | -4.78 | 1.31        | 1.37     |
| 14  | bA    | 3120 | CL7  | C4B-NB  | -4.78 | 1.31        | 1.37     |
| 14  | bB    | 827  | CL7  | C4C-C3C | -4.78 | 1.36        | 1.45     |
| 14  | bA    | 3104 | CL7  | C4B-NB  | -4.78 | 1.31        | 1.37     |
| 14  | bA    | 3109 | CL7  | C1C-C2C | -4.78 | 1.35        | 1.45     |
| 14  | aB    | 3010 | CL7  | MG-NA   | -4.77 | 1.96        | 2.05     |
| 14  | aA    | 3116 | CL7  | MG-ND   | -4.77 | 1.96        | 2.05     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | cA    | 3128 | CL7  | MG-NC   | -4.77 | 1.96        | 2.05     |
| 17  | aB    | 3027 | PQN  | C10-C1  | -4.77 | 1.39        | 1.48     |
| 14  | bA    | 3102 | CL7  | C3A-C4A | -4.77 | 1.43        | 1.52     |
| 14  | aB    | 3020 | CL7  | C1C-C2C | -4.77 | 1.35        | 1.45     |
| 17  | cB    | 828  | PQN  | C6-C5   | 4.77  | 1.47        | 1.39     |
| 14  | bA    | 3133 | CL7  | MG-ND   | -4.77 | 1.96        | 2.05     |
| 14  | cB    | 821  | CL7  | C1C-C2C | -4.77 | 1.35        | 1.45     |
| 14  | cB    | 821  | CL7  | MG-NA   | -4.76 | 1.96        | 2.05     |
| 13  | cB    | 805  | PHO  | C4B-NB  | -4.76 | 1.29        | 1.38     |
| 14  | bB    | 807  | CL7  | MG-NB   | -4.76 | 1.96        | 2.05     |
| 14  | aB    | 3009 | CL7  | C4B-NB  | -4.76 | 1.31        | 1.37     |
| 14  | bB    | 821  | CL7  | C1C-C2C | -4.76 | 1.35        | 1.45     |
| 14  | bA    | 3145 | CL7  | MG-ND   | -4.76 | 1.96        | 2.05     |
| 14  | aA    | 3107 | CL7  | MG-NC   | -4.76 | 1.96        | 2.05     |
| 14  | aB    | 3020 | CL7  | MG-NA   | -4.76 | 1.96        | 2.05     |
| 14  | cB    | 815  | CL7  | C4B-NB  | -4.76 | 1.31        | 1.37     |
| 14  | cL    | 203  | CL7  | MG-ND   | -4.75 | 1.96        | 2.05     |
| 14  | cB    | 817  | CL7  | MG-ND   | -4.75 | 1.96        | 2.05     |
| 14  | cB    | 823  | CL7  | C1C-C2C | -4.75 | 1.35        | 1.45     |
| 14  | cA    | 3144 | CL7  | MG-ND   | -4.75 | 1.96        | 2.05     |
| 14  | cB    | 804  | CL7  | C1C-C2C | -4.75 | 1.35        | 1.45     |
| 14  | cA    | 3121 | CL7  | C2A-C1A | -4.75 | 1.43        | 1.52     |
| 14  | bA    | 3119 | CL7  | MG-NC   | -4.75 | 1.96        | 2.05     |
| 14  | aA    | 3115 | CL7  | C4B-NB  | -4.75 | 1.31        | 1.37     |
| 14  | bB    | 818  | CL7  | C1C-C2C | -4.75 | 1.36        | 1.45     |
| 14  | cA    | 3110 | CL7  | C1C-C2C | -4.74 | 1.36        | 1.45     |
| 14  | aB    | 3019 | CL7  | MG-NA   | -4.74 | 1.96        | 2.05     |
| 14  | cA    | 3115 | CL7  | MG-ND   | -4.74 | 1.96        | 2.05     |
| 14  | aA    | 3110 | CL7  | C1C-C2C | -4.74 | 1.36        | 1.45     |
| 14  | bA    | 3106 | CL7  | C1B-C2B | -4.73 | 1.32        | 1.43     |
| 14  | aA    | 3146 | CL7  | C1C-C2C | -4.73 | 1.36        | 1.45     |
| 14  | bA    | 3111 | CL7  | C1C-C2C | -4.73 | 1.36        | 1.45     |
| 14  | bA    | 3102 | CL7  | C2A-C1A | -4.73 | 1.43        | 1.50     |
| 14  | aB    | 3014 | CL7  | MG-ND   | -4.73 | 1.96        | 2.05     |
| 13  | aB    | 3004 | PHO  | C3D-CAD | -4.73 | 1.37        | 1.47     |
| 14  | bB    | 820  | CL7  | MG-NA   | -4.73 | 1.96        | 2.05     |
| 14  | cJ    | 101  | CL7  | C4B-NB  | -4.73 | 1.32        | 1.37     |
| 14  | bA    | 3102 | CL7  | C1B-C2B | -4.73 | 1.32        | 1.43     |
| 14  | cB    | 819  | CL7  | C4C-NC  | 4.73  | 1.43        | 1.37     |
| 14  | bA    | 3117 | CL7  | C4B-NB  | -4.72 | 1.32        | 1.37     |
| 14  | cA    | 3107 | CL7  | C4B-NB  | -4.72 | 1.32        | 1.37     |
| 14  | cA    | 3103 | CL7  | C1C-C2C | -4.72 | 1.36        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | aA    | 3118 | CL7  | C1C-C2C | -4.72 | 1.36        | 1.45     |
| 14  | aB    | 3003 | CL7  | C1C-C2C | -4.72 | 1.36        | 1.45     |
| 14  | bA    | 3104 | CL7  | C1C-C2C | -4.72 | 1.36        | 1.45     |
| 14  | cB    | 814  | CL7  | MG-ND   | -4.72 | 1.96        | 2.05     |
| 14  | bA    | 3132 | CL7  | CAA-C2A | -4.72 | 1.45        | 1.54     |
| 14  | bA    | 3126 | CL7  | C1C-C2C | -4.72 | 1.36        | 1.45     |
| 14  | bJ    | 101  | CL7  | C1C-C2C | -4.71 | 1.36        | 1.45     |
| 14  | bB    | 817  | CL7  | MG-ND   | -4.71 | 1.96        | 2.05     |
| 14  | bA    | 3109 | CL7  | MG-NB   | -4.71 | 1.96        | 2.05     |
| 14  | aA    | 3134 | CL7  | MG-ND   | -4.71 | 1.96        | 2.05     |
| 14  | bB    | 814  | CL7  | C1C-C2C | -4.70 | 1.36        | 1.45     |
| 14  | bK    | 101  | CL7  | C1C-C2C | -4.70 | 1.36        | 1.45     |
| 14  | cA    | 3111 | CL7  | C1C-C2C | -4.70 | 1.36        | 1.45     |
| 14  | aB    | 3018 | CL7  | C1C-C2C | -4.70 | 1.36        | 1.45     |
| 14  | cA    | 3104 | CL7  | MG-NA   | -4.70 | 1.96        | 2.05     |
| 14  | cA    | 3111 | CL7  | C4B-NB  | -4.70 | 1.32        | 1.37     |
| 14  | bA    | 3103 | CL7  | C1C-C2C | -4.70 | 1.36        | 1.45     |
| 14  | aB    | 3005 | CL7  | OBD-CAD | -4.70 | 1.14        | 1.22     |
| 14  | cB    | 818  | CL7  | MG-ND   | -4.70 | 1.96        | 2.05     |
| 14  | bA    | 3124 | CL7  | C1D-C2D | -4.70 | 1.32        | 1.43     |
| 14  | aA    | 3104 | CL7  | MG-ND   | -4.69 | 1.96        | 2.05     |
| 14  | bA    | 3125 | CL7  | C4C-NC  | 4.69  | 1.43        | 1.37     |
| 14  | aA    | 3111 | CL7  | MG-NA   | -4.69 | 1.96        | 2.05     |
| 14  | bA    | 3145 | CL7  | C1C-C2C | -4.69 | 1.36        | 1.45     |
| 14  | aA    | 3123 | CL7  | MG-NA   | -4.69 | 1.96        | 2.05     |
| 14  | cA    | 3139 | CL7  | C4B-NB  | -4.69 | 1.32        | 1.37     |
| 14  | aA    | 3131 | CL7  | MG-NA   | -4.69 | 1.96        | 2.05     |
| 14  | aB    | 3013 | CL7  | C1C-C2C | -4.69 | 1.36        | 1.45     |
| 14  | aB    | 3026 | CL7  | MG-ND   | -4.69 | 1.96        | 2.05     |
| 14  | cA    | 3132 | CL7  | CBA-CGA | -4.69 | 1.37        | 1.50     |
| 14  | bA    | 3114 | CL7  | C1C-C2C | -4.69 | 1.36        | 1.45     |
| 14  | cA    | 3104 | CL7  | C1C-C2C | -4.69 | 1.36        | 1.45     |
| 14  | cB    | 814  | CL7  | C1C-C2C | -4.68 | 1.36        | 1.45     |
| 14  | cB    | 821  | CL7  | MG-ND   | -4.68 | 1.96        | 2.05     |
| 14  | cA    | 3120 | CL7  | MG-ND   | -4.68 | 1.96        | 2.05     |
| 14  | aA    | 3125 | CL7  | MG-NC   | -4.68 | 1.96        | 2.05     |
| 14  | bA    | 3129 | CL7  | OBD-CAD | -4.68 | 1.14        | 1.22     |
| 14  | cA    | 3116 | CL7  | C1C-C2C | -4.68 | 1.36        | 1.45     |
| 14  | bB    | 827  | CL7  | MG-ND   | -4.68 | 1.96        | 2.05     |
| 14  | bA    | 3117 | CL7  | MG-NA   | -4.68 | 1.96        | 2.05     |
| 14  | aB    | 3017 | CL7  | C1C-C2C | -4.68 | 1.36        | 1.45     |
| 13  | bB    | 805  | PHO  | C1B-C2B | 4.68  | 1.44        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | aB    | 3006 | CL7  | MG-ND   | -4.68 | 1.96        | 2.05     |
| 14  | aB    | 3010 | CL7  | MG-ND   | -4.68 | 1.96        | 2.05     |
| 14  | aA    | 3129 | CL7  | OBD-CAD | -4.67 | 1.14        | 1.22     |
| 14  | aA    | 3111 | CL7  | MG-ND   | -4.67 | 1.96        | 2.05     |
| 14  | bB    | 814  | CL7  | MG-ND   | -4.67 | 1.96        | 2.05     |
| 14  | bA    | 3115 | CL7  | MG-ND   | -4.67 | 1.96        | 2.05     |
| 14  | bB    | 808  | CL7  | C1C-C2C | -4.67 | 1.36        | 1.45     |
| 14  | aA    | 3146 | CL7  | MG-ND   | -4.67 | 1.96        | 2.05     |
| 14  | cB    | 823  | CL7  | MG-ND   | -4.67 | 1.96        | 2.05     |
| 14  | bA    | 3103 | CL7  | MG-ND   | -4.67 | 1.96        | 2.05     |
| 14  | aA    | 3117 | CL7  | C1C-C2C | -4.67 | 1.36        | 1.45     |
| 14  | bB    | 815  | CL7  | C4B-NB  | -4.67 | 1.32        | 1.37     |
| 14  | bB    | 819  | CL7  | C1C-C2C | -4.66 | 1.36        | 1.45     |
| 14  | cA    | 3144 | CL7  | C1C-C2C | -4.66 | 1.36        | 1.45     |
| 14  | cA    | 3119 | CL7  | C1C-C2C | -4.66 | 1.36        | 1.45     |
| 13  | cB    | 801  | PHO  | C4D-ND  | -4.66 | 1.32        | 1.38     |
| 14  | aA    | 3118 | CL7  | C4B-NB  | -4.66 | 1.32        | 1.37     |
| 14  | cA    | 3106 | CL7  | C1B-C2B | -4.66 | 1.32        | 1.43     |
| 14  | aA    | 3113 | CL7  | C1C-C2C | -4.66 | 1.36        | 1.45     |
| 14  | bB    | 821  | CL7  | MG-ND   | -4.65 | 1.96        | 2.05     |
| 14  | aA    | 3141 | CL7  | MG-ND   | -4.65 | 1.96        | 2.05     |
| 14  | aA    | 3128 | CL7  | C4C-NC  | 4.65  | 1.43        | 1.37     |
| 14  | bA    | 3106 | CL7  | MG-NA   | -4.65 | 1.96        | 2.05     |
| 14  | bB    | 831  | CL7  | C4B-NB  | -4.65 | 1.32        | 1.37     |
| 14  | bB    | 809  | CL7  | C4B-NB  | -4.65 | 1.32        | 1.37     |
| 14  | aB    | 3009 | CL7  | MG-NB   | -4.65 | 1.96        | 2.05     |
| 14  | bB    | 821  | CL7  | MG-NA   | -4.65 | 1.96        | 2.05     |
| 14  | bA    | 3111 | CL7  | C4B-NB  | -4.64 | 1.32        | 1.37     |
| 14  | aB    | 3013 | CL7  | MG-ND   | -4.64 | 1.96        | 2.05     |
| 14  | bB    | 813  | CL7  | MG-ND   | -4.64 | 1.96        | 2.05     |
| 14  | aA    | 3141 | CL7  | C4B-NB  | -4.64 | 1.32        | 1.37     |
| 14  | cB    | 826  | CL7  | MG-NB   | -4.64 | 1.96        | 2.05     |
| 14  | bA    | 3130 | CL7  | MG-NA   | -4.64 | 1.96        | 2.05     |
| 14  | cA    | 3117 | CL7  | C4B-NB  | -4.64 | 1.32        | 1.37     |
| 14  | bL    | 204  | CL7  | MG-NA   | -4.64 | 1.96        | 2.05     |
| 14  | cB    | 807  | CL7  | MG-ND   | -4.63 | 1.96        | 2.05     |
| 14  | aB    | 3006 | CL7  | MG-NB   | -4.63 | 1.96        | 2.05     |
| 14  | bA    | 3125 | CL7  | MG-ND   | -4.63 | 1.96        | 2.05     |
| 14  | aA    | 3121 | CL7  | C1C-C2C | -4.63 | 1.36        | 1.45     |
| 12  | cA    | 3101 | G9R  | OBB-CAB | 4.63  | 1.32        | 1.22     |
| 14  | aB    | 3030 | CL7  | C4B-NB  | -4.63 | 1.32        | 1.37     |
| 14  | cA    | 3130 | CL7  | MG-NA   | -4.63 | 1.96        | 2.05     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | aB    | 3005 | CL7  | CAA-C2A | -4.63 | 1.45        | 1.54     |
| 14  | bA    | 3115 | CL7  | C4B-NB  | -4.63 | 1.32        | 1.37     |
| 17  | aB    | 3027 | PQN  | C9-C10  | -4.63 | 1.32        | 1.39     |
| 14  | cA    | 3124 | CL7  | C1D-C2D | -4.62 | 1.32        | 1.43     |
| 14  | cA    | 3130 | CL7  | MG-ND   | -4.62 | 1.96        | 2.05     |
| 14  | aB    | 3012 | CL7  | MG-ND   | -4.62 | 1.96        | 2.05     |
| 14  | bB    | 826  | CL7  | C1D-ND  | -4.62 | 1.32        | 1.37     |
| 14  | cA    | 3123 | CL7  | MG-NB   | -4.62 | 1.96        | 2.05     |
| 14  | aA    | 3131 | CL7  | MG-ND   | -4.62 | 1.96        | 2.05     |
| 14  | aA    | 3106 | CL7  | C4C-C3C | -4.62 | 1.37        | 1.45     |
| 12  | bA    | 3101 | G9R  | CHC-C1C | 4.62  | 1.47        | 1.38     |
| 14  | bA    | 3141 | CL7  | C4B-NB  | -4.62 | 1.32        | 1.37     |
| 14  | aA    | 3105 | CL7  | C1C-C2C | -4.62 | 1.36        | 1.45     |
| 14  | aB    | 3010 | CL7  | MG-NC   | -4.62 | 1.96        | 2.05     |
| 14  | cB    | 813  | CL7  | MG-ND   | -4.62 | 1.96        | 2.05     |
| 14  | bJ    | 101  | CL7  | MG-ND   | -4.61 | 1.96        | 2.05     |
| 14  | aL    | 202  | CL7  | MG-ND   | -4.61 | 1.96        | 2.05     |
| 14  | cB    | 804  | CL7  | OBD-CAD | -4.61 | 1.14        | 1.22     |
| 14  | cA    | 3119 | CL7  | MG-NC   | -4.61 | 1.96        | 2.05     |
| 14  | cA    | 3142 | CL7  | C4C-NC  | 4.61  | 1.43        | 1.37     |
| 14  | cB    | 807  | CL7  | MG-NB   | -4.61 | 1.96        | 2.05     |
| 14  | aB    | 3022 | CL7  | MG-ND   | -4.61 | 1.96        | 2.05     |
| 14  | bB    | 823  | CL7  | MG-ND   | -4.60 | 1.96        | 2.05     |
| 14  | aB    | 3020 | CL7  | MG-ND   | -4.60 | 1.96        | 2.05     |
| 14  | cA    | 3103 | CL7  | C4B-NB  | -4.60 | 1.32        | 1.37     |
| 13  | bB    | 801  | PHO  | C4D-ND  | -4.60 | 1.32        | 1.38     |
| 14  | bL    | 203  | CL7  | MG-ND   | -4.60 | 1.96        | 2.05     |
| 14  | cA    | 3109 | CL7  | MG-NB   | -4.59 | 1.96        | 2.05     |
| 14  | aA    | 3130 | CL7  | CAA-C2A | 4.59  | 1.63        | 1.53     |
| 14  | aA    | 3120 | CL7  | C1C-C2C | -4.59 | 1.36        | 1.45     |
| 14  | aB    | 3021 | CL7  | MG-NC   | -4.59 | 1.96        | 2.05     |
| 14  | aA    | 3122 | CL7  | C2A-C1A | -4.59 | 1.43        | 1.52     |
| 14  | bB    | 820  | CL7  | MG-ND   | -4.58 | 1.96        | 2.05     |
| 14  | cA    | 3111 | CL7  | MG-ND   | -4.58 | 1.96        | 2.05     |
| 14  | bA    | 3130 | CL7  | MG-ND   | -4.58 | 1.96        | 2.05     |
| 14  | aA    | 3115 | CL7  | C1C-C2C | -4.58 | 1.36        | 1.45     |
| 14  | bB    | 807  | CL7  | MG-ND   | -4.58 | 1.96        | 2.05     |
| 14  | aB    | 3005 | CL7  | MG-NA   | -4.57 | 1.96        | 2.05     |
| 14  | aA    | 3112 | CL7  | C1C-C2C | -4.57 | 1.36        | 1.45     |
| 14  | bA    | 3132 | CL7  | CBA-CGA | -4.57 | 1.37        | 1.50     |
| 14  | bA    | 3122 | CL7  | MG-NA   | -4.57 | 1.96        | 2.05     |
| 14  | bA    | 3103 | CL7  | C4B-NB  | -4.56 | 1.32        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | cB    | 803  | CL7  | MG-ND   | -4.56 | 1.96        | 2.05     |
| 14  | cJ    | 101  | CL7  | MG-ND   | -4.56 | 1.96        | 2.05     |
| 12  | cA    | 3101 | G9R  | CHC-C1C | 4.56  | 1.47        | 1.38     |
| 14  | aA    | 3130 | CL7  | C4C-C3C | -4.55 | 1.37        | 1.45     |
| 14  | bK    | 101  | CL7  | MG-ND   | -4.55 | 1.96        | 2.05     |
| 14  | bB    | 806  | CL7  | C1C-C2C | -4.55 | 1.36        | 1.45     |
| 14  | aB    | 3002 | CL7  | CHB-C4A | -4.55 | 1.26        | 1.36     |
| 14  | cA    | 3102 | CL7  | C1B-C2B | -4.55 | 1.32        | 1.43     |
| 14  | bA    | 3131 | CL7  | C1C-C2C | -4.55 | 1.36        | 1.45     |
| 14  | bA    | 3111 | CL7  | MG-ND   | -4.55 | 1.96        | 2.05     |
| 14  | aB    | 3025 | CL7  | C1C-C2C | -4.55 | 1.36        | 1.45     |
| 14  | cA    | 3111 | CL7  | MG-NC   | -4.55 | 1.96        | 2.05     |
| 14  | aA    | 3110 | CL7  | C4B-NB  | -4.55 | 1.32        | 1.37     |
| 14  | bB    | 806  | CL7  | C4B-NB  | -4.54 | 1.32        | 1.37     |
| 14  | aK    | 101  | CL7  | C1C-C2C | -4.54 | 1.36        | 1.45     |
| 14  | bK    | 101  | CL7  | MG-NA   | -4.54 | 1.96        | 2.05     |
| 14  | bA    | 3107 | CL7  | MG-NB   | -4.54 | 1.96        | 2.05     |
| 14  | bL    | 205  | CL7  | OBD-CAD | -4.54 | 1.14        | 1.22     |
| 14  | bA    | 3139 | CL7  | MG-NB   | -4.54 | 1.96        | 2.05     |
| 14  | bA    | 3104 | CL7  | MG-NC   | -4.53 | 1.96        | 2.05     |
| 17  | aB    | 3027 | PQN  | C6-C5   | 4.53  | 1.47        | 1.39     |
| 14  | cA    | 3115 | CL7  | C4B-NB  | -4.53 | 1.32        | 1.37     |
| 14  | aA    | 3103 | CL7  | C1B-C2B | -4.53 | 1.32        | 1.43     |
| 14  | bA    | 3104 | CL7  | MG-NA   | -4.53 | 1.96        | 2.05     |
| 14  | aA    | 3109 | CL7  | MG-NB   | -4.53 | 1.96        | 2.05     |
| 14  | cB    | 826  | CL7  | C4B-NB  | -4.53 | 1.32        | 1.37     |
| 14  | aB    | 3007 | CL7  | C1C-C2C | -4.53 | 1.36        | 1.45     |
| 14  | aJ    | 101  | CL7  | MG-ND   | -4.52 | 1.96        | 2.05     |
| 14  | aA    | 3127 | CL7  | C4B-NB  | -4.52 | 1.32        | 1.37     |
| 14  | aB    | 3002 | CL7  | MG-ND   | -4.52 | 1.96        | 2.05     |
| 14  | bA    | 3115 | CL7  | C1C-C2C | -4.52 | 1.36        | 1.45     |
| 14  | cB    | 808  | CL7  | C2A-C1A | -4.52 | 1.44        | 1.50     |
| 14  | bB    | 811  | CL7  | MG-NA   | -4.52 | 1.96        | 2.05     |
| 14  | aA    | 3116 | CL7  | C1C-C2C | -4.52 | 1.36        | 1.45     |
| 14  | cA    | 3139 | CL7  | MG-NB   | -4.52 | 1.96        | 2.05     |
| 14  | aA    | 3146 | CL7  | C4B-NB  | -4.52 | 1.32        | 1.37     |
| 14  | aB    | 3025 | CL7  | MG-NB   | -4.52 | 1.96        | 2.05     |
| 14  | cB    | 833  | CL7  | C4B-NB  | -4.52 | 1.32        | 1.37     |
| 14  | aB    | 3010 | CL7  | MG-NB   | -4.51 | 1.96        | 2.05     |
| 14  | aA    | 3116 | CL7  | C4B-NB  | -4.51 | 1.32        | 1.37     |
| 14  | cB    | 806  | CL7  | OBD-CAD | -4.51 | 1.14        | 1.22     |
| 14  | bB    | 822  | CL7  | MG-NC   | -4.51 | 1.96        | 2.05     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | aB    | 3016 | CL7  | C1C-C2C | -4.51 | 1.36        | 1.45     |
| 14  | cB    | 806  | CL7  | C1C-C2C | -4.51 | 1.36        | 1.45     |
| 14  | cA    | 3117 | CL7  | MG-NC   | -4.51 | 1.96        | 2.05     |
| 14  | cF    | 201  | CL7  | C4B-NB  | -4.51 | 1.32        | 1.37     |
| 14  | bB    | 824  | CL7  | MG-ND   | -4.50 | 1.96        | 2.05     |
| 14  | cB    | 831  | CL7  | C4B-NB  | -4.50 | 1.32        | 1.37     |
| 14  | cA    | 3104 | CL7  | MG-NC   | -4.50 | 1.96        | 2.05     |
| 14  | bA    | 3110 | CL7  | MG-NC   | -4.50 | 1.96        | 2.05     |
| 14  | aB    | 3009 | CL7  | CAA-C2A | -4.50 | 1.45        | 1.54     |
| 14  | bA    | 3121 | CL7  | C1C-C2C | -4.50 | 1.36        | 1.45     |
| 14  | cA    | 3130 | CL7  | MG-NB   | -4.50 | 1.96        | 2.05     |
| 14  | aB    | 3012 | CL7  | MG-NB   | -4.50 | 1.96        | 2.05     |
| 14  | aA    | 3126 | CL7  | C4C-NC  | 4.49  | 1.43        | 1.37     |
| 14  | cA    | 3121 | CL7  | CAB-C3B | -4.49 | 1.35        | 1.45     |
| 14  | aA    | 3121 | CL7  | MG-ND   | -4.49 | 1.96        | 2.05     |
| 14  | bA    | 3117 | CL7  | MG-ND   | -4.49 | 1.96        | 2.05     |
| 14  | bF    | 201  | CL7  | C4B-NB  | -4.49 | 1.32        | 1.37     |
| 14  | cA    | 3103 | CL7  | MG-NB   | -4.48 | 1.96        | 2.05     |
| 14  | aA    | 3104 | CL7  | C1C-C2C | -4.48 | 1.36        | 1.45     |
| 14  | cA    | 3139 | CL7  | C1C-C2C | -4.48 | 1.36        | 1.45     |
| 17  | cB    | 828  | PQN  | C9-C10  | -4.48 | 1.32        | 1.39     |
| 14  | cB    | 818  | CL7  | MG-NC   | -4.48 | 1.96        | 2.05     |
| 14  | aA    | 3119 | CL7  | C1C-C2C | -4.48 | 1.36        | 1.45     |
| 14  | bB    | 813  | CL7  | MG-NB   | -4.48 | 1.96        | 2.05     |
| 14  | cA    | 3116 | CL7  | C4B-NB  | -4.48 | 1.32        | 1.37     |
| 14  | cA    | 3107 | CL7  | MG-NB   | -4.48 | 1.96        | 2.05     |
| 14  | aB    | 3024 | CL7  | MG-NC   | -4.47 | 1.96        | 2.05     |
| 14  | cB    | 810  | CL7  | C1C-C2C | -4.47 | 1.36        | 1.45     |
| 14  | aB    | 3014 | CL7  | C4B-NB  | -4.47 | 1.32        | 1.37     |
| 14  | bA    | 3116 | CL7  | C4B-NB  | -4.47 | 1.32        | 1.37     |
| 14  | bA    | 3118 | CL7  | MG-NA   | -4.47 | 1.96        | 2.05     |
| 14  | cB    | 813  | CL7  | MG-NB   | -4.47 | 1.96        | 2.05     |
| 14  | bA    | 3119 | CL7  | C1C-C2C | -4.47 | 1.36        | 1.45     |
| 14  | bA    | 3142 | CL7  | C4C-NC  | 4.47  | 1.43        | 1.37     |
| 14  | cB    | 803  | CL7  | CHB-C4A | -4.47 | 1.26        | 1.36     |
| 14  | cA    | 3118 | CL7  | C1C-C2C | -4.46 | 1.36        | 1.45     |
| 14  | cA    | 3131 | CL7  | C1C-C2C | -4.46 | 1.36        | 1.45     |
| 14  | bB    | 811  | CL7  | C1C-C2C | -4.46 | 1.36        | 1.45     |
| 14  | bA    | 3118 | CL7  | C4B-NB  | -4.46 | 1.32        | 1.37     |
| 14  | aL    | 204  | CL7  | OBD-CAD | -4.46 | 1.14        | 1.22     |
| 14  | bA    | 3116 | CL7  | C1C-C2C | -4.46 | 1.36        | 1.45     |
| 14  | aF    | 201  | CL7  | C4B-NB  | -4.46 | 1.32        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | aJ    | 101  | CL7  | MG-NC   | -4.46 | 1.97        | 2.05     |
| 14  | cB    | 824  | CL7  | MG-ND   | -4.46 | 1.97        | 2.05     |
| 14  | bF    | 201  | CL7  | MG-NB   | -4.45 | 1.97        | 2.05     |
| 14  | bB    | 813  | CL7  | MG-NC   | -4.45 | 1.97        | 2.05     |
| 14  | aA    | 3103 | CL7  | OBD-CAD | -4.45 | 1.14        | 1.22     |
| 14  | cA    | 3144 | CL7  | MG-NA   | -4.45 | 1.97        | 2.05     |
| 14  | cA    | 3113 | CL7  | MG-ND   | -4.45 | 1.97        | 2.05     |
| 14  | cA    | 3115 | CL7  | C1C-C2C | -4.45 | 1.36        | 1.45     |
| 14  | aB    | 3005 | CL7  | MG-ND   | -4.45 | 1.97        | 2.05     |
| 14  | aB    | 3025 | CL7  | C4B-NB  | -4.45 | 1.32        | 1.37     |
| 14  | aA    | 3112 | CL7  | MG-NC   | -4.45 | 1.97        | 2.05     |
| 14  | bA    | 3113 | CL7  | MG-ND   | -4.45 | 1.97        | 2.05     |
| 14  | bB    | 812  | CL7  | MG-NC   | -4.45 | 1.97        | 2.05     |
| 14  | cL    | 204  | CL7  | MG-NC   | -4.45 | 1.97        | 2.05     |
| 14  | cB    | 822  | CL7  | MG-NC   | -4.45 | 1.97        | 2.05     |
| 14  | cB    | 803  | CL7  | MG-NC   | -4.45 | 1.97        | 2.05     |
| 14  | cA    | 3110 | CL7  | MG-NC   | -4.44 | 1.97        | 2.05     |
| 14  | aA    | 3105 | CL7  | C4B-NB  | -4.44 | 1.32        | 1.37     |
| 14  | aA    | 3120 | CL7  | MG-NC   | -4.44 | 1.97        | 2.05     |
| 14  | bA    | 3130 | CL7  | MG-NB   | -4.44 | 1.97        | 2.05     |
| 14  | aB    | 3005 | CL7  | C1C-C2C | -4.44 | 1.36        | 1.45     |
| 14  | aA    | 3134 | CL7  | MG-NA   | -4.44 | 1.97        | 2.05     |
| 14  | cB    | 821  | CL7  | C4B-NB  | -4.44 | 1.32        | 1.37     |
| 12  | aA    | 3101 | G9R  | C4B-NB  | -4.43 | 1.32        | 1.37     |
| 14  | aA    | 3105 | CL7  | MG-NA   | -4.43 | 1.97        | 2.05     |
| 14  | aA    | 3110 | CL7  | MG-NB   | -4.43 | 1.97        | 2.05     |
| 14  | cB    | 813  | CL7  | MG-NC   | -4.43 | 1.97        | 2.05     |
| 14  | aA    | 3112 | CL7  | MG-ND   | -4.43 | 1.97        | 2.05     |
| 14  | bB    | 825  | CL7  | MG-NC   | -4.43 | 1.97        | 2.05     |
| 14  | aB    | 3011 | CL7  | MG-NC   | -4.43 | 1.97        | 2.05     |
| 14  | cA    | 3106 | CL7  | MG-NA   | -4.43 | 1.97        | 2.05     |
| 14  | aK    | 101  | CL7  | MG-NA   | -4.43 | 1.97        | 2.05     |
| 14  | bA    | 3117 | CL7  | MG-NC   | -4.43 | 1.97        | 2.05     |
| 14  | bB    | 818  | CL7  | MG-NC   | -4.42 | 1.97        | 2.05     |
| 14  | aA    | 3146 | CL7  | MG-NA   | -4.42 | 1.97        | 2.05     |
| 14  | aB    | 3012 | CL7  | MG-NC   | -4.42 | 1.97        | 2.05     |
| 14  | aB    | 3032 | CL7  | C4B-NB  | -4.42 | 1.32        | 1.37     |
| 14  | bA    | 3131 | CL7  | MG-NC   | -4.42 | 1.97        | 2.05     |
| 14  | aA    | 3118 | CL7  | MG-NC   | -4.41 | 1.97        | 2.05     |
| 14  | bB    | 821  | CL7  | C4B-NB  | -4.41 | 1.32        | 1.37     |
| 14  | cA    | 3131 | CL7  | MG-NB   | -4.41 | 1.97        | 2.05     |
| 14  | cF    | 201  | CL7  | MG-NB   | -4.41 | 1.97        | 2.05     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | cA    | 3129 | CL7  | C1B-C2B | -4.41 | 1.32        | 1.43     |
| 14  | aB    | 3023 | CL7  | MG-ND   | -4.41 | 1.97        | 2.05     |
| 14  | cA    | 3117 | CL7  | MG-ND   | -4.41 | 1.97        | 2.05     |
| 14  | bB    | 803  | CL7  | MG-ND   | -4.41 | 1.97        | 2.05     |
| 14  | aF    | 201  | CL7  | MG-NB   | -4.41 | 1.97        | 2.05     |
| 14  | aB    | 3005 | CL7  | C4B-NB  | -4.41 | 1.32        | 1.37     |
| 14  | bA    | 3145 | CL7  | MG-NA   | -4.40 | 1.97        | 2.05     |
| 14  | bA    | 3112 | CL7  | MG-NA   | -4.40 | 1.97        | 2.05     |
| 14  | cB    | 827  | CL7  | MG-NC   | -4.40 | 1.97        | 2.05     |
| 14  | bB    | 817  | CL7  | C1C-C2C | -4.40 | 1.36        | 1.45     |
| 14  | aA    | 3131 | CL7  | MG-NB   | -4.40 | 1.97        | 2.05     |
| 14  | bJ    | 101  | CL7  | MG-NC   | -4.40 | 1.97        | 2.05     |
| 13  | bB    | 805  | PHO  | C4B-NB  | -4.40 | 1.30        | 1.38     |
| 14  | aB    | 3017 | CL7  | MG-NC   | -4.40 | 1.97        | 2.05     |
| 14  | aL    | 204  | CL7  | C1C-C2C | -4.39 | 1.36        | 1.45     |
| 14  | aA    | 3106 | CL7  | C1C-NC  | 4.39  | 1.43        | 1.37     |
| 14  | aA    | 3124 | CL7  | MG-NC   | -4.39 | 1.97        | 2.05     |
| 14  | cB    | 812  | CL7  | MG-NC   | -4.39 | 1.97        | 2.05     |
| 14  | cA    | 3121 | CL7  | MG-NA   | -4.39 | 1.97        | 2.05     |
| 14  | bK    | 101  | CL7  | MG-NC   | -4.39 | 1.97        | 2.05     |
| 14  | cK    | 101  | CL7  | C4B-NB  | -4.39 | 1.32        | 1.37     |
| 14  | cA    | 3119 | CL7  | MG-ND   | -4.39 | 1.97        | 2.05     |
| 14  | cA    | 3126 | CL7  | MG-ND   | -4.39 | 1.97        | 2.05     |
| 14  | cB    | 817  | CL7  | C1C-C2C | -4.39 | 1.36        | 1.45     |
| 14  | bL    | 203  | CL7  | CAB-C3B | -4.39 | 1.35        | 1.45     |
| 14  | cA    | 3126 | CL7  | MG-NA   | -4.38 | 1.97        | 2.05     |
| 14  | bL    | 203  | CL7  | MG-NA   | -4.38 | 1.97        | 2.05     |
| 14  | aA    | 3104 | CL7  | C4B-NB  | -4.38 | 1.32        | 1.37     |
| 14  | bB    | 831  | CL7  | MG-ND   | -4.38 | 1.97        | 2.05     |
| 14  | bA    | 3126 | CL7  | C4B-NB  | -4.38 | 1.32        | 1.37     |
| 14  | bB    | 818  | CL7  | C4B-NB  | -4.38 | 1.32        | 1.37     |
| 14  | cK    | 101  | CL7  | MG-ND   | -4.38 | 1.97        | 2.05     |
| 14  | bB    | 833  | CL7  | C4B-NB  | -4.38 | 1.32        | 1.37     |
| 14  | cA    | 3131 | CL7  | MG-NC   | -4.38 | 1.97        | 2.05     |
| 14  | aA    | 3114 | CL7  | MG-ND   | -4.38 | 1.97        | 2.05     |
| 14  | bA    | 3120 | CL7  | MG-ND   | -4.38 | 1.97        | 2.05     |
| 14  | bA    | 3122 | CL7  | MG-ND   | -4.38 | 1.97        | 2.05     |
| 14  | cL    | 205  | CL7  | OBD-CAD | -4.38 | 1.14        | 1.22     |
| 14  | aB    | 3020 | CL7  | C4B-NB  | -4.37 | 1.32        | 1.37     |
| 14  | aA    | 3107 | CL7  | C1B-C2B | -4.37 | 1.33        | 1.43     |
| 14  | cB    | 811  | CL7  | C1C-C2C | -4.37 | 1.36        | 1.45     |
| 14  | cA    | 3124 | CL7  | C4B-NB  | -4.37 | 1.32        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | cA    | 3121 | CL7  | C1C-C2C | -4.37 | 1.36        | 1.45     |
| 14  | aA    | 3132 | CL7  | MG-NC   | -4.37 | 1.97        | 2.05     |
| 14  | aA    | 3132 | CL7  | MG-NB   | -4.37 | 1.97        | 2.05     |
| 13  | bB    | 805  | PHO  | C4A-C3A | -4.37 | 1.43        | 1.51     |
| 14  | aB    | 3010 | CL7  | C4C-NC  | 4.37  | 1.43        | 1.37     |
| 14  | bA    | 3114 | CL7  | MG-NA   | -4.36 | 1.97        | 2.05     |
| 12  | cA    | 3101 | G9R  | O2A-CGA | 4.36  | 1.46        | 1.33     |
| 14  | cB    | 814  | CL7  | C4B-NB  | -4.36 | 1.32        | 1.37     |
| 14  | aA    | 3111 | CL7  | MG-NC   | -4.36 | 1.97        | 2.05     |
| 14  | cB    | 806  | CL7  | CAB-C3B | -4.35 | 1.36        | 1.45     |
| 14  | cK    | 101  | CL7  | MG-NA   | -4.35 | 1.97        | 2.05     |
| 17  | bB    | 828  | PQN  | C6-C5   | 4.35  | 1.46        | 1.39     |
| 14  | cB    | 826  | CL7  | C1C-C2C | -4.35 | 1.36        | 1.45     |
| 14  | cA    | 3132 | CL7  | MG-NC   | -4.35 | 1.97        | 2.05     |
| 14  | aA    | 3118 | CL7  | MG-ND   | -4.34 | 1.97        | 2.05     |
| 14  | cA    | 3118 | CL7  | C4B-NB  | -4.34 | 1.32        | 1.37     |
| 14  | aB    | 3017 | CL7  | C4B-NB  | -4.34 | 1.32        | 1.37     |
| 14  | cB    | 823  | CL7  | MG-NC   | -4.33 | 1.97        | 2.05     |
| 14  | bA    | 3109 | CL7  | MG-NC   | -4.33 | 1.97        | 2.05     |
| 14  | aA    | 3132 | CL7  | C1C-C2C | -4.33 | 1.36        | 1.45     |
| 14  | aA    | 3121 | CL7  | MG-NB   | -4.33 | 1.97        | 2.05     |
| 14  | bA    | 3140 | CL7  | OBD-CAD | -4.32 | 1.15        | 1.22     |
| 14  | bA    | 3139 | CL7  | C1C-C2C | -4.32 | 1.36        | 1.45     |
| 14  | bA    | 3123 | CL7  | MG-NC   | -4.32 | 1.97        | 2.05     |
| 14  | bA    | 3113 | CL7  | C4B-NB  | -4.32 | 1.32        | 1.37     |
| 14  | bA    | 3119 | CL7  | MG-ND   | -4.32 | 1.97        | 2.05     |
| 14  | cB    | 817  | CL7  | MG-NA   | -4.32 | 1.97        | 2.05     |
| 14  | cB    | 831  | CL7  | MG-ND   | -4.32 | 1.97        | 2.05     |
| 14  | cJ    | 101  | CL7  | MG-NC   | -4.32 | 1.97        | 2.05     |
| 14  | cB    | 821  | CL7  | MG-NC   | -4.31 | 1.97        | 2.05     |
| 14  | bA    | 3130 | CL7  | MG-NC   | -4.31 | 1.97        | 2.05     |
| 14  | cA    | 3112 | CL7  | MG-NA   | -4.31 | 1.97        | 2.05     |
| 13  | aB    | 3004 | PHO  | C3A-C2A | -4.31 | 1.50        | 1.54     |
| 14  | bB    | 804  | CL7  | MG-NA   | -4.31 | 1.97        | 2.05     |
| 14  | bB    | 809  | CL7  | OBD-CAD | -4.31 | 1.15        | 1.22     |
| 14  | cL    | 204  | CL7  | MG-NA   | -4.31 | 1.97        | 2.05     |
| 14  | aB    | 3020 | CL7  | MG-NC   | -4.31 | 1.97        | 2.05     |
| 14  | aB    | 3022 | CL7  | MG-NC   | -4.31 | 1.97        | 2.05     |
| 14  | bA    | 3131 | CL7  | MG-NB   | -4.31 | 1.97        | 2.05     |
| 14  | bA    | 3123 | CL7  | C1C-C2C | -4.30 | 1.36        | 1.45     |
| 14  | bA    | 3121 | CL7  | MG-NA   | -4.30 | 1.97        | 2.05     |
| 14  | bA    | 3121 | CL7  | CAB-C3B | -4.30 | 1.36        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | bB    | 823  | CL7  | MG-NC   | -4.30 | 1.97        | 2.05     |
| 14  | aA    | 3140 | CL7  | MG-NB   | -4.29 | 1.97        | 2.05     |
| 14  | aA    | 3120 | CL7  | MG-ND   | -4.29 | 1.97        | 2.05     |
| 14  | aA    | 3133 | CL7  | MG-NB   | -4.29 | 1.97        | 2.05     |
| 14  | cB    | 804  | CL7  | MG-NB   | -4.29 | 1.97        | 2.05     |
| 14  | aA    | 3105 | CL7  | MG-NC   | -4.29 | 1.97        | 2.05     |
| 14  | bA    | 3124 | CL7  | C4B-NB  | -4.29 | 1.32        | 1.37     |
| 14  | aB    | 3032 | CL7  | MG-ND   | -4.29 | 1.97        | 2.05     |
| 14  | bA    | 3132 | CL7  | C4C-NC  | 4.29  | 1.43        | 1.37     |
| 14  | bB    | 810  | CL7  | C1C-C2C | -4.29 | 1.36        | 1.45     |
| 14  | bB    | 808  | CL7  | OBD-CAD | -4.29 | 1.15        | 1.22     |
| 14  | bB    | 810  | CL7  | CAA-C2A | -4.28 | 1.46        | 1.54     |
| 14  | aB    | 3010 | CL7  | C1C-C2C | -4.28 | 1.36        | 1.45     |
| 14  | aB    | 3003 | CL7  | C1C-NC  | 4.28  | 1.43        | 1.37     |
| 14  | aB    | 3016 | CL7  | MG-NA   | -4.28 | 1.97        | 2.05     |
| 14  | cA    | 3139 | CL7  | OBD-CAD | -4.28 | 1.15        | 1.22     |
| 14  | cA    | 3114 | CL7  | MG-NC   | -4.28 | 1.97        | 2.05     |
| 14  | cA    | 3124 | CL7  | C1C-C2C | -4.28 | 1.36        | 1.45     |
| 14  | bA    | 3103 | CL7  | MG-NB   | -4.27 | 1.97        | 2.05     |
| 12  | aA    | 3101 | G9R  | OBB-CAB | 4.27  | 1.31        | 1.22     |
| 14  | aB    | 3007 | CL7  | C2A-C1A | -4.27 | 1.44        | 1.50     |
| 14  | aB    | 3013 | CL7  | C4B-NB  | -4.27 | 1.32        | 1.37     |
| 14  | bA    | 3122 | CL7  | MG-NB   | -4.27 | 1.97        | 2.05     |
| 14  | cA    | 3130 | CL7  | MG-NC   | -4.27 | 1.97        | 2.05     |
| 14  | cB    | 809  | CL7  | OBD-CAD | -4.27 | 1.15        | 1.22     |
| 14  | aA    | 3134 | CL7  | C4B-NB  | -4.27 | 1.32        | 1.37     |
| 14  | bA    | 3129 | CL7  | C1B-C2B | -4.27 | 1.33        | 1.43     |
| 14  | aK    | 101  | CL7  | MG-ND   | -4.27 | 1.97        | 2.05     |
| 14  | cA    | 3109 | CL7  | MG-NC   | -4.27 | 1.97        | 2.05     |
| 14  | cA    | 3133 | CL7  | MG-NA   | -4.27 | 1.97        | 2.05     |
| 14  | cB    | 818  | CL7  | C4B-NB  | -4.26 | 1.32        | 1.37     |
| 14  | cA    | 3131 | CL7  | MG-NA   | -4.26 | 1.97        | 2.05     |
| 14  | cA    | 3113 | CL7  | C4B-NB  | -4.26 | 1.32        | 1.37     |
| 14  | aL    | 203  | CL7  | MG-NA   | -4.26 | 1.97        | 2.05     |
| 14  | cK    | 101  | CL7  | MG-NC   | -4.26 | 1.97        | 2.05     |
| 14  | bA    | 3104 | CL7  | MG-NB   | -4.26 | 1.97        | 2.05     |
| 14  | cB    | 825  | CL7  | C4B-NB  | -4.26 | 1.32        | 1.37     |
| 14  | bK    | 101  | CL7  | C4B-NB  | -4.26 | 1.32        | 1.37     |
| 14  | cA    | 3122 | CL7  | MG-ND   | -4.26 | 1.97        | 2.05     |
| 14  | aA    | 3131 | CL7  | MG-NC   | -4.26 | 1.97        | 2.05     |
| 14  | cA    | 3114 | CL7  | MG-NA   | -4.26 | 1.97        | 2.05     |
| 14  | aA    | 3125 | CL7  | C1D-C2D | -4.25 | 1.33        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | aA    | 3129 | CL7  | MG-NC   | -4.25 | 1.97        | 2.05     |
| 14  | cA    | 3120 | CL7  | MG-NB   | -4.25 | 1.97        | 2.05     |
| 14  | bB    | 826  | CL7  | C1C-C2C | -4.25 | 1.36        | 1.45     |
| 14  | bA    | 3139 | CL7  | OBD-CAD | -4.25 | 1.15        | 1.22     |
| 14  | bA    | 3114 | CL7  | MG-NC   | -4.25 | 1.97        | 2.05     |
| 14  | aB    | 3008 | CL7  | OBD-CAD | -4.25 | 1.15        | 1.22     |
| 14  | aB    | 3024 | CL7  | C4B-NB  | -4.25 | 1.32        | 1.37     |
| 14  | cA    | 3125 | CL7  | C4C-NC  | 4.25  | 1.43        | 1.37     |
| 14  | aB    | 3025 | CL7  | OBD-CAD | -4.24 | 1.15        | 1.22     |
| 14  | bB    | 827  | CL7  | MG-NA   | -4.24 | 1.97        | 2.05     |
| 14  | bB    | 814  | CL7  | C4B-NB  | -4.24 | 1.32        | 1.37     |
| 14  | cB    | 833  | CL7  | OBD-CAD | -4.24 | 1.15        | 1.22     |
| 14  | aK    | 101  | CL7  | C4B-NB  | -4.24 | 1.32        | 1.37     |
| 14  | cB    | 806  | CL7  | C4B-NB  | -4.24 | 1.32        | 1.37     |
| 14  | aA    | 3104 | CL7  | MG-NB   | -4.24 | 1.97        | 2.05     |
| 14  | bA    | 3120 | CL7  | MG-NB   | -4.24 | 1.97        | 2.05     |
| 14  | aL    | 202  | CL7  | MG-NA   | -4.24 | 1.97        | 2.05     |
| 14  | bB    | 825  | CL7  | C4B-NB  | -4.23 | 1.32        | 1.37     |
| 14  | cA    | 3107 | CL7  | C1C-C2C | -4.23 | 1.37        | 1.45     |
| 14  | aB    | 3026 | CL7  | CMA-C3A | 4.23  | 1.62        | 1.53     |
| 14  | bA    | 3103 | CL7  | MG-NC   | -4.23 | 1.97        | 2.05     |
| 14  | cA    | 3123 | CL7  | MG-ND   | -4.23 | 1.97        | 2.05     |
| 17  | bB    | 828  | PQN  | C9-C10  | -4.23 | 1.33        | 1.39     |
| 14  | aA    | 3113 | CL7  | MG-NA   | -4.23 | 1.97        | 2.05     |
| 14  | aB    | 3003 | CL7  | MG-NA   | -4.23 | 1.97        | 2.05     |
| 14  | bA    | 3131 | CL7  | MG-NA   | -4.22 | 1.97        | 2.05     |
| 12  | bA    | 3101 | G9R  | C4B-NB  | -4.22 | 1.32        | 1.37     |
| 14  | bA    | 3133 | CL7  | C4B-NB  | -4.22 | 1.32        | 1.37     |
| 14  | aA    | 3130 | CL7  | C1C-C2C | -4.22 | 1.37        | 1.45     |
| 14  | aB    | 3025 | CL7  | C4D-ND  | -4.22 | 1.31        | 1.37     |
| 14  | aA    | 3127 | CL7  | MG-ND   | -4.22 | 1.97        | 2.05     |
| 14  | bF    | 201  | CL7  | MG-ND   | -4.22 | 1.97        | 2.05     |
| 14  | bB    | 817  | CL7  | MG-NA   | -4.22 | 1.97        | 2.05     |
| 14  | bB    | 821  | CL7  | MG-NC   | -4.22 | 1.97        | 2.05     |
| 14  | cA    | 3104 | CL7  | MG-NB   | -4.22 | 1.97        | 2.05     |
| 14  | aA    | 3119 | CL7  | C4B-NB  | -4.21 | 1.32        | 1.37     |
| 14  | cA    | 3107 | CL7  | C1C-NC  | 4.21  | 1.43        | 1.37     |
| 14  | cB    | 808  | CL7  | C1C-C2C | -4.21 | 1.37        | 1.45     |
| 14  | bB    | 804  | CL7  | MG-NC   | -4.21 | 1.97        | 2.05     |
| 14  | cB    | 833  | CL7  | MG-NB   | -4.21 | 1.97        | 2.05     |
| 14  | aB    | 3005 | CL7  | CAB-C3B | -4.21 | 1.36        | 1.45     |
| 14  | bB    | 804  | CL7  | C1C-NC  | 4.21  | 1.43        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | aA    | 3126 | CL7  | MG-ND   | -4.21 | 1.97        | 2.05     |
| 14  | aA    | 3108 | CL7  | MG-NB   | -4.21 | 1.97        | 2.05     |
| 14  | aA    | 3121 | CL7  | OBD-CAD | -4.20 | 1.15        | 1.22     |
| 14  | bA    | 3123 | CL7  | C1C-NC  | 4.20  | 1.42        | 1.37     |
| 14  | cL    | 205  | CL7  | C1C-C2C | -4.20 | 1.37        | 1.45     |
| 14  | bA    | 3129 | CL7  | CAA-C2A | 4.20  | 1.62        | 1.53     |
| 14  | aK    | 101  | CL7  | MG-NC   | -4.20 | 1.97        | 2.05     |
| 14  | aA    | 3140 | CL7  | C1C-C2C | -4.19 | 1.37        | 1.45     |
| 14  | cA    | 3120 | CL7  | OBD-CAD | -4.19 | 1.15        | 1.22     |
| 14  | aB    | 3007 | CL7  | OBD-CAD | -4.19 | 1.15        | 1.22     |
| 14  | cA    | 3127 | CL7  | C4C-NC  | 4.19  | 1.42        | 1.37     |
| 14  | aB    | 3009 | CL7  | C1C-C2C | -4.19 | 1.37        | 1.45     |
| 14  | cA    | 3102 | CL7  | MG-NB   | -4.19 | 1.97        | 2.05     |
| 14  | cA    | 3109 | CL7  | MG-NA   | -4.18 | 1.97        | 2.05     |
| 14  | aA    | 3122 | CL7  | CAB-C3B | -4.18 | 1.36        | 1.45     |
| 14  | aB    | 3030 | CL7  | MG-NA   | -4.18 | 1.97        | 2.05     |
| 14  | aA    | 3122 | CL7  | C1C-C2C | -4.18 | 1.37        | 1.45     |
| 14  | bB    | 806  | CL7  | CAB-C3B | -4.18 | 1.36        | 1.45     |
| 14  | cB    | 810  | CL7  | C1D-C2D | -4.18 | 1.33        | 1.43     |
| 14  | cL    | 203  | CL7  | MG-NA   | -4.17 | 1.97        | 2.05     |
| 14  | aB    | 3013 | CL7  | MG-NC   | -4.17 | 1.97        | 2.05     |
| 14  | aA    | 3108 | CL7  | C1C-NC  | 4.17  | 1.42        | 1.37     |
| 14  | aA    | 3105 | CL7  | MG-NB   | -4.17 | 1.97        | 2.05     |
| 14  | aA    | 3119 | CL7  | MG-NA   | -4.17 | 1.97        | 2.05     |
| 14  | cA    | 3133 | CL7  | C4B-NB  | -4.17 | 1.32        | 1.37     |
| 14  | cF    | 201  | CL7  | MG-ND   | -4.17 | 1.97        | 2.05     |
| 14  | bA    | 3109 | CL7  | MG-NA   | -4.17 | 1.97        | 2.05     |
| 14  | bB    | 831  | CL7  | MG-NA   | -4.16 | 1.97        | 2.05     |
| 14  | bB    | 803  | CL7  | MG-NC   | -4.16 | 1.97        | 2.05     |
| 14  | cB    | 814  | CL7  | MG-NC   | -4.16 | 1.97        | 2.05     |
| 13  | bB    | 801  | PHO  | C1D-ND  | -4.16 | 1.30        | 1.38     |
| 14  | bA    | 3107 | CL7  | C1C-C2C | -4.16 | 1.37        | 1.45     |
| 14  | cL    | 203  | CL7  | MG-NC   | -4.16 | 1.97        | 2.05     |
| 13  | cB    | 805  | PHO  | CBD-CAD | -4.16 | 1.39        | 1.53     |
| 14  | aA    | 3133 | CL7  | MG-NC   | -4.16 | 1.97        | 2.05     |
| 14  | cB    | 809  | CL7  | C4B-NB  | -4.15 | 1.32        | 1.37     |
| 14  | aA    | 3124 | CL7  | MG-NB   | -4.15 | 1.97        | 2.05     |
| 14  | bB    | 814  | CL7  | MG-NC   | -4.14 | 1.97        | 2.05     |
| 14  | bA    | 3126 | CL7  | MG-ND   | -4.14 | 1.97        | 2.05     |
| 14  | cA    | 3106 | CL7  | CAB-C3B | -4.14 | 1.36        | 1.45     |
| 14  | bA    | 3127 | CL7  | C4C-NC  | 4.14  | 1.42        | 1.37     |
| 13  | bB    | 801  | PHO  | O2D-CGD | 4.14  | 1.43        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | bA    | 3126 | CL7  | MG-NA   | -4.14 | 1.97        | 2.05     |
| 14  | cA    | 3103 | CL7  | MG-NC   | -4.14 | 1.97        | 2.05     |
| 14  | cA    | 3132 | CL7  | CAA-CBA | -4.14 | 1.39        | 1.52     |
| 14  | bB    | 826  | CL7  | MG-NB   | -4.13 | 1.97        | 2.05     |
| 14  | bA    | 3120 | CL7  | MG-NC   | -4.13 | 1.97        | 2.05     |
| 14  | aF    | 201  | CL7  | MG-ND   | -4.13 | 1.97        | 2.05     |
| 14  | cA    | 3118 | CL7  | MG-NA   | -4.13 | 1.97        | 2.05     |
| 12  | bA    | 3101 | G9R  | OBB-CAB | 4.12  | 1.31        | 1.22     |
| 14  | cB    | 816  | CL7  | OBD-CAD | -4.12 | 1.15        | 1.22     |
| 14  | aA    | 3123 | CL7  | MG-NB   | -4.12 | 1.97        | 2.05     |
| 14  | cA    | 3111 | CL7  | MG-NB   | -4.12 | 1.97        | 2.05     |
| 14  | cB    | 808  | CL7  | MG-NA   | -4.12 | 1.97        | 2.05     |
| 13  | cB    | 805  | PHO  | C3B-C2B | -4.12 | 1.34        | 1.40     |
| 14  | aA    | 3107 | CL7  | MG-NA   | -4.12 | 1.97        | 2.05     |
| 14  | aA    | 3110 | CL7  | MG-NC   | -4.12 | 1.97        | 2.05     |
| 14  | aA    | 3124 | CL7  | MG-ND   | -4.11 | 1.97        | 2.05     |
| 14  | bA    | 3133 | CL7  | MG-NA   | -4.11 | 1.97        | 2.05     |
| 14  | cA    | 3125 | CL7  | MG-ND   | -4.11 | 1.97        | 2.05     |
| 14  | bA    | 3125 | CL7  | C4B-NB  | -4.11 | 1.32        | 1.37     |
| 14  | cA    | 3140 | CL7  | OBD-CAD | -4.11 | 1.15        | 1.22     |
| 17  | cA    | 3143 | PQN  | C10-C1  | -4.11 | 1.40        | 1.48     |
| 14  | cA    | 3118 | CL7  | MG-NB   | -4.11 | 1.97        | 2.05     |
| 14  | bB    | 803  | CL7  | CHC-C1C | -4.11 | 1.30        | 1.38     |
| 14  | cB    | 831  | CL7  | MG-NB   | -4.11 | 1.97        | 2.05     |
| 13  | aB    | 3004 | PHO  | C4A-C3A | -4.11 | 1.44        | 1.51     |
| 14  | bA    | 3140 | CL7  | MG-NB   | -4.11 | 1.97        | 2.05     |
| 14  | bB    | 833  | CL7  | MG-NB   | -4.11 | 1.97        | 2.05     |
| 14  | cB    | 806  | CL7  | C1C-NC  | 4.10  | 1.42        | 1.37     |
| 14  | aA    | 3130 | CL7  | C1B-C2B | -4.10 | 1.33        | 1.43     |
| 14  | aA    | 3132 | CL7  | MG-NA   | -4.10 | 1.97        | 2.05     |
| 14  | cA    | 3140 | CL7  | MG-NC   | -4.10 | 1.97        | 2.05     |
| 14  | aA    | 3104 | CL7  | MG-NC   | -4.10 | 1.97        | 2.05     |
| 14  | aA    | 3117 | CL7  | C4B-NB  | -4.10 | 1.32        | 1.37     |
| 14  | cB    | 826  | CL7  | OBD-CAD | -4.10 | 1.15        | 1.22     |
| 14  | cB    | 823  | CL7  | MG-NA   | -4.10 | 1.97        | 2.05     |
| 14  | bA    | 3141 | CL7  | MG-NB   | -4.10 | 1.97        | 2.05     |
| 14  | aB    | 3002 | CL7  | MG-NC   | -4.09 | 1.97        | 2.05     |
| 14  | aA    | 3110 | CL7  | MG-NA   | -4.09 | 1.97        | 2.05     |
| 13  | cB    | 801  | PHO  | C1D-ND  | -4.09 | 1.31        | 1.38     |
| 14  | cA    | 3113 | CL7  | MG-NC   | -4.09 | 1.97        | 2.05     |
| 13  | aA    | 3102 | PHO  | C4D-ND  | -4.09 | 1.32        | 1.38     |
| 14  | cA    | 3142 | CL7  | C1C-C2C | -4.09 | 1.37        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | bL    | 204  | CL7  | MG-NC   | -4.08 | 1.97        | 2.05     |
| 14  | cA    | 3140 | CL7  | MG-NB   | -4.08 | 1.97        | 2.05     |
| 14  | aA    | 3125 | CL7  | C1C-C2C | -4.08 | 1.37        | 1.45     |
| 14  | bB    | 815  | CL7  | MG-NC   | -4.08 | 1.97        | 2.05     |
| 14  | aA    | 3127 | CL7  | MG-NA   | -4.08 | 1.97        | 2.05     |
| 14  | bA    | 3145 | CL7  | MG-NC   | -4.08 | 1.97        | 2.05     |
| 14  | bB    | 806  | CL7  | MG-ND   | -4.08 | 1.97        | 2.05     |
| 14  | bA    | 3132 | CL7  | MG-NC   | -4.08 | 1.97        | 2.05     |
| 14  | cB    | 815  | CL7  | MG-NC   | -4.08 | 1.97        | 2.05     |
| 14  | bA    | 3125 | CL7  | C3B-C4B | -4.07 | 1.33        | 1.42     |
| 14  | bA    | 3108 | CL7  | OBD-CAD | -4.07 | 1.15        | 1.22     |
| 14  | cA    | 3112 | CL7  | C4B-NB  | -4.07 | 1.32        | 1.37     |
| 14  | aB    | 3030 | CL7  | MG-ND   | -4.07 | 1.97        | 2.05     |
| 14  | bA    | 3111 | CL7  | MG-NB   | -4.07 | 1.97        | 2.05     |
| 14  | bA    | 3140 | CL7  | MG-NA   | -4.07 | 1.97        | 2.05     |
| 14  | cA    | 3126 | CL7  | C2A-C1A | -4.07 | 1.47        | 1.52     |
| 14  | bA    | 3102 | CL7  | C3C-C2C | -4.07 | 1.28        | 1.36     |
| 14  | aB    | 3013 | CL7  | MG-NA   | -4.07 | 1.97        | 2.05     |
| 14  | bA    | 3112 | CL7  | C4B-NB  | -4.07 | 1.32        | 1.37     |
| 14  | aB    | 3006 | CL7  | MG-NC   | -4.06 | 1.97        | 2.05     |
| 14  | aB    | 3003 | CL7  | MG-NB   | -4.06 | 1.97        | 2.05     |
| 14  | bB    | 803  | CL7  | MG-NA   | -4.06 | 1.97        | 2.05     |
| 14  | cA    | 3124 | CL7  | MG-ND   | -4.06 | 1.97        | 2.05     |
| 14  | aA    | 3140 | CL7  | OBD-CAD | -4.06 | 1.15        | 1.22     |
| 14  | aA    | 3126 | CL7  | O1D-CGD | -4.06 | 1.11        | 1.21     |
| 14  | cA    | 3126 | CL7  | C4B-NB  | -4.06 | 1.32        | 1.37     |
| 14  | aB    | 3025 | CL7  | C3A-C4A | -4.06 | 1.45        | 1.52     |
| 14  | bB    | 810  | CL7  | C1D-C2D | -4.06 | 1.33        | 1.43     |
| 14  | aA    | 3114 | CL7  | C4B-NB  | -4.06 | 1.32        | 1.37     |
| 14  | bB    | 807  | CL7  | MG-NC   | -4.06 | 1.97        | 2.05     |
| 14  | cA    | 3122 | CL7  | MG-NB   | -4.06 | 1.97        | 2.05     |
| 14  | aA    | 3146 | CL7  | MG-NC   | -4.05 | 1.97        | 2.05     |
| 14  | bB    | 831  | CL7  | MG-NB   | -4.05 | 1.97        | 2.05     |
| 14  | bA    | 3128 | CL7  | C1C-NC  | 4.05  | 1.42        | 1.37     |
| 14  | aA    | 3129 | CL7  | C1C-C2C | -4.05 | 1.37        | 1.45     |
| 14  | cA    | 3119 | CL7  | MG-NB   | -4.05 | 1.97        | 2.05     |
| 14  | bA    | 3118 | CL7  | MG-NC   | -4.05 | 1.97        | 2.05     |
| 14  | bL    | 205  | CL7  | C1C-C2C | -4.04 | 1.37        | 1.45     |
| 14  | bA    | 3113 | CL7  | MG-NC   | -4.04 | 1.97        | 2.05     |
| 17  | cA    | 3143 | PQN  | O4-C4   | -4.04 | 1.14        | 1.23     |
| 14  | bA    | 3118 | CL7  | MG-NB   | -4.04 | 1.97        | 2.05     |
| 14  | aA    | 3122 | CL7  | MG-NA   | -4.04 | 1.97        | 2.05     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | bB    | 833  | CL7  | MG-ND   | -4.04 | 1.97        | 2.05     |
| 14  | cA    | 3144 | CL7  | MG-NC   | -4.04 | 1.97        | 2.05     |
| 14  | cL    | 205  | CL7  | MG-NA   | -4.04 | 1.97        | 2.05     |
| 14  | bA    | 3112 | CL7  | MG-NB   | -4.04 | 1.97        | 2.05     |
| 13  | aA    | 3102 | PHO  | O2D-CGD | 4.04  | 1.43        | 1.33     |
| 14  | bA    | 3124 | CL7  | C1C-C2C | -4.04 | 1.37        | 1.45     |
| 14  | cA    | 3105 | CL7  | C1C-NC  | 4.03  | 1.42        | 1.37     |
| 14  | cB    | 808  | CL7  | OBD-CAD | -4.03 | 1.15        | 1.22     |
| 14  | cA    | 3144 | CL7  | MG-NB   | -4.03 | 1.97        | 2.05     |
| 14  | bB    | 808  | CL7  | MG-NA   | -4.03 | 1.97        | 2.05     |
| 14  | aB    | 3005 | CL7  | C1C-NC  | 4.03  | 1.42        | 1.37     |
| 14  | cA    | 3112 | CL7  | MG-NB   | -4.02 | 1.97        | 2.05     |
| 14  | aA    | 3115 | CL7  | MG-NC   | -4.02 | 1.97        | 2.05     |
| 14  | bA    | 3140 | CL7  | MG-NC   | -4.02 | 1.97        | 2.05     |
| 14  | cB    | 804  | CL7  | MG-NC   | -4.01 | 1.97        | 2.05     |
| 14  | bA    | 3132 | CL7  | CAA-CBA | -4.01 | 1.40        | 1.52     |
| 17  | bA    | 3143 | PQN  | O4-C4   | -4.01 | 1.14        | 1.23     |
| 14  | aB    | 3015 | CL7  | OBD-CAD | -4.01 | 1.15        | 1.22     |
| 14  | aA    | 3133 | CL7  | C4C-NC  | 4.01  | 1.42        | 1.37     |
| 14  | aB    | 3031 | CL7  | MG-NC   | -4.01 | 1.97        | 2.05     |
| 14  | cB    | 806  | CL7  | MG-ND   | -4.01 | 1.97        | 2.05     |
| 14  | cA    | 3102 | CL7  | C3C-C2C | -4.00 | 1.28        | 1.36     |
| 14  | aA    | 3123 | CL7  | MG-ND   | -4.00 | 1.97        | 2.05     |
| 14  | cB    | 826  | CL7  | C4D-ND  | -4.00 | 1.32        | 1.37     |
| 14  | cB    | 833  | CL7  | CHB-C4A | -4.00 | 1.27        | 1.36     |
| 14  | aA    | 3141 | CL7  | MG-NB   | -4.00 | 1.97        | 2.05     |
| 14  | cA    | 3121 | CL7  | MG-NC   | -4.00 | 1.97        | 2.05     |
| 14  | cB    | 804  | CL7  | MG-NA   | -4.00 | 1.97        | 2.05     |
| 14  | aA    | 3108 | CL7  | C1C-C2C | -4.00 | 1.37        | 1.45     |
| 14  | bB    | 804  | CL7  | CHD-C4C | -4.00 | 1.30        | 1.38     |
| 14  | aA    | 3124 | CL7  | OBD-CAD | -3.99 | 1.15        | 1.22     |
| 14  | bA    | 3129 | CL7  | C1C-C2C | -3.99 | 1.37        | 1.45     |
| 14  | cA    | 3126 | CL7  | MG-NC   | -3.99 | 1.97        | 2.05     |
| 14  | cA    | 3140 | CL7  | MG-NA   | -3.99 | 1.97        | 2.05     |
| 13  | bB    | 805  | PHO  | CMB-C2B | -3.99 | 1.43        | 1.51     |
| 17  | aA    | 3144 | PQN  | C6-C5   | 3.99  | 1.46        | 1.39     |
| 14  | bA    | 3142 | CL7  | C1C-C2C | -3.99 | 1.37        | 1.45     |
| 14  | aA    | 3115 | CL7  | MG-NA   | -3.99 | 1.97        | 2.05     |
| 14  | aB    | 3022 | CL7  | MG-NA   | -3.99 | 1.97        | 2.05     |
| 14  | cB    | 814  | CL7  | MG-NA   | -3.99 | 1.97        | 2.05     |
| 14  | bA    | 3106 | CL7  | CAB-C3B | -3.99 | 1.36        | 1.45     |
| 14  | aB    | 3011 | CL7  | C4B-NB  | -3.98 | 1.32        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | aA    | 3113 | CL7  | MG-NB   | -3.98 | 1.97        | 2.05     |
| 14  | aB    | 3026 | CL7  | C1D-C2D | -3.98 | 1.33        | 1.43     |
| 17  | bA    | 3143 | PQN  | C10-C1  | -3.98 | 1.40        | 1.48     |
| 14  | bB    | 823  | CL7  | MG-NA   | -3.98 | 1.97        | 2.05     |
| 14  | bA    | 3118 | CL7  | MG-ND   | -3.98 | 1.97        | 2.05     |
| 14  | cA    | 3108 | CL7  | MG-NA   | -3.98 | 1.97        | 2.05     |
| 14  | cB    | 812  | CL7  | C4B-NB  | -3.98 | 1.32        | 1.37     |
| 14  | cA    | 3108 | CL7  | MG-NB   | -3.98 | 1.97        | 2.05     |
| 14  | aB    | 3007 | CL7  | MG-NA   | -3.98 | 1.97        | 2.05     |
| 13  | cB    | 805  | PHO  | C4A-C3A | -3.97 | 1.44        | 1.51     |
| 14  | aA    | 3114 | CL7  | MG-NC   | -3.97 | 1.97        | 2.05     |
| 13  | cB    | 801  | PHO  | O2D-CGD | 3.97  | 1.42        | 1.33     |
| 14  | bA    | 3121 | CL7  | MG-NC   | -3.97 | 1.97        | 2.05     |
| 14  | cA    | 3125 | CL7  | C3B-C4B | -3.97 | 1.33        | 1.42     |
| 14  | cB    | 833  | CL7  | MG-ND   | -3.97 | 1.97        | 2.05     |
| 14  | bB    | 804  | CL7  | MG-NB   | -3.97 | 1.97        | 2.05     |
| 14  | bB    | 815  | CL7  | MG-NB   | -3.96 | 1.97        | 2.05     |
| 14  | bA    | 3116 | CL7  | OBD-CAD | -3.96 | 1.15        | 1.22     |
| 14  | cA    | 3127 | CL7  | OBD-CAD | -3.96 | 1.15        | 1.22     |
| 14  | bA    | 3110 | CL7  | C4B-NB  | -3.96 | 1.32        | 1.37     |
| 14  | bA    | 3128 | CL7  | C1C-C2C | -3.96 | 1.37        | 1.45     |
| 14  | bB    | 827  | CL7  | C1D-C2D | -3.96 | 1.33        | 1.43     |
| 14  | cB    | 807  | CL7  | MG-NC   | -3.96 | 1.97        | 2.05     |
| 14  | aB    | 3016 | CL7  | MG-NC   | -3.96 | 1.97        | 2.05     |
| 13  | aA    | 3102 | PHO  | C1D-ND  | -3.96 | 1.31        | 1.38     |
| 14  | aA    | 3107 | CL7  | CAB-C3B | -3.96 | 1.36        | 1.45     |
| 14  | bA    | 3140 | CL7  | C2A-C1A | -3.96 | 1.44        | 1.50     |
| 14  | bA    | 3122 | CL7  | C1D-C2D | -3.95 | 1.33        | 1.43     |
| 14  | bA    | 3132 | CL7  | CHB-C4A | -3.95 | 1.28        | 1.36     |
| 14  | aA    | 3141 | CL7  | MG-NA   | -3.95 | 1.98        | 2.05     |
| 14  | bA    | 3110 | CL7  | MG-NB   | -3.95 | 1.98        | 2.05     |
| 14  | cA    | 3122 | CL7  | C1D-C2D | -3.95 | 1.33        | 1.43     |
| 14  | bB    | 832  | CL7  | MG-NB   | -3.95 | 1.98        | 2.05     |
| 14  | bA    | 3119 | CL7  | C1D-C2D | -3.95 | 1.34        | 1.43     |
| 14  | bB    | 826  | CL7  | OBD-CAD | -3.95 | 1.15        | 1.22     |
| 14  | cA    | 3129 | CL7  | C1C-C2C | -3.94 | 1.37        | 1.45     |
| 14  | cA    | 3102 | CL7  | C2A-C1A | -3.94 | 1.44        | 1.50     |
| 14  | aB    | 3008 | CL7  | C4C-NC  | 3.94  | 1.42        | 1.37     |
| 14  | cA    | 3125 | CL7  | O1D-CGD | -3.94 | 1.11        | 1.21     |
| 14  | bA    | 3123 | CL7  | MG-NB   | -3.94 | 1.98        | 2.05     |
| 14  | cB    | 832  | CL7  | MG-NC   | -3.93 | 1.98        | 2.05     |
| 14  | cB    | 803  | CL7  | CHC-C1C | -3.93 | 1.30        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | aB    | 3026 | CL7  | CHC-C1C | -3.93 | 1.30        | 1.38     |
| 14  | bK    | 101  | CL7  | C4D-CHA | -3.93 | 1.37        | 1.45     |
| 14  | cJ    | 101  | CL7  | MG-NB   | -3.93 | 1.98        | 2.05     |
| 14  | aA    | 3141 | CL7  | MG-NC   | -3.93 | 1.98        | 2.05     |
| 14  | aA    | 3123 | CL7  | C1D-C2D | -3.93 | 1.34        | 1.43     |
| 14  | aA    | 3119 | CL7  | MG-NB   | -3.93 | 1.98        | 2.05     |
| 13  | aB    | 3004 | PHO  | CBD-CAD | -3.93 | 1.40        | 1.53     |
| 14  | bB    | 803  | CL7  | CHB-C4A | -3.93 | 1.28        | 1.36     |
| 14  | cA    | 3123 | CL7  | MG-NA   | -3.93 | 1.98        | 2.05     |
| 14  | aA    | 3133 | CL7  | CAA-CBA | -3.93 | 1.40        | 1.52     |
| 14  | cB    | 827  | CL7  | C1D-C2D | -3.93 | 1.34        | 1.43     |
| 14  | bA    | 3127 | CL7  | OBD-CAD | -3.93 | 1.15        | 1.22     |
| 14  | bA    | 3107 | CL7  | C1C-NC  | 3.92  | 1.42        | 1.37     |
| 14  | aA    | 3126 | CL7  | C3B-C4B | -3.92 | 1.33        | 1.42     |
| 14  | aB    | 3032 | CL7  | MG-NB   | -3.92 | 1.98        | 2.05     |
| 14  | cB    | 817  | CL7  | MG-NC   | -3.92 | 1.98        | 2.05     |
| 14  | bB    | 814  | CL7  | MG-NA   | -3.92 | 1.98        | 2.05     |
| 14  | aA    | 3143 | CL7  | C1C-C2C | -3.92 | 1.37        | 1.45     |
| 14  | bA    | 3145 | CL7  | MG-NB   | -3.91 | 1.98        | 2.05     |
| 12  | cA    | 3101 | G9R  | C1B-NB  | -3.91 | 1.33        | 1.37     |
| 14  | aB    | 3003 | CL7  | MG-NC   | -3.91 | 1.98        | 2.05     |
| 14  | bB    | 812  | CL7  | C4B-NB  | -3.91 | 1.33        | 1.37     |
| 14  | aA    | 3146 | CL7  | MG-NB   | -3.91 | 1.98        | 2.05     |
| 14  | bB    | 817  | CL7  | MG-NC   | -3.91 | 1.98        | 2.05     |
| 14  | bB    | 806  | CL7  | CAA-C2A | -3.91 | 1.46        | 1.54     |
| 14  | bB    | 809  | CL7  | CHC-C1C | -3.91 | 1.30        | 1.38     |
| 14  | aB    | 3003 | CL7  | OBD-CAD | -3.90 | 1.15        | 1.22     |
| 14  | cA    | 3120 | CL7  | MG-NC   | -3.90 | 1.98        | 2.05     |
| 14  | bA    | 3128 | CL7  | C3C-C2C | -3.90 | 1.28        | 1.36     |
| 14  | bA    | 3113 | CL7  | MG-NB   | -3.90 | 1.98        | 2.05     |
| 14  | bB    | 833  | CL7  | OBD-CAD | -3.90 | 1.15        | 1.22     |
| 14  | bB    | 832  | CL7  | MG-NC   | -3.90 | 1.98        | 2.05     |
| 14  | cA    | 3124 | CL7  | MG-NB   | -3.90 | 1.98        | 2.05     |
| 14  | bB    | 821  | CL7  | MG-NB   | -3.90 | 1.98        | 2.05     |
| 14  | bB    | 810  | CL7  | C3A-C4A | -3.90 | 1.45        | 1.52     |
| 14  | cA    | 3139 | CL7  | MG-NC   | -3.89 | 1.98        | 2.05     |
| 14  | cA    | 3116 | CL7  | OBD-CAD | -3.89 | 1.15        | 1.22     |
| 14  | aA    | 3142 | CL7  | MG-NB   | -3.89 | 1.98        | 2.05     |
| 14  | bB    | 816  | CL7  | OBD-CAD | -3.89 | 1.15        | 1.22     |
| 14  | bA    | 3120 | CL7  | MG-NA   | -3.89 | 1.98        | 2.05     |
| 14  | cB    | 826  | CL7  | C3A-C4A | -3.89 | 1.45        | 1.52     |
| 14  | bA    | 3124 | CL7  | CAB-C3B | -3.89 | 1.37        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | aJ    | 101  | CL7  | MG-NB   | -3.89 | 1.98        | 2.05     |
| 14  | bA    | 3124 | CL7  | MG-ND   | -3.89 | 1.98        | 2.05     |
| 14  | bA    | 3115 | CL7  | C1C-NC  | 3.89  | 1.42        | 1.37     |
| 14  | aL    | 204  | CL7  | MG-NA   | -3.89 | 1.98        | 2.05     |
| 14  | cB    | 815  | CL7  | MG-NB   | -3.89 | 1.98        | 2.05     |
| 14  | aA    | 3111 | CL7  | C4B-NB  | -3.88 | 1.33        | 1.37     |
| 14  | bA    | 3124 | CL7  | MG-NB   | -3.88 | 1.98        | 2.05     |
| 14  | cB    | 831  | CL7  | MG-NA   | -3.88 | 1.98        | 2.05     |
| 14  | bB    | 826  | CL7  | C4D-ND  | -3.88 | 1.32        | 1.37     |
| 14  | aA    | 3112 | CL7  | MG-NB   | -3.88 | 1.98        | 2.05     |
| 14  | bL    | 203  | CL7  | MG-NC   | -3.88 | 1.98        | 2.05     |
| 14  | bA    | 3120 | CL7  | OBD-CAD | -3.88 | 1.15        | 1.22     |
| 14  | cB    | 826  | CL7  | C1D-C2D | -3.88 | 1.34        | 1.43     |
| 14  | cA    | 3113 | CL7  | MG-NB   | -3.88 | 1.98        | 2.05     |
| 14  | cA    | 3119 | CL7  | C1D-C2D | -3.88 | 1.34        | 1.43     |
| 14  | aA    | 3103 | CL7  | MG-NB   | -3.88 | 1.98        | 2.05     |
| 14  | bJ    | 101  | CL7  | MG-NB   | -3.88 | 1.98        | 2.05     |
| 14  | cA    | 3141 | CL7  | MG-NB   | -3.87 | 1.98        | 2.05     |
| 14  | bA    | 3119 | CL7  | CHB-C4A | -3.87 | 1.28        | 1.36     |
| 14  | bB    | 810  | CL7  | O2D-CED | -3.87 | 1.36        | 1.45     |
| 14  | aA    | 3127 | CL7  | MG-NB   | -3.87 | 1.98        | 2.05     |
| 14  | aA    | 3109 | CL7  | MG-NA   | -3.87 | 1.98        | 2.05     |
| 14  | aB    | 3016 | CL7  | MG-NB   | -3.87 | 1.98        | 2.05     |
| 14  | aA    | 3116 | CL7  | C1C-NC  | 3.87  | 1.42        | 1.37     |
| 14  | bA    | 3125 | CL7  | O1D-CGD | -3.87 | 1.11        | 1.21     |
| 14  | cA    | 3128 | CL7  | C3C-C2C | -3.87 | 1.28        | 1.36     |
| 14  | aB    | 3003 | CL7  | OBB-CAB | 3.86  | 1.31        | 1.22     |
| 14  | cA    | 3125 | CL7  | C4B-NB  | -3.86 | 1.33        | 1.37     |
| 12  | aA    | 3101 | G9R  | O2A-CGA | 3.86  | 1.44        | 1.33     |
| 14  | cB    | 821  | CL7  | MG-NB   | -3.86 | 1.98        | 2.05     |
| 14  | cB    | 807  | CL7  | CAB-C3B | -3.86 | 1.37        | 1.45     |
| 14  | aB    | 3030 | CL7  | MG-NC   | -3.85 | 1.98        | 2.05     |
| 14  | bA    | 3107 | CL7  | OBD-CAD | -3.85 | 1.15        | 1.22     |
| 14  | cB    | 817  | CL7  | MG-NB   | -3.85 | 1.98        | 2.05     |
| 14  | cA    | 3115 | CL7  | C1C-NC  | 3.85  | 1.42        | 1.37     |
| 14  | bA    | 3114 | CL7  | MG-NB   | -3.85 | 1.98        | 2.05     |
| 14  | cA    | 3110 | CL7  | C4B-NB  | -3.85 | 1.33        | 1.37     |
| 14  | aA    | 3122 | CL7  | MG-NC   | -3.85 | 1.98        | 2.05     |
| 14  | aB    | 3002 | CL7  | MG-NA   | -3.85 | 1.98        | 2.05     |
| 14  | aA    | 3133 | CL7  | C2A-C1A | -3.85 | 1.45        | 1.50     |
| 14  | bA    | 3119 | CL7  | MG-NB   | -3.85 | 1.98        | 2.05     |
| 14  | cA    | 3105 | CL7  | C1C-C2C | -3.85 | 1.37        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | bA    | 3105 | CL7  | C1C-NC  | 3.85  | 1.42        | 1.37     |
| 14  | cA    | 3110 | CL7  | MG-NB   | -3.85 | 1.98        | 2.05     |
| 14  | aB    | 3018 | CL7  | CMD-C2D | -3.85 | 1.42        | 1.50     |
| 14  | bA    | 3132 | CL7  | MG-ND   | -3.85 | 1.98        | 2.05     |
| 12  | aA    | 3101 | G9R  | C1D-ND  | 3.84  | 1.42        | 1.37     |
| 14  | aA    | 3127 | CL7  | C1C-NC  | 3.84  | 1.42        | 1.37     |
| 14  | bB    | 809  | CL7  | MG-ND   | -3.83 | 1.98        | 2.05     |
| 14  | cB    | 832  | CL7  | MG-NB   | -3.83 | 1.98        | 2.05     |
| 14  | bB    | 804  | CL7  | C2A-C1A | -3.83 | 1.45        | 1.50     |
| 14  | bA    | 3102 | CL7  | MG-NB   | -3.83 | 1.98        | 2.05     |
| 14  | bB    | 826  | CL7  | C1D-C2D | -3.83 | 1.34        | 1.43     |
| 14  | cA    | 3130 | CL7  | OBD-CAD | -3.83 | 1.15        | 1.22     |
| 13  | bB    | 805  | PHO  | CBD-CAD | -3.83 | 1.40        | 1.53     |
| 14  | aA    | 3140 | CL7  | MG-NC   | -3.83 | 1.98        | 2.05     |
| 14  | cA    | 3110 | CL7  | C1C-NC  | 3.83  | 1.42        | 1.37     |
| 14  | aA    | 3120 | CL7  | C1D-C2D | -3.83 | 1.34        | 1.43     |
| 14  | aB    | 3025 | CL7  | MG-ND   | -3.82 | 1.98        | 2.05     |
| 14  | cB    | 806  | CL7  | CAA-C2A | -3.82 | 1.47        | 1.54     |
| 14  | bA    | 3126 | CL7  | MG-NB   | -3.82 | 1.98        | 2.05     |
| 14  | cB    | 827  | CL7  | C1C-NC  | 3.82  | 1.42        | 1.37     |
| 14  | aA    | 3128 | CL7  | OBD-CAD | -3.82 | 1.15        | 1.22     |
| 14  | cB    | 819  | CL7  | CAA-C2A | -3.82 | 1.47        | 1.54     |
| 14  | cA    | 3129 | CL7  | MG-NA   | -3.81 | 1.98        | 2.05     |
| 14  | cB    | 823  | CL7  | MG-NB   | -3.81 | 1.98        | 2.05     |
| 14  | aB    | 3030 | CL7  | MG-NB   | -3.81 | 1.98        | 2.05     |
| 14  | bB    | 809  | CL7  | C4C-NC  | 3.81  | 1.42        | 1.37     |
| 14  | bB    | 806  | CL7  | C1C-NC  | 3.81  | 1.42        | 1.37     |
| 14  | aB    | 3023 | CL7  | MG-NC   | -3.81 | 1.98        | 2.05     |
| 14  | bA    | 3110 | CL7  | C1C-NC  | 3.81  | 1.42        | 1.37     |
| 14  | aL    | 202  | CL7  | MG-NC   | -3.81 | 1.98        | 2.05     |
| 14  | aB    | 3020 | CL7  | MG-NB   | -3.80 | 1.98        | 2.05     |
| 17  | cA    | 3143 | PQN  | O1-C1   | -3.80 | 1.15        | 1.23     |
| 14  | bB    | 823  | CL7  | MG-NB   | -3.80 | 1.98        | 2.05     |
| 14  | cA    | 3105 | CL7  | CHB-C4A | -3.80 | 1.28        | 1.36     |
| 14  | bA    | 3119 | CL7  | CAB-C3B | -3.80 | 1.37        | 1.45     |
| 14  | bB    | 817  | CL7  | MG-NB   | -3.80 | 1.98        | 2.05     |
| 13  | aB    | 3004 | PHO  | CMB-C2B | -3.80 | 1.43        | 1.51     |
| 17  | aA    | 3144 | PQN  | O4-C4   | -3.80 | 1.15        | 1.23     |
| 14  | cB    | 833  | CL7  | MG-NC   | -3.80 | 1.98        | 2.05     |
| 14  | aB    | 3003 | CL7  | C2A-C1A | -3.80 | 1.45        | 1.50     |
| 14  | aB    | 3022 | CL7  | MG-NB   | -3.80 | 1.98        | 2.05     |
| 14  | aA    | 3141 | CL7  | OBD-CAD | -3.80 | 1.15        | 1.22     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 12  | aA    | 3101 | G9R  | CHC-C1C | 3.79  | 1.46        | 1.38     |
| 14  | bB    | 824  | CL7  | MG-NC   | -3.79 | 1.98        | 2.05     |
| 14  | aA    | 3111 | CL7  | C1C-NC  | 3.79  | 1.42        | 1.37     |
| 14  | cA    | 3123 | CL7  | OBD-CAD | -3.79 | 1.15        | 1.22     |
| 14  | cB    | 811  | CL7  | C4C-NC  | 3.79  | 1.42        | 1.37     |
| 14  | aA    | 3126 | CL7  | C4B-NB  | -3.78 | 1.33        | 1.37     |
| 14  | aB    | 3007 | CL7  | C1D-C2D | -3.78 | 1.34        | 1.43     |
| 14  | cB    | 819  | CL7  | CMD-C2D | -3.78 | 1.42        | 1.50     |
| 14  | bA    | 3139 | CL7  | MG-NC   | -3.78 | 1.98        | 2.05     |
| 14  | aB    | 3013 | CL7  | MG-NB   | -3.78 | 1.98        | 2.05     |
| 14  | aA    | 3131 | CL7  | OBD-CAD | -3.78 | 1.16        | 1.22     |
| 14  | aB    | 3023 | CL7  | OBD-CAD | -3.78 | 1.16        | 1.22     |
| 14  | aB    | 3025 | CL7  | C1D-C2D | -3.78 | 1.34        | 1.43     |
| 14  | aL    | 202  | CL7  | CAB-C3B | -3.78 | 1.37        | 1.45     |
| 14  | aA    | 3117 | CL7  | MG-NA   | -3.78 | 1.98        | 2.05     |
| 14  | cA    | 3114 | CL7  | MG-NB   | -3.78 | 1.98        | 2.05     |
| 14  | bA    | 3105 | CL7  | C1C-C2C | -3.77 | 1.37        | 1.45     |
| 14  | bB    | 827  | CL7  | CHC-C1C | -3.77 | 1.31        | 1.38     |
| 14  | cA    | 3118 | CL7  | MG-ND   | -3.77 | 1.98        | 2.05     |
| 14  | aA    | 3127 | CL7  | MG-NC   | -3.77 | 1.98        | 2.05     |
| 14  | cL    | 204  | CL7  | C1D-C2D | -3.77 | 1.34        | 1.43     |
| 14  | cB    | 804  | CL7  | CHD-C4C | -3.77 | 1.31        | 1.38     |
| 14  | cA    | 3102 | CL7  | C3B-C4B | -3.77 | 1.34        | 1.42     |
| 14  | aB    | 3032 | CL7  | OBD-CAD | -3.77 | 1.16        | 1.22     |
| 14  | bA    | 3109 | CL7  | OBD-CAD | -3.76 | 1.16        | 1.22     |
| 14  | bA    | 3114 | CL7  | OBD-CAD | -3.76 | 1.16        | 1.22     |
| 14  | cA    | 3116 | CL7  | MG-NA   | -3.76 | 1.98        | 2.05     |
| 14  | cB    | 824  | CL7  | OBD-CAD | -3.76 | 1.16        | 1.22     |
| 14  | cB    | 804  | CL7  | C1C-NC  | 3.76  | 1.42        | 1.37     |
| 14  | aB    | 3014 | CL7  | MG-NC   | -3.76 | 1.98        | 2.05     |
| 14  | aB    | 3009 | CL7  | C1D-C2D | -3.76 | 1.34        | 1.43     |
| 14  | aA    | 3114 | CL7  | MG-NB   | -3.76 | 1.98        | 2.05     |
| 14  | aB    | 3011 | CL7  | MG-NB   | -3.76 | 1.98        | 2.05     |
| 14  | bA    | 3133 | CL7  | MG-NB   | -3.76 | 1.98        | 2.05     |
| 14  | aA    | 3113 | CL7  | C4B-NB  | -3.76 | 1.33        | 1.37     |
| 14  | cA    | 3103 | CL7  | OBD-CAD | -3.76 | 1.16        | 1.22     |
| 14  | bB    | 807  | CL7  | CAB-C3B | -3.76 | 1.37        | 1.45     |
| 14  | aB    | 3006 | CL7  | CAB-C3B | -3.76 | 1.37        | 1.45     |
| 14  | bB    | 824  | CL7  | OBD-CAD | -3.75 | 1.16        | 1.22     |
| 14  | cA    | 3133 | CL7  | MG-NB   | -3.75 | 1.98        | 2.05     |
| 14  | cA    | 3117 | CL7  | MG-NB   | -3.75 | 1.98        | 2.05     |
| 17  | bA    | 3143 | PQN  | C6-C5   | 3.75  | 1.45        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | cB    | 804  | CL7  | OBB-CAB | 3.75  | 1.30        | 1.22     |
| 14  | cK    | 101  | CL7  | C4D-CHA | -3.75 | 1.37        | 1.45     |
| 17  | bA    | 3143 | PQN  | O1-C1   | -3.75 | 1.15        | 1.23     |
| 14  | cA    | 3119 | CL7  | C1D-ND  | -3.74 | 1.33        | 1.37     |
| 12  | bA    | 3101 | G9R  | C1B-NB  | -3.74 | 1.33        | 1.37     |
| 17  | aA    | 3144 | PQN  | C10-C1  | -3.74 | 1.41        | 1.48     |
| 14  | bB    | 804  | CL7  | OBB-CAB | 3.74  | 1.30        | 1.22     |
| 14  | bB    | 814  | CL7  | MG-NB   | -3.74 | 1.98        | 2.05     |
| 14  | aA    | 3133 | CL7  | MG-NA   | -3.74 | 1.98        | 2.05     |
| 14  | aA    | 3115 | CL7  | MG-NB   | -3.74 | 1.98        | 2.05     |
| 14  | bA    | 3103 | CL7  | OBD-CAD | -3.73 | 1.16        | 1.22     |
| 14  | bA    | 3112 | CL7  | OBD-CAD | -3.73 | 1.16        | 1.22     |
| 14  | bA    | 3126 | CL7  | C1C-NC  | 3.73  | 1.42        | 1.37     |
| 14  | cA    | 3118 | CL7  | C4C-NC  | 3.73  | 1.42        | 1.37     |
| 14  | cB    | 810  | CL7  | OBD-CAD | -3.73 | 1.16        | 1.22     |
| 14  | bB    | 806  | CL7  | CHC-C1C | -3.73 | 1.31        | 1.38     |
| 14  | bA    | 3133 | CL7  | MG-NC   | -3.73 | 1.98        | 2.05     |
| 14  | cL    | 203  | CL7  | C4C-NC  | 3.73  | 1.42        | 1.37     |
| 14  | bA    | 3130 | CL7  | OBD-CAD | -3.73 | 1.16        | 1.22     |
| 14  | cA    | 3107 | CL7  | OBD-CAD | -3.73 | 1.16        | 1.22     |
| 14  | cA    | 3128 | CL7  | C1C-C2C | -3.73 | 1.38        | 1.45     |
| 14  | bB    | 833  | CL7  | CHB-C4A | -3.72 | 1.28        | 1.36     |
| 14  | bA    | 3117 | CL7  | MG-NB   | -3.72 | 1.98        | 2.05     |
| 14  | cA    | 3140 | CL7  | C2A-C1A | -3.72 | 1.45        | 1.50     |
| 14  | aB    | 3031 | CL7  | MG-NB   | -3.72 | 1.98        | 2.05     |
| 14  | bA    | 3132 | CL7  | MG-NA   | -3.72 | 1.98        | 2.05     |
| 14  | aL    | 203  | CL7  | C1D-C2D | -3.72 | 1.34        | 1.43     |
| 14  | bA    | 3117 | CL7  | OBD-CAD | -3.72 | 1.16        | 1.22     |
| 14  | bA    | 3108 | CL7  | MG-NA   | -3.72 | 1.98        | 2.05     |
| 17  | cA    | 3143 | PQN  | C6-C5   | 3.72  | 1.45        | 1.39     |
| 14  | aB    | 3008 | CL7  | C4B-NB  | -3.72 | 1.33        | 1.37     |
| 14  | cB    | 803  | CL7  | CAB-C3B | -3.72 | 1.37        | 1.45     |
| 14  | aA    | 3111 | CL7  | MG-NB   | -3.72 | 1.98        | 2.05     |
| 14  | bA    | 3129 | CL7  | CMB-C2B | -3.71 | 1.42        | 1.50     |
| 14  | bB    | 819  | CL7  | CMD-C2D | -3.71 | 1.42        | 1.50     |
| 14  | cA    | 3116 | CL7  | MG-NC   | -3.71 | 1.98        | 2.05     |
| 14  | aB    | 3032 | CL7  | MG-NC   | -3.71 | 1.98        | 2.05     |
| 14  | cB    | 810  | CL7  | C3A-C4A | -3.71 | 1.45        | 1.52     |
| 14  | bB    | 826  | CL7  | C3A-C4A | -3.71 | 1.45        | 1.52     |
| 14  | bK    | 101  | CL7  | MG-NB   | -3.71 | 1.98        | 2.05     |
| 14  | cB    | 812  | CL7  | MG-NB   | -3.71 | 1.98        | 2.05     |
| 14  | aB    | 3002 | CL7  | CHC-C1C | -3.71 | 1.31        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 13  | bB    | 805  | PHO  | C3B-C2B | -3.71 | 1.35        | 1.40     |
| 17  | bB    | 828  | PQN  | O1-C1   | -3.71 | 1.15        | 1.23     |
| 14  | cA    | 3124 | CL7  | CAB-C3B | -3.71 | 1.37        | 1.45     |
| 14  | cB    | 831  | CL7  | MG-NC   | -3.71 | 1.98        | 2.05     |
| 12  | aA    | 3101 | G9R  | CHB-C1B | 3.71  | 1.47        | 1.39     |
| 14  | bL    | 203  | CL7  | C4C-NC  | 3.70  | 1.42        | 1.37     |
| 14  | bA    | 3126 | CL7  | MG-NC   | -3.70 | 1.98        | 2.05     |
| 14  | aB    | 3006 | CL7  | MG-NA   | -3.70 | 1.98        | 2.05     |
| 14  | aB    | 3008 | CL7  | MG-NC   | -3.70 | 1.98        | 2.05     |
| 14  | bA    | 3105 | CL7  | CHB-C4A | -3.70 | 1.28        | 1.36     |
| 13  | aB    | 3004 | PHO  | CBB-CAB | 3.70  | 1.53        | 1.29     |
| 14  | aB    | 3009 | CL7  | O2D-CED | -3.70 | 1.36        | 1.45     |
| 17  | aB    | 3027 | PQN  | C5-C4   | -3.70 | 1.41        | 1.48     |
| 14  | bB    | 831  | CL7  | MG-NC   | -3.70 | 1.98        | 2.05     |
| 12  | cA    | 3101 | G9R  | C1D-ND  | 3.70  | 1.42        | 1.37     |
| 14  | cB    | 810  | CL7  | C2A-C1A | -3.70 | 1.45        | 1.50     |
| 14  | cB    | 803  | CL7  | MG-NA   | -3.70 | 1.98        | 2.05     |
| 14  | bA    | 3116 | CL7  | MG-NC   | -3.70 | 1.98        | 2.05     |
| 14  | aA    | 3130 | CL7  | CHB-C4A | -3.70 | 1.28        | 1.36     |
| 16  | aA    | 3139 | LHG  | O7-C5   | -3.70 | 1.40        | 1.47     |
| 14  | bB    | 810  | CL7  | C2A-C1A | -3.69 | 1.45        | 1.50     |
| 14  | bB    | 827  | CL7  | C1C-NC  | 3.69  | 1.42        | 1.37     |
| 14  | cA    | 3105 | CL7  | C3C-C2C | -3.69 | 1.28        | 1.36     |
| 14  | cA    | 3122 | CL7  | C4C-NC  | 3.69  | 1.42        | 1.37     |
| 14  | cB    | 814  | CL7  | MG-NB   | -3.69 | 1.98        | 2.05     |
| 14  | aA    | 3104 | CL7  | OBD-CAD | -3.69 | 1.16        | 1.22     |
| 14  | aA    | 3119 | CL7  | C4C-NC  | 3.69  | 1.42        | 1.37     |
| 14  | bB    | 827  | CL7  | C1B-NB  | 3.69  | 1.42        | 1.37     |
| 14  | aB    | 3014 | CL7  | MG-NB   | -3.69 | 1.98        | 2.05     |
| 14  | aB    | 3019 | CL7  | OBD-CAD | -3.69 | 1.16        | 1.22     |
| 14  | bB    | 826  | CL7  | MG-ND   | -3.69 | 1.98        | 2.05     |
| 14  | cA    | 3119 | CL7  | CHB-C4A | -3.68 | 1.28        | 1.36     |
| 14  | bB    | 808  | CL7  | C1D-C2D | -3.68 | 1.34        | 1.43     |
| 14  | cB    | 807  | CL7  | MG-NA   | -3.68 | 1.98        | 2.05     |
| 14  | bA    | 3128 | CL7  | C3A-C4A | -3.68 | 1.45        | 1.52     |
| 13  | bB    | 805  | PHO  | CBB-CAB | 3.68  | 1.53        | 1.29     |
| 14  | cA    | 3118 | CL7  | MG-NC   | -3.68 | 1.98        | 2.05     |
| 14  | bL    | 204  | CL7  | CHC-C1C | -3.68 | 1.31        | 1.38     |
| 17  | cB    | 828  | PQN  | O1-C1   | -3.67 | 1.15        | 1.23     |
| 13  | aB    | 3004 | PHO  | O2D-CGD | 3.67  | 1.42        | 1.33     |
| 14  | aA    | 3130 | CL7  | C3A-C4A | -3.67 | 1.45        | 1.52     |
| 14  | aB    | 3005 | CL7  | CHD-C4C | -3.67 | 1.31        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | bB    | 833  | CL7  | MG-NC   | -3.67 | 1.98        | 2.05     |
| 14  | cA    | 3123 | CL7  | C1D-C2D | -3.67 | 1.34        | 1.43     |
| 14  | bA    | 3129 | CL7  | C3A-C4A | -3.66 | 1.45        | 1.52     |
| 14  | bA    | 3122 | CL7  | OBD-CAD | -3.66 | 1.16        | 1.22     |
| 14  | cB    | 817  | CL7  | C1C-NC  | 3.66  | 1.42        | 1.37     |
| 14  | aL    | 202  | CL7  | CHC-C1C | -3.66 | 1.31        | 1.38     |
| 14  | aA    | 3103 | CL7  | C3C-C2C | -3.66 | 1.28        | 1.36     |
| 14  | bB    | 812  | CL7  | MG-NB   | -3.66 | 1.98        | 2.05     |
| 14  | cA    | 3120 | CL7  | MG-NA   | -3.66 | 1.98        | 2.05     |
| 14  | cA    | 3115 | CL7  | MG-NC   | -3.66 | 1.98        | 2.05     |
| 14  | bB    | 807  | CL7  | MG-NA   | -3.66 | 1.98        | 2.05     |
| 14  | aA    | 3119 | CL7  | MG-ND   | -3.65 | 1.98        | 2.05     |
| 14  | aB    | 3031 | CL7  | C3A-C4A | -3.65 | 1.45        | 1.52     |
| 14  | bA    | 3102 | CL7  | C3B-C4B | -3.65 | 1.34        | 1.42     |
| 14  | bB    | 826  | CL7  | C4C-NC  | 3.65  | 1.42        | 1.37     |
| 14  | bA    | 3127 | CL7  | MG-NC   | -3.64 | 1.98        | 2.05     |
| 13  | cB    | 805  | PHO  | CMB-C2B | -3.64 | 1.44        | 1.51     |
| 14  | bA    | 3105 | CL7  | C3C-C2C | -3.64 | 1.28        | 1.36     |
| 14  | cA    | 3116 | CL7  | C1C-NC  | 3.64  | 1.42        | 1.37     |
| 14  | aA    | 3123 | CL7  | OBD-CAD | -3.64 | 1.16        | 1.22     |
| 14  | bB    | 827  | CL7  | CMA-C3A | 3.64  | 1.61        | 1.53     |
| 14  | cA    | 3109 | CL7  | OBD-CAD | -3.64 | 1.16        | 1.22     |
| 14  | bB    | 818  | CL7  | MG-NB   | -3.63 | 1.98        | 2.05     |
| 14  | aA    | 3125 | CL7  | OBB-CAB | 3.63  | 1.30        | 1.22     |
| 14  | aA    | 3125 | CL7  | CHC-C1C | -3.63 | 1.31        | 1.38     |
| 14  | cA    | 3133 | CL7  | MG-NC   | -3.63 | 1.98        | 2.05     |
| 17  | aB    | 3027 | PQN  | O1-C1   | -3.63 | 1.15        | 1.23     |
| 14  | cA    | 3112 | CL7  | OBD-CAD | -3.63 | 1.16        | 1.22     |
| 14  | aA    | 3119 | CL7  | MG-NC   | -3.63 | 1.98        | 2.05     |
| 14  | cA    | 3122 | CL7  | OBD-CAD | -3.63 | 1.16        | 1.22     |
| 14  | aB    | 3026 | CL7  | C1B-NB  | 3.63  | 1.42        | 1.37     |
| 14  | bA    | 3116 | CL7  | MG-NA   | -3.62 | 1.98        | 2.05     |
| 14  | aL    | 204  | CL7  | CHC-C1C | -3.62 | 1.31        | 1.38     |
| 14  | cA    | 3125 | CL7  | C1D-C2D | -3.62 | 1.34        | 1.43     |
| 14  | aA    | 3125 | CL7  | MG-ND   | -3.62 | 1.98        | 2.05     |
| 14  | bB    | 815  | CL7  | OBD-CAD | -3.62 | 1.16        | 1.22     |
| 14  | bA    | 3110 | CL7  | OBD-CAD | -3.62 | 1.16        | 1.22     |
| 14  | bA    | 3123 | CL7  | MG-NA   | -3.62 | 1.98        | 2.05     |
| 14  | bL    | 204  | CL7  | C1D-C2D | -3.61 | 1.34        | 1.43     |
| 14  | cB    | 808  | CL7  | C1D-C2D | -3.61 | 1.34        | 1.43     |
| 14  | bL    | 205  | CL7  | CAB-C3B | -3.61 | 1.37        | 1.45     |
| 13  | cB    | 801  | PHO  | CBD-CAD | -3.61 | 1.41        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | cB    | 827  | CL7  | C1B-NB  | 3.61  | 1.42        | 1.37     |
| 14  | cF    | 201  | CL7  | MG-NC   | -3.61 | 1.98        | 2.05     |
| 14  | cA    | 3113 | CL7  | OBD-CAD | -3.61 | 1.16        | 1.22     |
| 14  | cB    | 820  | CL7  | OBD-CAD | -3.61 | 1.16        | 1.22     |
| 14  | aA    | 3117 | CL7  | C1C-NC  | 3.60  | 1.42        | 1.37     |
| 13  | bB    | 805  | PHO  | O2A-CGA | 3.60  | 1.43        | 1.33     |
| 14  | bA    | 3121 | CL7  | C4B-NB  | -3.60 | 1.33        | 1.37     |
| 14  | aA    | 3118 | CL7  | MG-NB   | -3.60 | 1.98        | 2.05     |
| 14  | cA    | 3121 | CL7  | OBD-CAD | -3.60 | 1.16        | 1.22     |
| 14  | cB    | 833  | CL7  | OBB-CAB | 3.60  | 1.30        | 1.22     |
| 14  | cL    | 205  | CL7  | CHC-C1C | -3.60 | 1.31        | 1.38     |
| 14  | cB    | 826  | CL7  | MG-ND   | -3.60 | 1.98        | 2.05     |
| 13  | aB    | 3004 | PHO  | C3B-C4B | 3.60  | 1.45        | 1.41     |
| 14  | cK    | 101  | CL7  | MG-NB   | -3.60 | 1.98        | 2.05     |
| 14  | bL    | 203  | CL7  | CHC-C1C | -3.59 | 1.31        | 1.38     |
| 14  | bB    | 820  | CL7  | OBD-CAD | -3.59 | 1.16        | 1.22     |
| 14  | cA    | 3114 | CL7  | OBD-CAD | -3.59 | 1.16        | 1.22     |
| 14  | bA    | 3128 | CL7  | C1D-ND  | -3.59 | 1.33        | 1.37     |
| 14  | aA    | 3116 | CL7  | MG-NC   | -3.59 | 1.98        | 2.05     |
| 14  | bB    | 806  | CL7  | CHD-C4C | -3.59 | 1.31        | 1.38     |
| 14  | cA    | 3117 | CL7  | OBD-CAD | -3.59 | 1.16        | 1.22     |
| 14  | aA    | 3128 | CL7  | MG-ND   | -3.59 | 1.98        | 2.05     |
| 14  | cA    | 3132 | CL7  | C2A-C1A | -3.59 | 1.45        | 1.50     |
| 14  | bA    | 3116 | CL7  | C1C-NC  | 3.59  | 1.42        | 1.37     |
| 14  | cL    | 203  | CL7  | CAB-C3B | -3.59 | 1.37        | 1.45     |
| 14  | cB    | 827  | CL7  | CHC-C1C | -3.59 | 1.31        | 1.38     |
| 14  | bB    | 831  | CL7  | OBD-CAD | -3.58 | 1.16        | 1.22     |
| 14  | cB    | 818  | CL7  | MG-NB   | -3.58 | 1.98        | 2.05     |
| 14  | aA    | 3130 | CL7  | OBD-CAD | -3.58 | 1.16        | 1.22     |
| 13  | cB    | 805  | PHO  | CBB-CAB | 3.58  | 1.53        | 1.29     |
| 14  | aL    | 202  | CL7  | C4C-NC  | 3.58  | 1.42        | 1.37     |
| 14  | bA    | 3125 | CL7  | C1D-C2D | -3.58 | 1.34        | 1.43     |
| 14  | aB    | 3009 | CL7  | C3A-C4A | -3.58 | 1.45        | 1.52     |
| 14  | aA    | 3129 | CL7  | C3C-C2C | -3.58 | 1.29        | 1.36     |
| 14  | bA    | 3121 | CL7  | OBD-CAD | -3.57 | 1.16        | 1.22     |
| 14  | bA    | 3123 | CL7  | OBB-CAB | 3.57  | 1.30        | 1.22     |
| 14  | bA    | 3115 | CL7  | MG-NC   | -3.57 | 1.98        | 2.05     |
| 14  | aA    | 3121 | CL7  | MG-NC   | -3.57 | 1.98        | 2.05     |
| 14  | aA    | 3110 | CL7  | OBD-CAD | -3.57 | 1.16        | 1.22     |
| 14  | bA    | 3105 | CL7  | OBD-CAD | -3.57 | 1.16        | 1.22     |
| 14  | cA    | 3105 | CL7  | OBD-CAD | -3.57 | 1.16        | 1.22     |
| 14  | bB    | 817  | CL7  | C1C-NC  | 3.57  | 1.42        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | cA    | 3123 | CL7  | O2D-CGD | -3.57 | 1.24        | 1.33     |
| 14  | cA    | 3127 | CL7  | MG-ND   | -3.57 | 1.98        | 2.05     |
| 13  | aB    | 3004 | PHO  | O2A-CGA | 3.57  | 1.43        | 1.33     |
| 14  | cA    | 3132 | CL7  | C4C-NC  | 3.57  | 1.42        | 1.37     |
| 14  | aA    | 3134 | CL7  | MG-NC   | -3.57 | 1.98        | 2.05     |
| 14  | bB    | 804  | CL7  | C3D-CAD | -3.57 | 1.33        | 1.45     |
| 14  | aB    | 3002 | CL7  | O2D-CGD | -3.56 | 1.24        | 1.33     |
| 14  | cA    | 3128 | CL7  | CHB-C4A | -3.56 | 1.28        | 1.36     |
| 14  | aF    | 201  | CL7  | MG-NC   | -3.56 | 1.98        | 2.05     |
| 14  | aL    | 204  | CL7  | C4C-NC  | 3.56  | 1.42        | 1.37     |
| 14  | cB    | 824  | CL7  | OBB-CAB | 3.56  | 1.30        | 1.22     |
| 14  | cA    | 3127 | CL7  | CAB-C3B | -3.56 | 1.37        | 1.45     |
| 14  | aB    | 3017 | CL7  | MG-NB   | -3.56 | 1.98        | 2.05     |
| 14  | aA    | 3134 | CL7  | C1C-NC  | 3.55  | 1.42        | 1.37     |
| 14  | bA    | 3113 | CL7  | OBD-CAD | -3.55 | 1.16        | 1.22     |
| 14  | aA    | 3133 | CL7  | MG-ND   | -3.55 | 1.98        | 2.05     |
| 14  | aB    | 3015 | CL7  | C1C-C2C | -3.55 | 1.38        | 1.45     |
| 13  | aA    | 3102 | PHO  | CBD-CAD | -3.55 | 1.41        | 1.53     |
| 14  | aA    | 3106 | CL7  | C1C-C2C | -3.55 | 1.38        | 1.45     |
| 14  | aK    | 101  | CL7  | MG-NB   | -3.55 | 1.98        | 2.05     |
| 14  | aK    | 101  | CL7  | C4D-CHA | -3.55 | 1.38        | 1.45     |
| 14  | cB    | 816  | CL7  | C2A-C1A | -3.54 | 1.45        | 1.50     |
| 14  | bB    | 819  | CL7  | C1D-C2D | -3.54 | 1.34        | 1.43     |
| 14  | aA    | 3128 | CL7  | MG-NC   | -3.54 | 1.98        | 2.05     |
| 14  | cB    | 819  | CL7  | C1B-NB  | 3.54  | 1.42        | 1.37     |
| 14  | aA    | 3120 | CL7  | MG-NB   | -3.54 | 1.98        | 2.05     |
| 14  | aB    | 3005 | CL7  | CHC-C1C | -3.54 | 1.31        | 1.38     |
| 14  | bB    | 811  | CL7  | C4C-NC  | 3.54  | 1.42        | 1.37     |
| 14  | cA    | 3132 | CL7  | MG-NA   | -3.54 | 1.98        | 2.05     |
| 14  | bL    | 204  | CL7  | CAB-C3B | -3.54 | 1.37        | 1.45     |
| 14  | cA    | 3132 | CL7  | CHB-C4A | -3.54 | 1.28        | 1.36     |
| 14  | aA    | 3117 | CL7  | MG-NC   | -3.54 | 1.98        | 2.05     |
| 14  | bF    | 201  | CL7  | MG-NC   | -3.54 | 1.98        | 2.05     |
| 14  | cB    | 812  | CL7  | C1C-NC  | 3.54  | 1.42        | 1.37     |
| 13  | bB    | 801  | PHO  | CBD-CAD | -3.54 | 1.41        | 1.53     |
| 14  | cB    | 824  | CL7  | MG-NC   | -3.54 | 1.98        | 2.05     |
| 14  | cB    | 806  | CL7  | C1D-ND  | -3.53 | 1.33        | 1.37     |
| 14  | bA    | 3141 | CL7  | MG-NC   | -3.53 | 1.98        | 2.05     |
| 14  | cA    | 3127 | CL7  | MG-NA   | -3.53 | 1.98        | 2.05     |
| 17  | bB    | 828  | PQN  | C5-C4   | -3.53 | 1.41        | 1.48     |
| 14  | aB    | 3016 | CL7  | C1C-NC  | 3.53  | 1.42        | 1.37     |
| 14  | aA    | 3130 | CL7  | CMB-C2B | -3.53 | 1.43        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | cA    | 3121 | CL7  | C4B-NB  | -3.53 | 1.33        | 1.37     |
| 14  | aA    | 3118 | CL7  | OBD-CAD | -3.53 | 1.16        | 1.22     |
| 14  | cA    | 3120 | CL7  | C1D-C2D | -3.53 | 1.34        | 1.43     |
| 14  | cA    | 3115 | CL7  | C4C-NC  | 3.53  | 1.42        | 1.37     |
| 14  | bB    | 816  | CL7  | C2A-C1A | -3.53 | 1.45        | 1.50     |
| 16  | bA    | 3138 | LHG  | O7-C5   | -3.52 | 1.41        | 1.47     |
| 14  | aB    | 3002 | CL7  | C4C-NC  | 3.52  | 1.42        | 1.37     |
| 14  | aA    | 3113 | CL7  | OBD-CAD | -3.52 | 1.16        | 1.22     |
| 14  | aA    | 3131 | CL7  | C4C-NC  | 3.52  | 1.42        | 1.37     |
| 14  | bA    | 3123 | CL7  | C4C-NC  | 3.52  | 1.42        | 1.37     |
| 14  | aB    | 3024 | CL7  | C1C-NC  | 3.52  | 1.42        | 1.37     |
| 14  | aA    | 3114 | CL7  | OBD-CAD | -3.52 | 1.16        | 1.22     |
| 14  | bB    | 832  | CL7  | C3A-C4A | -3.52 | 1.46        | 1.52     |
| 14  | cA    | 3119 | CL7  | CAB-C3B | -3.52 | 1.37        | 1.45     |
| 14  | cA    | 3132 | CL7  | MG-ND   | -3.51 | 1.98        | 2.05     |
| 14  | aB    | 3032 | CL7  | C1D-C2D | -3.51 | 1.35        | 1.43     |
| 14  | bB    | 806  | CL7  | C1D-ND  | -3.51 | 1.33        | 1.37     |
| 14  | cA    | 3128 | CL7  | C4D-ND  | -3.51 | 1.32        | 1.37     |
| 14  | bA    | 3102 | CL7  | MG-NC   | -3.51 | 1.98        | 2.05     |
| 14  | aA    | 3115 | CL7  | OBD-CAD | -3.51 | 1.16        | 1.22     |
| 14  | cB    | 827  | CL7  | MG-NA   | -3.51 | 1.98        | 2.05     |
| 14  | aJ    | 101  | CL7  | OBD-CAD | -3.51 | 1.16        | 1.22     |
| 14  | cA    | 3127 | CL7  | MG-NC   | -3.51 | 1.98        | 2.05     |
| 12  | aA    | 3101 | G9R  | C1B-NB  | -3.51 | 1.33        | 1.37     |
| 14  | cB    | 806  | CL7  | CHD-C4C | -3.51 | 1.31        | 1.38     |
| 14  | aB    | 3014 | CL7  | C4C-NC  | 3.50  | 1.42        | 1.37     |
| 14  | bL    | 205  | CL7  | CHC-C1C | -3.50 | 1.31        | 1.38     |
| 14  | bA    | 3123 | CL7  | OBD-CAD | -3.50 | 1.16        | 1.22     |
| 12  | bA    | 3101 | G9R  | CHB-C1B | 3.50  | 1.47        | 1.39     |
| 14  | aA    | 3113 | CL7  | C1C-NC  | 3.50  | 1.42        | 1.37     |
| 14  | cA    | 3128 | CL7  | MG-ND   | -3.50 | 1.98        | 2.05     |
| 14  | cB    | 816  | CL7  | OBB-CAB | 3.50  | 1.30        | 1.22     |
| 14  | aF    | 201  | CL7  | OBD-CAD | -3.50 | 1.16        | 1.22     |
| 14  | bA    | 3115 | CL7  | C4C-NC  | 3.50  | 1.42        | 1.37     |
| 14  | cA    | 3126 | CL7  | OBD-CAD | -3.50 | 1.16        | 1.22     |
| 14  | bA    | 3129 | CL7  | CHB-C4A | -3.50 | 1.29        | 1.36     |
| 14  | cA    | 3118 | CL7  | C1C-NC  | 3.49  | 1.42        | 1.37     |
| 14  | aB    | 3018 | CL7  | OBD-CAD | -3.49 | 1.16        | 1.22     |
| 14  | cA    | 3141 | CL7  | MG-NC   | -3.49 | 1.98        | 2.05     |
| 14  | cB    | 811  | CL7  | CHC-C1C | -3.49 | 1.31        | 1.38     |
| 14  | cL    | 204  | CL7  | C4D-ND  | -3.49 | 1.32        | 1.37     |
| 14  | bA    | 3129 | CL7  | OBB-CAB | 3.49  | 1.30        | 1.22     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | cA    | 3121 | CL7  | CHB-C4A | -3.49 | 1.29        | 1.36     |
| 14  | cB    | 806  | CL7  | CHC-C1C | -3.49 | 1.31        | 1.38     |
| 14  | bA    | 3111 | CL7  | C4C-NC  | 3.49  | 1.42        | 1.37     |
| 14  | cA    | 3102 | CL7  | MG-NC   | -3.49 | 1.98        | 2.05     |
| 14  | cA    | 3129 | CL7  | CMB-C2B | -3.49 | 1.43        | 1.50     |
| 14  | cA    | 3128 | CL7  | OBB-CAB | 3.49  | 1.30        | 1.22     |
| 14  | bB    | 822  | CL7  | C1C-NC  | 3.48  | 1.42        | 1.37     |
| 14  | bA    | 3132 | CL7  | C2A-C1A | -3.48 | 1.45        | 1.50     |
| 14  | bB    | 812  | CL7  | C1C-NC  | 3.48  | 1.42        | 1.37     |
| 14  | cA    | 3124 | CL7  | C4D-ND  | -3.48 | 1.32        | 1.37     |
| 14  | bB    | 816  | CL7  | C1C-C2C | -3.48 | 1.38        | 1.45     |
| 14  | bL    | 205  | CL7  | MG-NA   | -3.48 | 1.98        | 2.05     |
| 14  | bB    | 817  | CL7  | C4C-NC  | 3.48  | 1.42        | 1.37     |
| 14  | aB    | 3032 | CL7  | CHB-C4A | -3.48 | 1.29        | 1.36     |
| 14  | cA    | 3111 | CL7  | C4C-NC  | 3.48  | 1.42        | 1.37     |
| 14  | cB    | 817  | CL7  | C4C-NC  | 3.48  | 1.42        | 1.37     |
| 14  | aA    | 3106 | CL7  | C3C-C2C | -3.48 | 1.29        | 1.36     |
| 14  | cF    | 201  | CL7  | OBD-CAD | -3.48 | 1.16        | 1.22     |
| 14  | aK    | 101  | CL7  | C4C-NC  | 3.48  | 1.42        | 1.37     |
| 14  | aB    | 3010 | CL7  | CHC-C1C | -3.48 | 1.31        | 1.38     |
| 14  | aA    | 3122 | CL7  | MG-ND   | -3.47 | 1.98        | 2.05     |
| 14  | cB    | 822  | CL7  | C1C-NC  | 3.47  | 1.42        | 1.37     |
| 14  | aB    | 3005 | CL7  | C4C-NC  | 3.47  | 1.42        | 1.37     |
| 14  | aB    | 3032 | CL7  | CHD-C4C | -3.47 | 1.31        | 1.38     |
| 14  | cA    | 3114 | CL7  | CHB-C4A | -3.47 | 1.29        | 1.36     |
| 14  | aK    | 101  | CL7  | C1C-NC  | 3.47  | 1.42        | 1.37     |
| 14  | bB    | 816  | CL7  | CHB-C4A | -3.47 | 1.29        | 1.36     |
| 14  | cB    | 804  | CL7  | C2A-C1A | -3.47 | 1.45        | 1.50     |
| 14  | aB    | 3003 | CL7  | CHD-C4C | -3.47 | 1.31        | 1.38     |
| 14  | bB    | 819  | CL7  | OBD-CAD | -3.47 | 1.16        | 1.22     |
| 14  | aA    | 3133 | CL7  | CHB-C4A | -3.47 | 1.29        | 1.36     |
| 14  | cB    | 832  | CL7  | C3A-C4A | -3.46 | 1.46        | 1.52     |
| 14  | bF    | 201  | CL7  | OBD-CAD | -3.46 | 1.16        | 1.22     |
| 14  | aB    | 3026 | CL7  | CHD-C4C | -3.46 | 1.31        | 1.38     |
| 14  | aB    | 3016 | CL7  | C4C-NC  | 3.46  | 1.42        | 1.37     |
| 14  | bA    | 3145 | CL7  | OBD-CAD | -3.46 | 1.16        | 1.22     |
| 14  | aA    | 3123 | CL7  | C4C-NC  | 3.46  | 1.42        | 1.37     |
| 14  | cA    | 3105 | CL7  | MG-NA   | -3.46 | 1.98        | 2.05     |
| 14  | aB    | 3009 | CL7  | C2A-C1A | -3.46 | 1.45        | 1.50     |
| 14  | bA    | 3121 | CL7  | MG-ND   | -3.46 | 1.98        | 2.05     |
| 14  | aB    | 3031 | CL7  | CHC-C1C | -3.45 | 1.31        | 1.38     |
| 14  | cL    | 205  | CL7  | C4C-NC  | 3.45  | 1.42        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | cB    | 804  | CL7  | C3D-CAD | -3.45 | 1.33        | 1.45     |
| 14  | bB    | 809  | CL7  | O2D-CGD | -3.45 | 1.24        | 1.33     |
| 13  | cB    | 805  | PHO  | O2A-CGA | 3.45  | 1.43        | 1.33     |
| 14  | aA    | 3108 | CL7  | OBD-CAD | -3.45 | 1.16        | 1.22     |
| 14  | cA    | 3129 | CL7  | C3A-C4A | -3.45 | 1.46        | 1.52     |
| 14  | aB    | 3018 | CL7  | CAB-C3B | -3.45 | 1.37        | 1.45     |
| 14  | bA    | 3132 | CL7  | C1C-C2C | -3.45 | 1.38        | 1.45     |
| 14  | bA    | 3105 | CL7  | MG-NA   | -3.45 | 1.99        | 2.05     |
| 14  | bB    | 832  | CL7  | CHC-C1C | -3.45 | 1.31        | 1.38     |
| 14  | cA    | 3128 | CL7  | C1D-ND  | -3.44 | 1.33        | 1.37     |
| 14  | cA    | 3130 | CL7  | C4C-NC  | 3.44  | 1.42        | 1.37     |
| 14  | bB    | 810  | CL7  | OBD-CAD | -3.44 | 1.16        | 1.22     |
| 14  | bB    | 833  | CL7  | OBB-CAB | 3.44  | 1.30        | 1.22     |
| 14  | aA    | 3116 | CL7  | C4C-NC  | 3.44  | 1.42        | 1.37     |
| 12  | bA    | 3101 | G9R  | C1D-ND  | 3.44  | 1.42        | 1.37     |
| 14  | bA    | 3112 | CL7  | C1C-NC  | 3.44  | 1.42        | 1.37     |
| 14  | aB    | 3009 | CL7  | OBD-CAD | -3.44 | 1.16        | 1.22     |
| 14  | aA    | 3121 | CL7  | C4C-NC  | 3.44  | 1.42        | 1.37     |
| 14  | aA    | 3121 | CL7  | MG-NA   | -3.44 | 1.99        | 2.05     |
| 14  | bB    | 807  | CL7  | C4C-NC  | 3.43  | 1.42        | 1.37     |
| 17  | aA    | 3144 | PQN  | O1-C1   | -3.43 | 1.16        | 1.23     |
| 14  | bA    | 3105 | CL7  | C4B-NB  | -3.43 | 1.33        | 1.37     |
| 14  | cA    | 3118 | CL7  | OBB-CAB | 3.43  | 1.30        | 1.22     |
| 14  | aA    | 3134 | CL7  | MG-NB   | -3.43 | 1.99        | 2.05     |
| 14  | cB    | 820  | CL7  | C1D-C2D | -3.43 | 1.35        | 1.43     |
| 13  | bB    | 805  | PHO  | C3A-C2A | -3.43 | 1.51        | 1.54     |
| 14  | aA    | 3103 | CL7  | MG-NC   | -3.43 | 1.99        | 2.05     |
| 14  | aB    | 3002 | CL7  | C3A-C4A | -3.43 | 1.46        | 1.52     |
| 14  | aB    | 3018 | CL7  | C1B-NB  | 3.43  | 1.42        | 1.37     |
| 14  | aA    | 3120 | CL7  | CHB-C4A | -3.43 | 1.29        | 1.36     |
| 14  | bA    | 3142 | CL7  | OBD-CAD | -3.42 | 1.16        | 1.22     |
| 14  | bA    | 3130 | CL7  | C4C-NC  | 3.42  | 1.42        | 1.37     |
| 14  | aB    | 3023 | CL7  | OBB-CAB | 3.42  | 1.30        | 1.22     |
| 14  | bA    | 3127 | CL7  | MG-ND   | -3.42 | 1.99        | 2.05     |
| 14  | bA    | 3122 | CL7  | OBB-CAB | 3.42  | 1.29        | 1.22     |
| 14  | aA    | 3105 | CL7  | C4C-NC  | 3.42  | 1.42        | 1.37     |
| 14  | bB    | 831  | CL7  | C1D-C2D | -3.41 | 1.35        | 1.43     |
| 14  | cA    | 3126 | CL7  | C1C-NC  | 3.41  | 1.42        | 1.37     |
| 14  | aA    | 3105 | CL7  | OBD-CAD | -3.41 | 1.16        | 1.22     |
| 14  | cB    | 815  | CL7  | OBD-CAD | -3.41 | 1.16        | 1.22     |
| 14  | bB    | 819  | CL7  | CAA-C2A | -3.41 | 1.47        | 1.54     |
| 14  | aB    | 3025 | CL7  | CAB-C3B | -3.41 | 1.38        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | cB    | 809  | CL7  | MG-NC   | -3.41 | 1.99        | 2.05     |
| 14  | bB    | 817  | CL7  | OBD-CAD | -3.41 | 1.16        | 1.22     |
| 14  | cB    | 827  | CL7  | C2A-C1A | -3.41 | 1.45        | 1.50     |
| 14  | aA    | 3146 | CL7  | OBD-CAD | -3.41 | 1.16        | 1.22     |
| 14  | cA    | 3121 | CL7  | MG-ND   | -3.41 | 1.99        | 2.05     |
| 14  | bA    | 3141 | CL7  | C3A-C4A | -3.40 | 1.46        | 1.52     |
| 14  | bA    | 3128 | CL7  | MG-ND   | -3.40 | 1.99        | 2.05     |
| 14  | cB    | 826  | CL7  | CAB-C3B | -3.40 | 1.38        | 1.45     |
| 14  | cB    | 809  | CL7  | MG-ND   | -3.40 | 1.99        | 2.05     |
| 14  | bA    | 3145 | CL7  | C4C-NC  | 3.40  | 1.42        | 1.37     |
| 14  | aB    | 3016 | CL7  | OBD-CAD | -3.40 | 1.16        | 1.22     |
| 14  | cB    | 809  | CL7  | C4C-NC  | 3.40  | 1.42        | 1.37     |
| 14  | cB    | 826  | CL7  | C4C-NC  | 3.40  | 1.42        | 1.37     |
| 14  | cA    | 3141 | CL7  | C3A-C4A | -3.40 | 1.46        | 1.52     |
| 14  | cA    | 3105 | CL7  | C4B-NB  | -3.40 | 1.33        | 1.37     |
| 17  | cB    | 828  | PQN  | C5-C4   | -3.40 | 1.41        | 1.48     |
| 14  | cB    | 832  | CL7  | MG-NA   | -3.40 | 1.99        | 2.05     |
| 14  | cB    | 817  | CL7  | C1D-C2D | -3.40 | 1.35        | 1.43     |
| 14  | aA    | 3130 | CL7  | C3D-CAD | -3.39 | 1.33        | 1.45     |
| 14  | cF    | 201  | CL7  | C4C-NC  | 3.39  | 1.42        | 1.37     |
| 14  | cB    | 832  | CL7  | C4C-NC  | 3.39  | 1.42        | 1.37     |
| 14  | bB    | 812  | CL7  | OBD-CAD | -3.39 | 1.16        | 1.22     |
| 14  | aB    | 3015 | CL7  | OBB-CAB | 3.39  | 1.29        | 1.22     |
| 14  | aB    | 3011 | CL7  | C1C-NC  | 3.39  | 1.42        | 1.37     |
| 14  | cB    | 832  | CL7  | CHC-C1C | -3.39 | 1.31        | 1.38     |
| 12  | bA    | 3101 | G9R  | MG-NB   | -3.39 | 1.99        | 2.05     |
| 14  | bB    | 832  | CL7  | C1D-C2D | -3.39 | 1.35        | 1.43     |
| 14  | bB    | 803  | CL7  | CAB-C3B | -3.39 | 1.38        | 1.45     |
| 14  | bA    | 3124 | CL7  | C4D-ND  | -3.39 | 1.33        | 1.37     |
| 14  | cB    | 817  | CL7  | OBD-CAD | -3.39 | 1.16        | 1.22     |
| 14  | cB    | 818  | CL7  | OBD-CAD | -3.39 | 1.16        | 1.22     |
| 14  | bA    | 3142 | CL7  | C1C-NC  | 3.38  | 1.41        | 1.37     |
| 14  | aA    | 3125 | CL7  | MG-NB   | -3.38 | 1.99        | 2.05     |
| 14  | aA    | 3112 | CL7  | C4C-NC  | 3.38  | 1.41        | 1.37     |
| 14  | bA    | 3123 | CL7  | MG-ND   | -3.38 | 1.99        | 2.05     |
| 14  | aA    | 3103 | CL7  | C3B-C4B | -3.38 | 1.35        | 1.42     |
| 16  | cA    | 3138 | LHG  | O7-C5   | -3.38 | 1.41        | 1.47     |
| 14  | cB    | 819  | CL7  | OBD-CAD | -3.38 | 1.16        | 1.22     |
| 14  | aA    | 3106 | CL7  | MG-NA   | -3.38 | 1.99        | 2.05     |
| 14  | bA    | 3124 | CL7  | C1C-NC  | 3.38  | 1.41        | 1.37     |
| 13  | bB    | 801  | PHO  | CBB-CAB | 3.38  | 1.51        | 1.29     |
| 14  | cB    | 819  | CL7  | C1D-C2D | -3.38 | 1.35        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | aB    | 3021 | CL7  | C1C-NC  | 3.37  | 1.41        | 1.37     |
| 14  | aA    | 3146 | CL7  | C4C-NC  | 3.37  | 1.41        | 1.37     |
| 14  | bA    | 3120 | CL7  | C4C-NC  | 3.37  | 1.41        | 1.37     |
| 14  | bA    | 3120 | CL7  | C1D-C2D | -3.37 | 1.35        | 1.43     |
| 14  | aA    | 3142 | CL7  | MG-NC   | -3.37 | 1.99        | 2.05     |
| 14  | cL    | 205  | CL7  | CAB-C3B | -3.37 | 1.38        | 1.45     |
| 14  | cA    | 3142 | CL7  | CHD-C4C | -3.37 | 1.31        | 1.38     |
| 14  | aB    | 3018 | CL7  | C1D-C2D | -3.37 | 1.35        | 1.43     |
| 14  | cB    | 832  | CL7  | C1D-C2D | -3.37 | 1.35        | 1.43     |
| 14  | bB    | 811  | CL7  | CHC-C1C | -3.37 | 1.31        | 1.38     |
| 14  | bL    | 203  | CL7  | C1C-NC  | 3.37  | 1.41        | 1.37     |
| 14  | bB    | 809  | CL7  | MG-NC   | -3.37 | 1.99        | 2.05     |
| 14  | aB    | 3006 | CL7  | C4C-NC  | 3.37  | 1.41        | 1.37     |
| 14  | aB    | 3025 | CL7  | C4C-NC  | 3.36  | 1.41        | 1.37     |
| 14  | cB    | 807  | CL7  | C4C-NC  | 3.36  | 1.41        | 1.37     |
| 14  | bA    | 3121 | CL7  | CHB-C4A | -3.36 | 1.29        | 1.36     |
| 14  | bB    | 824  | CL7  | OBB-CAB | 3.36  | 1.29        | 1.22     |
| 13  | aA    | 3102 | PHO  | CBB-CAB | 3.36  | 1.51        | 1.29     |
| 14  | aA    | 3119 | CL7  | C1C-NC  | 3.36  | 1.41        | 1.37     |
| 14  | bA    | 3127 | CL7  | CAB-C3B | -3.36 | 1.38        | 1.45     |
| 14  | aA    | 3134 | CL7  | C4C-NC  | 3.36  | 1.41        | 1.37     |
| 14  | cA    | 3110 | CL7  | OBD-CAD | -3.36 | 1.16        | 1.22     |
| 13  | aB    | 3004 | PHO  | C3B-C2B | -3.36 | 1.35        | 1.40     |
| 14  | aF    | 201  | CL7  | C4C-NC  | 3.36  | 1.41        | 1.37     |
| 14  | cB    | 816  | CL7  | C1C-C2C | -3.36 | 1.38        | 1.45     |
| 14  | bA    | 3123 | CL7  | C1D-C2D | -3.36 | 1.35        | 1.43     |
| 14  | aL    | 204  | CL7  | CAB-C3B | -3.36 | 1.38        | 1.45     |
| 14  | aA    | 3122 | CL7  | C4C-NC  | 3.36  | 1.41        | 1.37     |
| 14  | aA    | 3119 | CL7  | OBB-CAB | 3.36  | 1.29        | 1.22     |
| 14  | aB    | 3031 | CL7  | MG-NA   | -3.36 | 1.99        | 2.05     |
| 14  | bA    | 3115 | CL7  | MG-NB   | -3.36 | 1.99        | 2.05     |
| 14  | cB    | 804  | CL7  | C1A-NA  | -3.35 | 1.29        | 1.38     |
| 14  | aB    | 3019 | CL7  | C1D-C2D | -3.35 | 1.35        | 1.43     |
| 14  | cA    | 3126 | CL7  | MG-NB   | -3.35 | 1.99        | 2.05     |
| 14  | bB    | 832  | CL7  | MG-NA   | -3.35 | 1.99        | 2.05     |
| 14  | bA    | 3128 | CL7  | CHB-C4A | -3.35 | 1.29        | 1.36     |
| 14  | aA    | 3116 | CL7  | MG-NB   | -3.35 | 1.99        | 2.05     |
| 14  | cA    | 3114 | CL7  | C1C-NC  | 3.35  | 1.41        | 1.37     |
| 14  | cB    | 825  | CL7  | C4C-NC  | 3.35  | 1.41        | 1.37     |
| 14  | aB    | 3032 | CL7  | OBB-CAB | 3.34  | 1.29        | 1.22     |
| 14  | aA    | 3142 | CL7  | C1C-NC  | 3.34  | 1.41        | 1.37     |
| 14  | aA    | 3132 | CL7  | C1C-NC  | 3.34  | 1.41        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | aA    | 3111 | CL7  | OBD-CAD | -3.34 | 1.16        | 1.22     |
| 14  | cA    | 3115 | CL7  | MG-NB   | -3.34 | 1.99        | 2.05     |
| 14  | bA    | 3104 | CL7  | OBD-CAD | -3.34 | 1.16        | 1.22     |
| 14  | cA    | 3108 | CL7  | CHC-C1C | -3.34 | 1.31        | 1.38     |
| 14  | aB    | 3011 | CL7  | OBD-CAD | -3.33 | 1.16        | 1.22     |
| 14  | cB    | 831  | CL7  | OBD-CAD | -3.33 | 1.16        | 1.22     |
| 14  | aA    | 3122 | CL7  | C4B-NB  | -3.33 | 1.33        | 1.37     |
| 14  | cB    | 819  | CL7  | CAB-C3B | -3.33 | 1.38        | 1.45     |
| 14  | cA    | 3132 | CL7  | C1C-C2C | -3.33 | 1.38        | 1.45     |
| 14  | bB    | 819  | CL7  | CAB-C3B | -3.33 | 1.38        | 1.45     |
| 14  | cA    | 3142 | CL7  | OBD-CAD | -3.33 | 1.16        | 1.22     |
| 14  | cA    | 3144 | CL7  | C1C-NC  | 3.33  | 1.41        | 1.37     |
| 14  | bB    | 818  | CL7  | OBD-CAD | -3.33 | 1.16        | 1.22     |
| 14  | bA    | 3132 | CL7  | CHD-C4C | -3.33 | 1.31        | 1.38     |
| 14  | bB    | 833  | CL7  | C1D-C2D | -3.33 | 1.35        | 1.43     |
| 14  | aA    | 3122 | CL7  | OBD-CAD | -3.33 | 1.16        | 1.22     |
| 14  | aB    | 3017 | CL7  | OBD-CAD | -3.33 | 1.16        | 1.22     |
| 14  | aB    | 3026 | CL7  | C3C-C2C | -3.32 | 1.29        | 1.36     |
| 14  | aB    | 3024 | CL7  | C4C-NC  | 3.32  | 1.41        | 1.37     |
| 14  | aL    | 203  | CL7  | C1C-NC  | 3.32  | 1.41        | 1.37     |
| 14  | cL    | 203  | CL7  | CHB-C4A | -3.32 | 1.29        | 1.36     |
| 14  | aB    | 3031 | CL7  | C1D-C2D | -3.32 | 1.35        | 1.43     |
| 14  | bB    | 803  | CL7  | C3A-C4A | -3.32 | 1.46        | 1.52     |
| 12  | cA    | 3101 | G9R  | MG-NB   | -3.32 | 1.99        | 2.05     |
| 14  | aB    | 3022 | CL7  | C4C-NC  | 3.32  | 1.41        | 1.37     |
| 14  | cB    | 803  | CL7  | O2D-CGD | -3.31 | 1.25        | 1.33     |
| 14  | bB    | 814  | CL7  | OBD-CAD | -3.31 | 1.16        | 1.22     |
| 14  | cA    | 3131 | CL7  | OBD-CAD | -3.31 | 1.16        | 1.22     |
| 14  | aA    | 3128 | CL7  | OBB-CAB | 3.31  | 1.29        | 1.22     |
| 14  | aB    | 3016 | CL7  | C1D-C2D | -3.31 | 1.35        | 1.43     |
| 14  | aA    | 3110 | CL7  | C4C-NC  | 3.31  | 1.41        | 1.37     |
| 14  | aB    | 3003 | CL7  | C4C-NC  | 3.31  | 1.41        | 1.37     |
| 14  | aB    | 3030 | CL7  | C1D-C2D | -3.31 | 1.35        | 1.43     |
| 14  | cB    | 816  | CL7  | CHB-C4A | -3.31 | 1.29        | 1.36     |
| 14  | bA    | 3118 | CL7  | OBB-CAB | 3.30  | 1.29        | 1.22     |
| 14  | aA    | 3121 | CL7  | C1D-C2D | -3.30 | 1.35        | 1.43     |
| 14  | aL    | 202  | CL7  | C1C-NC  | 3.30  | 1.41        | 1.37     |
| 14  | aB    | 3031 | CL7  | OBD-CAD | -3.30 | 1.16        | 1.22     |
| 14  | aA    | 3107 | CL7  | C1C-NC  | 3.30  | 1.41        | 1.37     |
| 14  | bL    | 205  | CL7  | C4C-NC  | 3.30  | 1.41        | 1.37     |
| 14  | bA    | 3131 | CL7  | OBD-CAD | -3.30 | 1.16        | 1.22     |
| 13  | cB    | 805  | PHO  | O2D-CGD | 3.30  | 1.41        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | cA    | 3130 | CL7  | C1D-C2D | -3.30 | 1.35        | 1.43     |
| 17  | cA    | 3143 | PQN  | C9-C10  | -3.30 | 1.34        | 1.39     |
| 14  | bB    | 817  | CL7  | C1D-C2D | -3.30 | 1.35        | 1.43     |
| 14  | bA    | 3106 | CL7  | C3D-CAD | -3.30 | 1.34        | 1.45     |
| 14  | cA    | 3112 | CL7  | C1C-NC  | 3.30  | 1.41        | 1.37     |
| 14  | bA    | 3130 | CL7  | C1D-C2D | -3.30 | 1.35        | 1.43     |
| 14  | cA    | 3106 | CL7  | C3D-CAD | -3.30 | 1.34        | 1.45     |
| 14  | aA    | 3106 | CL7  | CHB-C4A | -3.30 | 1.29        | 1.36     |
| 14  | cA    | 3122 | CL7  | CAA-C2A | -3.30 | 1.48        | 1.54     |
| 14  | cA    | 3133 | CL7  | C1C-NC  | 3.30  | 1.41        | 1.37     |
| 14  | cA    | 3129 | CL7  | C3D-CAD | -3.30 | 1.34        | 1.45     |
| 14  | bB    | 825  | CL7  | OBD-CAD | -3.29 | 1.16        | 1.22     |
| 14  | cB    | 831  | CL7  | C1D-C2D | -3.29 | 1.35        | 1.43     |
| 13  | cB    | 801  | PHO  | CBB-CAB | 3.29  | 1.51        | 1.29     |
| 14  | cB    | 812  | CL7  | OBD-CAD | -3.29 | 1.16        | 1.22     |
| 14  | cL    | 203  | CL7  | CHC-C1C | -3.29 | 1.32        | 1.38     |
| 14  | cB    | 811  | CL7  | OBD-CAD | -3.29 | 1.16        | 1.22     |
| 14  | aB    | 3019 | CL7  | MG-NC   | -3.29 | 1.99        | 2.05     |
| 14  | bA    | 3145 | CL7  | C1C-NC  | 3.29  | 1.41        | 1.37     |
| 14  | cA    | 3144 | CL7  | C4C-NC  | 3.29  | 1.41        | 1.37     |
| 14  | cA    | 3116 | CL7  | OBB-CAB | 3.29  | 1.29        | 1.22     |
| 14  | aB    | 3032 | CL7  | C3D-CAD | -3.29 | 1.34        | 1.45     |
| 14  | cB    | 820  | CL7  | CHB-C4A | -3.29 | 1.29        | 1.36     |
| 14  | aA    | 3126 | CL7  | C1D-C2D | -3.29 | 1.35        | 1.43     |
| 14  | cA    | 3104 | CL7  | OBD-CAD | -3.28 | 1.16        | 1.22     |
| 14  | bB    | 804  | CL7  | CMD-C2D | -3.28 | 1.43        | 1.50     |
| 14  | aA    | 3117 | CL7  | OBD-CAD | -3.28 | 1.16        | 1.22     |
| 14  | aA    | 3121 | CL7  | CAB-C3B | -3.28 | 1.38        | 1.45     |
| 14  | cA    | 3106 | CL7  | OBD-CAD | -3.28 | 1.16        | 1.22     |
| 14  | bA    | 3119 | CL7  | C1D-ND  | -3.28 | 1.33        | 1.37     |
| 14  | aA    | 3129 | CL7  | C3A-C4A | -3.28 | 1.46        | 1.52     |
| 14  | cB    | 819  | CL7  | CHC-C1C | -3.28 | 1.32        | 1.38     |
| 14  | bA    | 3129 | CL7  | C3D-CAD | -3.28 | 1.34        | 1.45     |
| 14  | cB    | 825  | CL7  | C1C-NC  | 3.28  | 1.41        | 1.37     |
| 14  | cB    | 821  | CL7  | OBD-CAD | -3.28 | 1.16        | 1.22     |
| 14  | aA    | 3130 | CL7  | CMA-C3A | -3.28 | 1.46        | 1.53     |
| 14  | bA    | 3133 | CL7  | C1C-NC  | 3.28  | 1.41        | 1.37     |
| 14  | cA    | 3119 | CL7  | C4B-NB  | -3.28 | 1.33        | 1.37     |
| 14  | aB    | 3025 | CL7  | CAA-C2A | -3.27 | 1.48        | 1.54     |
| 14  | bB    | 820  | CL7  | CHC-C1C | -3.27 | 1.32        | 1.38     |
| 14  | aA    | 3132 | CL7  | C4C-NC  | 3.27  | 1.41        | 1.37     |
| 14  | cA    | 3120 | CL7  | C4C-NC  | 3.27  | 1.41        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | aB    | 3031 | CL7  | C4C-NC  | 3.27  | 1.41        | 1.37     |
| 14  | aB    | 3003 | CL7  | C3D-CAD | -3.27 | 1.34        | 1.45     |
| 14  | bA    | 3118 | CL7  | C1C-NC  | 3.27  | 1.41        | 1.37     |
| 14  | bA    | 3118 | CL7  | C4C-NC  | 3.27  | 1.41        | 1.37     |
| 14  | aB    | 3008 | CL7  | MG-ND   | -3.27 | 1.99        | 2.05     |
| 14  | bA    | 3121 | CL7  | C4C-NC  | 3.27  | 1.41        | 1.37     |
| 14  | bJ    | 101  | CL7  | OBD-CAD | -3.27 | 1.16        | 1.22     |
| 14  | aB    | 3015 | CL7  | C4C-NC  | 3.26  | 1.41        | 1.37     |
| 14  | bB    | 821  | CL7  | OBD-CAD | -3.26 | 1.16        | 1.22     |
| 14  | bB    | 808  | CL7  | MG-NC   | -3.26 | 1.99        | 2.05     |
| 14  | cB    | 833  | CL7  | CHD-C4C | -3.26 | 1.32        | 1.38     |
| 14  | cB    | 814  | CL7  | OBD-CAD | -3.26 | 1.16        | 1.22     |
| 14  | aB    | 3030 | CL7  | C1C-NC  | 3.26  | 1.41        | 1.37     |
| 14  | cJ    | 101  | CL7  | C4C-NC  | 3.26  | 1.41        | 1.37     |
| 14  | cJ    | 101  | CL7  | OBD-CAD | -3.26 | 1.16        | 1.22     |
| 14  | aA    | 3115 | CL7  | C1C-NC  | 3.26  | 1.41        | 1.37     |
| 14  | aB    | 3015 | CL7  | C3D-CAD | -3.25 | 1.34        | 1.45     |
| 13  | bB    | 805  | PHO  | O2D-CGD | 3.25  | 1.41        | 1.33     |
| 14  | cB    | 820  | CL7  | CHC-C1C | -3.25 | 1.32        | 1.38     |
| 14  | bA    | 3106 | CL7  | CHC-C1C | -3.25 | 1.32        | 1.38     |
| 14  | bB    | 833  | CL7  | C3D-CAD | -3.25 | 1.34        | 1.45     |
| 14  | cB    | 820  | CL7  | MG-NC   | -3.24 | 1.99        | 2.05     |
| 14  | bB    | 816  | CL7  | OBB-CAB | 3.24  | 1.29        | 1.22     |
| 14  | cA    | 3130 | CL7  | CHB-C4A | -3.24 | 1.29        | 1.36     |
| 16  | bA    | 3138 | LHG  | O2-C2   | -3.24 | 1.33        | 1.43     |
| 14  | aA    | 3123 | CL7  | OBB-CAB | 3.24  | 1.29        | 1.22     |
| 14  | aB    | 3008 | CL7  | O2D-CGD | -3.24 | 1.25        | 1.33     |
| 14  | bB    | 813  | CL7  | OBD-CAD | -3.24 | 1.16        | 1.22     |
| 14  | aB    | 3013 | CL7  | OBD-CAD | -3.24 | 1.16        | 1.22     |
| 14  | bA    | 3131 | CL7  | C1C-NC  | 3.23  | 1.41        | 1.37     |
| 14  | aB    | 3002 | CL7  | CAB-C3B | -3.23 | 1.38        | 1.45     |
| 14  | cA    | 3116 | CL7  | CHD-C4C | -3.23 | 1.32        | 1.38     |
| 14  | bB    | 820  | CL7  | C1D-C2D | -3.23 | 1.35        | 1.43     |
| 14  | aA    | 3143 | CL7  | C1C-NC  | 3.23  | 1.41        | 1.37     |
| 14  | bB    | 823  | CL7  | C4C-NC  | 3.23  | 1.41        | 1.37     |
| 14  | cA    | 3144 | CL7  | OBD-CAD | -3.23 | 1.16        | 1.22     |
| 14  | aB    | 3018 | CL7  | CAA-C2A | -3.23 | 1.48        | 1.54     |
| 14  | aA    | 3143 | CL7  | CHC-C1C | -3.23 | 1.32        | 1.38     |
| 14  | aL    | 202  | CL7  | CHB-C4A | -3.23 | 1.29        | 1.36     |
| 14  | bB    | 820  | CL7  | MG-NC   | -3.23 | 1.99        | 2.05     |
| 14  | cA    | 3141 | CL7  | CAA-C2A | -3.23 | 1.48        | 1.54     |
| 14  | bL    | 203  | CL7  | CHB-C4A | -3.22 | 1.29        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 12  | bA    | 3101 | G9R  | C4D-CHA | 3.22  | 1.49        | 1.38     |
| 14  | aA    | 3141 | CL7  | C2A-C1A | -3.22 | 1.45        | 1.50     |
| 14  | bA    | 3124 | CL7  | CHB-C4A | -3.22 | 1.29        | 1.36     |
| 14  | cL    | 204  | CL7  | CAB-C3B | -3.22 | 1.38        | 1.45     |
| 14  | bJ    | 101  | CL7  | C4C-NC  | 3.22  | 1.41        | 1.37     |
| 14  | bA    | 3125 | CL7  | CHB-C4A | -3.22 | 1.29        | 1.36     |
| 14  | bB    | 825  | CL7  | C1C-NC  | 3.22  | 1.41        | 1.37     |
| 14  | bA    | 3142 | CL7  | CMD-C2D | -3.22 | 1.44        | 1.50     |
| 14  | aB    | 3019 | CL7  | CHC-C1C | -3.22 | 1.32        | 1.38     |
| 14  | bB    | 824  | CL7  | CHC-C1C | -3.21 | 1.32        | 1.38     |
| 14  | aA    | 3146 | CL7  | C1C-NC  | 3.21  | 1.41        | 1.37     |
| 14  | bA    | 3108 | CL7  | CHC-C1C | -3.21 | 1.32        | 1.38     |
| 14  | aB    | 3012 | CL7  | OBD-CAD | -3.21 | 1.16        | 1.22     |
| 14  | aA    | 3125 | CL7  | CAB-C3B | -3.21 | 1.38        | 1.45     |
| 14  | aA    | 3124 | CL7  | C4C-NC  | 3.21  | 1.41        | 1.37     |
| 14  | aB    | 3032 | CL7  | C4C-NC  | 3.21  | 1.41        | 1.37     |
| 14  | cB    | 813  | CL7  | OBD-CAD | -3.21 | 1.16        | 1.22     |
| 17  | bA    | 3143 | PQN  | C9-C10  | -3.21 | 1.34        | 1.39     |
| 14  | bB    | 810  | CL7  | C1D-ND  | -3.21 | 1.33        | 1.37     |
| 14  | aA    | 3117 | CL7  | OBB-CAB | 3.20  | 1.29        | 1.22     |
| 14  | cA    | 3129 | CL7  | CHC-C1C | -3.20 | 1.32        | 1.38     |
| 14  | aA    | 3117 | CL7  | C4C-NC  | 3.20  | 1.41        | 1.37     |
| 14  | aB    | 3020 | CL7  | C4C-NC  | 3.20  | 1.41        | 1.37     |
| 14  | aB    | 3003 | CL7  | C1A-NA  | -3.20 | 1.29        | 1.38     |
| 14  | bA    | 3109 | CL7  | C4C-NC  | 3.20  | 1.41        | 1.37     |
| 14  | bB    | 833  | CL7  | CHD-C4C | -3.20 | 1.32        | 1.38     |
| 14  | bA    | 3116 | CL7  | OBB-CAB | 3.20  | 1.29        | 1.22     |
| 14  | aA    | 3128 | CL7  | CAB-C3B | -3.20 | 1.38        | 1.45     |
| 14  | aA    | 3131 | CL7  | C1D-C2D | -3.20 | 1.35        | 1.43     |
| 14  | bA    | 3130 | CL7  | CHC-C1C | -3.20 | 1.32        | 1.38     |
| 14  | cB    | 833  | CL7  | C1D-C2D | -3.19 | 1.35        | 1.43     |
| 13  | bB    | 801  | PHO  | O2A-CGA | 3.19  | 1.42        | 1.33     |
| 14  | aB    | 3020 | CL7  | OBD-CAD | -3.19 | 1.17        | 1.22     |
| 14  | aJ    | 101  | CL7  | C4C-NC  | 3.19  | 1.41        | 1.37     |
| 14  | aA    | 3129 | CL7  | C1D-ND  | -3.19 | 1.33        | 1.37     |
| 14  | bB    | 820  | CL7  | C3A-C4A | -3.19 | 1.46        | 1.52     |
| 14  | bK    | 101  | CL7  | OBD-CAD | -3.19 | 1.16        | 1.23     |
| 14  | bA    | 3127 | CL7  | MG-NA   | -3.19 | 1.99        | 2.05     |
| 14  | aA    | 3120 | CL7  | C4B-NB  | -3.19 | 1.33        | 1.37     |
| 14  | aA    | 3107 | CL7  | CHC-C1C | -3.19 | 1.32        | 1.38     |
| 14  | cA    | 3111 | CL7  | OBD-CAD | -3.19 | 1.17        | 1.22     |
| 13  | cB    | 805  | PHO  | C3A-C2A | -3.19 | 1.51        | 1.54     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | cB    | 831  | CL7  | C1C-NC  | 3.19  | 1.41        | 1.37     |
| 14  | bA    | 3122 | CL7  | C4C-NC  | 3.18  | 1.41        | 1.37     |
| 14  | cB    | 821  | CL7  | C4C-NC  | 3.18  | 1.41        | 1.37     |
| 14  | bA    | 3105 | CL7  | C2A-C1A | -3.18 | 1.46        | 1.52     |
| 14  | bA    | 3141 | CL7  | C1C-NC  | 3.18  | 1.41        | 1.37     |
| 14  | cB    | 809  | CL7  | O2D-CGD | -3.18 | 1.25        | 1.33     |
| 14  | cA    | 3142 | CL7  | CHC-C1C | -3.18 | 1.32        | 1.38     |
| 13  | aA    | 3102 | PHO  | O2A-CGA | 3.17  | 1.42        | 1.33     |
| 14  | bB    | 809  | CL7  | C3D-C2D | -3.17 | 1.32        | 1.42     |
| 14  | cB    | 833  | CL7  | C3D-CAD | -3.17 | 1.34        | 1.45     |
| 14  | aB    | 3019 | CL7  | C4C-NC  | 3.17  | 1.41        | 1.37     |
| 14  | cA    | 3106 | CL7  | CHC-C1C | -3.17 | 1.32        | 1.38     |
| 14  | aA    | 3143 | CL7  | OBD-CAD | -3.17 | 1.17        | 1.22     |
| 14  | bB    | 819  | CL7  | C1B-NB  | 3.17  | 1.41        | 1.37     |
| 14  | aB    | 3007 | CL7  | MG-NB   | -3.17 | 1.99        | 2.05     |
| 14  | bB    | 820  | CL7  | CHD-C4C | -3.17 | 1.32        | 1.38     |
| 14  | aB    | 3005 | CL7  | C1D-ND  | -3.17 | 1.33        | 1.37     |
| 14  | aA    | 3124 | CL7  | C1D-C2D | -3.17 | 1.35        | 1.43     |
| 14  | aB    | 3015 | CL7  | CHB-C4A | -3.17 | 1.29        | 1.36     |
| 14  | aB    | 3023 | CL7  | CHB-C4A | -3.17 | 1.29        | 1.36     |
| 14  | cA    | 3131 | CL7  | C4C-NC  | 3.17  | 1.41        | 1.37     |
| 14  | cL    | 205  | CL7  | C2A-C1A | -3.17 | 1.46        | 1.50     |
| 14  | aA    | 3127 | CL7  | OBD-CAD | -3.16 | 1.17        | 1.22     |
| 14  | cA    | 3126 | CL7  | C4C-NC  | 3.16  | 1.41        | 1.37     |
| 14  | bA    | 3114 | CL7  | CHB-C4A | -3.16 | 1.29        | 1.36     |
| 14  | aB    | 3009 | CL7  | CAB-C3B | -3.16 | 1.38        | 1.45     |
| 14  | cB    | 826  | CL7  | CAA-C2A | -3.16 | 1.48        | 1.54     |
| 14  | aB    | 3019 | CL7  | CHD-C4C | -3.16 | 1.32        | 1.38     |
| 14  | cB    | 820  | CL7  | CHD-C4C | -3.16 | 1.32        | 1.38     |
| 14  | aA    | 3128 | CL7  | MG-NA   | -3.16 | 1.99        | 2.05     |
| 14  | bA    | 3126 | CL7  | C4C-NC  | 3.16  | 1.41        | 1.37     |
| 14  | aB    | 3009 | CL7  | MG-NA   | -3.16 | 1.99        | 2.05     |
| 14  | bA    | 3121 | CL7  | C1D-C2D | -3.16 | 1.35        | 1.43     |
| 14  | bA    | 3107 | CL7  | C4C-NC  | 3.16  | 1.41        | 1.37     |
| 14  | aB    | 3006 | CL7  | C1D-ND  | -3.16 | 1.33        | 1.37     |
| 14  | bF    | 201  | CL7  | C4C-NC  | 3.16  | 1.41        | 1.37     |
| 14  | aB    | 3023 | CL7  | CAB-C3B | -3.15 | 1.38        | 1.45     |
| 14  | cB    | 824  | CL7  | CHC-C1C | -3.15 | 1.32        | 1.38     |
| 14  | bA    | 3122 | CL7  | CAA-C2A | -3.15 | 1.48        | 1.54     |
| 14  | bB    | 819  | CL7  | CHC-C1C | -3.15 | 1.32        | 1.38     |
| 14  | aA    | 3125 | CL7  | C1C-NC  | 3.15  | 1.41        | 1.37     |
| 14  | cB    | 810  | CL7  | MG-NA   | -3.15 | 1.99        | 2.05     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | cB    | 804  | CL7  | C4C-NC  | 3.15  | 1.41        | 1.37     |
| 14  | bB    | 824  | CL7  | CAB-C3B | -3.15 | 1.38        | 1.45     |
| 14  | cB    | 810  | CL7  | CAB-C3B | -3.14 | 1.38        | 1.45     |
| 14  | bA    | 3130 | CL7  | CHB-C4A | -3.14 | 1.29        | 1.36     |
| 14  | aB    | 3026 | CL7  | C3B-C4B | -3.14 | 1.35        | 1.42     |
| 14  | bB    | 808  | CL7  | O2D-CGD | -3.14 | 1.25        | 1.33     |
| 16  | bA    | 3137 | LHG  | O7-C5   | -3.14 | 1.38        | 1.46     |
| 14  | bL    | 205  | CL7  | C3D-CAD | -3.14 | 1.34        | 1.45     |
| 14  | bA    | 3142 | CL7  | CHC-C1C | -3.14 | 1.32        | 1.38     |
| 14  | cA    | 3130 | CL7  | CHC-C1C | -3.14 | 1.32        | 1.38     |
| 14  | cB    | 823  | CL7  | C4C-NC  | 3.14  | 1.41        | 1.37     |
| 14  | aB    | 3030 | CL7  | OBD-CAD | -3.14 | 1.17        | 1.22     |
| 14  | cB    | 825  | CL7  | OBD-CAD | -3.14 | 1.17        | 1.22     |
| 14  | bB    | 821  | CL7  | C4C-NC  | 3.14  | 1.41        | 1.37     |
| 14  | cK    | 101  | CL7  | C4C-NC  | 3.14  | 1.41        | 1.37     |
| 14  | cA    | 3131 | CL7  | C1C-NC  | 3.14  | 1.41        | 1.37     |
| 14  | bA    | 3116 | CL7  | MG-NB   | -3.14 | 1.99        | 2.05     |
| 14  | aA    | 3142 | CL7  | C3A-C4A | -3.14 | 1.46        | 1.52     |
| 14  | bB    | 807  | CL7  | C1D-ND  | -3.13 | 1.33        | 1.37     |
| 14  | aA    | 3108 | CL7  | C4C-NC  | 3.13  | 1.41        | 1.37     |
| 14  | bA    | 3114 | CL7  | C1C-NC  | 3.13  | 1.41        | 1.37     |
| 14  | bB    | 831  | CL7  | C1C-NC  | 3.13  | 1.41        | 1.37     |
| 16  | bA    | 3138 | LHG  | O3-C3   | -3.13 | 1.32        | 1.44     |
| 12  | cA    | 3101 | G9R  | CHB-C1B | 3.13  | 1.46        | 1.39     |
| 14  | aA    | 3103 | CL7  | CHB-C4A | -3.13 | 1.29        | 1.36     |
| 14  | aA    | 3115 | CL7  | CHB-C4A | -3.13 | 1.29        | 1.36     |
| 14  | cB    | 811  | CL7  | OBB-CAB | 3.13  | 1.29        | 1.22     |
| 14  | aL    | 204  | CL7  | C3D-CAD | -3.13 | 1.34        | 1.45     |
| 14  | cB    | 823  | CL7  | OBD-CAD | -3.13 | 1.17        | 1.22     |
| 14  | aB    | 3017 | CL7  | C4C-NC  | 3.13  | 1.41        | 1.37     |
| 14  | bB    | 818  | CL7  | C1C-NC  | 3.13  | 1.41        | 1.37     |
| 14  | bB    | 810  | CL7  | MG-NA   | -3.13 | 1.99        | 2.05     |
| 14  | bB    | 827  | CL7  | CAA-C2A | -3.13 | 1.48        | 1.54     |
| 14  | bB    | 832  | CL7  | C4C-NC  | 3.13  | 1.41        | 1.37     |
| 14  | aA    | 3108 | CL7  | C2A-C1A | -3.13 | 1.46        | 1.50     |
| 14  | cA    | 3108 | CL7  | OBD-CAD | -3.13 | 1.17        | 1.22     |
| 14  | aA    | 3112 | CL7  | C1C-NC  | 3.13  | 1.41        | 1.37     |
| 14  | bB    | 825  | CL7  | C4C-NC  | 3.13  | 1.41        | 1.37     |
| 14  | cL    | 204  | CL7  | C2A-C1A | -3.13 | 1.46        | 1.50     |
| 14  | aF    | 201  | CL7  | CHB-C4A | -3.13 | 1.29        | 1.36     |
| 12  | bA    | 3101 | G9R  | CMD-C2D | -3.13 | 1.44        | 1.50     |
| 14  | aA    | 3126 | CL7  | OBB-CAB | 3.13  | 1.29        | 1.22     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | aB    | 3007 | CL7  | MG-NC   | -3.12 | 1.99        | 2.05     |
| 14  | cB    | 809  | CL7  | CHC-C1C | -3.12 | 1.32        | 1.38     |
| 13  | cB    | 805  | PHO  | C1-C2   | 3.12  | 1.58        | 1.49     |
| 14  | aB    | 3014 | CL7  | C1C-NC  | 3.12  | 1.41        | 1.37     |
| 14  | aA    | 3120 | CL7  | CAB-C3B | -3.12 | 1.38        | 1.45     |
| 13  | aA    | 3102 | PHO  | C3B-CAB | 3.12  | 1.54        | 1.47     |
| 14  | cA    | 3105 | CL7  | C2A-C1A | -3.12 | 1.46        | 1.52     |
| 14  | aA    | 3132 | CL7  | OBD-CAD | -3.12 | 1.17        | 1.22     |
| 14  | aA    | 3117 | CL7  | MG-NB   | -3.12 | 1.99        | 2.05     |
| 14  | bL    | 205  | CL7  | C1D-C2D | -3.12 | 1.35        | 1.43     |
| 14  | cL    | 205  | CL7  | C1D-C2D | -3.12 | 1.35        | 1.43     |
| 14  | cB    | 833  | CL7  | C1D-ND  | -3.12 | 1.34        | 1.37     |
| 14  | cA    | 3121 | CL7  | C1D-C2D | -3.11 | 1.35        | 1.43     |
| 14  | cA    | 3140 | CL7  | C3B-C4B | -3.11 | 1.35        | 1.42     |
| 14  | cB    | 809  | CL7  | C3D-C2D | -3.11 | 1.32        | 1.42     |
| 14  | bB    | 816  | CL7  | C4C-NC  | 3.11  | 1.41        | 1.37     |
| 14  | cB    | 807  | CL7  | CHB-C4A | -3.11 | 1.29        | 1.36     |
| 14  | bB    | 816  | CL7  | C3D-CAD | -3.11 | 1.34        | 1.45     |
| 14  | cA    | 3125 | CL7  | CHC-C1C | -3.11 | 1.32        | 1.38     |
| 14  | bB    | 822  | CL7  | OBD-CAD | -3.11 | 1.17        | 1.22     |
| 14  | aB    | 3026 | CL7  | C4D-ND  | -3.11 | 1.33        | 1.37     |
| 14  | aA    | 3115 | CL7  | OBB-CAB | 3.11  | 1.29        | 1.22     |
| 13  | cB    | 801  | PHO  | O2A-CGA | 3.11  | 1.42        | 1.33     |
| 14  | cF    | 201  | CL7  | CHB-C4A | -3.11 | 1.29        | 1.36     |
| 14  | bA    | 3120 | CL7  | CAB-C3B | -3.11 | 1.38        | 1.45     |
| 14  | bA    | 3106 | CL7  | C1C-NC  | 3.11  | 1.41        | 1.37     |
| 14  | aA    | 3134 | CL7  | OBD-CAD | -3.11 | 1.17        | 1.22     |
| 14  | aA    | 3109 | CL7  | OBD-CAD | -3.10 | 1.17        | 1.22     |
| 14  | aA    | 3109 | CL7  | CHC-C1C | -3.10 | 1.32        | 1.38     |
| 14  | cA    | 3140 | CL7  | CHC-C1C | -3.10 | 1.32        | 1.38     |
| 14  | aA    | 3130 | CL7  | C1C-NC  | 3.10  | 1.41        | 1.37     |
| 14  | cK    | 101  | CL7  | C1C-NC  | 3.10  | 1.41        | 1.37     |
| 14  | bA    | 3105 | CL7  | CMD-C2D | -3.10 | 1.44        | 1.50     |
| 14  | aB    | 3015 | CL7  | CAB-C3B | -3.10 | 1.38        | 1.45     |
| 14  | bB    | 832  | CL7  | CAB-C3B | -3.10 | 1.38        | 1.45     |
| 14  | cB    | 832  | CL7  | CAB-C3B | -3.10 | 1.38        | 1.45     |
| 14  | bA    | 3124 | CL7  | CAA-C2A | -3.10 | 1.48        | 1.54     |
| 14  | cB    | 819  | CL7  | C4D-ND  | -3.10 | 1.33        | 1.37     |
| 14  | aL    | 204  | CL7  | C1D-C2D | -3.10 | 1.36        | 1.43     |
| 14  | bB    | 827  | CL7  | C1D-ND  | -3.10 | 1.34        | 1.37     |
| 14  | aA    | 3127 | CL7  | C4C-NC  | 3.09  | 1.41        | 1.37     |
| 14  | bB    | 810  | CL7  | CAB-C3B | -3.09 | 1.38        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | cB    | 804  | CL7  | CAB-C3B | -3.09 | 1.38        | 1.45     |
| 14  | aA    | 3124 | CL7  | O2D-CGD | -3.09 | 1.25        | 1.33     |
| 14  | bA    | 3140 | CL7  | CHC-C1C | -3.09 | 1.32        | 1.38     |
| 14  | aA    | 3106 | CL7  | OBD-CAD | -3.09 | 1.17        | 1.22     |
| 14  | cB    | 818  | CL7  | C1C-NC  | 3.09  | 1.41        | 1.37     |
| 14  | bB    | 808  | CL7  | CHC-C1C | -3.09 | 1.32        | 1.38     |
| 14  | aB    | 3026 | CL7  | C1C-NC  | 3.09  | 1.41        | 1.37     |
| 12  | aA    | 3101 | G9R  | C1C-C2C | 3.09  | 1.50        | 1.44     |
| 14  | bB    | 809  | CL7  | CAA-C2A | -3.09 | 1.48        | 1.54     |
| 14  | bA    | 3119 | CL7  | C4B-NB  | -3.09 | 1.34        | 1.37     |
| 14  | bA    | 3123 | CL7  | O2D-CGD | -3.09 | 1.25        | 1.33     |
| 14  | cB    | 808  | CL7  | CHC-C1C | -3.09 | 1.32        | 1.38     |
| 14  | cB    | 810  | CL7  | C1D-ND  | -3.09 | 1.34        | 1.37     |
| 14  | aA    | 3133 | CL7  | C1C-C2C | -3.09 | 1.39        | 1.45     |
| 14  | cB    | 820  | CL7  | C1C-NC  | 3.08  | 1.41        | 1.37     |
| 14  | cB    | 807  | CL7  | C1D-ND  | -3.08 | 1.34        | 1.37     |
| 14  | cA    | 3105 | CL7  | CMD-C2D | -3.08 | 1.44        | 1.50     |
| 14  | cA    | 3109 | CL7  | C4C-NC  | 3.08  | 1.41        | 1.37     |
| 14  | bA    | 3111 | CL7  | OBD-CAD | -3.08 | 1.17        | 1.22     |
| 14  | cA    | 3113 | CL7  | C1D-C2D | -3.08 | 1.36        | 1.43     |
| 16  | cA    | 3138 | LHG  | O3-C3   | -3.08 | 1.32        | 1.44     |
| 14  | bA    | 3102 | CL7  | CAB-C3B | -3.08 | 1.38        | 1.45     |
| 14  | aB    | 3014 | CL7  | OBD-CAD | -3.08 | 1.17        | 1.22     |
| 14  | bK    | 101  | CL7  | C4C-NC  | 3.08  | 1.41        | 1.37     |
| 14  | bA    | 3104 | CL7  | C4C-NC  | 3.08  | 1.41        | 1.37     |
| 14  | bB    | 820  | CL7  | CHB-C4A | -3.08 | 1.29        | 1.36     |
| 14  | aA    | 3140 | CL7  | OBB-CAB | 3.08  | 1.29        | 1.22     |
| 14  | aB    | 3017 | CL7  | C1C-NC  | 3.08  | 1.41        | 1.37     |
| 14  | aA    | 3122 | CL7  | CHB-C4A | -3.07 | 1.29        | 1.36     |
| 14  | aB    | 3024 | CL7  | OBB-CAB | 3.07  | 1.29        | 1.22     |
| 14  | aB    | 3019 | CL7  | CHB-C4A | -3.07 | 1.30        | 1.36     |
| 14  | cB    | 816  | CL7  | CAB-C3B | -3.07 | 1.38        | 1.45     |
| 14  | bB    | 811  | CL7  | OBB-CAB | 3.07  | 1.29        | 1.22     |
| 14  | bB    | 825  | CL7  | OBB-CAB | 3.07  | 1.29        | 1.22     |
| 14  | cA    | 3124 | CL7  | C1C-NC  | 3.07  | 1.41        | 1.37     |
| 14  | bA    | 3140 | CL7  | CHD-C4C | -3.07 | 1.32        | 1.38     |
| 14  | cB    | 808  | CL7  | C1D-ND  | -3.07 | 1.34        | 1.37     |
| 14  | cA    | 3133 | CL7  | OBD-CAD | -3.07 | 1.17        | 1.22     |
| 14  | bA    | 3142 | CL7  | OBB-CAB | 3.07  | 1.29        | 1.22     |
| 14  | bA    | 3113 | CL7  | C1D-C2D | -3.07 | 1.36        | 1.43     |
| 14  | aA    | 3143 | CL7  | CHD-C4C | -3.07 | 1.32        | 1.38     |
| 14  | cB    | 832  | CL7  | CHB-C4A | -3.06 | 1.30        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | aA    | 3133 | CL7  | CHD-C4C | -3.06 | 1.32        | 1.38     |
| 14  | bB    | 806  | CL7  | OBB-CAB | 3.06  | 1.29        | 1.22     |
| 14  | aB    | 3003 | CL7  | CMD-C2D | -3.06 | 1.44        | 1.50     |
| 14  | cL    | 204  | CL7  | CHC-C1C | -3.06 | 1.32        | 1.38     |
| 14  | aA    | 3122 | CL7  | C1D-C2D | -3.06 | 1.36        | 1.43     |
| 14  | bB    | 804  | CL7  | C1A-NA  | -3.06 | 1.30        | 1.38     |
| 14  | cA    | 3142 | CL7  | OBB-CAB | 3.06  | 1.29        | 1.22     |
| 14  | bA    | 3107 | CL7  | C2A-C1A | -3.06 | 1.46        | 1.50     |
| 14  | bA    | 3111 | CL7  | C1C-NC  | 3.06  | 1.41        | 1.37     |
| 14  | aB    | 3030 | CL7  | CAA-C2A | -3.06 | 1.48        | 1.54     |
| 14  | cB    | 809  | CL7  | CAA-C2A | -3.06 | 1.48        | 1.54     |
| 14  | bB    | 816  | CL7  | CHD-C4C | -3.06 | 1.32        | 1.38     |
| 14  | bA    | 3124 | CL7  | CBD-CGD | -3.05 | 1.42        | 1.52     |
| 14  | bF    | 201  | CL7  | CHB-C4A | -3.05 | 1.30        | 1.36     |
| 14  | aA    | 3131 | CL7  | CHC-C1C | -3.05 | 1.32        | 1.38     |
| 14  | cA    | 3140 | CL7  | CHD-C4C | -3.05 | 1.32        | 1.38     |
| 14  | bB    | 807  | CL7  | CHB-C4A | -3.05 | 1.30        | 1.36     |
| 14  | aB    | 3026 | CL7  | C3D-C2D | -3.05 | 1.32        | 1.42     |
| 14  | cA    | 3128 | CL7  | C3A-C4A | -3.05 | 1.46        | 1.52     |
| 14  | aB    | 3015 | CL7  | CHD-C4C | -3.05 | 1.32        | 1.38     |
| 14  | cA    | 3131 | CL7  | C1D-C2D | -3.05 | 1.36        | 1.43     |
| 14  | bA    | 3106 | CL7  | OBD-CAD | -3.05 | 1.17        | 1.22     |
| 14  | bB    | 824  | CL7  | CHB-C4A | -3.05 | 1.30        | 1.36     |
| 14  | bA    | 3131 | CL7  | C1D-C2D | -3.05 | 1.36        | 1.43     |
| 14  | aB    | 3020 | CL7  | C1C-NC  | 3.05  | 1.41        | 1.37     |
| 14  | cB    | 818  | CL7  | OBB-CAB | 3.05  | 1.29        | 1.22     |
| 14  | bA    | 3139 | CL7  | CHC-C1C | -3.04 | 1.32        | 1.38     |
| 14  | bA    | 3133 | CL7  | OBD-CAD | -3.04 | 1.17        | 1.22     |
| 14  | cA    | 3124 | CL7  | OBB-CAB | 3.04  | 1.29        | 1.22     |
| 14  | bA    | 3116 | CL7  | CHD-C4C | -3.04 | 1.32        | 1.38     |
| 14  | aB    | 3021 | CL7  | OBD-CAD | -3.04 | 1.17        | 1.22     |
| 14  | cA    | 3106 | CL7  | C1C-NC  | 3.04  | 1.41        | 1.37     |
| 14  | cA    | 3120 | CL7  | C1C-NC  | 3.04  | 1.41        | 1.37     |
| 14  | cA    | 3142 | CL7  | C1C-NC  | 3.04  | 1.41        | 1.37     |
| 14  | aK    | 101  | CL7  | OBD-CAD | -3.04 | 1.16        | 1.23     |
| 14  | bB    | 826  | CL7  | CAB-C3B | -3.04 | 1.38        | 1.45     |
| 14  | aA    | 3140 | CL7  | C4C-NC  | 3.04  | 1.41        | 1.37     |
| 14  | cA    | 3128 | CL7  | C1C-NC  | 3.04  | 1.41        | 1.37     |
| 14  | cA    | 3133 | CL7  | OBB-CAB | 3.04  | 1.29        | 1.22     |
| 14  | bA    | 3126 | CL7  | OBD-CAD | -3.04 | 1.17        | 1.22     |
| 14  | aA    | 3143 | CL7  | OBB-CAB | 3.04  | 1.29        | 1.22     |
| 14  | aB    | 3024 | CL7  | OBD-CAD | -3.04 | 1.17        | 1.22     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | bB    | 821  | CL7  | C1C-NC  | 3.03  | 1.41        | 1.37     |
| 14  | bA    | 3128 | CL7  | C4D-ND  | -3.03 | 1.33        | 1.37     |
| 14  | cA    | 3129 | CL7  | C3D-C2D | -3.03 | 1.32        | 1.42     |
| 14  | cA    | 3129 | CL7  | CHB-C4A | -3.03 | 1.30        | 1.36     |
| 14  | cB    | 804  | CL7  | CAA-C2A | -3.03 | 1.48        | 1.54     |
| 14  | bA    | 3131 | CL7  | C4C-NC  | 3.03  | 1.41        | 1.37     |
| 14  | cA    | 3103 | CL7  | C1D-C2D | -3.03 | 1.36        | 1.43     |
| 14  | aB    | 3002 | CL7  | C1D-C2D | -3.03 | 1.36        | 1.43     |
| 14  | aB    | 3007 | CL7  | CHC-C1C | -3.03 | 1.32        | 1.38     |
| 14  | bA    | 3122 | CL7  | MG-NC   | -3.03 | 1.99        | 2.05     |
| 14  | bA    | 3140 | CL7  | C3B-C4B | -3.03 | 1.35        | 1.42     |
| 14  | bB    | 804  | CL7  | O2D-CGD | -3.03 | 1.25        | 1.33     |
| 14  | bA    | 3103 | CL7  | C1D-C2D | -3.03 | 1.36        | 1.43     |
| 14  | bB    | 816  | CL7  | CAB-C3B | -3.03 | 1.38        | 1.45     |
| 14  | cB    | 821  | CL7  | C1C-NC  | 3.03  | 1.41        | 1.37     |
| 14  | cA    | 3127 | CL7  | CHD-C4C | -3.03 | 1.32        | 1.38     |
| 14  | cA    | 3141 | CL7  | C1C-NC  | 3.03  | 1.41        | 1.37     |
| 14  | bB    | 810  | CL7  | CHD-C4C | -3.03 | 1.32        | 1.38     |
| 14  | cB    | 827  | CL7  | CHD-C4C | -3.03 | 1.32        | 1.38     |
| 14  | cA    | 3122 | CL7  | MG-NC   | -3.03 | 1.99        | 2.05     |
| 14  | aB    | 3022 | CL7  | OBD-CAD | -3.02 | 1.17        | 1.22     |
| 14  | bB    | 827  | CL7  | CHD-C4C | -3.02 | 1.32        | 1.38     |
| 14  | aA    | 3107 | CL7  | C3D-CAD | -3.02 | 1.34        | 1.45     |
| 14  | bA    | 3125 | CL7  | OBD-CAD | -3.02 | 1.17        | 1.22     |
| 14  | cB    | 808  | CL7  | MG-NB   | -3.02 | 1.99        | 2.05     |
| 14  | cL    | 205  | CL7  | C3D-CAD | -3.02 | 1.34        | 1.45     |
| 14  | aB    | 3031 | CL7  | CHB-C4A | -3.02 | 1.30        | 1.36     |
| 14  | cA    | 3105 | CL7  | C3D-CAD | -3.02 | 1.34        | 1.45     |
| 14  | cA    | 3102 | CL7  | CBD-CGD | -3.02 | 1.43        | 1.52     |
| 14  | bA    | 3139 | CL7  | OBB-CAB | 3.02  | 1.29        | 1.22     |
| 14  | bB    | 826  | CL7  | CAA-C2A | -3.02 | 1.48        | 1.54     |
| 14  | bB    | 832  | CL7  | CHB-C4A | -3.02 | 1.30        | 1.36     |
| 14  | cB    | 814  | CL7  | C4C-NC  | 3.02  | 1.41        | 1.37     |
| 14  | bB    | 823  | CL7  | C1D-C2D | -3.02 | 1.36        | 1.43     |
| 14  | bB    | 816  | CL7  | CHC-C1C | -3.02 | 1.32        | 1.38     |
| 12  | cA    | 3101 | G9R  | C3D-C4D | -3.02 | 1.37        | 1.44     |
| 14  | bA    | 3105 | CL7  | C3D-CAD | -3.02 | 1.34        | 1.45     |
| 14  | cB    | 804  | CL7  | CHC-C1C | -3.02 | 1.32        | 1.38     |
| 13  | aA    | 3102 | PHO  | C4B-NB  | -3.02 | 1.33        | 1.38     |
| 14  | cB    | 832  | CL7  | OBD-CAD | -3.01 | 1.17        | 1.22     |
| 14  | aA    | 3112 | CL7  | OBD-CAD | -3.01 | 1.17        | 1.22     |
| 14  | bA    | 3141 | CL7  | C1D-C2D | -3.01 | 1.36        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | cB    | 823  | CL7  | C1D-C2D | -3.01 | 1.36        | 1.43     |
| 14  | bA    | 3112 | CL7  | CHB-C4A | -3.01 | 1.30        | 1.36     |
| 14  | cB    | 824  | CL7  | CAB-C3B | -3.01 | 1.38        | 1.45     |
| 14  | bB    | 819  | CL7  | C3D-CAD | -3.01 | 1.34        | 1.45     |
| 13  | aB    | 3004 | PHO  | C1-C2   | 3.01  | 1.58        | 1.49     |
| 14  | aB    | 3008 | CL7  | C1C-NC  | 3.01  | 1.41        | 1.37     |
| 14  | aA    | 3106 | CL7  | C3D-CAD | -3.01 | 1.35        | 1.45     |
| 14  | aB    | 3022 | CL7  | CHC-C1C | -3.01 | 1.32        | 1.38     |
| 14  | bK    | 101  | CL7  | C1C-NC  | 3.00  | 1.41        | 1.37     |
| 14  | bB    | 818  | CL7  | C4C-NC  | 3.00  | 1.41        | 1.37     |
| 14  | bB    | 807  | CL7  | C3B-C4B | -3.00 | 1.35        | 1.42     |
| 14  | bB    | 819  | CL7  | C4D-ND  | -3.00 | 1.33        | 1.37     |
| 14  | bA    | 3128 | CL7  | OBB-CAB | 3.00  | 1.29        | 1.22     |
| 14  | cA    | 3107 | CL7  | C4C-NC  | 3.00  | 1.41        | 1.37     |
| 14  | bA    | 3102 | CL7  | C1A-NA  | -3.00 | 1.30        | 1.38     |
| 14  | cA    | 3124 | CL7  | CHC-C1C | -3.00 | 1.32        | 1.38     |
| 14  | bB    | 820  | CL7  | C1C-NC  | 3.00  | 1.41        | 1.37     |
| 14  | cA    | 3103 | CL7  | C1C-NC  | 3.00  | 1.41        | 1.37     |
| 14  | cA    | 3129 | CL7  | CAA-C2A | 3.00  | 1.59        | 1.53     |
| 14  | aB    | 3022 | CL7  | C1D-C2D | -2.99 | 1.36        | 1.43     |
| 14  | cB    | 808  | CL7  | MG-NC   | -2.99 | 1.99        | 2.05     |
| 14  | cB    | 827  | CL7  | CAB-C3B | -2.99 | 1.38        | 1.45     |
| 13  | bB    | 805  | PHO  | C3B-C4B | 2.99  | 1.44        | 1.41     |
| 14  | cB    | 809  | CL7  | C4D-ND  | -2.99 | 1.33        | 1.37     |
| 14  | cB    | 826  | CL7  | C3B-C4B | -2.99 | 1.35        | 1.42     |
| 17  | cB    | 828  | PQN  | C8-C9   | 2.99  | 1.45        | 1.38     |
| 14  | aB    | 3008 | CL7  | C3D-C2D | -2.99 | 1.32        | 1.42     |
| 14  | aB    | 3006 | CL7  | CHB-C4A | -2.99 | 1.30        | 1.36     |
| 14  | aA    | 3121 | CL7  | C1C-NC  | 2.99  | 1.41        | 1.37     |
| 14  | bA    | 3140 | CL7  | C1D-C2D | -2.99 | 1.36        | 1.43     |
| 14  | aA    | 3119 | CL7  | C1D-C2D | -2.99 | 1.36        | 1.43     |
| 14  | aB    | 3010 | CL7  | OBB-CAB | 2.99  | 1.29        | 1.22     |
| 14  | cB    | 826  | CL7  | O2D-CGD | -2.99 | 1.25        | 1.33     |
| 14  | cB    | 824  | CL7  | C1C-NC  | 2.99  | 1.41        | 1.37     |
| 14  | bA    | 3113 | CL7  | CAB-C3B | -2.99 | 1.38        | 1.45     |
| 14  | cB    | 804  | CL7  | O2D-CGD | -2.99 | 1.25        | 1.33     |
| 14  | aA    | 3128 | CL7  | C1D-C2D | -2.99 | 1.36        | 1.43     |
| 14  | bB    | 823  | CL7  | OBD-CAD | -2.99 | 1.17        | 1.22     |
| 14  | bB    | 826  | CL7  | C3C-C2C | -2.99 | 1.30        | 1.36     |
| 14  | cB    | 816  | CL7  | CHD-C4C | -2.99 | 1.32        | 1.38     |
| 14  | cA    | 3116 | CL7  | MG-NB   | -2.99 | 1.99        | 2.05     |
| 14  | aL    | 203  | CL7  | CAB-C3B | -2.99 | 1.38        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 12  | bA    | 3101 | G9R  | C1C-C2C | 2.99  | 1.50        | 1.44     |
| 14  | cA    | 3133 | CL7  | CHB-C4A | -2.98 | 1.30        | 1.36     |
| 14  | aA    | 3121 | CL7  | CHD-C4C | -2.98 | 1.32        | 1.38     |
| 14  | aA    | 3124 | CL7  | C1C-NC  | 2.98  | 1.41        | 1.37     |
| 14  | aB    | 3013 | CL7  | C4C-NC  | 2.98  | 1.41        | 1.37     |
| 14  | bA    | 3133 | CL7  | OBB-CAB | 2.98  | 1.28        | 1.22     |
| 14  | bA    | 3141 | CL7  | CHB-C4A | -2.98 | 1.30        | 1.36     |
| 14  | aB    | 3026 | CL7  | C2A-C1A | -2.98 | 1.46        | 1.50     |
| 14  | aA    | 3109 | CL7  | OBB-CAB | 2.98  | 1.28        | 1.22     |
| 13  | cB    | 801  | PHO  | C3D-C4D | -2.98 | 1.37        | 1.41     |
| 14  | cA    | 3103 | CL7  | CHB-C4A | -2.98 | 1.30        | 1.36     |
| 14  | bB    | 803  | CL7  | OBD-CAD | -2.98 | 1.17        | 1.22     |
| 14  | bA    | 3125 | CL7  | OBB-CAB | 2.98  | 1.28        | 1.22     |
| 14  | cA    | 3125 | CL7  | CHB-C4A | -2.98 | 1.30        | 1.36     |
| 14  | bB    | 808  | CL7  | MG-NB   | -2.98 | 1.99        | 2.05     |
| 14  | bB    | 823  | CL7  | CHC-C1C | -2.98 | 1.32        | 1.38     |
| 14  | cA    | 3111 | CL7  | C1C-NC  | 2.98  | 1.41        | 1.37     |
| 14  | bA    | 3114 | CL7  | C2A-C1A | -2.98 | 1.46        | 1.50     |
| 14  | cA    | 3120 | CL7  | CHC-C1C | -2.98 | 1.32        | 1.38     |
| 14  | aB    | 3025 | CL7  | O2D-CGD | -2.98 | 1.25        | 1.33     |
| 14  | bA    | 3127 | CL7  | C1D-C2D | -2.98 | 1.36        | 1.43     |
| 14  | cB    | 804  | CL7  | C4D-ND  | -2.97 | 1.33        | 1.37     |
| 14  | cA    | 3115 | CL7  | OBD-CAD | -2.97 | 1.17        | 1.22     |
| 14  | bA    | 3131 | CL7  | CHC-C1C | -2.97 | 1.32        | 1.38     |
| 14  | aB    | 3018 | CL7  | C4D-ND  | -2.97 | 1.33        | 1.37     |
| 14  | aB    | 3002 | CL7  | OBD-CAD | -2.97 | 1.17        | 1.22     |
| 14  | bB    | 814  | CL7  | C4C-NC  | 2.97  | 1.41        | 1.37     |
| 14  | aB    | 3026 | CL7  | CAA-C2A | -2.97 | 1.48        | 1.54     |
| 14  | bA    | 3118 | CL7  | OBD-CAD | -2.97 | 1.17        | 1.22     |
| 14  | bB    | 827  | CL7  | C3C-C2C | -2.97 | 1.30        | 1.36     |
| 12  | aA    | 3101 | G9R  | C4D-CHA | 2.97  | 1.48        | 1.38     |
| 14  | bB    | 825  | CL7  | CHB-C4A | -2.97 | 1.30        | 1.36     |
| 14  | aB    | 3019 | CL7  | C1C-NC  | 2.96  | 1.41        | 1.37     |
| 14  | bA    | 3115 | CL7  | OBD-CAD | -2.96 | 1.17        | 1.22     |
| 14  | aB    | 3018 | CL7  | C3D-CAD | -2.96 | 1.35        | 1.45     |
| 14  | cA    | 3124 | CL7  | CHB-C4A | -2.96 | 1.30        | 1.36     |
| 14  | aA    | 3118 | CL7  | C4C-NC  | 2.96  | 1.41        | 1.37     |
| 14  | aB    | 3013 | CL7  | C1C-NC  | 2.96  | 1.41        | 1.37     |
| 14  | bA    | 3125 | CL7  | MG-NC   | -2.96 | 1.99        | 2.05     |
| 14  | cA    | 3112 | CL7  | CHB-C4A | -2.96 | 1.30        | 1.36     |
| 14  | bA    | 3108 | CL7  | C3D-CAD | -2.96 | 1.35        | 1.45     |
| 14  | aB    | 3031 | CL7  | CAB-C3B | -2.96 | 1.38        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | aA    | 3103 | CL7  | O2A-C1  | 2.96  | 1.54        | 1.46     |
| 14  | aB    | 3015 | CL7  | CHC-C1C | -2.96 | 1.32        | 1.38     |
| 14  | bA    | 3108 | CL7  | OBB-CAB | 2.96  | 1.28        | 1.22     |
| 14  | bB    | 807  | CL7  | C1D-C2D | -2.96 | 1.36        | 1.43     |
| 14  | aA    | 3125 | CL7  | C4D-ND  | -2.96 | 1.33        | 1.37     |
| 14  | cB    | 815  | CL7  | C4C-NC  | 2.96  | 1.41        | 1.37     |
| 14  | cB    | 826  | CL7  | C3C-C2C | -2.96 | 1.30        | 1.36     |
| 14  | cB    | 806  | CL7  | C4C-NC  | 2.96  | 1.41        | 1.37     |
| 14  | bA    | 3109 | CL7  | C1D-C2D | -2.95 | 1.36        | 1.43     |
| 14  | bJ    | 101  | CL7  | C1C-NC  | 2.95  | 1.41        | 1.37     |
| 14  | cB    | 804  | CL7  | CMD-C2D | -2.95 | 1.44        | 1.50     |
| 14  | bA    | 3120 | CL7  | C1C-NC  | 2.95  | 1.41        | 1.37     |
| 14  | cB    | 825  | CL7  | C1D-C2D | -2.95 | 1.36        | 1.43     |
| 14  | bL    | 204  | CL7  | C4D-ND  | -2.95 | 1.33        | 1.37     |
| 14  | cA    | 3120 | CL7  | CAB-C3B | -2.95 | 1.39        | 1.45     |
| 12  | cA    | 3101 | G9R  | CMD-C2D | -2.95 | 1.44        | 1.50     |
| 16  | aA    | 3139 | LHG  | P-O6    | 2.95  | 1.71        | 1.59     |
| 14  | aA    | 3114 | CL7  | C1D-C2D | -2.95 | 1.36        | 1.43     |
| 14  | aA    | 3132 | CL7  | C1D-C2D | -2.95 | 1.36        | 1.43     |
| 14  | cB    | 827  | CL7  | CAA-C2A | -2.95 | 1.48        | 1.54     |
| 14  | aA    | 3104 | CL7  | CHB-C4A | -2.95 | 1.30        | 1.36     |
| 13  | bB    | 805  | PHO  | C1-C2   | 2.95  | 1.57        | 1.49     |
| 14  | aA    | 3104 | CL7  | C1C-NC  | 2.95  | 1.41        | 1.37     |
| 14  | cA    | 3127 | CL7  | C1D-C2D | -2.95 | 1.36        | 1.43     |
| 14  | aA    | 3133 | CL7  | C4-C3   | 2.94  | 1.58        | 1.50     |
| 16  | cA    | 3138 | LHG  | O2-C2   | -2.94 | 1.34        | 1.43     |
| 14  | bA    | 3128 | CL7  | CAB-C3B | -2.94 | 1.39        | 1.45     |
| 14  | cA    | 3128 | CL7  | C4B-NB  | -2.94 | 1.34        | 1.37     |
| 19  | cB    | 830  | LMG  | C3-C2   | 2.94  | 1.59        | 1.52     |
| 14  | bB    | 833  | CL7  | C4C-NC  | 2.94  | 1.41        | 1.37     |
| 14  | cK    | 101  | CL7  | OBD-CAD | -2.94 | 1.17        | 1.23     |
| 14  | aA    | 3126 | CL7  | MG-NC   | -2.94 | 2.00        | 2.05     |
| 14  | aB    | 3023 | CL7  | C1C-NC  | 2.94  | 1.41        | 1.37     |
| 14  | cA    | 3108 | CL7  | OBB-CAB | 2.94  | 1.28        | 1.22     |
| 14  | aB    | 3023 | CL7  | CHC-C1C | -2.94 | 1.32        | 1.38     |
| 14  | bB    | 826  | CL7  | C3B-C4B | -2.94 | 1.36        | 1.42     |
| 14  | aA    | 3141 | CL7  | CHD-C4C | -2.93 | 1.32        | 1.38     |
| 14  | aA    | 3130 | CL7  | OBB-CAB | 2.93  | 1.28        | 1.22     |
| 14  | cA    | 3142 | CL7  | CMD-C2D | -2.93 | 1.44        | 1.50     |
| 14  | bB    | 820  | CL7  | CAB-C3B | -2.93 | 1.39        | 1.45     |
| 14  | cA    | 3116 | CL7  | C1D-C2D | -2.93 | 1.36        | 1.43     |
| 14  | bK    | 101  | CL7  | OBB-CAB | 2.93  | 1.28        | 1.22     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | bA    | 3102 | CL7  | C1C-NC  | 2.93  | 1.41        | 1.37     |
| 14  | aA    | 3131 | CL7  | CHB-C4A | -2.93 | 1.30        | 1.36     |
| 14  | aA    | 3114 | CL7  | C4C-NC  | 2.93  | 1.41        | 1.37     |
| 14  | cA    | 3141 | CL7  | C1D-C2D | -2.93 | 1.36        | 1.43     |
| 14  | bA    | 3102 | CL7  | CBD-CGD | -2.93 | 1.43        | 1.52     |
| 14  | bA    | 3118 | CL7  | C1D-C2D | -2.93 | 1.36        | 1.43     |
| 14  | aJ    | 101  | CL7  | C1C-NC  | 2.93  | 1.41        | 1.37     |
| 13  | bB    | 801  | PHO  | C4B-NB  | -2.93 | 1.33        | 1.38     |
| 17  | aA    | 3144 | PQN  | C9-C10  | -2.93 | 1.35        | 1.39     |
| 14  | aB    | 3012 | CL7  | C1D-C2D | -2.93 | 1.36        | 1.43     |
| 14  | cB    | 813  | CL7  | C1D-C2D | -2.93 | 1.36        | 1.43     |
| 14  | cA    | 3123 | CL7  | O1D-CGD | -2.93 | 1.13        | 1.21     |
| 14  | aA    | 3110 | CL7  | C1C-NC  | 2.92  | 1.41        | 1.37     |
| 14  | bA    | 3132 | CL7  | CMA-C3A | 2.92  | 1.59        | 1.53     |
| 14  | bB    | 815  | CL7  | C4C-NC  | 2.92  | 1.41        | 1.37     |
| 14  | cJ    | 101  | CL7  | C1C-NC  | 2.92  | 1.41        | 1.37     |
| 14  | cB    | 823  | CL7  | CHC-C1C | -2.92 | 1.32        | 1.38     |
| 14  | aB    | 3030 | CL7  | CAB-C3B | -2.92 | 1.39        | 1.45     |
| 14  | cB    | 807  | CL7  | C1D-C2D | -2.92 | 1.36        | 1.43     |
| 14  | bB    | 831  | CL7  | CAB-C3B | -2.92 | 1.39        | 1.45     |
| 14  | bA    | 3106 | CL7  | CHD-C4C | -2.92 | 1.32        | 1.38     |
| 14  | aB    | 3014 | CL7  | CHC-C1C | -2.92 | 1.32        | 1.38     |
| 14  | aA    | 3127 | CL7  | CAB-C3B | -2.92 | 1.39        | 1.45     |
| 14  | cA    | 3105 | CL7  | C1D-C2D | -2.92 | 1.36        | 1.43     |
| 14  | bA    | 3132 | CL7  | C4D-ND  | -2.92 | 1.33        | 1.37     |
| 14  | aB    | 3025 | CL7  | C3B-C4B | -2.92 | 1.36        | 1.42     |
| 14  | cA    | 3131 | CL7  | CHC-C1C | -2.92 | 1.32        | 1.38     |
| 14  | bB    | 804  | CL7  | CAB-C3B | -2.92 | 1.39        | 1.45     |
| 14  | bA    | 3142 | CL7  | CAB-C3B | -2.91 | 1.39        | 1.45     |
| 14  | cA    | 3109 | CL7  | C1D-C2D | -2.91 | 1.36        | 1.43     |
| 14  | bA    | 3142 | CL7  | CHD-C4C | -2.91 | 1.32        | 1.38     |
| 14  | cA    | 3114 | CL7  | OBB-CAB | 2.91  | 1.28        | 1.22     |
| 14  | cA    | 3108 | CL7  | C3A-C4A | -2.91 | 1.47        | 1.52     |
| 14  | cB    | 810  | CL7  | CHD-C4C | -2.91 | 1.32        | 1.38     |
| 14  | cB    | 824  | CL7  | CHB-C4A | -2.91 | 1.30        | 1.36     |
| 14  | cB    | 818  | CL7  | C4C-NC  | 2.91  | 1.41        | 1.37     |
| 14  | cA    | 3113 | CL7  | C4C-NC  | 2.91  | 1.41        | 1.37     |
| 14  | aB    | 3006 | CL7  | C3B-C4B | -2.91 | 1.36        | 1.42     |
| 14  | cA    | 3118 | CL7  | C1D-C2D | -2.91 | 1.36        | 1.43     |
| 14  | bA    | 3107 | CL7  | OBB-CAB | 2.91  | 1.28        | 1.22     |
| 14  | bB    | 809  | CL7  | C4D-ND  | -2.91 | 1.33        | 1.37     |
| 14  | bB    | 813  | CL7  | C1D-C2D | -2.91 | 1.36        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | bA    | 3103 | CL7  | CHB-C4A | -2.91 | 1.30        | 1.36     |
| 14  | cA    | 3107 | CL7  | C2A-C1A | -2.91 | 1.46        | 1.50     |
| 14  | bA    | 3125 | CL7  | CHC-C1C | -2.91 | 1.32        | 1.38     |
| 14  | bA    | 3116 | CL7  | C1D-C2D | -2.91 | 1.36        | 1.43     |
| 14  | bB    | 821  | CL7  | OBB-CAB | 2.90  | 1.28        | 1.22     |
| 14  | bB    | 832  | CL7  | OBD-CAD | -2.90 | 1.17        | 1.22     |
| 14  | aA    | 3103 | CL7  | CBD-CGD | -2.90 | 1.43        | 1.52     |
| 14  | aB    | 3008 | CL7  | C3D-CAD | -2.90 | 1.35        | 1.45     |
| 14  | cB    | 803  | CL7  | C3A-C4A | -2.90 | 1.47        | 1.52     |
| 14  | bB    | 814  | CL7  | C1C-NC  | 2.90  | 1.41        | 1.37     |
| 14  | bB    | 833  | CL7  | CAB-C3B | -2.90 | 1.39        | 1.45     |
| 14  | cB    | 815  | CL7  | CHC-C1C | -2.90 | 1.32        | 1.38     |
| 14  | cA    | 3129 | CL7  | C4B-NB  | -2.90 | 1.34        | 1.37     |
| 14  | bA    | 3125 | CL7  | CAA-C2A | -2.90 | 1.48        | 1.54     |
| 14  | cK    | 101  | CL7  | OBB-CAB | 2.90  | 1.28        | 1.22     |
| 14  | cA    | 3140 | CL7  | C1D-C2D | -2.90 | 1.36        | 1.43     |
| 14  | bB    | 803  | CL7  | O2D-CGD | -2.90 | 1.26        | 1.33     |
| 14  | aA    | 3105 | CL7  | C1C-NC  | 2.89  | 1.41        | 1.37     |
| 14  | bB    | 809  | CL7  | C3D-CAD | -2.89 | 1.35        | 1.45     |
| 14  | bA    | 3121 | CL7  | OBB-CAB | 2.89  | 1.28        | 1.22     |
| 14  | aA    | 3134 | CL7  | OBB-CAB | 2.89  | 1.28        | 1.22     |
| 14  | bB    | 806  | CL7  | C4C-NC  | 2.89  | 1.41        | 1.37     |
| 14  | cA    | 3102 | CL7  | CAB-C3B | -2.89 | 1.39        | 1.45     |
| 14  | aA    | 3106 | CL7  | CMD-C2D | -2.89 | 1.44        | 1.50     |
| 14  | aB    | 3021 | CL7  | C1D-C2D | -2.89 | 1.36        | 1.43     |
| 14  | aA    | 3142 | CL7  | CHB-C4A | -2.89 | 1.30        | 1.36     |
| 14  | cA    | 3141 | CL7  | CHB-C4A | -2.89 | 1.30        | 1.36     |
| 14  | aB    | 3014 | CL7  | OBB-CAB | 2.89  | 1.28        | 1.22     |
| 14  | aB    | 3021 | CL7  | CHD-C4C | -2.89 | 1.32        | 1.38     |
| 14  | aA    | 3129 | CL7  | C1C-NC  | 2.89  | 1.41        | 1.37     |
| 14  | cB    | 825  | CL7  | OBB-CAB | 2.89  | 1.28        | 1.22     |
| 14  | cA    | 3132 | CL7  | CHD-C4C | -2.89 | 1.32        | 1.38     |
| 14  | aA    | 3115 | CL7  | C2A-C1A | -2.88 | 1.46        | 1.50     |
| 14  | cA    | 3124 | CL7  | C3A-C4A | -2.88 | 1.47        | 1.52     |
| 14  | cA    | 3139 | CL7  | C4C-NC  | 2.88  | 1.41        | 1.37     |
| 14  | bA    | 3124 | CL7  | CBA-CGA | -2.88 | 1.42        | 1.50     |
| 14  | aB    | 3019 | CL7  | C3A-C4A | -2.88 | 1.47        | 1.52     |
| 14  | aB    | 3032 | CL7  | C3B-C4B | -2.88 | 1.36        | 1.42     |
| 14  | bA    | 3124 | CL7  | C3A-C4A | -2.88 | 1.47        | 1.52     |
| 14  | bB    | 824  | CL7  | C1C-NC  | 2.88  | 1.41        | 1.37     |
| 14  | cB    | 814  | CL7  | C1C-NC  | 2.88  | 1.41        | 1.37     |
| 14  | cA    | 3120 | CL7  | CHD-C4C | -2.88 | 1.32        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | bB    | 808  | CL7  | C3D-CAD | -2.88 | 1.35        | 1.45     |
| 14  | cA    | 3140 | CL7  | CAB-C3B | -2.88 | 1.39        | 1.45     |
| 12  | aA    | 3101 | G9R  | OBD-CAD | 2.88  | 1.27        | 1.22     |
| 12  | bA    | 3101 | G9R  | C3D-C4D | -2.87 | 1.37        | 1.44     |
| 14  | aB    | 3003 | CL7  | CHC-C1C | -2.87 | 1.32        | 1.38     |
| 13  | bB    | 801  | PHO  | C3B-CAB | 2.87  | 1.53        | 1.47     |
| 14  | bA    | 3124 | CL7  | CHC-C1C | -2.87 | 1.32        | 1.38     |
| 14  | cB    | 816  | CL7  | C3D-CAD | -2.87 | 1.35        | 1.45     |
| 14  | bB    | 812  | CL7  | C2A-C1A | -2.87 | 1.47        | 1.52     |
| 14  | cA    | 3132 | CL7  | CMA-C3A | 2.87  | 1.59        | 1.53     |
| 14  | bA    | 3115 | CL7  | OBB-CAB | 2.87  | 1.28        | 1.22     |
| 14  | cB    | 833  | CL7  | CAB-C3B | -2.87 | 1.39        | 1.45     |
| 14  | bA    | 3128 | CL7  | C3D-CAD | -2.87 | 1.35        | 1.45     |
| 14  | bB    | 827  | CL7  | CAB-C3B | -2.87 | 1.39        | 1.45     |
| 14  | bB    | 820  | CL7  | C4C-NC  | 2.87  | 1.41        | 1.37     |
| 14  | cA    | 3142 | CL7  | CAB-C3B | -2.87 | 1.39        | 1.45     |
| 14  | cA    | 3128 | CL7  | CAB-C3B | -2.87 | 1.39        | 1.45     |
| 14  | cA    | 3116 | CL7  | CHC-C1C | -2.87 | 1.32        | 1.38     |
| 14  | cB    | 820  | CL7  | CAB-C3B | -2.87 | 1.39        | 1.45     |
| 14  | bA    | 3120 | CL7  | CHD-C4C | -2.87 | 1.32        | 1.38     |
| 14  | bA    | 3114 | CL7  | CHC-C1C | -2.87 | 1.32        | 1.38     |
| 14  | cB    | 807  | CL7  | C3B-C4B | -2.87 | 1.36        | 1.42     |
| 16  | bA    | 3138 | LHG  | P-O6    | 2.86  | 1.70        | 1.59     |
| 14  | cA    | 3124 | CL7  | CBA-CGA | -2.86 | 1.42        | 1.50     |
| 14  | aB    | 3007 | CL7  | C3D-CAD | -2.86 | 1.35        | 1.45     |
| 14  | cA    | 3106 | CL7  | CHD-C4C | -2.86 | 1.32        | 1.38     |
| 14  | bB    | 804  | CL7  | CHC-C1C | -2.86 | 1.32        | 1.38     |
| 14  | cA    | 3121 | CL7  | C4C-NC  | 2.86  | 1.41        | 1.37     |
| 14  | aB    | 3007 | CL7  | O2D-CGD | -2.86 | 1.26        | 1.33     |
| 14  | bB    | 825  | CL7  | C1D-C2D | -2.86 | 1.36        | 1.43     |
| 14  | aA    | 3108 | CL7  | OBB-CAB | 2.86  | 1.28        | 1.22     |
| 14  | cA    | 3108 | CL7  | C1D-C2D | -2.86 | 1.36        | 1.43     |
| 14  | cA    | 3115 | CL7  | OBB-CAB | 2.86  | 1.28        | 1.22     |
| 14  | cA    | 3125 | CL7  | OBB-CAB | 2.86  | 1.28        | 1.22     |
| 14  | aF    | 201  | CL7  | CHC-C1C | -2.85 | 1.32        | 1.38     |
| 14  | bA    | 3107 | CL7  | C1D-C2D | -2.85 | 1.36        | 1.43     |
| 14  | aA    | 3113 | CL7  | CHB-C4A | -2.85 | 1.30        | 1.36     |
| 14  | bA    | 3132 | CL7  | C4-C3   | 2.85  | 1.58        | 1.50     |
| 14  | aA    | 3121 | CL7  | CHB-C4A | -2.85 | 1.30        | 1.36     |
| 14  | cA    | 3104 | CL7  | C4C-NC  | 2.85  | 1.41        | 1.37     |
| 14  | cA    | 3124 | CL7  | C3D-C2D | -2.85 | 1.33        | 1.42     |
| 14  | cB    | 827  | CL7  | C3A-C4A | -2.85 | 1.47        | 1.52     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | aB    | 3020 | CL7  | OBB-CAB | 2.85  | 1.28        | 1.22     |
| 14  | aA    | 3141 | CL7  | CHC-C1C | -2.85 | 1.32        | 1.38     |
| 14  | bF    | 201  | CL7  | CHC-C1C | -2.85 | 1.32        | 1.38     |
| 14  | bB    | 827  | CL7  | C3B-C4B | -2.84 | 1.36        | 1.42     |
| 14  | bB    | 831  | CL7  | CAA-C2A | -2.84 | 1.48        | 1.54     |
| 14  | bA    | 3117 | CL7  | C1C-NC  | 2.84  | 1.41        | 1.37     |
| 14  | aA    | 3122 | CL7  | OBB-CAB | 2.84  | 1.28        | 1.22     |
| 14  | aB    | 3006 | CL7  | C1D-C2D | -2.84 | 1.36        | 1.43     |
| 14  | aB    | 3017 | CL7  | OBB-CAB | 2.84  | 1.28        | 1.22     |
| 14  | cA    | 3127 | CL7  | CAA-C2A | -2.84 | 1.48        | 1.54     |
| 14  | bA    | 3141 | CL7  | CAA-C2A | -2.84 | 1.48        | 1.54     |
| 14  | cA    | 3114 | CL7  | C2A-C1A | -2.84 | 1.46        | 1.50     |
| 14  | aA    | 3126 | CL7  | CHC-C1C | -2.84 | 1.32        | 1.38     |
| 14  | bA    | 3142 | CL7  | C3D-CAD | -2.84 | 1.35        | 1.45     |
| 14  | bB    | 827  | CL7  | C3D-C2D | -2.84 | 1.33        | 1.42     |
| 14  | aA    | 3104 | CL7  | C1D-C2D | -2.84 | 1.36        | 1.43     |
| 14  | aB    | 3032 | CL7  | O2D-CGD | -2.83 | 1.26        | 1.33     |
| 14  | cB    | 827  | CL7  | C3B-C4B | -2.83 | 1.36        | 1.42     |
| 14  | cL    | 203  | CL7  | C1C-NC  | 2.83  | 1.41        | 1.37     |
| 14  | bA    | 3103 | CL7  | C1C-NC  | 2.83  | 1.41        | 1.37     |
| 13  | bB    | 801  | PHO  | C3D-C4D | -2.83 | 1.37        | 1.41     |
| 14  | bK    | 101  | CL7  | C3D-CAD | -2.83 | 1.37        | 1.45     |
| 14  | cB    | 831  | CL7  | CHB-C4A | -2.83 | 1.30        | 1.36     |
| 14  | bL    | 204  | CL7  | C2A-C1A | -2.83 | 1.46        | 1.50     |
| 14  | cB    | 825  | CL7  | CHB-C4A | -2.83 | 1.30        | 1.36     |
| 14  | bA    | 3116 | CL7  | C4C-NC  | 2.83  | 1.41        | 1.37     |
| 14  | aA    | 3116 | CL7  | OBB-CAB | 2.83  | 1.28        | 1.22     |
| 16  | cA    | 3138 | LHG  | P-O6    | 2.83  | 1.70        | 1.59     |
| 12  | bA    | 3101 | G9R  | CHD-C4C | 2.83  | 1.45        | 1.39     |
| 14  | bF    | 201  | CL7  | OBB-CAB | 2.82  | 1.28        | 1.22     |
| 14  | cA    | 3130 | CL7  | OBB-CAB | 2.82  | 1.28        | 1.22     |
| 14  | cB    | 803  | CL7  | CAA-C2A | -2.82 | 1.48        | 1.54     |
| 14  | aL    | 203  | CL7  | C4D-ND  | -2.82 | 1.33        | 1.37     |
| 14  | cB    | 822  | CL7  | C1D-C2D | -2.82 | 1.36        | 1.43     |
| 14  | cB    | 812  | CL7  | C2A-C1A | -2.82 | 1.47        | 1.52     |
| 14  | cA    | 3125 | CL7  | MG-NC   | -2.82 | 2.00        | 2.05     |
| 14  | aA    | 3141 | CL7  | C1D-C2D | -2.82 | 1.36        | 1.43     |
| 14  | aA    | 3141 | CL7  | C1C-NC  | 2.82  | 1.41        | 1.37     |
| 14  | cB    | 827  | CL7  | C3C-C2C | -2.82 | 1.30        | 1.36     |
| 14  | aA    | 3120 | CL7  | CMA-C3A | 2.82  | 1.59        | 1.53     |
| 14  | bL    | 203  | CL7  | C3A-C4A | -2.82 | 1.47        | 1.52     |
| 14  | cA    | 3109 | CL7  | C1C-NC  | 2.82  | 1.41        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | bA    | 3113 | CL7  | C4C-NC  | 2.82  | 1.41        | 1.37     |
| 14  | bB    | 818  | CL7  | OBB-CAB | 2.82  | 1.28        | 1.22     |
| 14  | bA    | 3117 | CL7  | C4C-NC  | 2.82  | 1.41        | 1.37     |
| 14  | cF    | 201  | CL7  | CHC-C1C | -2.82 | 1.32        | 1.38     |
| 14  | cB    | 823  | CL7  | CAB-C3B | -2.82 | 1.39        | 1.45     |
| 14  | aA    | 3118 | CL7  | C1C-NC  | 2.81  | 1.41        | 1.37     |
| 14  | cA    | 3122 | CL7  | CHB-C4A | -2.81 | 1.30        | 1.36     |
| 14  | bB    | 822  | CL7  | C1D-C2D | -2.81 | 1.36        | 1.43     |
| 14  | aA    | 3110 | CL7  | C1D-C2D | -2.81 | 1.36        | 1.43     |
| 14  | aA    | 3112 | CL7  | OBB-CAB | 2.81  | 1.28        | 1.22     |
| 14  | aA    | 3103 | CL7  | C1A-NA  | -2.81 | 1.30        | 1.38     |
| 14  | aA    | 3120 | CL7  | C1D-ND  | -2.81 | 1.34        | 1.37     |
| 14  | aB    | 3009 | CL7  | C1D-ND  | -2.81 | 1.34        | 1.37     |
| 14  | bA    | 3129 | CL7  | MG-NA   | -2.81 | 2.00        | 2.05     |
| 14  | cB    | 814  | CL7  | OBB-CAB | 2.81  | 1.28        | 1.22     |
| 14  | aB    | 3025 | CL7  | C3C-C2C | -2.81 | 1.30        | 1.36     |
| 14  | aB    | 3024 | CL7  | CHB-C4A | -2.81 | 1.30        | 1.36     |
| 14  | aB    | 3009 | CL7  | CHD-C4C | -2.81 | 1.32        | 1.38     |
| 14  | bB    | 814  | CL7  | CHC-C1C | -2.81 | 1.32        | 1.38     |
| 12  | cA    | 3101 | G9R  | C1C-C2C | 2.81  | 1.50        | 1.44     |
| 14  | cB    | 819  | CL7  | C3D-CAD | -2.81 | 1.35        | 1.45     |
| 14  | cA    | 3133 | CL7  | CHC-C1C | -2.81 | 1.32        | 1.38     |
| 14  | cB    | 827  | CL7  | C3D-C2D | -2.80 | 1.33        | 1.42     |
| 14  | cA    | 3107 | CL7  | OBB-CAB | 2.80  | 1.28        | 1.22     |
| 14  | bA    | 3108 | CL7  | C1D-C2D | -2.80 | 1.36        | 1.43     |
| 14  | bA    | 3122 | CL7  | CHB-C4A | -2.80 | 1.30        | 1.36     |
| 14  | aA    | 3107 | CL7  | OBD-CAD | -2.80 | 1.17        | 1.22     |
| 14  | cL    | 204  | CL7  | C1A-NA  | -2.80 | 1.30        | 1.38     |
| 14  | cA    | 3117 | CL7  | C1C-NC  | 2.80  | 1.41        | 1.37     |
| 14  | cA    | 3118 | CL7  | OBD-CAD | -2.80 | 1.17        | 1.22     |
| 14  | cB    | 827  | CL7  | C4D-ND  | -2.80 | 1.33        | 1.37     |
| 14  | bB    | 822  | CL7  | CHC-C1C | -2.80 | 1.32        | 1.38     |
| 14  | cB    | 803  | CL7  | OBD-CAD | -2.80 | 1.17        | 1.22     |
| 14  | bA    | 3126 | CL7  | CAB-C3B | -2.80 | 1.39        | 1.45     |
| 14  | bA    | 3102 | CL7  | C1D-C2D | -2.80 | 1.36        | 1.43     |
| 14  | aA    | 3142 | CL7  | OBD-CAD | -2.80 | 1.17        | 1.22     |
| 14  | aF    | 201  | CL7  | OBB-CAB | 2.80  | 1.28        | 1.22     |
| 14  | bB    | 803  | CL7  | CAA-C2A | -2.80 | 1.48        | 1.54     |
| 14  | cB    | 810  | CL7  | OBB-CAB | 2.80  | 1.28        | 1.22     |
| 14  | aA    | 3142 | CL7  | C1D-C2D | -2.80 | 1.36        | 1.43     |
| 16  | aA    | 3139 | LHG  | O3-C3   | -2.80 | 1.34        | 1.44     |
| 14  | cB    | 820  | CL7  | O1D-CGD | -2.79 | 1.14        | 1.21     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | cB    | 820  | CL7  | C4C-NC  | 2.79  | 1.41        | 1.37     |
| 17  | aB    | 3027 | PQN  | C8-C9   | 2.79  | 1.44        | 1.38     |
| 14  | cA    | 3117 | CL7  | C4C-NC  | 2.79  | 1.41        | 1.37     |
| 14  | cB    | 826  | CL7  | C3D-CAD | -2.79 | 1.35        | 1.45     |
| 14  | bA    | 3129 | CL7  | C2A-C1A | -2.79 | 1.47        | 1.52     |
| 16  | bA    | 3137 | LHG  | O8-C6   | -2.79 | 1.38        | 1.45     |
| 14  | aA    | 3117 | CL7  | CHC-C1C | -2.79 | 1.32        | 1.38     |
| 14  | cB    | 826  | CL7  | C3D-C4D | -2.79 | 1.32        | 1.39     |
| 14  | aB    | 3011 | CL7  | C2A-C1A | -2.79 | 1.47        | 1.52     |
| 14  | cA    | 3107 | CL7  | CHC-C1C | -2.79 | 1.32        | 1.38     |
| 14  | bB    | 833  | CL7  | C1C-NC  | 2.79  | 1.41        | 1.37     |
| 14  | bA    | 3107 | CL7  | CHC-C1C | -2.79 | 1.32        | 1.38     |
| 14  | cA    | 3106 | CL7  | C3B-C4B | -2.79 | 1.36        | 1.42     |
| 14  | bB    | 826  | CL7  | C3D-C4D | -2.79 | 1.32        | 1.39     |
| 14  | bA    | 3102 | CL7  | O2D-CGD | -2.79 | 1.26        | 1.33     |
| 14  | aA    | 3116 | CL7  | OBD-CAD | -2.79 | 1.17        | 1.22     |
| 14  | aB    | 3009 | CL7  | OBB-CAB | 2.79  | 1.28        | 1.22     |
| 14  | cA    | 3127 | CL7  | OBB-CAB | 2.79  | 1.28        | 1.22     |
| 14  | bA    | 3133 | CL7  | C4C-NC  | 2.79  | 1.41        | 1.37     |
| 14  | aB    | 3026 | CL7  | OBD-CAD | -2.79 | 1.17        | 1.22     |
| 14  | bB    | 806  | CL7  | C3D-C2D | -2.79 | 1.33        | 1.42     |
| 14  | aA    | 3117 | CL7  | C1D-C2D | -2.79 | 1.36        | 1.43     |
| 14  | aA    | 3131 | CL7  | OBB-CAB | 2.79  | 1.28        | 1.22     |
| 14  | aB    | 3026 | CL7  | C3A-C4A | -2.78 | 1.47        | 1.52     |
| 14  | aB    | 3002 | CL7  | CAA-C2A | -2.78 | 1.48        | 1.54     |
| 14  | aA    | 3112 | CL7  | CHC-C1C | -2.78 | 1.33        | 1.38     |
| 14  | cA    | 3119 | CL7  | C3D-CAD | -2.78 | 1.35        | 1.45     |
| 14  | cB    | 816  | CL7  | CHC-C1C | -2.78 | 1.33        | 1.38     |
| 14  | aA    | 3108 | CL7  | C1D-C2D | -2.78 | 1.36        | 1.43     |
| 14  | aB    | 3010 | CL7  | OBD-CAD | -2.78 | 1.17        | 1.22     |
| 14  | bB    | 814  | CL7  | OBB-CAB | 2.78  | 1.28        | 1.22     |
| 14  | bA    | 3127 | CL7  | C3D-C2D | -2.78 | 1.33        | 1.42     |
| 17  | aB    | 3027 | PQN  | C2M-C2  | -2.78 | 1.44        | 1.50     |
| 14  | aB    | 3026 | CL7  | C1D-ND  | -2.78 | 1.34        | 1.37     |
| 14  | cA    | 3102 | CL7  | CHC-C1C | -2.78 | 1.33        | 1.38     |
| 14  | bA    | 3119 | CL7  | CMA-C3A | 2.78  | 1.59        | 1.53     |
| 14  | bA    | 3127 | CL7  | CHD-C4C | -2.78 | 1.33        | 1.38     |
| 14  | aB    | 3022 | CL7  | CAB-C3B | -2.78 | 1.39        | 1.45     |
| 14  | bB    | 810  | CL7  | C3B-C4B | -2.78 | 1.36        | 1.42     |
| 14  | aA    | 3104 | CL7  | C4C-NC  | 2.78  | 1.41        | 1.37     |
| 14  | bA    | 3133 | CL7  | CHD-C4C | -2.78 | 1.33        | 1.38     |
| 14  | bA    | 3139 | CL7  | C4C-NC  | 2.77  | 1.41        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | bA    | 3106 | CL7  | CHB-C4A | -2.77 | 1.30        | 1.36     |
| 14  | bA    | 3145 | CL7  | OBB-CAB | 2.77  | 1.28        | 1.22     |
| 14  | bL    | 203  | CL7  | C1D-C2D | -2.77 | 1.36        | 1.43     |
| 14  | bL    | 204  | CL7  | CBD-CGD | -2.77 | 1.43        | 1.52     |
| 14  | aA    | 3108 | CL7  | CHC-C1C | -2.77 | 1.33        | 1.38     |
| 14  | cB    | 832  | CL7  | C1C-NC  | 2.77  | 1.41        | 1.37     |
| 14  | aA    | 3103 | CL7  | O2D-CGD | -2.77 | 1.26        | 1.33     |
| 14  | bB    | 810  | CL7  | C1C-NC  | 2.77  | 1.41        | 1.37     |
| 14  | bB    | 815  | CL7  | C1D-C2D | -2.77 | 1.36        | 1.43     |
| 14  | aB    | 3008 | CL7  | CAA-C2A | -2.77 | 1.49        | 1.54     |
| 14  | bA    | 3109 | CL7  | OBB-CAB | 2.77  | 1.28        | 1.22     |
| 14  | bA    | 3130 | CL7  | OBB-CAB | 2.77  | 1.28        | 1.22     |
| 14  | cA    | 3133 | CL7  | CHD-C4C | -2.77 | 1.33        | 1.38     |
| 14  | aA    | 3111 | CL7  | C4C-NC  | 2.77  | 1.41        | 1.37     |
| 14  | bA    | 3141 | CL7  | OBD-CAD | -2.76 | 1.17        | 1.22     |
| 14  | bA    | 3133 | CL7  | CHC-C1C | -2.76 | 1.33        | 1.38     |
| 14  | cA    | 3133 | CL7  | C4C-NC  | 2.76  | 1.41        | 1.37     |
| 14  | cK    | 101  | CL7  | C3D-CAD | -2.76 | 1.38        | 1.45     |
| 14  | aA    | 3129 | CL7  | MG-ND   | -2.76 | 2.00        | 2.05     |
| 14  | aB    | 3007 | CL7  | C3A-C4A | -2.76 | 1.47        | 1.52     |
| 14  | aA    | 3114 | CL7  | OBB-CAB | 2.76  | 1.28        | 1.22     |
| 14  | bA    | 3114 | CL7  | OBB-CAB | 2.76  | 1.28        | 1.22     |
| 14  | bA    | 3105 | CL7  | C1D-C2D | -2.76 | 1.36        | 1.43     |
| 14  | cA    | 3142 | CL7  | C3D-CAD | -2.76 | 1.35        | 1.45     |
| 14  | bA    | 3102 | CL7  | O2A-C1  | 2.76  | 1.53        | 1.46     |
| 14  | bB    | 831  | CL7  | O2D-CGD | -2.76 | 1.26        | 1.33     |
| 17  | bB    | 828  | PQN  | C2M-C2  | -2.76 | 1.45        | 1.50     |
| 14  | cA    | 3108 | CL7  | C3D-CAD | -2.76 | 1.35        | 1.45     |
| 14  | bB    | 807  | CL7  | CHD-C4C | -2.76 | 1.33        | 1.38     |
| 14  | cB    | 806  | CL7  | OBB-CAB | 2.76  | 1.28        | 1.22     |
| 14  | aA    | 3129 | CL7  | CHB-C4A | -2.76 | 1.30        | 1.36     |
| 14  | cB    | 822  | CL7  | CHC-C1C | -2.75 | 1.33        | 1.38     |
| 14  | cA    | 3116 | CL7  | C4C-NC  | 2.75  | 1.41        | 1.37     |
| 14  | cB    | 815  | CL7  | OBB-CAB | 2.75  | 1.28        | 1.22     |
| 14  | cB    | 808  | CL7  | C3D-CAD | -2.75 | 1.35        | 1.45     |
| 14  | aB    | 3019 | CL7  | CAB-C3B | -2.75 | 1.39        | 1.45     |
| 14  | bB    | 826  | CL7  | C3D-CAD | -2.75 | 1.35        | 1.45     |
| 14  | bA    | 3127 | CL7  | CHB-C4A | -2.75 | 1.30        | 1.36     |
| 14  | cB    | 831  | CL7  | CAA-C2A | -2.75 | 1.49        | 1.54     |
| 14  | bB    | 831  | CL7  | CHB-C4A | -2.75 | 1.30        | 1.36     |
| 14  | bB    | 811  | CL7  | OBD-CAD | -2.75 | 1.17        | 1.22     |
| 14  | aA    | 3129 | CL7  | CAB-C3B | -2.75 | 1.39        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | aA    | 3126 | CL7  | C3A-C4A | -2.75 | 1.47        | 1.52     |
| 17  | cB    | 828  | PQN  | C2M-C2  | -2.75 | 1.45        | 1.50     |
| 14  | cA    | 3123 | CL7  | CHC-C1C | -2.75 | 1.33        | 1.38     |
| 14  | aL    | 203  | CL7  | CBD-CGD | -2.74 | 1.43        | 1.52     |
| 14  | cB    | 803  | CL7  | C1D-ND  | -2.74 | 1.34        | 1.37     |
| 14  | cA    | 3104 | CL7  | OBB-CAB | 2.74  | 1.28        | 1.22     |
| 14  | bB    | 822  | CL7  | CAB-C3B | -2.74 | 1.39        | 1.45     |
| 14  | aA    | 3103 | CL7  | C1C-NC  | 2.74  | 1.41        | 1.37     |
| 13  | cB    | 805  | PHO  | O1D-CGD | -2.74 | 1.14        | 1.21     |
| 14  | aB    | 3006 | CL7  | C1C-NC  | 2.74  | 1.41        | 1.37     |
| 14  | cB    | 833  | CL7  | C1C-NC  | 2.74  | 1.41        | 1.37     |
| 14  | bB    | 833  | CL7  | C3B-C4B | -2.74 | 1.36        | 1.42     |
| 14  | bA    | 3126 | CL7  | OBB-CAB | 2.74  | 1.28        | 1.22     |
| 14  | cA    | 3142 | CL7  | C1D-C2D | -2.74 | 1.36        | 1.43     |
| 14  | aJ    | 101  | CL7  | OBB-CAB | 2.74  | 1.28        | 1.22     |
| 14  | cA    | 3106 | CL7  | C3A-C4A | -2.73 | 1.47        | 1.52     |
| 14  | cB    | 807  | CL7  | C3A-C4A | -2.73 | 1.47        | 1.52     |
| 14  | bA    | 3104 | CL7  | OBB-CAB | 2.73  | 1.28        | 1.22     |
| 14  | cA    | 3109 | CL7  | OBB-CAB | 2.73  | 1.28        | 1.22     |
| 14  | cB    | 807  | CL7  | CHD-C4C | -2.73 | 1.33        | 1.38     |
| 14  | aB    | 3008 | CL7  | C4D-ND  | -2.73 | 1.33        | 1.37     |
| 14  | bB    | 831  | CL7  | C3B-C4B | -2.73 | 1.36        | 1.42     |
| 14  | aF    | 201  | CL7  | C1C-NC  | 2.73  | 1.41        | 1.37     |
| 14  | bA    | 3140 | CL7  | CAB-C3B | -2.73 | 1.39        | 1.45     |
| 14  | cB    | 803  | CL7  | C1D-C2D | -2.73 | 1.36        | 1.43     |
| 14  | bB    | 813  | CL7  | OBB-CAB | 2.73  | 1.28        | 1.22     |
| 14  | aB    | 3024 | CL7  | C1D-C2D | -2.73 | 1.36        | 1.43     |
| 14  | bA    | 3109 | CL7  | C1C-NC  | 2.73  | 1.41        | 1.37     |
| 14  | bA    | 3129 | CL7  | C3D-C2D | -2.73 | 1.33        | 1.42     |
| 14  | cA    | 3144 | CL7  | OBB-CAB | 2.73  | 1.28        | 1.22     |
| 14  | aB    | 3005 | CL7  | C3D-C2D | -2.73 | 1.33        | 1.42     |
| 12  | aA    | 3101 | G9R  | CHD-C4C | 2.73  | 1.45        | 1.39     |
| 14  | bL    | 203  | CL7  | OBD-CAD | -2.73 | 1.17        | 1.22     |
| 14  | aA    | 3143 | CL7  | CMD-C2D | -2.73 | 1.45        | 1.50     |
| 14  | bB    | 823  | CL7  | CAB-C3B | -2.72 | 1.39        | 1.45     |
| 14  | bB    | 818  | CL7  | C1D-C2D | -2.72 | 1.36        | 1.43     |
| 14  | cB    | 827  | CL7  | C1D-ND  | -2.72 | 1.34        | 1.37     |
| 14  | aB    | 3013 | CL7  | CHC-C1C | -2.72 | 1.33        | 1.38     |
| 14  | bB    | 815  | CL7  | CHC-C1C | -2.72 | 1.33        | 1.38     |
| 14  | cL    | 204  | CL7  | C3C-C2C | -2.72 | 1.30        | 1.36     |
| 14  | cB    | 809  | CL7  | C3D-CAD | -2.72 | 1.35        | 1.45     |
| 14  | cB    | 821  | CL7  | OBB-CAB | 2.72  | 1.28        | 1.22     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | aA    | 3109 | CL7  | C1D-C2D | -2.72 | 1.36        | 1.43     |
| 14  | aB    | 3012 | CL7  | OBB-CAB | 2.72  | 1.28        | 1.22     |
| 14  | bA    | 3104 | CL7  | C1C-NC  | 2.72  | 1.41        | 1.37     |
| 14  | bA    | 3129 | CL7  | C1C-NC  | 2.72  | 1.41        | 1.37     |
| 14  | cA    | 3111 | CL7  | CHC-C1C | -2.72 | 1.33        | 1.38     |
| 14  | bA    | 3124 | CL7  | C3D-C2D | -2.72 | 1.33        | 1.42     |
| 14  | bB    | 807  | CL7  | OBD-CAD | -2.72 | 1.17        | 1.22     |
| 14  | cB    | 807  | CL7  | OBD-CAD | -2.72 | 1.17        | 1.22     |
| 14  | cA    | 3117 | CL7  | C2A-C1A | -2.71 | 1.47        | 1.52     |
| 14  | aA    | 3146 | CL7  | OBB-CAB | 2.71  | 1.28        | 1.22     |
| 14  | aL    | 202  | CL7  | C1D-C2D | -2.71 | 1.36        | 1.43     |
| 14  | cA    | 3124 | CL7  | CAA-C2A | -2.71 | 1.49        | 1.54     |
| 14  | cA    | 3107 | CL7  | C1D-C2D | -2.71 | 1.36        | 1.43     |
| 14  | cA    | 3126 | CL7  | OBB-CAB | 2.71  | 1.28        | 1.22     |
| 14  | bB    | 812  | CL7  | CHB-C4A | -2.71 | 1.30        | 1.36     |
| 14  | bJ    | 101  | CL7  | CHC-C1C | -2.71 | 1.33        | 1.38     |
| 14  | cB    | 820  | CL7  | C3D-CAD | -2.71 | 1.36        | 1.45     |
| 14  | cA    | 3129 | CL7  | C1D-C2D | -2.71 | 1.36        | 1.43     |
| 14  | cB    | 831  | CL7  | CAB-C3B | -2.71 | 1.39        | 1.45     |
| 14  | cA    | 3109 | CL7  | CHC-C1C | -2.71 | 1.33        | 1.38     |
| 14  | cB    | 822  | CL7  | CHD-C4C | -2.71 | 1.33        | 1.38     |
| 12  | cA    | 3101 | G9R  | C4D-CHA | 2.71  | 1.48        | 1.38     |
| 14  | bA    | 3120 | CL7  | CHC-C1C | -2.71 | 1.33        | 1.38     |
| 14  | cB    | 814  | CL7  | CHC-C1C | -2.71 | 1.33        | 1.38     |
| 14  | aB    | 3032 | CL7  | C1C-NC  | 2.71  | 1.41        | 1.37     |
| 14  | bJ    | 101  | CL7  | OBB-CAB | 2.71  | 1.28        | 1.22     |
| 14  | aB    | 3032 | CL7  | C1D-ND  | -2.71 | 1.34        | 1.37     |
| 14  | aB    | 3021 | CL7  | CAB-C3B | -2.71 | 1.39        | 1.45     |
| 14  | aL    | 202  | CL7  | OBD-CAD | -2.71 | 1.17        | 1.22     |
| 14  | aB    | 3024 | CL7  | CHC-C1C | -2.70 | 1.33        | 1.38     |
| 14  | aL    | 204  | CL7  | C2A-C1A | -2.70 | 1.46        | 1.50     |
| 14  | bA    | 3142 | CL7  | C1D-C2D | -2.70 | 1.36        | 1.43     |
| 14  | bB    | 825  | CL7  | CHC-C1C | -2.70 | 1.33        | 1.38     |
| 14  | bA    | 3117 | CL7  | OBB-CAB | 2.70  | 1.28        | 1.22     |
| 14  | aB    | 3017 | CL7  | C1D-C2D | -2.70 | 1.36        | 1.43     |
| 14  | aA    | 3114 | CL7  | CAB-C3B | -2.70 | 1.39        | 1.45     |
| 14  | cA    | 3125 | CL7  | CAB-C3B | -2.70 | 1.39        | 1.45     |
| 14  | aA    | 3107 | CL7  | CHD-C4C | -2.70 | 1.33        | 1.38     |
| 14  | cF    | 201  | CL7  | OBB-CAB | 2.70  | 1.28        | 1.22     |
| 14  | cA    | 3140 | CL7  | O2D-CGD | -2.70 | 1.26        | 1.33     |
| 14  | aB    | 3013 | CL7  | OBB-CAB | 2.70  | 1.28        | 1.22     |
| 14  | bB    | 810  | CL7  | C3C-C2C | -2.70 | 1.30        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | aB    | 3002 | CL7  | C3D-CAD | -2.70 | 1.36        | 1.45     |
| 14  | cL    | 204  | CL7  | CBD-CGD | -2.70 | 1.44        | 1.52     |
| 14  | cA    | 3102 | CL7  | C1C-NC  | 2.70  | 1.41        | 1.37     |
| 14  | cA    | 3120 | CL7  | C1D-ND  | -2.70 | 1.34        | 1.37     |
| 14  | aB    | 3021 | CL7  | CHC-C1C | -2.70 | 1.33        | 1.38     |
| 14  | cB    | 808  | CL7  | O2D-CGD | -2.70 | 1.26        | 1.33     |
| 14  | cA    | 3114 | CL7  | CHC-C1C | -2.70 | 1.33        | 1.38     |
| 14  | cA    | 3116 | CL7  | C3D-CAD | -2.70 | 1.36        | 1.45     |
| 14  | cA    | 3102 | CL7  | C1A-NA  | -2.69 | 1.31        | 1.38     |
| 14  | aB    | 3012 | CL7  | C4C-NC  | 2.69  | 1.41        | 1.37     |
| 14  | aA    | 3133 | CL7  | CMA-C3A | 2.69  | 1.59        | 1.53     |
| 14  | cB    | 812  | CL7  | CHB-C4A | -2.69 | 1.30        | 1.36     |
| 12  | aA    | 3101 | G9R  | C3D-C4D | -2.69 | 1.38        | 1.44     |
| 14  | cA    | 3123 | CL7  | C4C-NC  | 2.69  | 1.41        | 1.37     |
| 14  | cA    | 3127 | CL7  | C3D-C2D | -2.69 | 1.33        | 1.42     |
| 14  | aB    | 3030 | CL7  | O2D-CGD | -2.69 | 1.26        | 1.33     |
| 14  | bB    | 815  | CL7  | OBB-CAB | 2.69  | 1.28        | 1.22     |
| 14  | aB    | 3008 | CL7  | CHC-C1C | -2.69 | 1.33        | 1.38     |
| 14  | aJ    | 101  | CL7  | CHC-C1C | -2.69 | 1.33        | 1.38     |
| 14  | aA    | 3118 | CL7  | OBB-CAB | 2.69  | 1.28        | 1.22     |
| 14  | cB    | 806  | CL7  | C3D-C2D | -2.69 | 1.33        | 1.42     |
| 14  | bA    | 3118 | CL7  | C3B-C4B | -2.69 | 1.36        | 1.42     |
| 14  | cB    | 810  | CL7  | C3B-C4B | -2.69 | 1.36        | 1.42     |
| 14  | bA    | 3116 | CL7  | CHC-C1C | -2.69 | 1.33        | 1.38     |
| 14  | cA    | 3110 | CL7  | CHD-C4C | -2.69 | 1.33        | 1.38     |
| 14  | aA    | 3128 | CL7  | CHD-C4C | -2.69 | 1.33        | 1.38     |
| 14  | bB    | 822  | CL7  | CHD-C4C | -2.69 | 1.33        | 1.38     |
| 14  | cB    | 806  | CL7  | CHB-C4A | -2.69 | 1.30        | 1.36     |
| 14  | aA    | 3141 | CL7  | C3B-C4B | -2.69 | 1.36        | 1.42     |
| 14  | cB    | 813  | CL7  | OBB-CAB | 2.69  | 1.28        | 1.22     |
| 14  | cB    | 807  | CL7  | C1C-NC  | 2.69  | 1.41        | 1.37     |
| 14  | bB    | 804  | CL7  | C1D-C2D | -2.68 | 1.36        | 1.43     |
| 14  | aA    | 3131 | CL7  | C1C-NC  | 2.68  | 1.41        | 1.37     |
| 14  | bB    | 808  | CL7  | CHB-C4A | -2.68 | 1.30        | 1.36     |
| 14  | aB    | 3003 | CL7  | CAB-C3B | -2.68 | 1.39        | 1.45     |
| 14  | bA    | 3110 | CL7  | CHB-C4A | -2.68 | 1.30        | 1.36     |
| 14  | bB    | 803  | CL7  | C1D-ND  | -2.68 | 1.34        | 1.37     |
| 14  | bB    | 803  | CL7  | C1D-C2D | -2.68 | 1.36        | 1.43     |
| 14  | bA    | 3139 | CL7  | C3B-C4B | -2.68 | 1.36        | 1.42     |
| 14  | aA    | 3113 | CL7  | C4C-NC  | 2.68  | 1.41        | 1.37     |
| 14  | aB    | 3032 | CL7  | CAB-C3B | -2.68 | 1.39        | 1.45     |
| 14  | aB    | 3006 | CL7  | OBD-CAD | -2.68 | 1.17        | 1.22     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | cA    | 3117 | CL7  | OBB-CAB | 2.68  | 1.28        | 1.22     |
| 14  | cB    | 827  | CL7  | OBD-CAD | -2.68 | 1.17        | 1.22     |
| 14  | aA    | 3140 | CL7  | CHC-C1C | -2.68 | 1.33        | 1.38     |
| 14  | bA    | 3119 | CL7  | C3D-CAD | -2.67 | 1.36        | 1.45     |
| 14  | bA    | 3104 | CL7  | C1D-C2D | -2.67 | 1.37        | 1.43     |
| 14  | bA    | 3133 | CL7  | CHB-C4A | -2.67 | 1.30        | 1.36     |
| 14  | aA    | 3125 | CL7  | CBA-CGA | -2.67 | 1.42        | 1.50     |
| 14  | bL    | 205  | CL7  | C2A-C1A | -2.67 | 1.46        | 1.50     |
| 14  | bB    | 824  | CL7  | C1D-C2D | -2.67 | 1.37        | 1.43     |
| 14  | cB    | 815  | CL7  | C1D-C2D | -2.67 | 1.37        | 1.43     |
| 14  | bB    | 820  | CL7  | C3D-CAD | -2.67 | 1.36        | 1.45     |
| 14  | cB    | 803  | CL7  | C3D-CAD | -2.67 | 1.36        | 1.45     |
| 14  | cB    | 813  | CL7  | C4C-NC  | 2.67  | 1.41        | 1.37     |
| 14  | aA    | 3109 | CL7  | C2A-C1A | -2.67 | 1.46        | 1.50     |
| 14  | bA    | 3133 | CL7  | C1D-C2D | -2.67 | 1.37        | 1.43     |
| 14  | bA    | 3110 | CL7  | CHD-C4C | -2.67 | 1.33        | 1.38     |
| 14  | aA    | 3129 | CL7  | C4D-ND  | -2.67 | 1.34        | 1.37     |
| 14  | bB    | 823  | CL7  | OBB-CAB | 2.67  | 1.28        | 1.22     |
| 14  | aK    | 101  | CL7  | C3D-CAD | -2.67 | 1.38        | 1.45     |
| 14  | cA    | 3125 | CL7  | OBD-CAD | -2.66 | 1.17        | 1.22     |
| 14  | aA    | 3130 | CL7  | CHC-C1C | -2.66 | 1.33        | 1.38     |
| 14  | aB    | 3011 | CL7  | CHB-C4A | -2.66 | 1.30        | 1.36     |
| 14  | cB    | 833  | CL7  | C4C-NC  | 2.66  | 1.41        | 1.37     |
| 14  | cA    | 3128 | CL7  | C3D-CAD | -2.66 | 1.36        | 1.45     |
| 14  | cB    | 804  | CL7  | C1D-C2D | -2.66 | 1.37        | 1.43     |
| 14  | aB    | 3025 | CL7  | C3D-C4D | -2.66 | 1.32        | 1.39     |
| 14  | aA    | 3104 | CL7  | CHC-C1C | -2.66 | 1.33        | 1.38     |
| 14  | bA    | 3119 | CL7  | C3B-C4B | -2.66 | 1.36        | 1.42     |
| 14  | bA    | 3128 | CL7  | O2A-CGA | 2.66  | 1.41        | 1.33     |
| 14  | aA    | 3111 | CL7  | CHB-C4A | -2.66 | 1.30        | 1.36     |
| 14  | bA    | 3129 | CL7  | CHC-C1C | -2.66 | 1.33        | 1.38     |
| 14  | bB    | 831  | CL7  | C4C-NC  | 2.66  | 1.41        | 1.37     |
| 14  | bB    | 803  | CL7  | C3D-CAD | -2.66 | 1.36        | 1.45     |
| 14  | cB    | 831  | CL7  | C3B-C4B | -2.66 | 1.36        | 1.42     |
| 14  | cA    | 3141 | CL7  | OBD-CAD | -2.66 | 1.17        | 1.22     |
| 14  | aB    | 3019 | CL7  | C4D-ND  | -2.66 | 1.34        | 1.37     |
| 14  | aB    | 3031 | CL7  | O2D-CED | -2.66 | 1.39        | 1.45     |
| 14  | cJ    | 101  | CL7  | CHC-C1C | -2.66 | 1.33        | 1.38     |
| 14  | aK    | 101  | CL7  | OBB-CAB | 2.66  | 1.28        | 1.22     |
| 14  | aB    | 3007 | CL7  | CHB-C4A | -2.66 | 1.30        | 1.36     |
| 14  | cA    | 3102 | CL7  | CHB-C4A | -2.66 | 1.30        | 1.36     |
| 14  | aL    | 203  | CL7  | CHC-C1C | -2.66 | 1.33        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | bB    | 817  | CL7  | OBB-CAB | 2.66  | 1.28        | 1.22     |
| 14  | bB    | 808  | CL7  | C3A-C4A | -2.66 | 1.47        | 1.52     |
| 14  | cA    | 3103 | CL7  | CHC-C1C | -2.65 | 1.33        | 1.38     |
| 14  | aA    | 3130 | CL7  | C1D-C2D | -2.65 | 1.37        | 1.43     |
| 14  | bA    | 3117 | CL7  | C2A-C1A | -2.65 | 1.47        | 1.52     |
| 14  | bB    | 809  | CL7  | MG-NB   | -2.65 | 2.00        | 2.05     |
| 14  | aB    | 3019 | CL7  | C3D-CAD | -2.65 | 1.36        | 1.45     |
| 14  | aB    | 3016 | CL7  | OBB-CAB | 2.65  | 1.28        | 1.22     |
| 12  | cA    | 3101 | G9R  | CMB-C2B | -2.65 | 1.45        | 1.50     |
| 14  | bA    | 3139 | CL7  | C3D-CAD | -2.65 | 1.36        | 1.45     |
| 14  | aA    | 3114 | CL7  | C1C-NC  | 2.65  | 1.41        | 1.37     |
| 14  | aL    | 203  | CL7  | C3C-C2C | -2.65 | 1.31        | 1.36     |
| 14  | bB    | 816  | CL7  | CBD-CGD | -2.65 | 1.44        | 1.52     |
| 14  | cF    | 201  | CL7  | C1D-C2D | -2.65 | 1.37        | 1.43     |
| 14  | aA    | 3141 | CL7  | CAB-C3B | -2.65 | 1.39        | 1.45     |
| 14  | bB    | 814  | CL7  | C1D-C2D | -2.65 | 1.37        | 1.43     |
| 14  | aA    | 3129 | CL7  | OBB-CAB | 2.65  | 1.28        | 1.22     |
| 14  | bA    | 3102 | CL7  | CHB-C4A | -2.65 | 1.30        | 1.36     |
| 14  | bA    | 3127 | CL7  | CAA-C2A | -2.65 | 1.49        | 1.54     |
| 14  | cA    | 3104 | CL7  | C1C-NC  | 2.65  | 1.41        | 1.37     |
| 14  | cA    | 3132 | CL7  | C4-C3   | 2.65  | 1.57        | 1.50     |
| 14  | bB    | 810  | CL7  | CMA-C3A | 2.65  | 1.58        | 1.53     |
| 14  | cB    | 833  | CL7  | CAA-C2A | -2.65 | 1.49        | 1.54     |
| 14  | aB    | 3030 | CL7  | CHD-C4C | -2.65 | 1.33        | 1.38     |
| 14  | aA    | 3120 | CL7  | C3D-CAD | -2.65 | 1.36        | 1.45     |
| 14  | bB    | 832  | CL7  | C3D-CAD | -2.65 | 1.36        | 1.45     |
| 14  | cA    | 3110 | CL7  | CHB-C4A | -2.65 | 1.30        | 1.36     |
| 14  | cA    | 3123 | CL7  | CHB-C4A | -2.65 | 1.30        | 1.36     |
| 14  | cB    | 814  | CL7  | C1D-C2D | -2.64 | 1.37        | 1.43     |
| 16  | aA    | 3138 | LHG  | O7-C5   | -2.64 | 1.40        | 1.46     |
| 12  | aA    | 3101 | G9R  | MG-NB   | -2.64 | 2.00        | 2.05     |
| 14  | aB    | 3005 | CL7  | OBB-CAB | 2.64  | 1.28        | 1.22     |
| 14  | bB    | 803  | CL7  | C4C-NC  | 2.64  | 1.41        | 1.37     |
| 17  | cA    | 3143 | PQN  | C5-C4   | -2.64 | 1.43        | 1.48     |
| 14  | bA    | 3125 | CL7  | CAB-C3B | -2.64 | 1.39        | 1.45     |
| 14  | aA    | 3126 | CL7  | CBD-CGD | -2.64 | 1.44        | 1.52     |
| 14  | bA    | 3145 | CL7  | CHC-C1C | -2.64 | 1.33        | 1.38     |
| 14  | cB    | 822  | CL7  | O2D-CGD | -2.64 | 1.26        | 1.33     |
| 14  | bB    | 818  | CL7  | CHC-C1C | -2.64 | 1.33        | 1.38     |
| 13  | cB    | 801  | PHO  | C3B-CAB | 2.64  | 1.53        | 1.47     |
| 14  | cB    | 822  | CL7  | C2A-C1A | -2.64 | 1.47        | 1.52     |
| 14  | aB    | 3007 | CL7  | C1D-ND  | -2.64 | 1.34        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | cB    | 832  | CL7  | C3D-CAD | -2.64 | 1.36        | 1.45     |
| 12  | aA    | 3101 | G9R  | CMD-C2D | -2.64 | 1.45        | 1.50     |
| 14  | bA    | 3110 | CL7  | C1D-C2D | -2.64 | 1.37        | 1.43     |
| 14  | cA    | 3127 | CL7  | CHC-C1C | -2.64 | 1.33        | 1.38     |
| 14  | aA    | 3110 | CL7  | CHC-C1C | -2.64 | 1.33        | 1.38     |
| 14  | bA    | 3103 | CL7  | CHC-C1C | -2.63 | 1.33        | 1.38     |
| 14  | cA    | 3107 | CL7  | C3A-C4A | -2.63 | 1.47        | 1.52     |
| 14  | cA    | 3132 | CL7  | O2A-CGA | 2.63  | 1.41        | 1.33     |
| 14  | cB    | 809  | CL7  | MG-NB   | -2.63 | 2.00        | 2.05     |
| 14  | cB    | 833  | CL7  | C3B-C4B | -2.63 | 1.36        | 1.42     |
| 14  | aB    | 3005 | CL7  | C3D-CAD | -2.63 | 1.36        | 1.45     |
| 14  | aA    | 3110 | CL7  | OBB-CAB | 2.63  | 1.28        | 1.22     |
| 14  | cB    | 825  | CL7  | CHC-C1C | -2.63 | 1.33        | 1.38     |
| 14  | aL    | 203  | CL7  | C2A-C1A | -2.63 | 1.46        | 1.50     |
| 14  | aA    | 3119 | CL7  | OBD-CAD | -2.63 | 1.17        | 1.22     |
| 14  | bA    | 3110 | CL7  | OBB-CAB | 2.63  | 1.28        | 1.22     |
| 14  | cB    | 816  | CL7  | C3A-C4A | -2.63 | 1.47        | 1.52     |
| 14  | aA    | 3130 | CL7  | C2A-C1A | -2.63 | 1.47        | 1.52     |
| 14  | aA    | 3115 | CL7  | CHC-C1C | -2.63 | 1.33        | 1.38     |
| 14  | bB    | 815  | CL7  | C1C-NC  | 2.63  | 1.41        | 1.37     |
| 14  | cF    | 201  | CL7  | C1C-NC  | 2.63  | 1.41        | 1.37     |
| 14  | aB    | 3022 | CL7  | OBB-CAB | 2.63  | 1.28        | 1.22     |
| 14  | bB    | 806  | CL7  | C1D-C2D | -2.63 | 1.37        | 1.43     |
| 14  | cJ    | 101  | CL7  | OBB-CAB | 2.62  | 1.28        | 1.22     |
| 14  | bB    | 813  | CL7  | C4C-NC  | 2.62  | 1.41        | 1.37     |
| 14  | cA    | 3112 | CL7  | CHC-C1C | -2.62 | 1.33        | 1.38     |
| 14  | bB    | 816  | CL7  | C3A-C4A | -2.62 | 1.47        | 1.52     |
| 14  | bA    | 3109 | CL7  | CHC-C1C | -2.62 | 1.33        | 1.38     |
| 14  | bF    | 201  | CL7  | C1D-C2D | -2.62 | 1.37        | 1.43     |
| 14  | aA    | 3125 | CL7  | C3D-C2D | -2.62 | 1.34        | 1.42     |
| 14  | cB    | 804  | CL7  | C3D-C2D | -2.62 | 1.34        | 1.42     |
| 14  | bB    | 832  | CL7  | C1C-NC  | 2.62  | 1.41        | 1.37     |
| 14  | aA    | 3129 | CL7  | C4B-NB  | -2.62 | 1.34        | 1.37     |
| 14  | bB    | 811  | CL7  | C2A-C1A | -2.62 | 1.47        | 1.52     |
| 14  | cB    | 806  | CL7  | C1D-C2D | -2.62 | 1.37        | 1.43     |
| 14  | aA    | 3128 | CL7  | CHC-C1C | -2.62 | 1.33        | 1.38     |
| 14  | aB    | 3026 | CL7  | CAB-C3B | -2.62 | 1.39        | 1.45     |
| 14  | aA    | 3121 | CL7  | CHC-C1C | -2.62 | 1.33        | 1.38     |
| 14  | cA    | 3106 | CL7  | CHB-C4A | -2.62 | 1.30        | 1.36     |
| 14  | aB    | 3013 | CL7  | C1D-C2D | -2.62 | 1.37        | 1.43     |
| 14  | bA    | 3111 | CL7  | CHC-C1C | -2.61 | 1.33        | 1.38     |
| 14  | bF    | 201  | CL7  | C1C-NC  | 2.61  | 1.41        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | cA    | 3108 | CL7  | C3B-C4B | -2.61 | 1.36        | 1.42     |
| 14  | cL    | 203  | CL7  | C1D-C2D | -2.61 | 1.37        | 1.43     |
| 14  | aB    | 3018 | CL7  | CHC-C1C | -2.61 | 1.33        | 1.38     |
| 14  | aB    | 3009 | CL7  | C3B-C4B | -2.61 | 1.36        | 1.42     |
| 14  | bB    | 813  | CL7  | CHC-C1C | -2.61 | 1.33        | 1.38     |
| 14  | cB    | 810  | CL7  | C3C-C2C | -2.61 | 1.31        | 1.36     |
| 14  | cA    | 3104 | CL7  | C1D-C2D | -2.61 | 1.37        | 1.43     |
| 14  | bB    | 831  | CL7  | CHD-C4C | -2.61 | 1.33        | 1.38     |
| 14  | bA    | 3120 | CL7  | CAA-C2A | -2.61 | 1.49        | 1.54     |
| 14  | bA    | 3124 | CL7  | C2A-C1A | -2.61 | 1.46        | 1.50     |
| 14  | bA    | 3130 | CL7  | C1C-NC  | 2.61  | 1.41        | 1.37     |
| 14  | cA    | 3130 | CL7  | CHD-C4C | -2.61 | 1.33        | 1.38     |
| 14  | bA    | 3130 | CL7  | CHD-C4C | -2.61 | 1.33        | 1.38     |
| 14  | bA    | 3132 | CL7  | O2A-CGA | 2.61  | 1.41        | 1.33     |
| 14  | aB    | 3017 | CL7  | CHC-C1C | -2.61 | 1.33        | 1.38     |
| 14  | cA    | 3133 | CL7  | C1D-C2D | -2.61 | 1.37        | 1.43     |
| 13  | cB    | 805  | PHO  | C4C-NC  | -2.61 | 1.29        | 1.37     |
| 14  | aA    | 3132 | CL7  | CHC-C1C | -2.61 | 1.33        | 1.38     |
| 14  | bB    | 808  | CL7  | C3C-C2C | -2.61 | 1.31        | 1.36     |
| 14  | aB    | 3009 | CL7  | C3C-C2C | -2.61 | 1.31        | 1.36     |
| 14  | cA    | 3114 | CL7  | C3A-C4A | -2.60 | 1.47        | 1.52     |
| 14  | cB    | 823  | CL7  | OBB-CAB | 2.60  | 1.28        | 1.22     |
| 14  | cA    | 3127 | CL7  | CHB-C4A | -2.60 | 1.31        | 1.36     |
| 14  | cA    | 3123 | CL7  | C1C-NC  | 2.60  | 1.41        | 1.37     |
| 14  | cB    | 831  | CL7  | OBB-CAB | 2.60  | 1.28        | 1.22     |
| 14  | bB    | 833  | CL7  | O2D-CGD | -2.60 | 1.26        | 1.33     |
| 14  | aA    | 3142 | CL7  | OBB-CAB | 2.60  | 1.28        | 1.22     |
| 14  | aB    | 3015 | CL7  | C1C-NC  | 2.60  | 1.41        | 1.37     |
| 14  | bB    | 804  | CL7  | C4C-NC  | 2.60  | 1.41        | 1.37     |
| 14  | bL    | 203  | CL7  | C3D-CAD | -2.60 | 1.36        | 1.45     |
| 14  | cF    | 201  | CL7  | CAB-C3B | -2.60 | 1.39        | 1.45     |
| 14  | cA    | 3119 | CL7  | C3B-C4B | -2.60 | 1.36        | 1.42     |
| 14  | bA    | 3116 | CL7  | C3D-CAD | -2.60 | 1.36        | 1.45     |
| 14  | bA    | 3106 | CL7  | C1D-ND  | -2.60 | 1.34        | 1.37     |
| 14  | cB    | 822  | CL7  | OBD-CAD | -2.60 | 1.18        | 1.22     |
| 14  | bA    | 3127 | CL7  | OBB-CAB | 2.60  | 1.28        | 1.22     |
| 14  | cJ    | 101  | CL7  | CHB-C4A | -2.60 | 1.31        | 1.36     |
| 14  | aA    | 3106 | CL7  | C1D-C2D | -2.60 | 1.37        | 1.43     |
| 14  | cB    | 815  | CL7  | C1C-NC  | 2.60  | 1.41        | 1.37     |
| 14  | cA    | 3139 | CL7  | C3D-CAD | -2.60 | 1.36        | 1.45     |
| 14  | bB    | 827  | CL7  | C2A-C1A | -2.60 | 1.46        | 1.50     |
| 14  | cB    | 820  | CL7  | C4D-ND  | -2.59 | 1.34        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | aB    | 3030 | CL7  | CHB-C4A | -2.59 | 1.31        | 1.36     |
| 14  | cA    | 3114 | CL7  | C1D-ND  | -2.59 | 1.34        | 1.37     |
| 14  | aB    | 3031 | CL7  | C3D-CAD | -2.59 | 1.36        | 1.45     |
| 14  | aA    | 3105 | CL7  | CHC-C1C | -2.59 | 1.33        | 1.38     |
| 14  | bA    | 3140 | CL7  | C1C-NC  | 2.59  | 1.41        | 1.37     |
| 14  | cL    | 203  | CL7  | OBD-CAD | -2.59 | 1.18        | 1.22     |
| 14  | bA    | 3110 | CL7  | C3D-CAD | -2.59 | 1.36        | 1.45     |
| 14  | bA    | 3139 | CL7  | C1D-C2D | -2.59 | 1.37        | 1.43     |
| 14  | cB    | 831  | CL7  | O2D-CGD | -2.59 | 1.26        | 1.33     |
| 14  | cB    | 831  | CL7  | C4C-NC  | 2.59  | 1.41        | 1.37     |
| 14  | cA    | 3132 | CL7  | C3A-C4A | -2.59 | 1.47        | 1.52     |
| 14  | cA    | 3131 | CL7  | CHD-C4C | -2.59 | 1.33        | 1.38     |
| 14  | cA    | 3110 | CL7  | C1D-C2D | -2.59 | 1.37        | 1.43     |
| 14  | aA    | 3128 | CL7  | C3D-C2D | -2.59 | 1.34        | 1.42     |
| 14  | bB    | 825  | CL7  | C3D-CAD | -2.59 | 1.36        | 1.45     |
| 14  | aA    | 3109 | CL7  | C1C-NC  | 2.59  | 1.41        | 1.37     |
| 14  | aB    | 3003 | CL7  | O2D-CGD | -2.59 | 1.26        | 1.33     |
| 14  | aA    | 3128 | CL7  | C1B-NB  | 2.58  | 1.41        | 1.37     |
| 14  | bA    | 3117 | CL7  | CHB-C4A | -2.58 | 1.31        | 1.36     |
| 14  | cA    | 3107 | CL7  | C3D-CAD | -2.58 | 1.36        | 1.45     |
| 14  | aA    | 3112 | CL7  | C1D-C2D | -2.58 | 1.37        | 1.43     |
| 14  | aB    | 3014 | CL7  | CAB-C3B | -2.58 | 1.39        | 1.45     |
| 14  | bF    | 201  | CL7  | CAB-C3B | -2.58 | 1.39        | 1.45     |
| 14  | aB    | 3025 | CL7  | MG-NA   | -2.58 | 2.00        | 2.05     |
| 14  | aF    | 201  | CL7  | C1D-C2D | -2.58 | 1.37        | 1.43     |
| 14  | bB    | 827  | CL7  | C4D-ND  | -2.58 | 1.34        | 1.37     |
| 14  | aA    | 3109 | CL7  | C3D-CAD | -2.58 | 1.36        | 1.45     |
| 14  | cB    | 817  | CL7  | OBB-CAB | 2.58  | 1.28        | 1.22     |
| 14  | cA    | 3102 | CL7  | O2A-C1  | 2.58  | 1.53        | 1.46     |
| 14  | aA    | 3143 | CL7  | C3D-CAD | -2.58 | 1.36        | 1.45     |
| 14  | aB    | 3008 | CL7  | OBB-CAB | 2.58  | 1.28        | 1.22     |
| 14  | cA    | 3144 | CL7  | CHC-C1C | -2.58 | 1.33        | 1.38     |
| 14  | aA    | 3146 | CL7  | CHC-C1C | -2.58 | 1.33        | 1.38     |
| 14  | cB    | 803  | CL7  | C4C-NC  | 2.58  | 1.41        | 1.37     |
| 14  | bB    | 812  | CL7  | OBB-CAB | 2.58  | 1.28        | 1.22     |
| 14  | bB    | 806  | CL7  | CHB-C4A | -2.58 | 1.31        | 1.36     |
| 14  | aA    | 3105 | CL7  | C1D-C2D | -2.58 | 1.37        | 1.43     |
| 14  | cA    | 3116 | CL7  | CHB-C4A | -2.58 | 1.31        | 1.36     |
| 14  | aB    | 3014 | CL7  | C1D-C2D | -2.57 | 1.37        | 1.43     |
| 14  | bB    | 820  | CL7  | C4D-ND  | -2.57 | 1.34        | 1.37     |
| 14  | cA    | 3109 | CL7  | CHB-C4A | -2.57 | 1.31        | 1.36     |
| 14  | cA    | 3106 | CL7  | OBB-CAB | 2.57  | 1.28        | 1.22     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | aB    | 3023 | CL7  | C1D-C2D | -2.57 | 1.37        | 1.43     |
| 14  | cA    | 3113 | CL7  | CAB-C3B | -2.57 | 1.39        | 1.45     |
| 14  | aB    | 3022 | CL7  | CHB-C4A | -2.57 | 1.31        | 1.36     |
| 14  | cA    | 3141 | CL7  | C3D-CAD | -2.57 | 1.36        | 1.45     |
| 14  | bB    | 810  | CL7  | CHC-C1C | -2.57 | 1.33        | 1.38     |
| 14  | cA    | 3105 | CL7  | C3A-C4A | -2.57 | 1.47        | 1.52     |
| 14  | cA    | 3119 | CL7  | CMA-C3A | 2.57  | 1.58        | 1.53     |
| 14  | aB    | 3011 | CL7  | OBB-CAB | 2.57  | 1.28        | 1.22     |
| 14  | aB    | 3003 | CL7  | O2A-C1  | 2.57  | 1.53        | 1.46     |
| 14  | aA    | 3124 | CL7  | C1D-ND  | -2.56 | 1.34        | 1.37     |
| 14  | aA    | 3111 | CL7  | C1D-C2D | -2.56 | 1.37        | 1.43     |
| 13  | cB    | 805  | PHO  | C3B-C4B | 2.56  | 1.44        | 1.41     |
| 14  | aB    | 3005 | CL7  | CHB-C4A | -2.56 | 1.31        | 1.36     |
| 14  | cA    | 3110 | CL7  | OBB-CAB | 2.56  | 1.28        | 1.22     |
| 14  | aB    | 3009 | CL7  | C1C-NC  | 2.56  | 1.40        | 1.37     |
| 14  | bK    | 101  | CL7  | C1D-C2D | -2.56 | 1.37        | 1.43     |
| 14  | cA    | 3126 | CL7  | CAB-C3B | -2.56 | 1.39        | 1.45     |
| 14  | aB    | 3024 | CL7  | C3D-CAD | -2.56 | 1.36        | 1.45     |
| 14  | cB    | 831  | CL7  | CHD-C4C | -2.56 | 1.33        | 1.38     |
| 14  | bA    | 3128 | CL7  | C4B-NB  | -2.56 | 1.34        | 1.37     |
| 17  | bB    | 828  | PQN  | C8-C9   | 2.56  | 1.44        | 1.38     |
| 14  | aA    | 3143 | CL7  | CAB-C3B | -2.56 | 1.39        | 1.45     |
| 14  | aA    | 3117 | CL7  | CHD-C4C | -2.56 | 1.33        | 1.38     |
| 14  | bB    | 806  | CL7  | C3D-CAD | -2.56 | 1.36        | 1.45     |
| 14  | bA    | 3117 | CL7  | CHC-C1C | -2.56 | 1.33        | 1.38     |
| 14  | cA    | 3112 | CL7  | OBB-CAB | 2.56  | 1.28        | 1.22     |
| 14  | cA    | 3140 | CL7  | C1C-NC  | 2.56  | 1.40        | 1.37     |
| 14  | bA    | 3125 | CL7  | C3A-C4A | -2.56 | 1.47        | 1.52     |
| 14  | bB    | 817  | CL7  | CHC-C1C | -2.56 | 1.33        | 1.38     |
| 14  | aB    | 3025 | CL7  | C3D-CAD | -2.56 | 1.36        | 1.45     |
| 14  | cB    | 824  | CL7  | C1D-C2D | -2.56 | 1.37        | 1.43     |
| 14  | bB    | 807  | CL7  | C3A-C4A | -2.55 | 1.47        | 1.52     |
| 14  | aA    | 3130 | CL7  | MG-NA   | -2.55 | 2.00        | 2.05     |
| 14  | bA    | 3112 | CL7  | OBB-CAB | 2.55  | 1.27        | 1.22     |
| 14  | cB    | 818  | CL7  | C1D-C2D | -2.55 | 1.37        | 1.43     |
| 14  | bA    | 3114 | CL7  | C6-C5   | -2.55 | 1.42        | 1.52     |
| 14  | cB    | 816  | CL7  | C1C-NC  | 2.55  | 1.40        | 1.37     |
| 14  | cA    | 3125 | CL7  | C3A-C4A | -2.55 | 1.47        | 1.52     |
| 14  | aF    | 201  | CL7  | CAB-C3B | -2.55 | 1.39        | 1.45     |
| 14  | bA    | 3112 | CL7  | CHC-C1C | -2.55 | 1.33        | 1.38     |
| 14  | bB    | 804  | CL7  | CHB-C4A | -2.55 | 1.31        | 1.36     |
| 14  | aA    | 3109 | CL7  | CHB-C4A | -2.55 | 1.31        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | bA    | 3118 | CL7  | CHC-C1C | -2.55 | 1.33        | 1.38     |
| 14  | cA    | 3125 | CL7  | C3D-C4D | -2.55 | 1.33        | 1.39     |
| 14  | aA    | 3126 | CL7  | CHB-C4A | -2.55 | 1.31        | 1.36     |
| 14  | aB    | 3026 | CL7  | CMD-C2D | -2.55 | 1.45        | 1.50     |
| 14  | aA    | 3140 | CL7  | C3D-CAD | -2.55 | 1.36        | 1.45     |
| 14  | bA    | 3116 | CL7  | CBD-CGD | -2.55 | 1.44        | 1.52     |
| 14  | bA    | 3105 | CL7  | C3A-C4A | -2.55 | 1.47        | 1.52     |
| 19  | bB    | 830  | LMG  | C3-C2   | 2.54  | 1.58        | 1.52     |
| 14  | bA    | 3132 | CL7  | CBD-CGD | -2.54 | 1.44        | 1.52     |
| 14  | cB    | 813  | CL7  | CHB-C4A | -2.54 | 1.31        | 1.36     |
| 14  | aA    | 3125 | CL7  | C4C-NC  | 2.54  | 1.40        | 1.37     |
| 14  | cA    | 3104 | CL7  | CHC-C1C | -2.54 | 1.33        | 1.38     |
| 14  | cJ    | 101  | CL7  | C1D-C2D | -2.54 | 1.37        | 1.43     |
| 14  | aA    | 3108 | CL7  | C3A-C4A | -2.54 | 1.47        | 1.52     |
| 14  | bA    | 3112 | CL7  | C4C-NC  | 2.54  | 1.40        | 1.37     |
| 14  | aA    | 3133 | CL7  | C4D-ND  | -2.54 | 1.34        | 1.37     |
| 14  | cA    | 3103 | CL7  | C4C-NC  | 2.54  | 1.40        | 1.37     |
| 14  | cB    | 809  | CL7  | CHD-C4C | -2.54 | 1.33        | 1.38     |
| 14  | bA    | 3131 | CL7  | CHD-C4C | -2.54 | 1.33        | 1.38     |
| 14  | bB    | 822  | CL7  | C2A-C1A | -2.54 | 1.47        | 1.52     |
| 14  | aA    | 3111 | CL7  | CHD-C4C | -2.54 | 1.33        | 1.38     |
| 14  | bA    | 3109 | CL7  | CHB-C4A | -2.54 | 1.31        | 1.36     |
| 14  | cA    | 3117 | CL7  | CHB-C4A | -2.54 | 1.31        | 1.36     |
| 14  | bB    | 810  | CL7  | OBb-CAB | 2.54  | 1.27        | 1.22     |
| 14  | aB    | 3006 | CL7  | C3A-C4A | -2.54 | 1.47        | 1.52     |
| 14  | cB    | 818  | CL7  | CHC-C1C | -2.54 | 1.33        | 1.38     |
| 14  | bB    | 821  | CL7  | CHC-C1C | -2.54 | 1.33        | 1.38     |
| 14  | cA    | 3130 | CL7  | C1C-NC  | 2.54  | 1.40        | 1.37     |
| 14  | cB    | 826  | CL7  | MG-NA   | -2.54 | 2.00        | 2.05     |
| 14  | bL    | 205  | CL7  | C1A-NA  | -2.54 | 1.31        | 1.38     |
| 17  | cB    | 828  | PQN  | C3-C4   | -2.53 | 1.40        | 1.47     |
| 14  | bB    | 826  | CL7  | O2D-CGD | -2.53 | 1.27        | 1.33     |
| 14  | aA    | 3123 | CL7  | CHC-C1C | -2.53 | 1.33        | 1.38     |
| 14  | cB    | 821  | CL7  | CHC-C1C | -2.53 | 1.33        | 1.38     |
| 14  | bB    | 813  | CL7  | CHB-C4A | -2.53 | 1.31        | 1.36     |
| 14  | bB    | 823  | CL7  | CHB-C4A | -2.53 | 1.31        | 1.36     |
| 14  | cB    | 813  | CL7  | CHC-C1C | -2.53 | 1.33        | 1.38     |
| 14  | bA    | 3129 | CL7  | C1D-C2D | -2.53 | 1.37        | 1.43     |
| 14  | cA    | 3110 | CL7  | C4C-NC  | 2.53  | 1.40        | 1.37     |
| 14  | aB    | 3020 | CL7  | C1D-C2D | -2.53 | 1.37        | 1.43     |
| 14  | cA    | 3111 | CL7  | CAB-C3B | -2.53 | 1.39        | 1.45     |
| 14  | bB    | 821  | CL7  | C1D-C2D | -2.53 | 1.37        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | bJ    | 101  | CL7  | C1D-C2D | -2.53 | 1.37        | 1.43     |
| 14  | aA    | 3106 | CL7  | C3A-C4A | -2.53 | 1.47        | 1.52     |
| 14  | bA    | 3112 | CL7  | C2A-C1A | -2.53 | 1.47        | 1.52     |
| 14  | aB    | 3012 | CL7  | CHC-C1C | -2.53 | 1.33        | 1.38     |
| 14  | bB    | 808  | CL7  | OBB-CAB | 2.53  | 1.27        | 1.22     |
| 14  | aA    | 3118 | CL7  | C2A-C1A | -2.53 | 1.47        | 1.52     |
| 14  | bA    | 3125 | CL7  | C3D-C4D | -2.53 | 1.33        | 1.39     |
| 14  | aA    | 3125 | CL7  | CHB-C4A | -2.53 | 1.31        | 1.36     |
| 14  | aL    | 202  | CL7  | C3A-C4A | -2.53 | 1.47        | 1.52     |
| 13  | aA    | 3102 | PHO  | C1-C2   | 2.52  | 1.56        | 1.49     |
| 14  | cB    | 823  | CL7  | CHB-C4A | -2.52 | 1.31        | 1.36     |
| 14  | aB    | 3021 | CL7  | C4C-NC  | 2.52  | 1.40        | 1.37     |
| 14  | aJ    | 101  | CL7  | CHB-C4A | -2.52 | 1.31        | 1.36     |
| 14  | bA    | 3130 | CL7  | CAB-C3B | -2.52 | 1.39        | 1.45     |
| 14  | bB    | 808  | CL7  | C1D-ND  | -2.52 | 1.34        | 1.37     |
| 14  | aB    | 3016 | CL7  | CHC-C1C | -2.52 | 1.33        | 1.38     |
| 14  | bA    | 3109 | CL7  | C3D-CAD | -2.52 | 1.36        | 1.45     |
| 16  | bA    | 3137 | LHG  | O3-C3   | -2.52 | 1.35        | 1.44     |
| 14  | cL    | 205  | CL7  | O2D-CGD | -2.52 | 1.27        | 1.33     |
| 14  | bA    | 3123 | CL7  | CHB-C4A | -2.52 | 1.31        | 1.36     |
| 14  | bB    | 804  | CL7  | O2A-C1  | 2.52  | 1.53        | 1.46     |
| 14  | cA    | 3112 | CL7  | C4C-NC  | 2.52  | 1.40        | 1.37     |
| 14  | aB    | 3011 | CL7  | CAB-C3B | -2.52 | 1.39        | 1.45     |
| 14  | cA    | 3117 | CL7  | CHC-C1C | -2.52 | 1.33        | 1.38     |
| 14  | aB    | 3019 | CL7  | CMD-C2D | -2.52 | 1.45        | 1.50     |
| 14  | aA    | 3123 | CL7  | CAA-C2A | -2.52 | 1.49        | 1.54     |
| 14  | bB    | 811  | CL7  | C1D-C2D | -2.52 | 1.37        | 1.43     |
| 14  | cB    | 812  | CL7  | OBB-CAB | 2.52  | 1.27        | 1.22     |
| 17  | bA    | 3143 | PQN  | C7-C6   | -2.52 | 1.33        | 1.38     |
| 14  | bB    | 804  | CL7  | C4D-ND  | -2.52 | 1.34        | 1.37     |
| 14  | aB    | 3030 | CL7  | C3B-C4B | -2.52 | 1.37        | 1.42     |
| 14  | aA    | 3127 | CL7  | OBB-CAB | 2.52  | 1.27        | 1.22     |
| 14  | bA    | 3108 | CL7  | C3A-C4A | -2.51 | 1.47        | 1.52     |
| 14  | cA    | 3132 | CL7  | CBD-CGD | -2.51 | 1.44        | 1.52     |
| 14  | aA    | 3133 | CL7  | C1C-NC  | 2.51  | 1.40        | 1.37     |
| 14  | cB    | 817  | CL7  | CHC-C1C | -2.51 | 1.33        | 1.38     |
| 14  | bA    | 3122 | CL7  | C3D-CAD | -2.51 | 1.36        | 1.45     |
| 14  | bA    | 3122 | CL7  | C1D-ND  | -2.51 | 1.34        | 1.37     |
| 14  | bB    | 822  | CL7  | C4C-NC  | 2.51  | 1.40        | 1.37     |
| 14  | bA    | 3125 | CL7  | C4D-ND  | -2.51 | 1.34        | 1.37     |
| 14  | cA    | 3141 | CL7  | CHD-C4C | -2.51 | 1.33        | 1.38     |
| 14  | cA    | 3120 | CL7  | CAA-C2A | -2.51 | 1.49        | 1.54     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | cA    | 3124 | CL7  | CBD-CGD | -2.51 | 1.44        | 1.52     |
| 14  | aB    | 3031 | CL7  | C1C-NC  | 2.51  | 1.40        | 1.37     |
| 17  | cA    | 3143 | PQN  | C2M-C2  | -2.51 | 1.45        | 1.50     |
| 14  | aA    | 3110 | CL7  | CHB-C4A | -2.51 | 1.31        | 1.36     |
| 14  | aA    | 3143 | CL7  | C1D-C2D | -2.51 | 1.37        | 1.43     |
| 14  | bA    | 3110 | CL7  | CAB-C3B | -2.51 | 1.39        | 1.45     |
| 14  | cA    | 3130 | CL7  | CAB-C3B | -2.51 | 1.39        | 1.45     |
| 14  | aA    | 3113 | CL7  | OBb-CAB | 2.51  | 1.27        | 1.22     |
| 14  | aL    | 203  | CL7  | C1A-NA  | -2.51 | 1.31        | 1.38     |
| 14  | bA    | 3111 | CL7  | C1D-C2D | -2.50 | 1.37        | 1.43     |
| 14  | cA    | 3112 | CL7  | C2A-C1A | -2.50 | 1.47        | 1.52     |
| 14  | cB    | 813  | CL7  | C1C-NC  | 2.50  | 1.40        | 1.37     |
| 14  | bA    | 3111 | CL7  | C2A-C1A | -2.50 | 1.47        | 1.52     |
| 17  | aB    | 3027 | PQN  | C3-C4   | -2.50 | 1.40        | 1.47     |
| 14  | aA    | 3133 | CL7  | CBD-CGD | -2.50 | 1.44        | 1.52     |
| 14  | cB    | 809  | CL7  | C1C-NC  | 2.50  | 1.40        | 1.37     |
| 14  | bA    | 3128 | CL7  | CMB-C2B | -2.50 | 1.45        | 1.50     |
| 14  | bB    | 815  | CL7  | CAB-C3B | -2.50 | 1.39        | 1.45     |
| 14  | cB    | 816  | CL7  | C4C-NC  | 2.50  | 1.40        | 1.37     |
| 14  | cA    | 3140 | CL7  | O1D-CGD | -2.50 | 1.15        | 1.21     |
| 14  | bA    | 3106 | CL7  | C3B-C4B | -2.50 | 1.37        | 1.42     |
| 14  | cB    | 811  | CL7  | C3D-CAD | -2.50 | 1.36        | 1.45     |
| 14  | cA    | 3111 | CL7  | C2A-C1A | -2.50 | 1.47        | 1.52     |
| 14  | bB    | 804  | CL7  | C3D-C2D | -2.50 | 1.34        | 1.42     |
| 14  | bA    | 3114 | CL7  | CHD-C4C | -2.50 | 1.33        | 1.38     |
| 14  | aB    | 3007 | CL7  | C3B-C4B | -2.50 | 1.37        | 1.42     |
| 14  | bB    | 827  | CL7  | CMD-C2D | -2.49 | 1.45        | 1.50     |
| 14  | bA    | 3130 | CL7  | C3D-CAD | -2.49 | 1.36        | 1.45     |
| 14  | cB    | 824  | CL7  | C3D-CAD | -2.49 | 1.36        | 1.45     |
| 14  | cB    | 833  | CL7  | O2D-CGD | -2.49 | 1.27        | 1.33     |
| 14  | aB    | 3010 | CL7  | C1D-C2D | -2.49 | 1.37        | 1.43     |
| 14  | aB    | 3011 | CL7  | C1D-C2D | -2.49 | 1.37        | 1.43     |
| 14  | aA    | 3117 | CL7  | C3D-CAD | -2.49 | 1.36        | 1.45     |
| 16  | cA    | 3137 | LHG  | O8-C6   | -2.49 | 1.39        | 1.45     |
| 14  | bB    | 826  | CL7  | MG-NA   | -2.49 | 2.00        | 2.05     |
| 14  | aB    | 3007 | CL7  | C3C-C2C | -2.49 | 1.31        | 1.36     |
| 14  | bA    | 3124 | CL7  | C4C-NC  | 2.49  | 1.40        | 1.37     |
| 14  | aA    | 3129 | CL7  | C3D-CAD | -2.49 | 1.36        | 1.45     |
| 14  | cB    | 806  | CL7  | C3D-CAD | -2.49 | 1.36        | 1.45     |
| 14  | cK    | 101  | CL7  | CHB-C4A | -2.49 | 1.31        | 1.36     |
| 14  | cA    | 3113 | CL7  | C2A-C1A | -2.49 | 1.47        | 1.52     |
| 14  | aA    | 3131 | CL7  | CAB-C3B | -2.49 | 1.39        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | cA    | 3109 | CL7  | C3D-CAD | -2.49 | 1.36        | 1.45     |
| 14  | bA    | 3113 | CL7  | CHB-C4A | -2.49 | 1.31        | 1.36     |
| 14  | cB    | 810  | CL7  | CHB-C4A | -2.49 | 1.31        | 1.36     |
| 14  | bA    | 3121 | CL7  | C3D-CAD | -2.49 | 1.36        | 1.45     |
| 14  | bA    | 3116 | CL7  | CHB-C4A | -2.49 | 1.31        | 1.36     |
| 14  | aL    | 203  | CL7  | C4C-NC  | 2.49  | 1.40        | 1.37     |
| 14  | bA    | 3110 | CL7  | C4C-NC  | 2.49  | 1.40        | 1.37     |
| 14  | cB    | 822  | CL7  | CAB-C3B | -2.49 | 1.39        | 1.45     |
| 14  | aA    | 3119 | CL7  | C3B-C4B | -2.49 | 1.37        | 1.42     |
| 14  | aA    | 3143 | CL7  | CHB-C4A | -2.49 | 1.31        | 1.36     |
| 14  | bL    | 205  | CL7  | C1C-NC  | 2.48  | 1.40        | 1.37     |
| 14  | cA    | 3106 | CL7  | C1D-ND  | -2.48 | 1.34        | 1.37     |
| 14  | bB    | 820  | CL7  | CMD-C2D | -2.48 | 1.45        | 1.50     |
| 14  | aB    | 3020 | CL7  | CHC-C1C | -2.48 | 1.33        | 1.38     |
| 14  | bA    | 3104 | CL7  | CHC-C1C | -2.48 | 1.33        | 1.38     |
| 14  | aA    | 3111 | CL7  | OBb-CAB | 2.48  | 1.27        | 1.22     |
| 14  | bA    | 3103 | CL7  | C4C-NC  | 2.48  | 1.40        | 1.37     |
| 14  | cB    | 810  | CL7  | C1C-NC  | 2.48  | 1.40        | 1.37     |
| 14  | cA    | 3123 | CL7  | CHD-C4C | -2.48 | 1.33        | 1.38     |
| 14  | bB    | 815  | CL7  | CHB-C4A | -2.48 | 1.31        | 1.36     |
| 14  | aB    | 3006 | CL7  | CHD-C4C | -2.48 | 1.33        | 1.38     |
| 14  | aB    | 3009 | CL7  | CMA-C3A | 2.48  | 1.58        | 1.53     |
| 14  | cB    | 815  | CL7  | CHB-C4A | -2.48 | 1.31        | 1.36     |
| 14  | cA    | 3132 | CL7  | C4D-ND  | -2.48 | 1.34        | 1.37     |
| 14  | bA    | 3133 | CL7  | C3D-CAD | -2.48 | 1.36        | 1.45     |
| 14  | aB    | 3012 | CL7  | CHB-C4A | -2.48 | 1.31        | 1.36     |
| 14  | aB    | 3007 | CL7  | C1C-NC  | 2.48  | 1.40        | 1.37     |
| 14  | cB    | 810  | CL7  | O2D-CED | -2.48 | 1.39        | 1.45     |
| 14  | aA    | 3105 | CL7  | CAB-C3B | -2.48 | 1.40        | 1.45     |
| 14  | bA    | 3107 | CL7  | C3D-CAD | -2.48 | 1.36        | 1.45     |
| 14  | bA    | 3114 | CL7  | C3D-CAD | -2.48 | 1.36        | 1.45     |
| 14  | bB    | 832  | CL7  | C3C-C2C | -2.48 | 1.31        | 1.36     |
| 14  | aA    | 3134 | CL7  | C1D-C2D | -2.47 | 1.37        | 1.43     |
| 14  | cB    | 816  | CL7  | CBD-CGD | -2.47 | 1.44        | 1.52     |
| 14  | cA    | 3140 | CL7  | C3D-CAD | -2.47 | 1.36        | 1.45     |
| 14  | bB    | 820  | CL7  | CAA-C2A | -2.47 | 1.49        | 1.54     |
| 14  | cB    | 811  | CL7  | C1D-C2D | -2.47 | 1.37        | 1.43     |
| 14  | cA    | 3130 | CL7  | C3D-CAD | -2.47 | 1.36        | 1.45     |
| 14  | aA    | 3103 | CL7  | O1D-CGD | -2.47 | 1.15        | 1.21     |
| 14  | bA    | 3142 | CL7  | CHB-C4A | -2.47 | 1.31        | 1.36     |
| 14  | bB    | 811  | CL7  | CHD-C4C | -2.47 | 1.33        | 1.38     |
| 14  | bA    | 3140 | CL7  | O2D-CGD | -2.47 | 1.27        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | bB    | 831  | CL7  | C3D-CAD | -2.47 | 1.36        | 1.45     |
| 14  | cA    | 3122 | CL7  | C3D-C2D | -2.47 | 1.34        | 1.42     |
| 14  | cA    | 3116 | CL7  | CBD-CGD | -2.47 | 1.44        | 1.52     |
| 14  | cA    | 3127 | CL7  | C4D-ND  | -2.47 | 1.34        | 1.37     |
| 14  | aB    | 3021 | CL7  | C2A-C1A | -2.47 | 1.47        | 1.52     |
| 14  | cA    | 3125 | CL7  | CBD-CGD | -2.47 | 1.44        | 1.52     |
| 14  | aB    | 3025 | CL7  | CHB-C4A | -2.47 | 1.31        | 1.36     |
| 14  | cA    | 3129 | CL7  | C1A-CHA | -2.47 | 1.27        | 1.38     |
| 14  | aB    | 3018 | CL7  | C3D-C2D | -2.47 | 1.34        | 1.42     |
| 14  | cA    | 3108 | CL7  | C1C-NC  | 2.47  | 1.40        | 1.37     |
| 14  | bB    | 803  | CL7  | C3C-C2C | -2.47 | 1.31        | 1.36     |
| 14  | bB    | 824  | CL7  | C3D-CAD | -2.47 | 1.36        | 1.45     |
| 14  | aB    | 3005 | CL7  | C1D-C2D | -2.47 | 1.37        | 1.43     |
| 14  | bK    | 101  | CL7  | C2A-C1A | -2.46 | 1.47        | 1.52     |
| 14  | aA    | 3134 | CL7  | CHB-C4A | -2.46 | 1.31        | 1.36     |
| 14  | aB    | 3019 | CL7  | C3B-C4B | -2.46 | 1.37        | 1.42     |
| 12  | cA    | 3101 | G9R  | CHD-C4C | 2.46  | 1.44        | 1.39     |
| 14  | aL    | 204  | CL7  | C1A-NA  | -2.46 | 1.31        | 1.38     |
| 13  | aB    | 3004 | PHO  | O1D-CGD | -2.46 | 1.15        | 1.21     |
| 13  | aA    | 3102 | PHO  | C3D-C4D | -2.46 | 1.37        | 1.41     |
| 14  | cL    | 204  | CL7  | CBA-CGA | -2.46 | 1.43        | 1.50     |
| 14  | bL    | 203  | CL7  | CHD-C4C | -2.46 | 1.33        | 1.38     |
| 17  | bB    | 828  | PQN  | C3-C4   | -2.46 | 1.41        | 1.47     |
| 14  | cB    | 818  | CL7  | CHB-C4A | -2.46 | 1.31        | 1.36     |
| 14  | cA    | 3104 | CL7  | C2A-C1A | -2.46 | 1.48        | 1.52     |
| 14  | bK    | 101  | CL7  | CHB-C4A | -2.46 | 1.31        | 1.36     |
| 14  | aL    | 202  | CL7  | CHD-C4C | -2.46 | 1.33        | 1.38     |
| 14  | aB    | 3030 | CL7  | C3A-C4A | -2.46 | 1.48        | 1.52     |
| 14  | cB    | 812  | CL7  | C1D-C2D | -2.46 | 1.37        | 1.43     |
| 14  | aA    | 3140 | CL7  | C3B-C4B | -2.46 | 1.37        | 1.42     |
| 14  | aA    | 3127 | CL7  | C3B-C4B | -2.46 | 1.37        | 1.42     |
| 14  | cA    | 3121 | CL7  | OBb-CAB | 2.46  | 1.27        | 1.22     |
| 14  | bA    | 3121 | CL7  | O1D-CGD | -2.46 | 1.15        | 1.21     |
| 14  | cA    | 3113 | CL7  | CHC-C1C | -2.46 | 1.33        | 1.38     |
| 16  | aA    | 3138 | LHG  | O8-C6   | -2.46 | 1.39        | 1.45     |
| 14  | aB    | 3023 | CL7  | C3D-CAD | -2.46 | 1.36        | 1.45     |
| 14  | cL    | 204  | CL7  | C3B-C4B | -2.45 | 1.37        | 1.42     |
| 14  | aA    | 3132 | CL7  | CHD-C4C | -2.45 | 1.33        | 1.38     |
| 14  | cB    | 820  | CL7  | C3A-C4A | -2.45 | 1.48        | 1.52     |
| 14  | aA    | 3133 | CL7  | O2A-CGA | 2.45  | 1.40        | 1.33     |
| 14  | cA    | 3125 | CL7  | CAA-C2A | -2.45 | 1.49        | 1.54     |
| 14  | bA    | 3126 | CL7  | C1D-C2D | -2.45 | 1.37        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | cA    | 3129 | CL7  | O2D-CGD | -2.45 | 1.27        | 1.33     |
| 14  | aA    | 3118 | CL7  | CHB-C4A | -2.45 | 1.31        | 1.36     |
| 14  | cB    | 815  | CL7  | CAB-C3B | -2.45 | 1.40        | 1.45     |
| 14  | bB    | 812  | CL7  | CAB-C3B | -2.45 | 1.40        | 1.45     |
| 14  | bA    | 3127 | CL7  | CHC-C1C | -2.45 | 1.33        | 1.38     |
| 14  | aA    | 3132 | CL7  | OBB-CAB | 2.45  | 1.27        | 1.22     |
| 14  | bA    | 3126 | CL7  | CHC-C1C | -2.45 | 1.33        | 1.38     |
| 14  | cA    | 3122 | CL7  | C3D-CAD | -2.45 | 1.36        | 1.45     |
| 14  | bB    | 807  | CL7  | C1C-NC  | 2.45  | 1.40        | 1.37     |
| 14  | bA    | 3129 | CL7  | C1A-CHA | -2.45 | 1.27        | 1.38     |
| 14  | aJ    | 101  | CL7  | C1D-C2D | -2.45 | 1.37        | 1.43     |
| 14  | aA    | 3123 | CL7  | MG-NC   | -2.45 | 2.00        | 2.05     |
| 19  | cB    | 830  | LMG  | O7-C8   | -2.45 | 1.40        | 1.46     |
| 17  | bA    | 3143 | PQN  | C5-C4   | -2.45 | 1.43        | 1.48     |
| 14  | cB    | 812  | CL7  | C4C-NC  | 2.45  | 1.40        | 1.37     |
| 14  | bA    | 3106 | CL7  | C1D-C2D | -2.45 | 1.37        | 1.43     |
| 14  | bA    | 3113 | CL7  | C3D-CAD | -2.44 | 1.36        | 1.45     |
| 14  | cA    | 3123 | CL7  | C4D-ND  | -2.44 | 1.34        | 1.37     |
| 14  | cA    | 3133 | CL7  | C3D-CAD | -2.44 | 1.36        | 1.45     |
| 14  | cK    | 101  | CL7  | C1D-C2D | -2.44 | 1.37        | 1.43     |
| 14  | aB    | 3011 | CL7  | CHD-C4C | -2.44 | 1.33        | 1.38     |
| 14  | cA    | 3120 | CL7  | C3D-CAD | -2.44 | 1.36        | 1.45     |
| 14  | aB    | 3005 | CL7  | CMD-C2D | -2.44 | 1.45        | 1.50     |
| 14  | bA    | 3106 | CL7  | C3C-C2C | -2.44 | 1.31        | 1.36     |
| 14  | aB    | 3017 | CL7  | CHB-C4A | -2.44 | 1.31        | 1.36     |
| 14  | bA    | 3141 | CL7  | C3D-CAD | -2.44 | 1.36        | 1.45     |
| 14  | aA    | 3127 | CL7  | C1D-C2D | -2.44 | 1.37        | 1.43     |
| 14  | aL    | 204  | CL7  | C1C-NC  | 2.44  | 1.40        | 1.37     |
| 14  | cA    | 3142 | CL7  | CHB-C4A | -2.44 | 1.31        | 1.36     |
| 14  | bB    | 812  | CL7  | C4C-NC  | 2.44  | 1.40        | 1.37     |
| 14  | bB    | 813  | CL7  | C1C-NC  | 2.44  | 1.40        | 1.37     |
| 14  | cA    | 3113 | CL7  | C1C-NC  | 2.44  | 1.40        | 1.37     |
| 14  | aA    | 3134 | CL7  | CHC-C1C | -2.44 | 1.33        | 1.38     |
| 14  | aB    | 3010 | CL7  | C2A-C1A | -2.44 | 1.48        | 1.52     |
| 14  | cB    | 812  | CL7  | CAB-C3B | -2.44 | 1.40        | 1.45     |
| 14  | bB    | 804  | CL7  | CAA-C2A | -2.44 | 1.49        | 1.54     |
| 14  | aA    | 3103 | CL7  | MG-NA   | -2.44 | 2.01        | 2.05     |
| 14  | bA    | 3141 | CL7  | CHD-C4C | -2.44 | 1.33        | 1.38     |
| 14  | aA    | 3107 | CL7  | C4C-NC  | 2.44  | 1.40        | 1.37     |
| 14  | aA    | 3105 | CL7  | C3D-CAD | -2.44 | 1.36        | 1.45     |
| 14  | aA    | 3124 | CL7  | C2A-C1A | -2.44 | 1.47        | 1.50     |
| 14  | bA    | 3114 | CL7  | C1D-ND  | -2.44 | 1.34        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 13  | bB    | 805  | PHO  | C4C-NC  | -2.44 | 1.30        | 1.37     |
| 14  | aB    | 3003 | CL7  | C1D-C2D | -2.44 | 1.37        | 1.43     |
| 14  | cB    | 810  | CL7  | C3D-CAD | -2.44 | 1.36        | 1.45     |
| 14  | cA    | 3107 | CL7  | CAB-C3B | -2.44 | 1.40        | 1.45     |
| 14  | bA    | 3140 | CL7  | C3D-CAD | -2.44 | 1.36        | 1.45     |
| 14  | bA    | 3120 | CL7  | C3D-CAD | -2.44 | 1.36        | 1.45     |
| 14  | aB    | 3016 | CL7  | CHB-C4A | -2.44 | 1.31        | 1.36     |
| 14  | bB    | 826  | CL7  | CHB-C4A | -2.43 | 1.31        | 1.36     |
| 14  | cA    | 3106 | CL7  | C3C-C2C | -2.43 | 1.31        | 1.36     |
| 14  | cA    | 3114 | CL7  | CHD-C4C | -2.43 | 1.33        | 1.38     |
| 14  | cB    | 832  | CL7  | O2D-CED | -2.43 | 1.39        | 1.45     |
| 14  | aA    | 3142 | CL7  | C3D-CAD | -2.43 | 1.36        | 1.45     |
| 13  | bB    | 801  | PHO  | C1-C2   | 2.43  | 1.56        | 1.49     |
| 14  | aA    | 3108 | CL7  | C3D-CAD | -2.43 | 1.36        | 1.45     |
| 14  | bB    | 804  | CL7  | CBD-CGD | -2.43 | 1.44        | 1.52     |
| 14  | aA    | 3142 | CL7  | CAA-C2A | -2.43 | 1.49        | 1.54     |
| 14  | cB    | 819  | CL7  | C3D-C2D | -2.43 | 1.34        | 1.42     |
| 14  | cA    | 3125 | CL7  | C4D-ND  | -2.43 | 1.34        | 1.37     |
| 14  | bL    | 205  | CL7  | O2D-CGD | -2.43 | 1.27        | 1.33     |
| 14  | cA    | 3114 | CL7  | C3D-CAD | -2.43 | 1.36        | 1.45     |
| 14  | cB    | 822  | CL7  | C4C-NC  | 2.43  | 1.40        | 1.37     |
| 14  | bB    | 804  | CL7  | O1D-CGD | -2.43 | 1.15        | 1.21     |
| 13  | bB    | 801  | PHO  | C3D-CAD | -2.43 | 1.42        | 1.47     |
| 14  | bB    | 803  | CL7  | C3B-C4B | -2.43 | 1.37        | 1.42     |
| 14  | bB    | 812  | CL7  | CHD-C4C | -2.43 | 1.33        | 1.38     |
| 14  | aJ    | 101  | CL7  | CAA-C2A | -2.43 | 1.49        | 1.54     |
| 14  | cB    | 803  | CL7  | C3B-C4B | -2.43 | 1.37        | 1.42     |
| 14  | bA    | 3140 | CL7  | OBB-CAB | 2.43  | 1.27        | 1.22     |
| 14  | aL    | 202  | CL7  | C3D-CAD | -2.43 | 1.36        | 1.45     |
| 14  | aB    | 3030 | CL7  | C3D-CAD | -2.43 | 1.36        | 1.45     |
| 14  | aA    | 3130 | CL7  | C3D-C2D | -2.43 | 1.34        | 1.42     |
| 14  | cB    | 821  | CL7  | C1D-C2D | -2.42 | 1.37        | 1.43     |
| 13  | cB    | 801  | PHO  | C1-C2   | 2.42  | 1.56        | 1.49     |
| 14  | cB    | 806  | CL7  | CMD-C2D | -2.42 | 1.45        | 1.50     |
| 14  | bA    | 3124 | CL7  | C3D-CAD | -2.42 | 1.36        | 1.45     |
| 14  | bA    | 3103 | CL7  | C2A-C1A | -2.42 | 1.48        | 1.52     |
| 14  | bA    | 3112 | CL7  | CHD-C4C | -2.42 | 1.33        | 1.38     |
| 14  | bB    | 809  | CL7  | CHC-C4B | -2.42 | 1.34        | 1.39     |
| 14  | bA    | 3131 | CL7  | C3D-CAD | -2.42 | 1.36        | 1.45     |
| 14  | cB    | 820  | CL7  | OBB-CAB | 2.42  | 1.27        | 1.22     |
| 14  | bA    | 3128 | CL7  | C3B-C4B | -2.42 | 1.37        | 1.42     |
| 14  | cA    | 3110 | CL7  | C2A-C1A | -2.42 | 1.48        | 1.52     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | bA    | 3133 | CL7  | CAB-C3B | -2.42 | 1.40        | 1.45     |
| 14  | bA    | 3113 | CL7  | OBB-CAB | 2.42  | 1.27        | 1.22     |
| 14  | bL    | 205  | CL7  | C3A-C4A | -2.42 | 1.48        | 1.52     |
| 14  | bA    | 3140 | CL7  | CAA-C2A | -2.42 | 1.49        | 1.54     |
| 14  | cL    | 205  | CL7  | CMD-C2D | -2.42 | 1.45        | 1.50     |
| 14  | aA    | 3120 | CL7  | C3B-C4B | -2.42 | 1.37        | 1.42     |
| 14  | cB    | 807  | CL7  | O2D-CGD | -2.42 | 1.27        | 1.33     |
| 14  | aB    | 3008 | CL7  | MG-NB   | -2.42 | 2.01        | 2.05     |
| 14  | bA    | 3113 | CL7  | C1C-NC  | 2.42  | 1.40        | 1.37     |
| 14  | bJ    | 101  | CL7  | CHB-C4A | -2.42 | 1.31        | 1.36     |
| 14  | bA    | 3111 | CL7  | CAB-C3B | -2.42 | 1.40        | 1.45     |
| 14  | cB    | 804  | CL7  | C3A-C4A | -2.42 | 1.48        | 1.52     |
| 14  | aA    | 3120 | CL7  | C1C-NC  | 2.42  | 1.40        | 1.37     |
| 14  | aA    | 3127 | CL7  | CHC-C1C | -2.42 | 1.33        | 1.38     |
| 14  | bA    | 3132 | CL7  | C3A-C4A | -2.42 | 1.48        | 1.52     |
| 14  | bA    | 3114 | CL7  | C3A-C4A | -2.42 | 1.48        | 1.52     |
| 14  | cA    | 3125 | CL7  | CAC-C3C | -2.42 | 1.44        | 1.51     |
| 14  | cA    | 3111 | CL7  | C1D-C2D | -2.42 | 1.37        | 1.43     |
| 14  | cB    | 825  | CL7  | C3D-CAD | -2.42 | 1.37        | 1.45     |
| 14  | bB    | 807  | CL7  | C3D-CAD | -2.41 | 1.37        | 1.45     |
| 14  | bL    | 204  | CL7  | C1A-NA  | -2.41 | 1.31        | 1.38     |
| 14  | aB    | 3015 | CL7  | O2A-C1  | 2.41  | 1.53        | 1.46     |
| 14  | cB    | 804  | CL7  | C3B-C4B | -2.41 | 1.37        | 1.42     |
| 14  | bA    | 3114 | CL7  | CMD-C2D | -2.41 | 1.45        | 1.50     |
| 14  | aA    | 3113 | CL7  | C1D-C2D | -2.41 | 1.37        | 1.43     |
| 14  | cA    | 3105 | CL7  | OBB-CAB | 2.41  | 1.27        | 1.22     |
| 14  | cA    | 3113 | CL7  | CHB-C4A | -2.41 | 1.31        | 1.36     |
| 14  | cB    | 823  | CL7  | C1C-NC  | 2.41  | 1.40        | 1.37     |
| 14  | cL    | 205  | CL7  | C1C-NC  | 2.41  | 1.40        | 1.37     |
| 14  | aA    | 3113 | CL7  | C2A-C1A | -2.41 | 1.48        | 1.52     |
| 14  | aA    | 3126 | CL7  | CAB-C3B | -2.41 | 1.40        | 1.45     |
| 14  | bA    | 3141 | CL7  | C1D-ND  | -2.41 | 1.34        | 1.37     |
| 14  | cA    | 3141 | CL7  | C1D-ND  | -2.41 | 1.34        | 1.37     |
| 14  | cA    | 3104 | CL7  | C3D-CAD | -2.41 | 1.37        | 1.45     |
| 14  | aB    | 3002 | CL7  | C1D-ND  | -2.41 | 1.34        | 1.37     |
| 14  | aB    | 3022 | CL7  | C3B-C4B | -2.41 | 1.37        | 1.42     |
| 14  | cL    | 205  | CL7  | C3A-C4A | -2.41 | 1.48        | 1.52     |
| 14  | cA    | 3106 | CL7  | CMD-C2D | -2.41 | 1.45        | 1.50     |
| 14  | bB    | 814  | CL7  | CHB-C4A | -2.41 | 1.31        | 1.36     |
| 19  | bB    | 830  | LMG  | O6-C5   | -2.41 | 1.38        | 1.44     |
| 14  | bA    | 3113 | CL7  | CHC-C1C | -2.41 | 1.33        | 1.38     |
| 14  | aA    | 3131 | CL7  | C3D-CAD | -2.41 | 1.37        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | aA    | 3114 | CL7  | CHC-C1C | -2.41 | 1.33        | 1.38     |
| 14  | aA    | 3117 | CL7  | CBD-CGD | -2.41 | 1.44        | 1.52     |
| 14  | aA    | 3106 | CL7  | C2A-C1A | -2.40 | 1.48        | 1.52     |
| 14  | cK    | 101  | CL7  | CHC-C1C | -2.40 | 1.33        | 1.38     |
| 14  | aA    | 3115 | CL7  | C3A-C4A | -2.40 | 1.48        | 1.52     |
| 14  | cA    | 3132 | CL7  | C3D-CAD | -2.40 | 1.37        | 1.45     |
| 14  | cB    | 826  | CL7  | CHB-C4A | -2.40 | 1.31        | 1.36     |
| 14  | cL    | 203  | CL7  | C3D-CAD | -2.40 | 1.37        | 1.45     |
| 14  | bA    | 3125 | CL7  | CAC-C3C | -2.40 | 1.45        | 1.51     |
| 14  | aB    | 3023 | CL7  | O2A-C1  | 2.40  | 1.52        | 1.46     |
| 14  | cA    | 3113 | CL7  | C3D-CAD | -2.40 | 1.37        | 1.45     |
| 14  | cB    | 823  | CL7  | C3B-C4B | -2.40 | 1.37        | 1.42     |
| 14  | cA    | 3103 | CL7  | CAB-C3B | -2.40 | 1.40        | 1.45     |
| 14  | cA    | 3110 | CL7  | C3D-CAD | -2.40 | 1.37        | 1.45     |
| 14  | bB    | 827  | CL7  | OBD-CAD | -2.40 | 1.18        | 1.22     |
| 14  | cA    | 3118 | CL7  | C3B-C4B | -2.40 | 1.37        | 1.42     |
| 14  | cA    | 3139 | CL7  | OBB-CAB | 2.40  | 1.27        | 1.22     |
| 14  | aA    | 3115 | CL7  | C3D-CAD | -2.40 | 1.37        | 1.45     |
| 14  | cA    | 3119 | CL7  | OBB-CAB | 2.40  | 1.27        | 1.22     |
| 16  | cA    | 3137 | LHG  | O3-C3   | -2.40 | 1.35        | 1.44     |
| 14  | bA    | 3123 | CL7  | CHD-C4C | -2.40 | 1.33        | 1.38     |
| 14  | aB    | 3011 | CL7  | C3B-C4B | -2.40 | 1.37        | 1.42     |
| 14  | bB    | 833  | CL7  | C1D-ND  | -2.40 | 1.34        | 1.37     |
| 14  | cB    | 816  | CL7  | C1D-ND  | -2.40 | 1.34        | 1.37     |
| 14  | aB    | 3003 | CL7  | CAA-C2A | -2.40 | 1.49        | 1.54     |
| 14  | aA    | 3131 | CL7  | CHD-C4C | -2.40 | 1.33        | 1.38     |
| 14  | cB    | 813  | CL7  | CAB-C3B | -2.40 | 1.40        | 1.45     |
| 14  | bA    | 3141 | CL7  | C3B-C4B | -2.40 | 1.37        | 1.42     |
| 14  | bB    | 809  | CL7  | C2A-C1A | -2.39 | 1.47        | 1.50     |
| 14  | cA    | 3131 | CL7  | C3D-CAD | -2.39 | 1.37        | 1.45     |
| 14  | bA    | 3104 | CL7  | C3D-CAD | -2.39 | 1.37        | 1.45     |
| 14  | bA    | 3123 | CL7  | O1D-CGD | -2.39 | 1.15        | 1.21     |
| 14  | cA    | 3126 | CL7  | C1D-C2D | -2.39 | 1.37        | 1.43     |
| 14  | bB    | 833  | CL7  | C3D-C2D | -2.39 | 1.34        | 1.42     |
| 14  | aB    | 3011 | CL7  | C4C-NC  | 2.39  | 1.40        | 1.37     |
| 14  | aA    | 3134 | CL7  | CAB-C3B | -2.39 | 1.40        | 1.45     |
| 14  | aB    | 3015 | CL7  | C3A-C4A | -2.39 | 1.48        | 1.52     |
| 14  | cA    | 3131 | CL7  | OBB-CAB | 2.39  | 1.27        | 1.22     |
| 14  | bA    | 3124 | CL7  | C1D-ND  | -2.39 | 1.34        | 1.37     |
| 14  | aA    | 3103 | CL7  | CBA-CGA | -2.39 | 1.43        | 1.50     |
| 14  | cB    | 812  | CL7  | C3B-C4B | -2.39 | 1.37        | 1.42     |
| 14  | bA    | 3110 | CL7  | CHC-C1C | -2.39 | 1.33        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | aB    | 3003 | CL7  | C3B-C4B | -2.39 | 1.37        | 1.42     |
| 14  | bA    | 3107 | CL7  | CHD-C4C | -2.39 | 1.33        | 1.38     |
| 14  | bA    | 3106 | CL7  | CBD-CGD | -2.39 | 1.44        | 1.52     |
| 17  | aA    | 3144 | PQN  | C5-C4   | -2.39 | 1.43        | 1.48     |
| 14  | cA    | 3141 | CL7  | OBB-CAB | 2.39  | 1.27        | 1.22     |
| 14  | aB    | 3015 | CL7  | C3C-C2C | -2.39 | 1.31        | 1.36     |
| 14  | aL    | 204  | CL7  | C3A-C4A | -2.39 | 1.48        | 1.52     |
| 14  | cL    | 205  | CL7  | C3D-C2D | -2.38 | 1.34        | 1.42     |
| 14  | aB    | 3003 | CL7  | CBD-CGD | -2.38 | 1.44        | 1.52     |
| 14  | cB    | 808  | CL7  | CHB-C4A | -2.38 | 1.31        | 1.36     |
| 14  | cL    | 205  | CL7  | C1A-NA  | -2.38 | 1.32        | 1.38     |
| 14  | bA    | 3119 | CL7  | CHD-C1D | -2.38 | 1.34        | 1.39     |
| 14  | cA    | 3117 | CL7  | C1D-C2D | -2.38 | 1.37        | 1.43     |
| 14  | aB    | 3013 | CL7  | CHB-C4A | -2.38 | 1.31        | 1.36     |
| 14  | cA    | 3110 | CL7  | CAB-C3B | -2.38 | 1.40        | 1.45     |
| 14  | aB    | 3009 | CL7  | CHC-C1C | -2.38 | 1.33        | 1.38     |
| 14  | bB    | 833  | CL7  | CBD-CGD | -2.38 | 1.45        | 1.52     |
| 14  | bB    | 826  | CL7  | C3D-C2D | -2.38 | 1.34        | 1.42     |
| 14  | cB    | 822  | CL7  | OBB-CAB | 2.38  | 1.27        | 1.22     |
| 17  | cA    | 3143 | PQN  | C7-C6   | -2.38 | 1.33        | 1.38     |
| 14  | bB    | 812  | CL7  | C1D-C2D | -2.38 | 1.37        | 1.43     |
| 14  | bB    | 832  | CL7  | CMD-C2D | -2.38 | 1.45        | 1.50     |
| 14  | bL    | 204  | CL7  | C3C-C2C | -2.38 | 1.31        | 1.36     |
| 14  | aB    | 3012 | CL7  | C2A-C1A | -2.38 | 1.48        | 1.52     |
| 14  | aA    | 3122 | CL7  | C3D-CAD | -2.38 | 1.37        | 1.45     |
| 14  | aA    | 3114 | CL7  | CHB-C4A | -2.38 | 1.31        | 1.36     |
| 14  | cB    | 813  | CL7  | C2A-C1A | -2.38 | 1.48        | 1.52     |
| 14  | cA    | 3121 | CL7  | C3D-CAD | -2.38 | 1.37        | 1.45     |
| 14  | bA    | 3106 | CL7  | C3A-C4A | -2.38 | 1.48        | 1.52     |
| 14  | cA    | 3144 | CL7  | CHB-C4A | -2.38 | 1.31        | 1.36     |
| 14  | cA    | 3124 | CL7  | C4C-NC  | 2.38  | 1.40        | 1.37     |
| 14  | aL    | 203  | CL7  | C3D-CAD | -2.38 | 1.37        | 1.45     |
| 14  | cA    | 3122 | CL7  | OBB-CAB | 2.38  | 1.27        | 1.22     |
| 17  | bB    | 828  | PQN  | C24-C23 | -2.38 | 1.45        | 1.52     |
| 14  | aA    | 3142 | CL7  | CHD-C4C | -2.38 | 1.33        | 1.38     |
| 14  | bA    | 3113 | CL7  | C2A-C1A | -2.37 | 1.48        | 1.52     |
| 14  | aA    | 3124 | CL7  | CAB-C3B | -2.37 | 1.40        | 1.45     |
| 14  | cA    | 3144 | CL7  | C1D-C2D | -2.37 | 1.37        | 1.43     |
| 14  | aL    | 204  | CL7  | C3C-C2C | -2.37 | 1.31        | 1.36     |
| 14  | cB    | 832  | CL7  | C3C-C2C | -2.37 | 1.31        | 1.36     |
| 14  | aA    | 3134 | CL7  | CHD-C4C | -2.37 | 1.33        | 1.38     |
| 14  | aB    | 3017 | CL7  | C3D-CAD | -2.37 | 1.37        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | bB    | 833  | CL7  | CHC-C1C | -2.37 | 1.33        | 1.38     |
| 14  | aA    | 3105 | CL7  | OBB-CAB | 2.37  | 1.27        | 1.22     |
| 14  | aB    | 3030 | CL7  | C4C-NC  | 2.37  | 1.40        | 1.37     |
| 14  | bB    | 833  | CL7  | CAA-C2A | -2.37 | 1.49        | 1.54     |
| 19  | aB    | 3029 | LMG  | C3-C2   | 2.37  | 1.58        | 1.52     |
| 14  | bA    | 3117 | CL7  | C1D-C2D | -2.37 | 1.37        | 1.43     |
| 14  | aA    | 3107 | CL7  | CHB-C4A | -2.37 | 1.31        | 1.36     |
| 14  | cA    | 3130 | CL7  | C2A-C1A | -2.37 | 1.48        | 1.52     |
| 14  | bA    | 3131 | CL7  | OBB-CAB | 2.37  | 1.27        | 1.22     |
| 14  | cB    | 820  | CL7  | C3B-C4B | -2.37 | 1.37        | 1.42     |
| 14  | aB    | 3031 | CL7  | C3C-C2C | -2.37 | 1.31        | 1.36     |
| 14  | aB    | 3012 | CL7  | C1C-NC  | 2.37  | 1.40        | 1.37     |
| 14  | aA    | 3125 | CL7  | CBD-CGD | -2.37 | 1.45        | 1.52     |
| 14  | cA    | 3106 | CL7  | CBD-CGD | -2.37 | 1.45        | 1.52     |
| 14  | cB    | 817  | CL7  | C3D-CAD | -2.37 | 1.37        | 1.45     |
| 14  | cB    | 807  | CL7  | C3D-CAD | -2.36 | 1.37        | 1.45     |
| 14  | cB    | 825  | CL7  | C1D-ND  | -2.36 | 1.34        | 1.37     |
| 14  | cA    | 3128 | CL7  | C3D-C2D | -2.36 | 1.34        | 1.42     |
| 14  | bB    | 823  | CL7  | C3B-C4B | -2.36 | 1.37        | 1.42     |
| 14  | aB    | 3008 | CL7  | C2A-C1A | -2.36 | 1.47        | 1.50     |
| 14  | aB    | 3015 | CL7  | C1D-ND  | -2.36 | 1.34        | 1.37     |
| 14  | cB    | 812  | CL7  | CHD-C4C | -2.36 | 1.33        | 1.38     |
| 14  | cB    | 804  | CL7  | O2A-C1  | 2.36  | 1.52        | 1.46     |
| 14  | bA    | 3127 | CL7  | C3D-CAD | -2.36 | 1.37        | 1.45     |
| 14  | bB    | 817  | CL7  | C3D-CAD | -2.36 | 1.37        | 1.45     |
| 14  | cA    | 3133 | CL7  | CAB-C3B | -2.36 | 1.40        | 1.45     |
| 14  | bB    | 824  | CL7  | C3B-C4B | -2.36 | 1.37        | 1.42     |
| 14  | bA    | 3128 | CL7  | C1D-C2D | -2.36 | 1.37        | 1.43     |
| 14  | bA    | 3126 | CL7  | C3B-C4B | -2.36 | 1.37        | 1.42     |
| 14  | aB    | 3010 | CL7  | C3D-CAD | -2.36 | 1.37        | 1.45     |
| 14  | aB    | 3024 | CL7  | CAB-C3B | -2.36 | 1.40        | 1.45     |
| 14  | bB    | 808  | CL7  | CMD-C2D | -2.36 | 1.45        | 1.50     |
| 14  | cB    | 820  | CL7  | CMD-C2D | -2.36 | 1.45        | 1.50     |
| 14  | cJ    | 101  | CL7  | CAB-C3B | -2.36 | 1.40        | 1.45     |
| 14  | bA    | 3112 | CL7  | C1D-C2D | -2.36 | 1.37        | 1.43     |
| 14  | cA    | 3128 | CL7  | CMB-C2B | -2.36 | 1.45        | 1.50     |
| 12  | bA    | 3101 | G9R  | C1C-NC  | -2.36 | 1.34        | 1.37     |
| 14  | bL    | 205  | CL7  | C3C-C2C | -2.36 | 1.31        | 1.36     |
| 14  | aA    | 3123 | CL7  | C1D-ND  | -2.36 | 1.34        | 1.37     |
| 16  | aA    | 3138 | LHG  | O3-C3   | -2.36 | 1.35        | 1.44     |
| 14  | cB    | 803  | CL7  | CBD-CGD | -2.35 | 1.45        | 1.52     |
| 14  | bA    | 3139 | CL7  | C3C-C2C | -2.35 | 1.31        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | aA    | 3114 | CL7  | C3D-CAD | -2.35 | 1.37        | 1.45     |
| 14  | cA    | 3127 | CL7  | C3D-CAD | -2.35 | 1.37        | 1.45     |
| 14  | cB    | 815  | CL7  | C3D-CAD | -2.35 | 1.37        | 1.45     |
| 14  | cA    | 3122 | CL7  | O1D-CGD | -2.35 | 1.15        | 1.21     |
| 14  | cB    | 819  | CL7  | O2A-C1  | 2.35  | 1.52        | 1.46     |
| 14  | bA    | 3145 | CL7  | C1D-C2D | -2.35 | 1.37        | 1.43     |
| 14  | bB    | 818  | CL7  | CHB-C4A | -2.35 | 1.31        | 1.36     |
| 14  | bL    | 205  | CL7  | CMD-C2D | -2.35 | 1.45        | 1.50     |
| 14  | aB    | 3016 | CL7  | CAB-C3B | -2.35 | 1.40        | 1.45     |
| 14  | cB    | 810  | CL7  | CHC-C1C | -2.35 | 1.33        | 1.38     |
| 14  | bB    | 812  | CL7  | C3B-C4B | -2.35 | 1.37        | 1.42     |
| 14  | aA    | 3133 | CL7  | C1D-C2D | -2.35 | 1.37        | 1.43     |
| 14  | bA    | 3120 | CL7  | O2D-CGD | -2.35 | 1.27        | 1.33     |
| 14  | cB    | 824  | CL7  | C3B-C4B | -2.35 | 1.37        | 1.42     |
| 14  | aA    | 3133 | CL7  | OBB-CAB | 2.35  | 1.27        | 1.22     |
| 14  | aB    | 3032 | CL7  | CHC-C1C | -2.35 | 1.33        | 1.38     |
| 14  | aB    | 3003 | CL7  | C3A-C4A | -2.35 | 1.48        | 1.52     |
| 14  | bA    | 3145 | CL7  | CHB-C4A | -2.35 | 1.31        | 1.36     |
| 14  | cB    | 827  | CL7  | CMD-C2D | -2.35 | 1.45        | 1.50     |
| 14  | aA    | 3113 | CL7  | CHC-C1C | -2.35 | 1.33        | 1.38     |
| 14  | aA    | 3146 | CL7  | CHB-C4A | -2.35 | 1.31        | 1.36     |
| 14  | aL    | 204  | CL7  | CMD-C2D | -2.35 | 1.45        | 1.50     |
| 14  | aA    | 3110 | CL7  | C3D-CAD | -2.35 | 1.37        | 1.45     |
| 14  | cA    | 3115 | CL7  | C2A-C1A | -2.35 | 1.48        | 1.52     |
| 14  | aA    | 3112 | CL7  | C3B-C4B | -2.35 | 1.37        | 1.42     |
| 14  | aB    | 3031 | CL7  | CMD-C2D | -2.34 | 1.45        | 1.50     |
| 14  | aB    | 3012 | CL7  | CAB-C3B | -2.34 | 1.40        | 1.45     |
| 14  | cA    | 3112 | CL7  | C1D-C2D | -2.34 | 1.37        | 1.43     |
| 14  | bA    | 3122 | CL7  | CHC-C1C | -2.34 | 1.33        | 1.38     |
| 14  | aA    | 3124 | CL7  | O1D-CGD | -2.34 | 1.15        | 1.21     |
| 14  | bB    | 818  | CL7  | C3D-CAD | -2.34 | 1.37        | 1.45     |
| 14  | aA    | 3114 | CL7  | C2A-C1A | -2.34 | 1.48        | 1.52     |
| 14  | bB    | 816  | CL7  | C1D-ND  | -2.34 | 1.34        | 1.37     |
| 14  | bA    | 3123 | CL7  | C2A-C1A | -2.34 | 1.47        | 1.50     |
| 14  | aA    | 3126 | CL7  | C3D-C4D | -2.34 | 1.33        | 1.39     |
| 14  | bL    | 205  | CL7  | CAA-C2A | -2.34 | 1.49        | 1.54     |
| 14  | aA    | 3128 | CL7  | CHB-C4A | -2.34 | 1.31        | 1.36     |
| 14  | aB    | 3015 | CL7  | CBD-CGD | -2.34 | 1.45        | 1.52     |
| 14  | cA    | 3132 | CL7  | C1C-NC  | 2.34  | 1.40        | 1.37     |
| 14  | bJ    | 101  | CL7  | CAB-C3B | -2.34 | 1.40        | 1.45     |
| 14  | cB    | 823  | CL7  | C3D-CAD | -2.34 | 1.37        | 1.45     |
| 14  | aB    | 3032 | CL7  | C3D-C2D | -2.34 | 1.35        | 1.42     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | aB    | 3018 | CL7  | O2A-C1  | 2.34  | 1.52        | 1.46     |
| 14  | cA    | 3139 | CL7  | CAB-C3B | -2.34 | 1.40        | 1.45     |
| 14  | cB    | 824  | CL7  | C4C-NC  | 2.34  | 1.40        | 1.37     |
| 14  | aA    | 3118 | CL7  | C1D-C2D | -2.34 | 1.37        | 1.43     |
| 14  | bA    | 3132 | CL7  | C1D-C2D | -2.34 | 1.37        | 1.43     |
| 14  | cA    | 3124 | CL7  | C3C-C2C | -2.34 | 1.31        | 1.36     |
| 14  | cA    | 3106 | CL7  | C1D-C2D | -2.34 | 1.37        | 1.43     |
| 14  | bB    | 825  | CL7  | CAB-C3B | -2.34 | 1.40        | 1.45     |
| 14  | bA    | 3107 | CL7  | C3A-C4A | -2.34 | 1.48        | 1.52     |
| 14  | cA    | 3124 | CL7  | C3D-CAD | -2.34 | 1.37        | 1.45     |
| 14  | aA    | 3118 | CL7  | CHC-C1C | -2.34 | 1.33        | 1.38     |
| 14  | cA    | 3102 | CL7  | O2D-CGD | -2.34 | 1.27        | 1.33     |
| 14  | aA    | 3111 | CL7  | CHC-C1C | -2.33 | 1.33        | 1.38     |
| 14  | bA    | 3132 | CL7  | C3D-CAD | -2.33 | 1.37        | 1.45     |
| 14  | bB    | 823  | CL7  | C3D-CAD | -2.33 | 1.37        | 1.45     |
| 12  | aA    | 3101 | G9R  | CMB-C2B | -2.33 | 1.45        | 1.50     |
| 14  | cL    | 205  | CL7  | C1D-ND  | -2.33 | 1.34        | 1.37     |
| 14  | aA    | 3126 | CL7  | CAC-C3C | -2.33 | 1.45        | 1.51     |
| 14  | cA    | 3103 | CL7  | C2A-C1A | -2.33 | 1.48        | 1.52     |
| 14  | cA    | 3112 | CL7  | CAB-C3B | -2.33 | 1.40        | 1.45     |
| 14  | aB    | 3006 | CL7  | C3D-CAD | -2.33 | 1.37        | 1.45     |
| 14  | bJ    | 101  | CL7  | C3D-CAD | -2.33 | 1.37        | 1.45     |
| 14  | bA    | 3130 | CL7  | C2A-C1A | -2.33 | 1.48        | 1.52     |
| 14  | bF    | 201  | CL7  | C3B-C4B | -2.33 | 1.37        | 1.42     |
| 14  | bL    | 205  | CL7  | C3D-C2D | -2.33 | 1.35        | 1.42     |
| 14  | cL    | 205  | CL7  | C3C-C2C | -2.33 | 1.31        | 1.36     |
| 14  | aF    | 201  | CL7  | C2A-C1A | -2.33 | 1.48        | 1.52     |
| 14  | cB    | 831  | CL7  | C3D-CAD | -2.33 | 1.37        | 1.45     |
| 14  | cA    | 3139 | CL7  | CHC-C1C | -2.33 | 1.33        | 1.38     |
| 14  | aB    | 3023 | CL7  | C4C-NC  | 2.33  | 1.40        | 1.37     |
| 14  | aA    | 3113 | CL7  | CHD-C4C | -2.32 | 1.33        | 1.38     |
| 14  | aA    | 3125 | CL7  | C3C-C2C | -2.32 | 1.31        | 1.36     |
| 14  | bB    | 817  | CL7  | CHD-C4C | -2.32 | 1.33        | 1.38     |
| 14  | bB    | 831  | CL7  | OBB-CAB | 2.32  | 1.27        | 1.22     |
| 14  | aA    | 3104 | CL7  | CAB-C3B | -2.32 | 1.40        | 1.45     |
| 14  | cA    | 3139 | CL7  | C1D-C2D | -2.32 | 1.37        | 1.43     |
| 14  | aA    | 3119 | CL7  | CHC-C1C | -2.32 | 1.33        | 1.38     |
| 14  | bA    | 3102 | CL7  | O1D-CGD | -2.32 | 1.15        | 1.21     |
| 14  | cA    | 3104 | CL7  | CAB-C3B | -2.32 | 1.40        | 1.45     |
| 14  | bA    | 3104 | CL7  | C2A-C1A | -2.32 | 1.48        | 1.52     |
| 14  | aA    | 3134 | CL7  | C3D-CAD | -2.32 | 1.37        | 1.45     |
| 14  | bB    | 811  | CL7  | C3D-CAD | -2.32 | 1.37        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | cB    | 808  | CL7  | CMD-C2D | -2.32 | 1.45        | 1.50     |
| 14  | bA    | 3115 | CL7  | C2A-C1A | -2.32 | 1.48        | 1.52     |
| 14  | aA    | 3111 | CL7  | C3D-CAD | -2.32 | 1.37        | 1.45     |
| 14  | aA    | 3132 | CL7  | CHB-C4A | -2.32 | 1.31        | 1.36     |
| 14  | bB    | 808  | CL7  | C1C-NC  | 2.32  | 1.40        | 1.37     |
| 14  | aA    | 3103 | CL7  | CHC-C1C | -2.32 | 1.33        | 1.38     |
| 14  | aB    | 3022 | CL7  | C3D-CAD | -2.32 | 1.37        | 1.45     |
| 19  | cB    | 830  | LMG  | O6-C5   | -2.32 | 1.38        | 1.44     |
| 14  | cA    | 3112 | CL7  | CHD-C4C | -2.32 | 1.33        | 1.38     |
| 17  | bA    | 3143 | PQN  | C2M-C2  | -2.32 | 1.45        | 1.50     |
| 14  | cF    | 201  | CL7  | C3B-C4B | -2.32 | 1.37        | 1.42     |
| 14  | cA    | 3123 | CL7  | CBD-CGD | -2.31 | 1.45        | 1.52     |
| 14  | aA    | 3103 | CL7  | C1D-C2D | -2.31 | 1.37        | 1.43     |
| 14  | bB    | 815  | CL7  | C3D-CAD | -2.31 | 1.37        | 1.45     |
| 14  | bA    | 3110 | CL7  | C3B-C4B | -2.31 | 1.37        | 1.42     |
| 13  | cB    | 801  | PHO  | C3D-CAD | -2.31 | 1.42        | 1.47     |
| 14  | aA    | 3125 | CL7  | C3A-C4A | -2.31 | 1.48        | 1.52     |
| 14  | cB    | 808  | CL7  | C3C-C2C | -2.31 | 1.31        | 1.36     |
| 14  | cB    | 814  | CL7  | CHB-C4A | -2.31 | 1.31        | 1.36     |
| 14  | aB    | 3011 | CL7  | C3A-C4A | -2.31 | 1.48        | 1.52     |
| 14  | bB    | 825  | CL7  | C1D-ND  | -2.31 | 1.34        | 1.37     |
| 14  | bB    | 813  | CL7  | CAB-C3B | -2.31 | 1.40        | 1.45     |
| 14  | cA    | 3123 | CL7  | CAB-C3B | -2.31 | 1.40        | 1.45     |
| 14  | aB    | 3019 | CL7  | O1D-CGD | -2.31 | 1.15        | 1.21     |
| 14  | bA    | 3129 | CL7  | O2D-CGD | -2.31 | 1.27        | 1.33     |
| 14  | bA    | 3132 | CL7  | O2A-C1  | 2.31  | 1.52        | 1.46     |
| 14  | bA    | 3123 | CL7  | CBD-CGD | -2.31 | 1.45        | 1.52     |
| 14  | cA    | 3122 | CL7  | CHC-C1C | -2.31 | 1.33        | 1.38     |
| 14  | bB    | 810  | CL7  | C3D-CAD | -2.31 | 1.37        | 1.45     |
| 14  | aA    | 3122 | CL7  | O1D-CGD | -2.31 | 1.15        | 1.21     |
| 14  | cA    | 3126 | CL7  | CHC-C1C | -2.31 | 1.33        | 1.38     |
| 14  | aA    | 3116 | CL7  | C2A-C1A | -2.31 | 1.48        | 1.52     |
| 14  | bA    | 3103 | CL7  | OBB-CAB | 2.31  | 1.27        | 1.22     |
| 14  | aA    | 3107 | CL7  | CBD-CGD | -2.31 | 1.45        | 1.52     |
| 14  | aA    | 3107 | CL7  | OBB-CAB | 2.31  | 1.27        | 1.22     |
| 14  | cA    | 3121 | CL7  | C1C-NC  | 2.31  | 1.40        | 1.37     |
| 14  | bA    | 3108 | CL7  | CAB-C3B | -2.31 | 1.40        | 1.45     |
| 14  | aA    | 3115 | CL7  | CMD-C2D | -2.31 | 1.45        | 1.50     |
| 14  | cB    | 832  | CL7  | CMD-C2D | -2.31 | 1.45        | 1.50     |
| 14  | bA    | 3112 | CL7  | CAB-C3B | -2.31 | 1.40        | 1.45     |
| 14  | cA    | 3114 | CL7  | CMD-C2D | -2.30 | 1.45        | 1.50     |
| 14  | bB    | 811  | CL7  | CHB-C4A | -2.30 | 1.31        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 14  | aA    | 3142 | CL7  | CMA-C3A  | 2.30  | 1.58        | 1.53     |
| 14  | aB    | 3022 | CL7  | C1C-NC   | 2.30  | 1.40        | 1.37     |
| 14  | aA    | 3106 | CL7  | C4B-NB   | -2.30 | 1.35        | 1.37     |
| 14  | cB    | 819  | CL7  | C1A-NA   | -2.30 | 1.32        | 1.38     |
| 14  | bB    | 813  | CL7  | C2A-C1A  | -2.30 | 1.48        | 1.52     |
| 14  | bA    | 3132 | CL7  | C3B-C4B  | -2.30 | 1.37        | 1.42     |
| 14  | aA    | 3141 | CL7  | O2D-CGD  | -2.30 | 1.27        | 1.33     |
| 14  | cB    | 817  | CL7  | CHD-C4C  | -2.30 | 1.33        | 1.38     |
| 14  | cJ    | 101  | CL7  | C3D-CAD  | -2.30 | 1.37        | 1.45     |
| 14  | bA    | 3120 | CL7  | C2A-C1A  | -2.30 | 1.47        | 1.50     |
| 14  | aK    | 101  | CL7  | C1D-C2D  | -2.30 | 1.37        | 1.43     |
| 14  | aA    | 3113 | CL7  | CAB-C3B  | -2.30 | 1.40        | 1.45     |
| 14  | aB    | 3008 | CL7  | C1D-C2D  | -2.30 | 1.37        | 1.43     |
| 14  | bA    | 3125 | CL7  | CBD-CGD  | -2.30 | 1.45        | 1.52     |
| 14  | cL    | 203  | CL7  | CHD-C4C  | -2.30 | 1.33        | 1.38     |
| 14  | aA    | 3117 | CL7  | CHB-C4A  | -2.30 | 1.31        | 1.36     |
| 14  | aL    | 204  | CL7  | C3D-C2D  | -2.30 | 1.35        | 1.42     |
| 14  | cA    | 3114 | CL7  | C6-C5    | -2.30 | 1.43        | 1.52     |
| 14  | bK    | 101  | CL7  | CHC-C1C  | -2.30 | 1.33        | 1.38     |
| 14  | cA    | 3120 | CL7  | CHB-C4A  | -2.30 | 1.31        | 1.36     |
| 14  | aB    | 3007 | CL7  | OB B-CAB | 2.30  | 1.27        | 1.22     |
| 14  | bB    | 804  | CL7  | C3B-C4B  | -2.29 | 1.37        | 1.42     |
| 14  | cA    | 3129 | CL7  | C4D-ND   | -2.29 | 1.34        | 1.37     |
| 14  | cA    | 3111 | CL7  | CHB-C4A  | -2.29 | 1.31        | 1.36     |
| 14  | cB    | 818  | CL7  | C3D-CAD  | -2.29 | 1.37        | 1.45     |
| 14  | aA    | 3133 | CL7  | C3D-CAD  | -2.29 | 1.37        | 1.45     |
| 14  | aA    | 3146 | CL7  | C1D-C2D  | -2.29 | 1.37        | 1.43     |
| 14  | cB    | 809  | CL7  | CHC-C4B  | -2.29 | 1.34        | 1.39     |
| 14  | bB    | 809  | CL7  | CHD-C4C  | -2.29 | 1.33        | 1.38     |
| 14  | bA    | 3108 | CL7  | CHD-C4C  | -2.29 | 1.33        | 1.38     |
| 14  | cB    | 817  | CL7  | CAB-C3B  | -2.29 | 1.40        | 1.45     |
| 14  | aB    | 3005 | CL7  | O2A-C1   | 2.29  | 1.52        | 1.46     |
| 14  | bB    | 832  | CL7  | O2D-CGD  | -2.29 | 1.27        | 1.33     |
| 14  | aB    | 3009 | CL7  | C3D-CAD  | -2.29 | 1.37        | 1.45     |
| 14  | aA    | 3106 | CL7  | C3B-C4B  | -2.29 | 1.37        | 1.42     |
| 14  | bB    | 806  | CL7  | CMD-C2D  | -2.29 | 1.45        | 1.50     |
| 14  | aA    | 3124 | CL7  | CHD-C4C  | -2.29 | 1.33        | 1.38     |
| 14  | bB    | 820  | CL7  | OB B-CAB | 2.29  | 1.27        | 1.22     |
| 14  | aB    | 3021 | CL7  | C3D-CAD  | -2.29 | 1.37        | 1.45     |
| 14  | aA    | 3115 | CL7  | CHD-C4C  | -2.29 | 1.33        | 1.38     |
| 14  | cA    | 3118 | CL7  | CHC-C1C  | -2.29 | 1.33        | 1.38     |
| 14  | aB    | 3015 | CL7  | C2A-C1A  | -2.29 | 1.47        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | bA    | 3102 | CL7  | CHC-C1C | -2.29 | 1.33        | 1.38     |
| 14  | bB    | 824  | CL7  | CHD-C4C | -2.29 | 1.33        | 1.38     |
| 14  | bA    | 3122 | CL7  | C3D-C2D | -2.29 | 1.35        | 1.42     |
| 14  | cA    | 3123 | CL7  | C1D-ND  | -2.29 | 1.35        | 1.37     |
| 14  | bB    | 824  | CL7  | C1D-ND  | -2.28 | 1.35        | 1.37     |
| 14  | cB    | 824  | CL7  | C1D-ND  | -2.28 | 1.35        | 1.37     |
| 14  | bB    | 818  | CL7  | CAB-C3B | -2.28 | 1.40        | 1.45     |
| 14  | cB    | 827  | CL7  | CMA-C3A | 2.28  | 1.58        | 1.53     |
| 14  | aB    | 3002 | CL7  | C3C-C2C | -2.28 | 1.31        | 1.36     |
| 14  | aF    | 201  | CL7  | C3B-C4B | -2.28 | 1.37        | 1.42     |
| 14  | aA    | 3122 | CL7  | C3A-C4A | -2.28 | 1.48        | 1.52     |
| 14  | bA    | 3132 | CL7  | C1C-NC  | 2.28  | 1.40        | 1.37     |
| 14  | aA    | 3104 | CL7  | OBB-CAB | 2.28  | 1.27        | 1.22     |
| 14  | bA    | 3128 | CL7  | O2A-C1  | 2.28  | 1.52        | 1.46     |
| 14  | aB    | 3016 | CL7  | C3D-CAD | -2.28 | 1.37        | 1.45     |
| 12  | aA    | 3101 | G9R  | C3D-C2D | 2.28  | 1.45        | 1.39     |
| 14  | cA    | 3110 | CL7  | CHC-C1C | -2.28 | 1.33        | 1.38     |
| 14  | bA    | 3142 | CL7  | C3D-C2D | -2.28 | 1.35        | 1.42     |
| 14  | bA    | 3103 | CL7  | CAB-C3B | -2.28 | 1.40        | 1.45     |
| 14  | aB    | 3007 | CL7  | CHD-C4C | -2.28 | 1.33        | 1.38     |
| 14  | aA    | 3134 | CL7  | C2A-C1A | -2.28 | 1.48        | 1.52     |
| 14  | bA    | 3106 | CL7  | CMD-C2D | -2.28 | 1.46        | 1.50     |
| 14  | cA    | 3103 | CL7  | OBB-CAB | 2.28  | 1.27        | 1.22     |
| 14  | bB    | 820  | CL7  | O2D-CGD | -2.28 | 1.27        | 1.33     |
| 14  | aB    | 3023 | CL7  | C3B-C4B | -2.28 | 1.37        | 1.42     |
| 14  | aB    | 3017 | CL7  | CAB-C3B | -2.28 | 1.40        | 1.45     |
| 14  | aA    | 3126 | CL7  | OBD-CAD | -2.28 | 1.18        | 1.22     |
| 14  | bB    | 822  | CL7  | C3D-CAD | -2.28 | 1.37        | 1.45     |
| 14  | aB    | 3009 | CL7  | CHB-C4A | -2.28 | 1.31        | 1.36     |
| 14  | aA    | 3122 | CL7  | C1C-NC  | 2.28  | 1.40        | 1.37     |
| 14  | cB    | 825  | CL7  | CAB-C3B | -2.28 | 1.40        | 1.45     |
| 14  | cB    | 808  | CL7  | C3A-C4A | -2.28 | 1.48        | 1.52     |
| 14  | cA    | 3102 | CL7  | C1D-C2D | -2.28 | 1.37        | 1.43     |
| 14  | aK    | 101  | CL7  | CHC-C1C | -2.27 | 1.34        | 1.38     |
| 14  | cB    | 811  | CL7  | CHD-C4C | -2.27 | 1.34        | 1.38     |
| 14  | bB    | 811  | CL7  | O1D-CGD | -2.27 | 1.15        | 1.21     |
| 14  | bA    | 3105 | CL7  | C3B-C4B | -2.27 | 1.37        | 1.42     |
| 14  | bA    | 3127 | CL7  | C4D-ND  | -2.27 | 1.34        | 1.37     |
| 14  | cB    | 824  | CL7  | CHD-C4C | -2.27 | 1.34        | 1.38     |
| 14  | cA    | 3120 | CL7  | C3B-C4B | -2.27 | 1.37        | 1.42     |
| 14  | cA    | 3128 | CL7  | CBD-CGD | -2.27 | 1.45        | 1.52     |
| 14  | cA    | 3121 | CL7  | C3C-C2C | -2.27 | 1.31        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 17  | cB    | 828  | PQN  | C12-C13  | 2.27  | 1.38        | 1.33     |
| 14  | aA    | 3123 | CL7  | C3D-C2D  | -2.27 | 1.35        | 1.42     |
| 14  | bB    | 807  | CL7  | O2D-CGD  | -2.27 | 1.27        | 1.33     |
| 14  | aL    | 204  | CL7  | C1D-ND   | -2.27 | 1.35        | 1.37     |
| 14  | cA    | 3103 | CL7  | C3D-CAD  | -2.27 | 1.37        | 1.45     |
| 14  | bA    | 3132 | CL7  | O1A-CGA  | 2.27  | 1.29        | 1.22     |
| 14  | aB    | 3007 | CL7  | CMD-C2D  | -2.27 | 1.46        | 1.50     |
| 14  | aA    | 3121 | CL7  | C3D-CAD  | -2.27 | 1.37        | 1.45     |
| 19  | bB    | 830  | LMG  | O7-C8    | -2.27 | 1.40        | 1.46     |
| 14  | bB    | 819  | CL7  | C3D-C2D  | -2.27 | 1.35        | 1.42     |
| 14  | bA    | 3108 | CL7  | C3B-C4B  | -2.27 | 1.37        | 1.42     |
| 14  | bB    | 803  | CL7  | CHD-C4C  | -2.27 | 1.34        | 1.38     |
| 14  | aA    | 3113 | CL7  | C1B-NB   | 2.27  | 1.40        | 1.37     |
| 17  | cB    | 828  | PQN  | C24-C23  | -2.27 | 1.45        | 1.52     |
| 14  | aA    | 3104 | CL7  | C3D-CAD  | -2.27 | 1.37        | 1.45     |
| 14  | aA    | 3123 | CL7  | C3D-CAD  | -2.26 | 1.37        | 1.45     |
| 14  | aA    | 3132 | CL7  | C3D-CAD  | -2.26 | 1.37        | 1.45     |
| 14  | bA    | 3125 | CL7  | C3D-CAD  | -2.26 | 1.37        | 1.45     |
| 14  | aA    | 3107 | CL7  | C3B-C4B  | -2.26 | 1.37        | 1.42     |
| 14  | bA    | 3129 | CL7  | CMA-C3A  | -2.26 | 1.48        | 1.53     |
| 14  | cA    | 3104 | CL7  | CHD-C4C  | -2.26 | 1.34        | 1.38     |
| 14  | aA    | 3140 | CL7  | C1D-C2D  | -2.26 | 1.37        | 1.43     |
| 14  | aA    | 3106 | CL7  | O2D-CGD  | -2.26 | 1.27        | 1.33     |
| 14  | aJ    | 101  | CL7  | CAB-C3B  | -2.26 | 1.40        | 1.45     |
| 14  | cA    | 3123 | CL7  | O2A-CGA  | 2.26  | 1.39        | 1.33     |
| 14  | aB    | 3014 | CL7  | C3D-CAD  | -2.26 | 1.37        | 1.45     |
| 14  | aA    | 3105 | CL7  | CHB-C4A  | -2.26 | 1.31        | 1.36     |
| 14  | cA    | 3132 | CL7  | CHC-C1C  | -2.26 | 1.34        | 1.38     |
| 14  | bB    | 816  | CL7  | O1D-CGD  | -2.26 | 1.15        | 1.21     |
| 14  | cA    | 3132 | CL7  | C1D-C2D  | -2.26 | 1.37        | 1.43     |
| 14  | cA    | 3120 | CL7  | O2D-CED  | -2.26 | 1.40        | 1.45     |
| 14  | cB    | 809  | CL7  | OB B-CAB | 2.26  | 1.27        | 1.22     |
| 14  | bB    | 820  | CL7  | C3B-C4B  | -2.26 | 1.37        | 1.42     |
| 14  | aA    | 3125 | CL7  | C3D-CAD  | -2.26 | 1.37        | 1.45     |
| 14  | aA    | 3128 | CL7  | C3D-CAD  | -2.26 | 1.37        | 1.45     |
| 14  | aB    | 3002 | CL7  | CBD-CGD  | -2.26 | 1.45        | 1.52     |
| 14  | aL    | 204  | CL7  | O2D-CGD  | -2.26 | 1.27        | 1.33     |
| 14  | aB    | 3023 | CL7  | C1D-ND   | -2.26 | 1.35        | 1.37     |
| 14  | aA    | 3112 | CL7  | C2A-C1A  | -2.26 | 1.48        | 1.52     |
| 14  | aB    | 3008 | CL7  | O2A-C1   | 2.26  | 1.52        | 1.46     |
| 14  | bA    | 3122 | CL7  | C1C-NC   | 2.26  | 1.40        | 1.37     |
| 14  | cA    | 3121 | CL7  | C3D-C2D  | -2.26 | 1.35        | 1.42     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | bL    | 204  | CL7  | CBA-CGA | -2.26 | 1.44        | 1.50     |
| 14  | cA    | 3126 | CL7  | CHD-C4C | -2.25 | 1.34        | 1.38     |
| 14  | bA    | 3104 | CL7  | CAB-C3B | -2.25 | 1.40        | 1.45     |
| 14  | cB    | 803  | CL7  | CHD-C4C | -2.25 | 1.34        | 1.38     |
| 17  | cA    | 3143 | PQN  | C2-C1   | -2.25 | 1.43        | 1.48     |
| 14  | aB    | 3024 | CL7  | C1D-ND  | -2.25 | 1.35        | 1.37     |
| 14  | aA    | 3141 | CL7  | C3D-CAD | -2.25 | 1.37        | 1.45     |
| 14  | bB    | 819  | CL7  | O2A-C1  | 2.25  | 1.52        | 1.46     |
| 14  | bB    | 832  | CL7  | CHD-C4C | -2.25 | 1.34        | 1.38     |
| 14  | bA    | 3108 | CL7  | C1C-NC  | 2.25  | 1.40        | 1.37     |
| 14  | bA    | 3110 | CL7  | C2A-C1A | -2.25 | 1.48        | 1.52     |
| 14  | aA    | 3123 | CL7  | CHB-C4A | -2.25 | 1.31        | 1.36     |
| 14  | bB    | 817  | CL7  | CHB-C4A | -2.25 | 1.31        | 1.36     |
| 14  | aA    | 3141 | CL7  | C1D-ND  | -2.25 | 1.35        | 1.37     |
| 14  | bB    | 826  | CL7  | O2D-CED | -2.25 | 1.40        | 1.45     |
| 14  | aB    | 3006 | CL7  | O1D-CGD | -2.25 | 1.15        | 1.21     |
| 14  | bB    | 819  | CL7  | O2D-CED | -2.25 | 1.40        | 1.45     |
| 14  | cA    | 3123 | CL7  | C3D-CAD | -2.25 | 1.37        | 1.45     |
| 14  | cB    | 812  | CL7  | CHC-C1C | -2.25 | 1.34        | 1.38     |
| 14  | aB    | 3021 | CL7  | OBb-CAB | 2.25  | 1.27        | 1.22     |
| 14  | cA    | 3120 | CL7  | O2D-CGD | -2.25 | 1.27        | 1.33     |
| 14  | bB    | 809  | CL7  | C1D-ND  | -2.25 | 1.35        | 1.37     |
| 14  | bA    | 3120 | CL7  | CHB-C4A | -2.25 | 1.31        | 1.36     |
| 14  | bA    | 3111 | CL7  | OBb-CAB | 2.25  | 1.27        | 1.22     |
| 14  | cB    | 810  | CL7  | CMA-C3A | 2.25  | 1.58        | 1.53     |
| 14  | cB    | 817  | CL7  | CHB-C4A | -2.25 | 1.31        | 1.36     |
| 14  | cB    | 831  | CL7  | C1D-ND  | -2.25 | 1.35        | 1.37     |
| 14  | cB    | 809  | CL7  | C1D-C2D | -2.25 | 1.38        | 1.43     |
| 14  | aB    | 3006 | CL7  | CHC-C1C | -2.25 | 1.34        | 1.38     |
| 14  | aB    | 3013 | CL7  | CHD-C4C | -2.25 | 1.34        | 1.38     |
| 12  | bA    | 3101 | G9R  | CMB-C2B | -2.25 | 1.46        | 1.50     |
| 14  | aA    | 3127 | CL7  | O2A-C1  | 2.25  | 1.52        | 1.46     |
| 14  | bA    | 3107 | CL7  | CAB-C3B | -2.24 | 1.40        | 1.45     |
| 14  | aB    | 3003 | CL7  | C3D-C2D | -2.24 | 1.35        | 1.42     |
| 14  | bB    | 809  | CL7  | C1C-NC  | 2.24  | 1.40        | 1.37     |
| 14  | bA    | 3121 | CL7  | C3C-C2C | -2.24 | 1.31        | 1.36     |
| 14  | cA    | 3132 | CL7  | O2A-C1  | 2.24  | 1.52        | 1.46     |
| 14  | bA    | 3131 | CL7  | CHB-C4A | -2.24 | 1.31        | 1.36     |
| 14  | aA    | 3103 | CL7  | CAB-C3B | -2.24 | 1.40        | 1.45     |
| 14  | aA    | 3107 | CL7  | C1D-C2D | -2.24 | 1.38        | 1.43     |
| 14  | cA    | 3128 | CL7  | C1D-C2D | -2.24 | 1.38        | 1.43     |
| 14  | aB    | 3017 | CL7  | CHD-C4C | -2.24 | 1.34        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | bA    | 3120 | CL7  | C3B-C4B | -2.24 | 1.37        | 1.42     |
| 14  | cA    | 3119 | CL7  | C1A-CHA | -2.24 | 1.28        | 1.38     |
| 14  | aA    | 3125 | CL7  | O2A-C1  | 2.24  | 1.52        | 1.46     |
| 14  | cB    | 821  | CL7  | C3D-CAD | -2.24 | 1.37        | 1.45     |
| 14  | bL    | 204  | CL7  | C3B-C4B | -2.24 | 1.37        | 1.42     |
| 14  | cA    | 3106 | CL7  | C3D-C2D | -2.24 | 1.35        | 1.42     |
| 14  | bB    | 823  | CL7  | CHD-C4C | -2.24 | 1.34        | 1.38     |
| 17  | aA    | 3144 | PQN  | C10-C5  | 2.24  | 1.44        | 1.40     |
| 14  | bB    | 808  | CL7  | C3B-C4B | -2.24 | 1.37        | 1.42     |
| 14  | bA    | 3102 | CL7  | C4D-ND  | -2.24 | 1.34        | 1.37     |
| 14  | aA    | 3128 | CL7  | CAA-CBA | -2.24 | 1.45        | 1.52     |
| 14  | cB    | 817  | CL7  | O2D-CGD | -2.24 | 1.27        | 1.33     |
| 14  | cB    | 813  | CL7  | C3D-CAD | -2.24 | 1.37        | 1.45     |
| 17  | aA    | 3144 | PQN  | C2M-C2  | -2.24 | 1.46        | 1.50     |
| 14  | cB    | 832  | CL7  | CAA-C2A | -2.24 | 1.49        | 1.54     |
| 14  | aL    | 203  | CL7  | C3B-C4B | -2.24 | 1.37        | 1.42     |
| 14  | bA    | 3129 | CL7  | C4B-NB  | -2.24 | 1.35        | 1.37     |
| 14  | bA    | 3139 | CL7  | CAB-C3B | -2.24 | 1.40        | 1.45     |
| 14  | aA    | 3130 | CL7  | C4B-NB  | -2.24 | 1.35        | 1.37     |
| 14  | aB    | 3016 | CL7  | CHD-C4C | -2.24 | 1.34        | 1.38     |
| 12  | cA    | 3101 | G9R  | C4D-ND  | -2.24 | 1.34        | 1.37     |
| 14  | cB    | 811  | CL7  | C2A-C1A | -2.24 | 1.48        | 1.52     |
| 14  | cA    | 3122 | CL7  | C1D-ND  | -2.23 | 1.35        | 1.37     |
| 14  | bA    | 3112 | CL7  | C3D-CAD | -2.23 | 1.37        | 1.45     |
| 14  | bA    | 3132 | CL7  | CHC-C1C | -2.23 | 1.34        | 1.38     |
| 14  | aB    | 3007 | CL7  | CMA-C3A | 2.23  | 1.58        | 1.53     |
| 14  | aA    | 3142 | CL7  | C1D-ND  | -2.23 | 1.35        | 1.37     |
| 14  | bA    | 3105 | CL7  | OBB-CAB | 2.23  | 1.27        | 1.22     |
| 14  | aA    | 3107 | CL7  | CMD-C2D | -2.23 | 1.46        | 1.50     |
| 14  | aB    | 3006 | CL7  | O2D-CGD | -2.23 | 1.27        | 1.33     |
| 14  | cA    | 3124 | CL7  | C2A-C1A | -2.23 | 1.47        | 1.50     |
| 17  | bA    | 3143 | PQN  | C2-C1   | -2.23 | 1.43        | 1.48     |
| 14  | aB    | 3030 | CL7  | OBB-CAB | 2.23  | 1.27        | 1.22     |
| 14  | aA    | 3130 | CL7  | C1A-CHA | -2.23 | 1.28        | 1.38     |
| 14  | cA    | 3105 | CL7  | C3B-C4B | -2.23 | 1.37        | 1.42     |
| 14  | bB    | 823  | CL7  | C1C-NC  | 2.23  | 1.40        | 1.37     |
| 14  | bB    | 819  | CL7  | O2D-CGD | -2.23 | 1.27        | 1.33     |
| 14  | cA    | 3110 | CL7  | C3B-C4B | -2.23 | 1.37        | 1.42     |
| 14  | cA    | 3128 | CL7  | CHD-C4C | -2.23 | 1.34        | 1.38     |
| 14  | cA    | 3114 | CL7  | CBD-CGD | -2.23 | 1.45        | 1.52     |
| 14  | aB    | 3032 | CL7  | CBD-CGD | -2.22 | 1.45        | 1.52     |
| 14  | aB    | 3020 | CL7  | C3D-CAD | -2.22 | 1.37        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | aA    | 3122 | CL7  | C3C-C2C | -2.22 | 1.32        | 1.36     |
| 14  | cA    | 3142 | CL7  | O2D-CGD | -2.22 | 1.27        | 1.33     |
| 14  | bA    | 3111 | CL7  | CHB-C4A | -2.22 | 1.31        | 1.36     |
| 14  | aA    | 3111 | CL7  | CAB-C3B | -2.22 | 1.40        | 1.45     |
| 14  | cA    | 3139 | CL7  | CHB-C4A | -2.22 | 1.31        | 1.36     |
| 14  | cA    | 3113 | CL7  | OBB-CAB | 2.22  | 1.27        | 1.22     |
| 14  | cA    | 3115 | CL7  | CHC-C1C | -2.22 | 1.34        | 1.38     |
| 14  | aA    | 3107 | CL7  | C3C-C2C | -2.22 | 1.32        | 1.36     |
| 14  | cA    | 3118 | CL7  | CMD-C2D | -2.22 | 1.46        | 1.50     |
| 14  | cB    | 823  | CL7  | CHD-C4C | -2.22 | 1.34        | 1.38     |
| 14  | cL    | 204  | CL7  | C3D-CAD | -2.22 | 1.37        | 1.45     |
| 14  | cA    | 3132 | CL7  | OBB-CAB | 2.22  | 1.27        | 1.22     |
| 14  | cB    | 831  | CL7  | C3A-C4A | -2.22 | 1.48        | 1.52     |
| 13  | aB    | 3004 | PHO  | C4C-NC  | -2.22 | 1.30        | 1.37     |
| 14  | cB    | 803  | CL7  | C3C-C2C | -2.22 | 1.32        | 1.36     |
| 14  | aJ    | 101  | CL7  | C3D-CAD | -2.22 | 1.37        | 1.45     |
| 14  | bA    | 3102 | CL7  | MG-NA   | -2.22 | 2.01        | 2.05     |
| 14  | bA    | 3104 | CL7  | CHD-C4C | -2.22 | 1.34        | 1.38     |
| 14  | cF    | 201  | CL7  | C2A-C1A | -2.22 | 1.48        | 1.52     |
| 14  | aB    | 3012 | CL7  | C3D-CAD | -2.22 | 1.37        | 1.45     |
| 14  | bA    | 3141 | CL7  | CAB-C3B | -2.22 | 1.40        | 1.45     |
| 14  | aB    | 3025 | CL7  | C3D-C2D | -2.22 | 1.35        | 1.42     |
| 14  | aB    | 3031 | CL7  | CAA-C2A | -2.22 | 1.50        | 1.54     |
| 14  | bA    | 3105 | CL7  | O2D-CGD | -2.22 | 1.27        | 1.33     |
| 14  | aB    | 3003 | CL7  | CHB-C4A | -2.22 | 1.31        | 1.36     |
| 14  | cA    | 3131 | CL7  | CHB-C4A | -2.22 | 1.31        | 1.36     |
| 14  | bB    | 818  | CL7  | CHD-C4C | -2.22 | 1.34        | 1.38     |
| 14  | cA    | 3127 | CL7  | C3B-C4B | -2.22 | 1.37        | 1.42     |
| 14  | bA    | 3108 | CL7  | C3D-C2D | -2.22 | 1.35        | 1.42     |
| 14  | aB    | 3023 | CL7  | CHD-C4C | -2.22 | 1.34        | 1.38     |
| 14  | bB    | 822  | CL7  | OBB-CAB | 2.22  | 1.27        | 1.22     |
| 14  | cA    | 3140 | CL7  | C3A-C4A | -2.22 | 1.48        | 1.52     |
| 14  | aA    | 3132 | CL7  | CAB-C3B | -2.22 | 1.40        | 1.45     |
| 14  | aB    | 3009 | CL7  | C6-C5   | -2.22 | 1.44        | 1.52     |
| 14  | cA    | 3132 | CL7  | C1D-ND  | -2.22 | 1.35        | 1.37     |
| 14  | bB    | 809  | CL7  | CAB-C3B | -2.22 | 1.40        | 1.45     |
| 14  | bB    | 806  | CL7  | C6-C5   | -2.22 | 1.44        | 1.52     |
| 14  | bA    | 3121 | CL7  | C3D-C2D | -2.22 | 1.35        | 1.42     |
| 14  | bA    | 3139 | CL7  | C3D-C2D | -2.22 | 1.35        | 1.42     |
| 14  | bA    | 3115 | CL7  | CHC-C1C | -2.22 | 1.34        | 1.38     |
| 14  | bL    | 205  | CL7  | C1D-ND  | -2.22 | 1.35        | 1.37     |
| 14  | cL    | 203  | CL7  | C3A-C4A | -2.22 | 1.48        | 1.52     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | aA    | 3131 | CL7  | C2A-C1A | -2.22 | 1.48        | 1.52     |
| 14  | cA    | 3108 | CL7  | O1D-CGD | -2.21 | 1.15        | 1.21     |
| 14  | bA    | 3127 | CL7  | C3A-C2A | -2.21 | 1.48        | 1.54     |
| 14  | bA    | 3103 | CL7  | C3D-CAD | -2.21 | 1.37        | 1.45     |
| 14  | aB    | 3031 | CL7  | CHD-C4C | -2.21 | 1.34        | 1.38     |
| 14  | aA    | 3124 | CL7  | C3A-C4A | -2.21 | 1.48        | 1.52     |
| 14  | aA    | 3126 | CL7  | C4D-ND  | -2.21 | 1.34        | 1.37     |
| 14  | bA    | 3103 | CL7  | C3A-C4A | -2.21 | 1.48        | 1.52     |
| 14  | aB    | 3002 | CL7  | OBB-CAB | 2.21  | 1.27        | 1.22     |
| 14  | cB    | 812  | CL7  | C3A-C4A | -2.21 | 1.48        | 1.52     |
| 14  | aA    | 3124 | CL7  | C4D-ND  | -2.21 | 1.34        | 1.37     |
| 14  | bA    | 3106 | CL7  | C3D-C2D | -2.21 | 1.35        | 1.42     |
| 14  | bB    | 814  | CL7  | C2A-C1A | -2.21 | 1.48        | 1.52     |
| 14  | cB    | 814  | CL7  | CHD-C4C | -2.21 | 1.34        | 1.38     |
| 14  | cB    | 811  | CL7  | CHB-C4A | -2.21 | 1.31        | 1.36     |
| 14  | cA    | 3124 | CL7  | CHD-C4C | -2.21 | 1.34        | 1.38     |
| 14  | aA    | 3146 | CL7  | C3D-CAD | -2.21 | 1.37        | 1.45     |
| 14  | bB    | 820  | CL7  | C3D-C2D | -2.21 | 1.35        | 1.42     |
| 12  | bA    | 3101 | G9R  | CMA-C3A | -2.21 | 1.48        | 1.53     |
| 14  | aB    | 3002 | CL7  | CHD-C4C | -2.21 | 1.34        | 1.38     |
| 14  | bB    | 814  | CL7  | CHD-C4C | -2.21 | 1.34        | 1.38     |
| 14  | aB    | 3013 | CL7  | C3D-CAD | -2.21 | 1.37        | 1.45     |
| 14  | cB    | 804  | CL7  | CHB-C4A | -2.21 | 1.31        | 1.36     |
| 14  | cB    | 804  | CL7  | CBD-CGD | -2.21 | 1.45        | 1.52     |
| 14  | bA    | 3145 | CL7  | C2A-C1A | -2.21 | 1.48        | 1.52     |
| 14  | bB    | 816  | CL7  | C3C-C2C | -2.21 | 1.32        | 1.36     |
| 14  | aA    | 3121 | CL7  | C1D-ND  | -2.21 | 1.35        | 1.37     |
| 14  | cA    | 3123 | CL7  | C3D-C2D | -2.21 | 1.35        | 1.42     |
| 14  | bF    | 201  | CL7  | C2A-C1A | -2.21 | 1.48        | 1.52     |
| 14  | cA    | 3132 | CL7  | C3B-C4B | -2.21 | 1.37        | 1.42     |
| 14  | bA    | 3120 | CL7  | OBB-CAB | 2.20  | 1.27        | 1.22     |
| 14  | bA    | 3124 | CL7  | OBB-CAB | 2.20  | 1.27        | 1.22     |
| 14  | cA    | 3103 | CL7  | C3A-C4A | -2.20 | 1.48        | 1.52     |
| 14  | bB    | 807  | CL7  | CBD-CGD | -2.20 | 1.45        | 1.52     |
| 14  | bB    | 821  | CL7  | C3D-CAD | -2.20 | 1.37        | 1.45     |
| 14  | cA    | 3139 | CL7  | C3D-C2D | -2.20 | 1.35        | 1.42     |
| 14  | bA    | 3141 | CL7  | O2A-C1  | 2.20  | 1.52        | 1.46     |
| 14  | cB    | 807  | CL7  | CBD-CGD | -2.20 | 1.45        | 1.52     |
| 14  | bB    | 819  | CL7  | CHB-C4A | -2.20 | 1.31        | 1.36     |
| 14  | cB    | 814  | CL7  | C3D-CAD | -2.20 | 1.37        | 1.45     |
| 14  | aA    | 3125 | CL7  | C2A-C1A | -2.20 | 1.47        | 1.50     |
| 16  | aA    | 3138 | LHG  | P-O3    | 2.20  | 1.68        | 1.59     |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 14  | bL    | 203  | CL7  | C3B-C4B  | -2.20 | 1.37        | 1.42     |
| 14  | cB    | 809  | CL7  | C1D-ND   | -2.20 | 1.35        | 1.37     |
| 14  | bB    | 813  | CL7  | C3D-CAD  | -2.20 | 1.37        | 1.45     |
| 14  | bB    | 814  | CL7  | C3D-CAD  | -2.20 | 1.37        | 1.45     |
| 14  | aB    | 3019 | CL7  | C3D-C2D  | -2.20 | 1.35        | 1.42     |
| 14  | cA    | 3126 | CL7  | C3D-CAD  | -2.20 | 1.37        | 1.45     |
| 14  | aB    | 3007 | CL7  | CAB-C3B  | -2.20 | 1.40        | 1.45     |
| 14  | cA    | 3111 | CL7  | OB B-CAB | 2.20  | 1.27        | 1.22     |
| 14  | bL    | 204  | CL7  | C3D-CAD  | -2.20 | 1.37        | 1.45     |
| 14  | bA    | 3145 | CL7  | C3D-CAD  | -2.20 | 1.37        | 1.45     |
| 14  | aA    | 3128 | CL7  | C4D-ND   | -2.20 | 1.34        | 1.37     |
| 14  | bB    | 817  | CL7  | CAB-C3B  | -2.20 | 1.40        | 1.45     |
| 14  | cB    | 833  | CL7  | CHC-C1C  | -2.19 | 1.34        | 1.38     |
| 14  | cA    | 3131 | CL7  | C3B-C4B  | -2.19 | 1.37        | 1.42     |
| 14  | bA    | 3119 | CL7  | C1C-NC   | 2.19  | 1.40        | 1.37     |
| 14  | aA    | 3116 | CL7  | CHC-C1C  | -2.19 | 1.34        | 1.38     |
| 14  | aK    | 101  | CL7  | CHB-C4A  | -2.19 | 1.31        | 1.36     |
| 14  | bA    | 3118 | CL7  | CHB-C4A  | -2.19 | 1.31        | 1.36     |
| 14  | cA    | 3142 | CL7  | C3D-C2D  | -2.19 | 1.35        | 1.42     |
| 14  | cA    | 3112 | CL7  | C3D-CAD  | -2.19 | 1.37        | 1.45     |
| 14  | bA    | 3121 | CL7  | C3B-C4B  | -2.19 | 1.37        | 1.42     |
| 14  | bB    | 809  | CL7  | C3B-C4B  | -2.19 | 1.37        | 1.42     |
| 14  | aA    | 3141 | CL7  | C4C-NC   | 2.19  | 1.40        | 1.37     |
| 14  | aB    | 3030 | CL7  | C1D-ND   | -2.19 | 1.35        | 1.37     |
| 14  | aA    | 3130 | CL7  | C1D-ND   | -2.19 | 1.35        | 1.37     |
| 14  | aB    | 3026 | CL7  | CMC-C2C  | -2.19 | 1.46        | 1.50     |
| 14  | aA    | 3120 | CL7  | CAA-CBA  | -2.19 | 1.46        | 1.52     |
| 14  | bA    | 3123 | CL7  | C3D-C2D  | -2.19 | 1.35        | 1.42     |
| 14  | bB    | 812  | CL7  | CHC-C1C  | -2.19 | 1.34        | 1.38     |
| 14  | cA    | 3113 | CL7  | CHD-C4C  | -2.19 | 1.34        | 1.38     |
| 14  | aA    | 3111 | CL7  | C3B-C4B  | -2.19 | 1.37        | 1.42     |
| 14  | cA    | 3139 | CL7  | C3B-C4B  | -2.19 | 1.37        | 1.42     |
| 14  | bB    | 812  | CL7  | C3A-C4A  | -2.19 | 1.48        | 1.52     |
| 14  | cA    | 3107 | CL7  | CHB-C4A  | -2.19 | 1.31        | 1.36     |
| 14  | cA    | 3123 | CL7  | C2A-C1A  | -2.19 | 1.47        | 1.50     |
| 14  | cB    | 815  | CL7  | O2D-CGD  | -2.19 | 1.27        | 1.33     |
| 14  | aL    | 202  | CL7  | C1A-NA   | -2.19 | 1.32        | 1.38     |
| 17  | aB    | 3027 | PQN  | C11-C3   | 2.19  | 1.55        | 1.51     |
| 14  | cB    | 817  | CL7  | C2A-C1A  | -2.19 | 1.48        | 1.52     |
| 14  | aB    | 3016 | CL7  | O2D-CGD  | -2.19 | 1.27        | 1.33     |
| 14  | cB    | 833  | CL7  | C3A-C4A  | -2.18 | 1.48        | 1.52     |
| 14  | aB    | 3032 | CL7  | C1B-NB   | -2.18 | 1.35        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | bB    | 824  | CL7  | C4C-NC  | 2.18  | 1.40        | 1.37     |
| 16  | bA    | 3137 | LHG  | O6-C4   | -2.18 | 1.36        | 1.44     |
| 14  | aA    | 3143 | CL7  | C1B-NB  | 2.18  | 1.40        | 1.37     |
| 14  | aA    | 3120 | CL7  | OBB-CAB | 2.18  | 1.27        | 1.22     |
| 14  | bB    | 809  | CL7  | C1D-C2D | -2.18 | 1.38        | 1.43     |
| 14  | bB    | 832  | CL7  | CAA-C2A | -2.18 | 1.50        | 1.54     |
| 14  | cB    | 808  | CL7  | C3D-C2D | -2.18 | 1.35        | 1.42     |
| 14  | bA    | 3124 | CL7  | C3C-C2C | -2.18 | 1.32        | 1.36     |
| 14  | aA    | 3143 | CL7  | CAA-C2A | -2.18 | 1.50        | 1.54     |
| 14  | aA    | 3133 | CL7  | O1A-CGA | 2.18  | 1.29        | 1.22     |
| 14  | bA    | 3113 | CL7  | C4D-ND  | -2.18 | 1.34        | 1.37     |
| 14  | cB    | 820  | CL7  | C2A-C1A | -2.18 | 1.47        | 1.50     |
| 14  | cB    | 833  | CL7  | C3D-C2D | -2.18 | 1.35        | 1.42     |
| 14  | cB    | 815  | CL7  | C3B-C4B | -2.18 | 1.37        | 1.42     |
| 14  | bL    | 204  | CL7  | C1D-ND  | -2.18 | 1.35        | 1.37     |
| 14  | aB    | 3013 | CL7  | C2A-C1A | -2.18 | 1.48        | 1.52     |
| 14  | bB    | 817  | CL7  | O2D-CGD | -2.18 | 1.27        | 1.33     |
| 14  | cA    | 3126 | CL7  | O2D-CGD | -2.18 | 1.27        | 1.33     |
| 14  | bA    | 3141 | CL7  | CMA-C3A | 2.18  | 1.57        | 1.53     |
| 14  | cB    | 810  | CL7  | C6-C5   | -2.18 | 1.44        | 1.52     |
| 14  | aA    | 3104 | CL7  | C2A-C1A | -2.18 | 1.48        | 1.52     |
| 14  | cA    | 3102 | CL7  | CBA-CGA | -2.17 | 1.44        | 1.50     |
| 14  | cA    | 3104 | CL7  | CHB-C4A | -2.17 | 1.31        | 1.36     |
| 14  | bA    | 3145 | CL7  | C3B-C4B | -2.17 | 1.37        | 1.42     |
| 14  | aB    | 3020 | CL7  | C2A-C1A | -2.17 | 1.48        | 1.52     |
| 14  | bA    | 3126 | CL7  | CHB-C4A | -2.17 | 1.30        | 1.36     |
| 14  | cB    | 803  | CL7  | CMA-C3A | 2.17  | 1.57        | 1.53     |
| 14  | aL    | 203  | CL7  | C1D-ND  | -2.17 | 1.35        | 1.37     |
| 14  | bB    | 803  | CL7  | CBD-CGD | -2.17 | 1.45        | 1.52     |
| 14  | bL    | 203  | CL7  | C1A-NA  | -2.17 | 1.32        | 1.38     |
| 14  | bB    | 831  | CL7  | CHC-C1C | -2.17 | 1.34        | 1.38     |
| 14  | bA    | 3108 | CL7  | CHB-C4A | -2.17 | 1.31        | 1.36     |
| 14  | cA    | 3124 | CL7  | C1D-ND  | -2.17 | 1.35        | 1.37     |
| 17  | aB    | 3027 | PQN  | C24-C23 | -2.17 | 1.45        | 1.52     |
| 14  | bA    | 3127 | CL7  | CAA-CBA | -2.17 | 1.46        | 1.52     |
| 17  | aB    | 3027 | PQN  | C10-C5  | 2.17  | 1.44        | 1.40     |
| 14  | aB    | 3020 | CL7  | CHB-C4A | -2.17 | 1.31        | 1.36     |
| 14  | cB    | 822  | CL7  | C3B-C4B | -2.16 | 1.37        | 1.42     |
| 14  | cB    | 832  | CL7  | CHD-C4C | -2.16 | 1.34        | 1.38     |
| 14  | cL    | 203  | CL7  | C1A-NA  | -2.16 | 1.32        | 1.38     |
| 14  | bA    | 3140 | CL7  | C4C-NC  | 2.16  | 1.40        | 1.37     |
| 14  | cA    | 3144 | CL7  | C2A-C1A | -2.16 | 1.48        | 1.52     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | cA    | 3105 | CL7  | O2D-CGD | -2.16 | 1.27        | 1.33     |
| 14  | bA    | 3121 | CL7  | CMD-C2D | -2.16 | 1.46        | 1.50     |
| 14  | bB    | 827  | CL7  | C3A-C4A | -2.16 | 1.48        | 1.52     |
| 14  | aB    | 3006 | CL7  | CBD-CGD | -2.16 | 1.45        | 1.52     |
| 14  | aA    | 3124 | CL7  | CAA-C2A | -2.16 | 1.50        | 1.54     |
| 14  | cB    | 806  | CL7  | O2A-C1  | 2.16  | 1.52        | 1.46     |
| 14  | cL    | 204  | CL7  | C4C-NC  | 2.16  | 1.40        | 1.37     |
| 14  | bA    | 3128 | CL7  | C3D-C2D | -2.16 | 1.35        | 1.42     |
| 14  | aB    | 3014 | CL7  | CHB-C4A | -2.16 | 1.31        | 1.36     |
| 14  | bA    | 3117 | CL7  | C3D-CAD | -2.16 | 1.37        | 1.45     |
| 14  | aA    | 3113 | CL7  | C3D-CAD | -2.16 | 1.37        | 1.45     |
| 14  | cF    | 201  | CL7  | C3D-CAD | -2.16 | 1.37        | 1.45     |
| 14  | bB    | 816  | CL7  | C1C-NC  | 2.16  | 1.40        | 1.37     |
| 14  | aL    | 203  | CL7  | C3A-C4A | -2.16 | 1.48        | 1.52     |
| 14  | bA    | 3102 | CL7  | CBA-CGA | -2.16 | 1.44        | 1.50     |
| 14  | cB    | 819  | CL7  | C3A-C4A | -2.16 | 1.48        | 1.52     |
| 14  | bB    | 803  | CL7  | C1C-NC  | 2.16  | 1.40        | 1.37     |
| 14  | aB    | 3002 | CL7  | C3B-C4B | -2.16 | 1.37        | 1.42     |
| 14  | cA    | 3127 | CL7  | C3A-C2A | -2.16 | 1.48        | 1.54     |
| 14  | aB    | 3008 | CL7  | CHC-C4B | -2.16 | 1.34        | 1.39     |
| 14  | aA    | 3110 | CL7  | CAB-C3B | -2.16 | 1.40        | 1.45     |
| 14  | cA    | 3113 | CL7  | C4D-ND  | -2.16 | 1.34        | 1.37     |
| 14  | bA    | 3112 | CL7  | C1D-ND  | -2.16 | 1.35        | 1.37     |
| 14  | cA    | 3106 | CL7  | C4C-NC  | 2.16  | 1.40        | 1.37     |
| 14  | aA    | 3126 | CL7  | C3D-CAD | -2.15 | 1.37        | 1.45     |
| 14  | aA    | 3140 | CL7  | CAB-C3B | -2.15 | 1.40        | 1.45     |
| 14  | aA    | 3146 | CL7  | C2A-C1A | -2.15 | 1.48        | 1.52     |
| 14  | bB    | 811  | CL7  | O2D-CGD | -2.15 | 1.28        | 1.33     |
| 14  | cA    | 3141 | CL7  | CHC-C1C | -2.15 | 1.34        | 1.38     |
| 14  | aA    | 3105 | CL7  | C2A-C1A | -2.15 | 1.48        | 1.52     |
| 14  | aB    | 3016 | CL7  | C2A-C1A | -2.15 | 1.48        | 1.52     |
| 12  | bA    | 3101 | G9R  | OBD-CAD | 2.15  | 1.26        | 1.22     |
| 14  | cA    | 3104 | CL7  | C3B-C4B | -2.15 | 1.37        | 1.42     |
| 14  | cA    | 3112 | CL7  | C1B-NB  | 2.15  | 1.40        | 1.37     |
| 14  | cB    | 826  | CL7  | C3D-C2D | -2.15 | 1.35        | 1.42     |
| 14  | bB    | 821  | CL7  | CHB-C4A | -2.15 | 1.32        | 1.36     |
| 14  | bB    | 821  | CL7  | CHD-C4C | -2.15 | 1.34        | 1.38     |
| 14  | cB    | 808  | CL7  | CHD-C4C | -2.15 | 1.34        | 1.38     |
| 14  | bB    | 815  | CL7  | C3B-C4B | -2.15 | 1.37        | 1.42     |
| 14  | cA    | 3108 | CL7  | CAB-C3B | -2.15 | 1.40        | 1.45     |
| 14  | cA    | 3103 | CL7  | CHD-C4C | -2.15 | 1.34        | 1.38     |
| 14  | cA    | 3128 | CL7  | C3B-C4B | -2.15 | 1.37        | 1.42     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | bA    | 3107 | CL7  | C3C-C2C | -2.15 | 1.32        | 1.36     |
| 14  | bA    | 3119 | CL7  | OBB-CAB | 2.15  | 1.27        | 1.22     |
| 14  | aA    | 3107 | CL7  | C2A-C1A | -2.15 | 1.47        | 1.50     |
| 13  | cB    | 801  | PHO  | C4B-NB  | -2.15 | 1.34        | 1.38     |
| 14  | cB    | 833  | CL7  | CBD-CGD | -2.15 | 1.45        | 1.52     |
| 14  | cA    | 3144 | CL7  | C3D-CAD | -2.15 | 1.37        | 1.45     |
| 14  | aB    | 3011 | CL7  | CHC-C1C | -2.15 | 1.34        | 1.38     |
| 14  | aA    | 3127 | CL7  | C3D-CAD | -2.15 | 1.37        | 1.45     |
| 14  | cB    | 818  | CL7  | CAB-C3B | -2.15 | 1.40        | 1.45     |
| 14  | aB    | 3010 | CL7  | CHB-C4A | -2.15 | 1.32        | 1.36     |
| 14  | aF    | 201  | CL7  | C4D-ND  | -2.14 | 1.34        | 1.37     |
| 14  | bA    | 3129 | CL7  | C4D-ND  | -2.14 | 1.34        | 1.37     |
| 14  | cA    | 3141 | CL7  | C3B-C4B | -2.14 | 1.37        | 1.42     |
| 17  | aB    | 3027 | PQN  | C12-C13 | 2.14  | 1.38        | 1.33     |
| 16  | bA    | 3137 | LHG  | P-O3    | 2.14  | 1.68        | 1.59     |
| 14  | cA    | 3121 | CL7  | C3A-C4A | -2.14 | 1.48        | 1.52     |
| 14  | aA    | 3129 | CL7  | O2A-CGA | 2.14  | 1.39        | 1.33     |
| 12  | bA    | 3101 | G9R  | CAB-C3B | 2.14  | 1.49        | 1.45     |
| 14  | aA    | 3132 | CL7  | C3B-C4B | -2.14 | 1.37        | 1.42     |
| 14  | aA    | 3116 | CL7  | CAB-C3B | -2.14 | 1.40        | 1.45     |
| 14  | bA    | 3141 | CL7  | CHC-C1C | -2.14 | 1.34        | 1.38     |
| 14  | cB    | 807  | CL7  | CHC-C1C | -2.14 | 1.34        | 1.38     |
| 14  | bB    | 831  | CL7  | C3A-C4A | -2.14 | 1.48        | 1.52     |
| 14  | cA    | 3122 | CL7  | C4D-ND  | -2.14 | 1.34        | 1.37     |
| 14  | aA    | 3146 | CL7  | CAB-C3B | -2.14 | 1.40        | 1.45     |
| 14  | aB    | 3022 | CL7  | CHD-C4C | -2.14 | 1.34        | 1.38     |
| 14  | cA    | 3139 | CL7  | C3C-C2C | -2.14 | 1.32        | 1.36     |
| 14  | bA    | 3131 | CL7  | CAB-C3B | -2.14 | 1.40        | 1.45     |
| 14  | bA    | 3114 | CL7  | CAB-C3B | -2.14 | 1.40        | 1.45     |
| 14  | bB    | 814  | CL7  | CAB-C3B | -2.13 | 1.40        | 1.45     |
| 14  | aB    | 3030 | CL7  | CHC-C1C | -2.13 | 1.34        | 1.38     |
| 14  | cB    | 831  | CL7  | CHC-C1C | -2.13 | 1.34        | 1.38     |
| 14  | aB    | 3019 | CL7  | C2A-C1A | -2.13 | 1.47        | 1.50     |
| 14  | bA    | 3113 | CL7  | CHD-C4C | -2.13 | 1.34        | 1.38     |
| 14  | cA    | 3117 | CL7  | C3D-CAD | -2.13 | 1.37        | 1.45     |
| 14  | cB    | 820  | CL7  | C3D-C2D | -2.13 | 1.35        | 1.42     |
| 17  | bB    | 828  | PQN  | C10-C5  | 2.13  | 1.44        | 1.40     |
| 14  | cA    | 3133 | CL7  | C3A-C4A | -2.13 | 1.48        | 1.52     |
| 14  | bB    | 807  | CL7  | CHC-C1C | -2.13 | 1.34        | 1.38     |
| 14  | aB    | 3011 | CL7  | C3D-CAD | -2.13 | 1.37        | 1.45     |
| 14  | bA    | 3126 | CL7  | C3D-CAD | -2.13 | 1.37        | 1.45     |
| 14  | cA    | 3125 | CL7  | C3D-CAD | -2.13 | 1.37        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 17  | cB    | 828  | PQN  | C10-C5  | 2.13  | 1.44        | 1.40     |
| 14  | bB    | 808  | CL7  | CMA-C3A | 2.13  | 1.57        | 1.53     |
| 14  | aB    | 3003 | CL7  | O1D-CGD | -2.13 | 1.15        | 1.21     |
| 14  | bA    | 3127 | CL7  | C1B-NB  | 2.13  | 1.40        | 1.37     |
| 14  | cB    | 821  | CL7  | C2A-C1A | -2.13 | 1.48        | 1.52     |
| 14  | aA    | 3124 | CL7  | CHC-C1C | -2.13 | 1.34        | 1.38     |
| 14  | aA    | 3118 | CL7  | C3D-CAD | -2.13 | 1.37        | 1.45     |
| 14  | bB    | 822  | CL7  | C3B-C4B | -2.13 | 1.37        | 1.42     |
| 14  | cA    | 3111 | CL7  | C3B-C4B | -2.13 | 1.37        | 1.42     |
| 14  | bA    | 3122 | CL7  | CAB-C3B | -2.13 | 1.40        | 1.45     |
| 14  | bA    | 3131 | CL7  | C3B-C4B | -2.13 | 1.37        | 1.42     |
| 14  | bA    | 3121 | CL7  | O2D-CGD | -2.13 | 1.28        | 1.33     |
| 14  | aA    | 3133 | CL7  | CHC-C1C | -2.13 | 1.34        | 1.38     |
| 14  | bA    | 3145 | CL7  | CAB-C3B | -2.13 | 1.40        | 1.45     |
| 14  | aB    | 3031 | CL7  | O2D-CGD | -2.13 | 1.28        | 1.33     |
| 14  | aB    | 3032 | CL7  | C4D-ND  | -2.13 | 1.34        | 1.37     |
| 14  | aB    | 3014 | CL7  | C3B-C4B | -2.13 | 1.37        | 1.42     |
| 14  | cA    | 3141 | CL7  | O2A-C1  | 2.13  | 1.52        | 1.46     |
| 14  | cA    | 3114 | CL7  | CAB-C3B | -2.13 | 1.40        | 1.45     |
| 14  | aA    | 3109 | CL7  | C3B-C4B | -2.13 | 1.37        | 1.42     |
| 14  | cA    | 3139 | CL7  | C1A-CHA | -2.13 | 1.28        | 1.38     |
| 14  | aA    | 3128 | CL7  | C3A-C2A | -2.12 | 1.48        | 1.54     |
| 14  | aA    | 3105 | CL7  | CHD-C4C | -2.12 | 1.34        | 1.38     |
| 14  | cA    | 3144 | CL7  | C3B-C4B | -2.12 | 1.37        | 1.42     |
| 14  | aA    | 3121 | CL7  | O2D-CED | -2.12 | 1.40        | 1.45     |
| 14  | bB    | 809  | CL7  | O2A-C1  | 2.12  | 1.52        | 1.46     |
| 16  | cA    | 3137 | LHG  | P-O3    | 2.12  | 1.67        | 1.59     |
| 14  | aA    | 3107 | CL7  | C1D-ND  | -2.12 | 1.35        | 1.37     |
| 14  | bB    | 818  | CL7  | C3B-C4B | -2.12 | 1.37        | 1.42     |
| 14  | bA    | 3121 | CL7  | C3A-C4A | -2.12 | 1.48        | 1.52     |
| 14  | bA    | 3121 | CL7  | C1C-NC  | 2.12  | 1.40        | 1.37     |
| 14  | cF    | 201  | CL7  | C4D-ND  | -2.12 | 1.34        | 1.37     |
| 14  | cB    | 808  | CL7  | CMA-C3A | 2.12  | 1.57        | 1.53     |
| 14  | cB    | 803  | CL7  | OBb-CAB | 2.12  | 1.26        | 1.22     |
| 14  | bB    | 825  | CL7  | CHD-C4C | -2.12 | 1.34        | 1.38     |
| 14  | aA    | 3123 | CL7  | O1D-CGD | -2.12 | 1.15        | 1.21     |
| 14  | cB    | 808  | CL7  | C1C-NC  | 2.12  | 1.40        | 1.37     |
| 14  | aB    | 3020 | CL7  | CAB-C3B | -2.12 | 1.40        | 1.45     |
| 14  | bA    | 3106 | CL7  | C2A-C1A | -2.12 | 1.47        | 1.50     |
| 14  | bB    | 815  | CL7  | C4D-ND  | -2.12 | 1.34        | 1.37     |
| 14  | aA    | 3119 | CL7  | C3D-CAD | -2.12 | 1.38        | 1.45     |
| 14  | aA    | 3127 | CL7  | CHB-C4A | -2.12 | 1.30        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | cA    | 3120 | CL7  | C2A-C1A | -2.12 | 1.47        | 1.50     |
| 14  | bB    | 810  | CL7  | C3D-C2D | -2.12 | 1.35        | 1.42     |
| 14  | bF    | 201  | CL7  | C3D-CAD | -2.12 | 1.38        | 1.45     |
| 14  | cA    | 3132 | CL7  | O1D-CGD | -2.12 | 1.15        | 1.21     |
| 14  | bA    | 3104 | CL7  | CHB-C4A | -2.12 | 1.32        | 1.36     |
| 14  | cA    | 3106 | CL7  | C2A-C1A | -2.12 | 1.47        | 1.50     |
| 14  | cB    | 808  | CL7  | OBb-CAB | 2.12  | 1.26        | 1.22     |
| 14  | bA    | 3117 | CL7  | CHD-C4C | -2.12 | 1.34        | 1.38     |
| 14  | aB    | 3021 | CL7  | C3B-C4B | -2.11 | 1.37        | 1.42     |
| 14  | aA    | 3131 | CL7  | O2D-CGD | -2.11 | 1.28        | 1.33     |
| 14  | aA    | 3143 | CL7  | C3D-C2D | -2.11 | 1.35        | 1.42     |
| 14  | cB    | 819  | CL7  | O2D-CGD | -2.11 | 1.28        | 1.33     |
| 14  | cB    | 806  | CL7  | CBD-CGD | -2.11 | 1.45        | 1.52     |
| 14  | cB    | 826  | CL7  | C1B-NB  | 2.11  | 1.40        | 1.37     |
| 14  | bA    | 3121 | CL7  | CBD-CGD | -2.11 | 1.45        | 1.52     |
| 14  | aB    | 3013 | CL7  | CAB-C3B | -2.11 | 1.40        | 1.45     |
| 14  | cA    | 3144 | CL7  | CAB-C3B | -2.11 | 1.40        | 1.45     |
| 14  | aA    | 3109 | CL7  | O1D-CGD | -2.11 | 1.15        | 1.21     |
| 14  | cB    | 821  | CL7  | CAB-C3B | -2.11 | 1.40        | 1.45     |
| 14  | cA    | 3119 | CL7  | C1C-NC  | 2.11  | 1.40        | 1.37     |
| 14  | aA    | 3130 | CL7  | O2D-CGD | -2.11 | 1.28        | 1.33     |
| 14  | bA    | 3115 | CL7  | CAB-C3B | -2.11 | 1.40        | 1.45     |
| 14  | aA    | 3104 | CL7  | C3A-C4A | -2.11 | 1.48        | 1.52     |
| 14  | cB    | 827  | CL7  | O2D-CGD | -2.11 | 1.28        | 1.33     |
| 14  | cB    | 832  | CL7  | O2D-CGD | -2.11 | 1.28        | 1.33     |
| 14  | aA    | 3123 | CL7  | C1C-NC  | 2.11  | 1.40        | 1.37     |
| 14  | cB    | 827  | CL7  | CMC-C2C | -2.11 | 1.46        | 1.50     |
| 14  | bB    | 817  | CL7  | C2A-C1A | -2.11 | 1.48        | 1.52     |
| 14  | cB    | 818  | CL7  | CHD-C4C | -2.11 | 1.34        | 1.38     |
| 14  | cA    | 3115 | CL7  | CAB-C3B | -2.11 | 1.40        | 1.45     |
| 14  | cA    | 3119 | CL7  | CAA-CBA | -2.11 | 1.46        | 1.52     |
| 14  | aB    | 3018 | CL7  | C3B-C4B | -2.11 | 1.37        | 1.42     |
| 14  | bA    | 3115 | CL7  | C1D-ND  | -2.11 | 1.35        | 1.37     |
| 14  | aA    | 3115 | CL7  | C1D-ND  | -2.11 | 1.35        | 1.37     |
| 14  | aB    | 3002 | CL7  | C1C-NC  | 2.11  | 1.40        | 1.37     |
| 14  | cB    | 808  | CL7  | C3B-C4B | -2.11 | 1.37        | 1.42     |
| 14  | bA    | 3116 | CL7  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 14  | bA    | 3105 | CL7  | CAC-C3C | -2.11 | 1.45        | 1.51     |
| 14  | aA    | 3142 | CL7  | C3B-C4B | -2.11 | 1.37        | 1.42     |
| 14  | aB    | 3008 | CL7  | C1A-NA  | -2.11 | 1.32        | 1.38     |
| 14  | cB    | 814  | CL7  | C2A-C1A | -2.10 | 1.48        | 1.52     |
| 14  | cA    | 3118 | CL7  | C3D-CAD | -2.10 | 1.38        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 17  | aA    | 3144 | PQN  | C7-C6   | -2.10 | 1.34        | 1.38     |
| 14  | bB    | 812  | CL7  | C3D-CAD | -2.10 | 1.38        | 1.45     |
| 14  | cJ    | 101  | CL7  | CAA-C2A | -2.10 | 1.50        | 1.54     |
| 14  | aA    | 3104 | CL7  | CHD-C4C | -2.10 | 1.34        | 1.38     |
| 14  | bA    | 3119 | CL7  | CAA-CBA | -2.10 | 1.46        | 1.52     |
| 14  | aB    | 3015 | CL7  | CAA-C2A | 2.10  | 1.58        | 1.54     |
| 14  | cB    | 815  | CL7  | C4D-ND  | -2.10 | 1.34        | 1.37     |
| 14  | bA    | 3124 | CL7  | CMC-C2C | -2.10 | 1.46        | 1.50     |
| 14  | aA    | 3111 | CL7  | C2A-C1A | -2.10 | 1.48        | 1.52     |
| 14  | cB    | 816  | CL7  | O2A-C1  | 2.10  | 1.52        | 1.46     |
| 14  | aA    | 3121 | CL7  | CAA-C2A | -2.10 | 1.50        | 1.54     |
| 12  | cA    | 3101 | G9R  | CHB-C4A | -2.10 | 1.32        | 1.37     |
| 14  | aA    | 3108 | CL7  | CAB-C3B | -2.10 | 1.40        | 1.45     |
| 14  | bB    | 821  | CL7  | CAB-C3B | -2.10 | 1.40        | 1.45     |
| 14  | cB    | 819  | CL7  | O2D-CED | -2.10 | 1.40        | 1.45     |
| 14  | aB    | 3008 | CL7  | C3C-C2C | -2.10 | 1.32        | 1.36     |
| 14  | aA    | 3141 | CL7  | C3A-C4A | -2.10 | 1.48        | 1.52     |
| 14  | bA    | 3132 | CL7  | OBB-CAB | 2.10  | 1.26        | 1.22     |
| 14  | bA    | 3119 | CL7  | C1A-CHA | -2.10 | 1.29        | 1.38     |
| 14  | bB    | 803  | CL7  | C1A-NA  | -2.10 | 1.32        | 1.38     |
| 14  | bA    | 3114 | CL7  | C1D-C2D | -2.09 | 1.38        | 1.43     |
| 13  | cB    | 805  | PHO  | CAA-C2A | 2.09  | 1.58        | 1.54     |
| 14  | bA    | 3132 | CL7  | C1D-ND  | -2.09 | 1.35        | 1.37     |
| 12  | aA    | 3101 | G9R  | CAB-C3B | 2.09  | 1.49        | 1.45     |
| 14  | bB    | 807  | CL7  | O1D-CGD | -2.09 | 1.16        | 1.21     |
| 14  | cJ    | 101  | CL7  | C3A-C4A | -2.09 | 1.48        | 1.52     |
| 16  | cA    | 3137 | LHG  | O6-C4   | -2.09 | 1.36        | 1.44     |
| 14  | bB    | 820  | CL7  | O1D-CGD | -2.09 | 1.16        | 1.21     |
| 14  | cA    | 3108 | CL7  | CHB-C4A | -2.09 | 1.32        | 1.36     |
| 14  | bA    | 3118 | CL7  | C3A-C4A | -2.09 | 1.48        | 1.52     |
| 14  | bA    | 3118 | CL7  | C3D-CAD | -2.09 | 1.38        | 1.45     |
| 14  | cL    | 203  | CL7  | C3D-C2D | -2.09 | 1.35        | 1.42     |
| 14  | aB    | 3008 | CL7  | C1D-ND  | -2.09 | 1.35        | 1.37     |
| 14  | bB    | 821  | CL7  | C2A-C1A | -2.09 | 1.48        | 1.52     |
| 14  | cL    | 204  | CL7  | C1C-NC  | 2.09  | 1.40        | 1.37     |
| 14  | aB    | 3031 | CL7  | C3D-C2D | -2.09 | 1.35        | 1.42     |
| 14  | bA    | 3141 | CL7  | OBB-CAB | 2.09  | 1.26        | 1.22     |
| 14  | cA    | 3121 | CL7  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 14  | cA    | 3140 | CL7  | OBB-CAB | 2.09  | 1.26        | 1.22     |
| 14  | cB    | 821  | CL7  | CHB-C4A | -2.09 | 1.32        | 1.36     |
| 14  | aB    | 3006 | CL7  | C3C-C2C | -2.08 | 1.32        | 1.36     |
| 14  | cA    | 3122 | CL7  | C1C-NC  | 2.08  | 1.40        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | cA    | 3130 | CL7  | O2D-CGD | -2.08 | 1.28        | 1.33     |
| 14  | cL    | 204  | CL7  | C3D-C2D | -2.08 | 1.35        | 1.42     |
| 14  | cA    | 3121 | CL7  | CBD-CGD | -2.08 | 1.45        | 1.52     |
| 14  | bB    | 825  | CL7  | C3B-C4B | -2.08 | 1.38        | 1.42     |
| 14  | bB    | 832  | CL7  | C3D-C2D | -2.08 | 1.35        | 1.42     |
| 14  | bA    | 3133 | CL7  | C3B-C4B | -2.08 | 1.38        | 1.42     |
| 14  | aB    | 3020 | CL7  | CHD-C4C | -2.08 | 1.34        | 1.38     |
| 14  | cB    | 821  | CL7  | CHD-C4C | -2.08 | 1.34        | 1.38     |
| 14  | aA    | 3118 | CL7  | C3B-C4B | -2.08 | 1.38        | 1.42     |
| 14  | bA    | 3109 | CL7  | CAB-C3B | -2.08 | 1.40        | 1.45     |
| 14  | bA    | 3112 | CL7  | C1B-NB  | 2.08  | 1.40        | 1.37     |
| 14  | cB    | 807  | CL7  | O1D-CGD | -2.08 | 1.16        | 1.21     |
| 14  | aF    | 201  | CL7  | C3D-CAD | -2.08 | 1.38        | 1.45     |
| 14  | aK    | 101  | CL7  | CAB-C3B | -2.08 | 1.40        | 1.45     |
| 14  | bB    | 809  | CL7  | C1A-NA  | -2.08 | 1.32        | 1.38     |
| 14  | cB    | 826  | CL7  | O2D-CED | -2.08 | 1.40        | 1.45     |
| 14  | cA    | 3114 | CL7  | C1D-C2D | -2.08 | 1.38        | 1.43     |
| 14  | cA    | 3110 | CL7  | O1D-CGD | -2.08 | 1.16        | 1.21     |
| 14  | bB    | 827  | CL7  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 14  | bA    | 3111 | CL7  | C3B-C4B | -2.07 | 1.38        | 1.42     |
| 14  | cA    | 3102 | CL7  | MG-NA   | -2.07 | 2.01        | 2.05     |
| 14  | bA    | 3106 | CL7  | OBB-CAB | 2.07  | 1.26        | 1.22     |
| 14  | aA    | 3125 | CL7  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 14  | aA    | 3107 | CL7  | C3A-C4A | -2.07 | 1.48        | 1.52     |
| 14  | cA    | 3129 | CL7  | C2A-C1A | -2.07 | 1.48        | 1.52     |
| 14  | bA    | 3142 | CL7  | O2D-CGD | -2.07 | 1.28        | 1.33     |
| 14  | bA    | 3114 | CL7  | CBD-CGD | -2.07 | 1.45        | 1.52     |
| 14  | bA    | 3124 | CL7  | CHD-C4C | -2.07 | 1.34        | 1.38     |
| 14  | cA    | 3117 | CL7  | CHD-C4C | -2.07 | 1.34        | 1.38     |
| 17  | bA    | 3143 | PQN  | C3-C4   | -2.07 | 1.42        | 1.47     |
| 14  | aA    | 3146 | CL7  | C3B-C4B | -2.07 | 1.38        | 1.42     |
| 14  | cB    | 832  | CL7  | C3D-C2D | -2.07 | 1.35        | 1.42     |
| 14  | aB    | 3026 | CL7  | O2D-CGD | -2.07 | 1.28        | 1.33     |
| 14  | cA    | 3123 | CL7  | C3A-C4A | -2.07 | 1.48        | 1.52     |
| 14  | cA    | 3121 | CL7  | C3B-C4B | -2.07 | 1.38        | 1.42     |
| 14  | aA    | 3112 | CL7  | CHB-C4A | -2.07 | 1.32        | 1.36     |
| 14  | bB    | 820  | CL7  | CMA-C3A | 2.07  | 1.57        | 1.53     |
| 14  | cB    | 814  | CL7  | CAB-C3B | -2.07 | 1.40        | 1.45     |
| 14  | aA    | 3142 | CL7  | CHC-C1C | -2.07 | 1.34        | 1.38     |
| 14  | aB    | 3019 | CL7  | OBB-CAB | 2.07  | 1.26        | 1.22     |
| 14  | bL    | 205  | CL7  | CHB-C4A | -2.07 | 1.32        | 1.36     |
| 14  | cB    | 812  | CL7  | C3D-CAD | -2.07 | 1.38        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | aA    | 3119 | CL7  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 14  | bA    | 3128 | CL7  | CBD-CGD | -2.07 | 1.45        | 1.52     |
| 14  | aA    | 3122 | CL7  | C3D-C2D | -2.06 | 1.35        | 1.42     |
| 14  | bA    | 3125 | CL7  | MG-NB   | -2.06 | 2.01        | 2.05     |
| 14  | aA    | 3107 | CL7  | C3D-C2D | -2.06 | 1.35        | 1.42     |
| 12  | aA    | 3101 | G9R  | O2A-C1  | -2.06 | 1.40        | 1.46     |
| 14  | bA    | 3104 | CL7  | C3B-C4B | -2.06 | 1.38        | 1.42     |
| 14  | bA    | 3133 | CL7  | C3A-C4A | -2.06 | 1.48        | 1.52     |
| 14  | bA    | 3125 | CL7  | CAA-CBA | -2.06 | 1.46        | 1.52     |
| 14  | aA    | 3142 | CL7  | C4C-NC  | 2.06  | 1.40        | 1.37     |
| 14  | aB    | 3014 | CL7  | C3A-C4A | -2.06 | 1.48        | 1.52     |
| 14  | bA    | 3116 | CL7  | O2D-CGD | -2.06 | 1.28        | 1.33     |
| 14  | cA    | 3107 | CL7  | CHD-C4C | -2.06 | 1.34        | 1.38     |
| 14  | bA    | 3108 | CL7  | C4C-NC  | 2.06  | 1.40        | 1.37     |
| 14  | aA    | 3118 | CL7  | CHD-C4C | -2.06 | 1.34        | 1.38     |
| 14  | cA    | 3122 | CL7  | C3B-C4B | -2.06 | 1.38        | 1.42     |
| 17  | bA    | 3143 | PQN  | C10-C5  | 2.06  | 1.44        | 1.40     |
| 14  | aB    | 3032 | CL7  | C3A-C4A | -2.06 | 1.48        | 1.52     |
| 14  | bA    | 3120 | CL7  | C1D-ND  | -2.06 | 1.35        | 1.37     |
| 14  | bB    | 803  | CL7  | OBb-CAB | 2.06  | 1.26        | 1.22     |
| 14  | cB    | 825  | CL7  | CHD-C4C | -2.06 | 1.34        | 1.38     |
| 14  | aB    | 3008 | CL7  | C3B-C4B | -2.06 | 1.38        | 1.42     |
| 14  | cA    | 3127 | CL7  | CBA-CGA | -2.06 | 1.44        | 1.50     |
| 14  | aB    | 3018 | CL7  | O2D-CED | -2.06 | 1.40        | 1.45     |
| 14  | aB    | 3003 | CL7  | CBA-CGA | -2.05 | 1.44        | 1.50     |
| 14  | aB    | 3007 | CL7  | C3D-C2D | -2.05 | 1.35        | 1.42     |
| 14  | aA    | 3126 | CL7  | CAA-CBA | -2.05 | 1.46        | 1.52     |
| 14  | cA    | 3109 | CL7  | C2A-C1A | -2.05 | 1.48        | 1.52     |
| 14  | aB    | 3009 | CL7  | C3D-C2D | -2.05 | 1.35        | 1.42     |
| 14  | cA    | 3116 | CL7  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 14  | bA    | 3103 | CL7  | CHD-C4C | -2.05 | 1.34        | 1.38     |
| 14  | aB    | 3005 | CL7  | CBD-CGD | -2.05 | 1.46        | 1.52     |
| 13  | cB    | 801  | PHO  | CBC-CAC | 2.05  | 1.60        | 1.51     |
| 14  | cB    | 823  | CL7  | C3A-C4A | -2.05 | 1.48        | 1.52     |
| 14  | bK    | 101  | CL7  | CHD-C4C | -2.05 | 1.34        | 1.38     |
| 16  | cA    | 3137 | LHG  | O7-C5   | -2.05 | 1.41        | 1.46     |
| 14  | aB    | 3010 | CL7  | CHD-C4C | -2.05 | 1.34        | 1.38     |
| 14  | bA    | 3107 | CL7  | CHB-C4A | -2.05 | 1.32        | 1.36     |
| 14  | cA    | 3115 | CL7  | C1D-ND  | -2.05 | 1.35        | 1.37     |
| 14  | aA    | 3119 | CL7  | CHD-C4C | -2.05 | 1.34        | 1.38     |
| 14  | cA    | 3119 | CL7  | CHD-C1D | -2.05 | 1.34        | 1.39     |
| 14  | aA    | 3106 | CL7  | C4C-NC  | 2.05  | 1.40        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | bA    | 3122 | CL7  | O1D-CGD | -2.05 | 1.16        | 1.21     |
| 13  | aA    | 3102 | PHO  | C3D-CAD | -2.05 | 1.43        | 1.47     |
| 14  | bB    | 819  | CL7  | C1A-NA  | -2.05 | 1.32        | 1.38     |
| 14  | cA    | 3131 | CL7  | CAB-C3B | -2.05 | 1.40        | 1.45     |
| 14  | cA    | 3127 | CL7  | C1D-ND  | -2.05 | 1.35        | 1.37     |
| 14  | cA    | 3141 | CL7  | C3D-C2D | -2.05 | 1.35        | 1.42     |
| 13  | bB    | 805  | PHO  | C1C-NC  | -2.05 | 1.31        | 1.37     |
| 14  | aA    | 3108 | CL7  | CHD-C4C | -2.04 | 1.34        | 1.38     |
| 14  | cK    | 101  | CL7  | CAB-C3B | -2.04 | 1.40        | 1.45     |
| 14  | cB    | 817  | CL7  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 14  | bA    | 3115 | CL7  | C3D-CAD | -2.04 | 1.38        | 1.45     |
| 14  | bB    | 820  | CL7  | C2A-C1A | -2.04 | 1.47        | 1.50     |
| 14  | aL    | 203  | CL7  | C3D-C2D | -2.04 | 1.36        | 1.42     |
| 14  | bF    | 201  | CL7  | C4D-ND  | -2.04 | 1.34        | 1.37     |
| 14  | aB    | 3032 | CL7  | CAA-C2A | -2.04 | 1.50        | 1.54     |
| 14  | bB    | 807  | CL7  | C3C-C2C | -2.04 | 1.32        | 1.36     |
| 14  | cB    | 809  | CL7  | C2A-C1A | -2.04 | 1.47        | 1.50     |
| 14  | aA    | 3105 | CL7  | C3B-C4B | -2.04 | 1.38        | 1.42     |
| 14  | aA    | 3124 | CL7  | CBD-CGD | -2.04 | 1.46        | 1.52     |
| 14  | cA    | 3125 | CL7  | CAA-CBA | -2.04 | 1.46        | 1.52     |
| 14  | cA    | 3127 | CL7  | C1B-NB  | 2.04  | 1.40        | 1.37     |
| 14  | bA    | 3130 | CL7  | C3B-C4B | -2.04 | 1.38        | 1.42     |
| 14  | cA    | 3133 | CL7  | C3B-C4B | -2.04 | 1.38        | 1.42     |
| 14  | cA    | 3115 | CL7  | C3D-CAD | -2.04 | 1.38        | 1.45     |
| 14  | cB    | 820  | CL7  | CMA-C3A | 2.04  | 1.57        | 1.53     |
| 14  | aB    | 3018 | CL7  | C1A-NA  | -2.03 | 1.32        | 1.38     |
| 14  | aA    | 3140 | CL7  | C3C-C2C | -2.03 | 1.32        | 1.36     |
| 14  | cB    | 809  | CL7  | C1A-NA  | -2.03 | 1.32        | 1.38     |
| 14  | cA    | 3107 | CL7  | C3C-C2C | -2.03 | 1.32        | 1.36     |
| 14  | aA    | 3114 | CL7  | CHD-C4C | -2.03 | 1.34        | 1.38     |
| 14  | cB    | 807  | CL7  | C3D-C2D | -2.03 | 1.36        | 1.42     |
| 14  | cA    | 3123 | CL7  | CAA-C2A | -2.03 | 1.50        | 1.54     |
| 14  | aB    | 3018 | CL7  | CHB-C4A | -2.03 | 1.32        | 1.36     |
| 14  | aB    | 3024 | CL7  | CHD-C4C | -2.03 | 1.34        | 1.38     |
| 13  | aA    | 3102 | PHO  | CBC-CAC | 2.03  | 1.60        | 1.51     |
| 14  | cA    | 3117 | CL7  | C3B-C4B | -2.03 | 1.38        | 1.42     |
| 14  | bA    | 3130 | CL7  | O2D-CGD | -2.03 | 1.28        | 1.33     |
| 14  | aA    | 3116 | CL7  | C1D-ND  | -2.03 | 1.35        | 1.37     |
| 14  | cA    | 3118 | CL7  | CHD-C4C | -2.03 | 1.34        | 1.38     |
| 14  | cB    | 810  | CL7  | C1A-NA  | -2.03 | 1.32        | 1.38     |
| 14  | bA    | 3118 | CL7  | C3A-C2A | -2.03 | 1.52        | 1.54     |
| 14  | aA    | 3117 | CL7  | O2D-CGD | -2.03 | 1.28        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | bA    | 3131 | CL7  | C2A-C1A | -2.03 | 1.48        | 1.52     |
| 14  | bB    | 815  | CL7  | CHD-C4C | -2.03 | 1.34        | 1.38     |
| 14  | cA    | 3116 | CL7  | C3A-C4A | -2.02 | 1.48        | 1.52     |
| 14  | aB    | 3025 | CL7  | O2D-CED | -2.02 | 1.40        | 1.45     |
| 14  | cB    | 819  | CL7  | C3B-C4B | -2.02 | 1.38        | 1.42     |
| 14  | bB    | 818  | CL7  | C2A-C1A | -2.02 | 1.48        | 1.52     |
| 17  | aA    | 3144 | PQN  | C2-C1   | -2.02 | 1.43        | 1.48     |
| 14  | cB    | 803  | CL7  | C1A-NA  | -2.02 | 1.33        | 1.38     |
| 14  | cA    | 3126 | CL7  | C4D-ND  | -2.02 | 1.34        | 1.37     |
| 14  | cB    | 804  | CL7  | C3C-C2C | -2.02 | 1.32        | 1.36     |
| 14  | aA    | 3115 | CL7  | C1D-C2D | -2.02 | 1.38        | 1.43     |
| 14  | bA    | 3141 | CL7  | C3D-C2D | -2.02 | 1.36        | 1.42     |
| 14  | cA    | 3119 | CL7  | O2A-C1  | 2.02  | 1.50        | 1.45     |
| 14  | aB    | 3018 | CL7  | C3A-C4A | -2.02 | 1.48        | 1.52     |
| 14  | aB    | 3019 | CL7  | CAA-C2A | -2.02 | 1.50        | 1.54     |
| 14  | bA    | 3102 | CL7  | C3D-C2D | -2.02 | 1.36        | 1.42     |
| 14  | aA    | 3124 | CL7  | C3B-C4B | -2.02 | 1.38        | 1.42     |
| 14  | bB    | 825  | CL7  | C3D-C2D | -2.02 | 1.36        | 1.42     |
| 14  | bB    | 817  | CL7  | CMD-C2D | -2.02 | 1.46        | 1.50     |
| 14  | aA    | 3122 | CL7  | CBD-CGD | -2.02 | 1.46        | 1.52     |
| 14  | cA    | 3123 | CL7  | C1A-NA  | -2.02 | 1.33        | 1.38     |
| 14  | bA    | 3123 | CL7  | C3D-CAD | -2.02 | 1.38        | 1.45     |
| 14  | cL    | 203  | CL7  | O2D-CGD | -2.02 | 1.28        | 1.33     |
| 14  | cB    | 825  | CL7  | C3B-C4B | -2.02 | 1.38        | 1.42     |
| 14  | bA    | 3118 | CL7  | CHD-C4C | -2.02 | 1.34        | 1.38     |
| 14  | cK    | 101  | CL7  | C3B-C4B | -2.02 | 1.38        | 1.42     |
| 14  | bB    | 831  | CL7  | C1D-ND  | -2.02 | 1.35        | 1.37     |
| 14  | bA    | 3141 | CL7  | C3C-C2C | -2.02 | 1.32        | 1.36     |
| 13  | bB    | 801  | PHO  | CMB-C2B | -2.02 | 1.47        | 1.51     |
| 14  | cB    | 804  | CL7  | CBA-CGA | -2.02 | 1.44        | 1.50     |
| 14  | aB    | 3006 | CL7  | CAA-C2A | -2.02 | 1.50        | 1.54     |
| 14  | bA    | 3108 | CL7  | O1D-CGD | -2.01 | 1.16        | 1.21     |
| 14  | aA    | 3133 | CL7  | O1D-CGD | -2.01 | 1.16        | 1.21     |
| 12  | bA    | 3101 | G9R  | C3D-C2D | 2.01  | 1.44        | 1.39     |
| 14  | bF    | 201  | CL7  | C3A-C4A | -2.01 | 1.48        | 1.52     |
| 14  | aA    | 3142 | CL7  | C3D-C2D | -2.01 | 1.36        | 1.42     |
| 14  | bA    | 3123 | CL7  | C3A-C4A | -2.01 | 1.48        | 1.52     |
| 14  | aL    | 202  | CL7  | C1D-ND  | -2.01 | 1.35        | 1.37     |
| 14  | aB    | 3024 | CL7  | C3B-C4B | -2.01 | 1.38        | 1.42     |
| 14  | cA    | 3118 | CL7  | CHB-C4A | -2.01 | 1.32        | 1.36     |
| 14  | aA    | 3133 | CL7  | C3A-C4A | -2.01 | 1.48        | 1.52     |
| 14  | cB    | 822  | CL7  | C3D-CAD | -2.01 | 1.38        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | aB    | 3010 | CL7  | C1C-NC  | 2.01  | 1.40        | 1.37     |
| 14  | aA    | 3114 | CL7  | C4D-ND  | -2.01 | 1.34        | 1.37     |
| 14  | aA    | 3107 | CL7  | O2A-C1  | 2.01  | 1.51        | 1.46     |
| 17  | bB    | 828  | PQN  | C12-C13 | 2.01  | 1.37        | 1.33     |
| 14  | aA    | 3133 | CL7  | C3B-C4B | -2.01 | 1.38        | 1.42     |
| 14  | cA    | 3121 | CL7  | O2D-CGD | -2.01 | 1.28        | 1.33     |
| 14  | cB    | 818  | CL7  | C2A-C1A | -2.01 | 1.48        | 1.52     |
| 14  | bB    | 815  | CL7  | C3A-C4A | -2.01 | 1.48        | 1.52     |
| 14  | bB    | 819  | CL7  | C3C-C2C | -2.01 | 1.32        | 1.36     |
| 14  | aA    | 3142 | CL7  | O2A-C1  | 2.01  | 1.51        | 1.46     |
| 14  | bA    | 3117 | CL7  | C3B-C4B | -2.01 | 1.38        | 1.42     |
| 14  | aB    | 3007 | CL7  | CAA-C2A | -2.01 | 1.50        | 1.54     |
| 14  | bA    | 3128 | CL7  | CHD-C4C | -2.01 | 1.34        | 1.38     |
| 14  | cF    | 201  | CL7  | C3A-C4A | -2.01 | 1.48        | 1.52     |
| 14  | bB    | 807  | CL7  | C3D-C2D | -2.01 | 1.36        | 1.42     |
| 14  | aA    | 3108 | CL7  | CHB-C4A | -2.01 | 1.32        | 1.36     |
| 14  | cA    | 3122 | CL7  | C2A-C1A | -2.01 | 1.47        | 1.50     |
| 14  | cB    | 821  | CL7  | C3B-C4B | -2.01 | 1.38        | 1.42     |
| 14  | aB    | 3015 | CL7  | O2A-CGA | 2.00  | 1.39        | 1.33     |
| 14  | cA    | 3108 | CL7  | C3D-C2D | -2.00 | 1.36        | 1.42     |
| 14  | aB    | 3013 | CL7  | C3B-C4B | -2.00 | 1.38        | 1.42     |
| 14  | aB    | 3022 | CL7  | O1D-CGD | -2.00 | 1.16        | 1.21     |
| 14  | aA    | 3125 | CL7  | CAA-C2A | -2.00 | 1.50        | 1.54     |
| 14  | cK    | 101  | CL7  | C2A-C1A | -2.00 | 1.48        | 1.52     |
| 14  | bB    | 833  | CL7  | O1D-CGD | -2.00 | 1.16        | 1.21     |
| 14  | bA    | 3133 | CL7  | C2A-C1A | -2.00 | 1.48        | 1.52     |
| 14  | bB    | 804  | CL7  | C3A-C4A | -2.00 | 1.48        | 1.52     |
| 13  | bB    | 805  | PHO  | CAA-C2A | 2.00  | 1.58        | 1.54     |

All (3705) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 12  | bA    | 3101 | G9R  | C1D-ND-C4D  | -14.07 | 96.34       | 106.33   |
| 12  | aA    | 3101 | G9R  | C1D-ND-C4D  | -12.96 | 97.13       | 106.33   |
| 12  | bA    | 3101 | G9R  | C4A-NA-C1A  | -12.94 | 100.89      | 106.71   |
| 12  | cA    | 3101 | G9R  | C4A-NA-C1A  | -11.27 | 101.64      | 106.71   |
| 13  | cB    | 805  | PHO  | C4D-CHA-CBD | -11.07 | 103.51      | 108.52   |
| 12  | cA    | 3101 | G9R  | C1D-ND-C4D  | -10.63 | 98.78       | 106.33   |
| 12  | aA    | 3101 | G9R  | C4A-NA-C1A  | -10.61 | 101.94      | 106.71   |
| 12  | cA    | 3101 | G9R  | CHD-C4C-C3C | -10.46 | 109.46      | 124.84   |
| 12  | aA    | 3101 | G9R  | CHD-C4C-C3C | -10.12 | 109.97      | 124.84   |
| 13  | bB    | 805  | PHO  | C4D-CHA-CBD | -10.12 | 103.94      | 108.52   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12  | bA    | 3101 | G9R  | CHD-C4C-C3C | -9.73 | 110.54      | 124.84   |
| 13  | aB    | 3004 | PHO  | C4D-CHA-CBD | -9.46 | 104.24      | 108.52   |
| 14  | cA    | 3124 | CL7  | O2D-CGD-O1D | -9.45 | 105.36      | 123.84   |
| 14  | cA    | 3119 | CL7  | C1A-NA-C4A  | -9.09 | 100.80      | 106.30   |
| 14  | bA    | 3124 | CL7  | O2D-CGD-O1D | -8.87 | 106.50      | 123.84   |
| 14  | bA    | 3119 | CL7  | C1A-NA-C4A  | -8.81 | 100.97      | 106.30   |
| 14  | aA    | 3120 | CL7  | C1A-NA-C4A  | -8.10 | 101.40      | 106.30   |
| 12  | bA    | 3101 | G9R  | C2D-C1D-ND  | 7.86  | 115.90      | 110.10   |
| 14  | cA    | 3123 | CL7  | O2D-CGD-CBD | 7.83  | 125.19      | 111.27   |
| 14  | bB    | 803  | CL7  | O2D-CGD-CBD | 7.81  | 125.14      | 111.27   |
| 14  | aA    | 3125 | CL7  | O2D-CGD-O1D | -7.65 | 108.88      | 123.84   |
| 14  | cB    | 803  | CL7  | O2D-CGD-CBD | 7.48  | 124.56      | 111.27   |
| 14  | cA    | 3125 | CL7  | O2D-CGD-O1D | -7.35 | 109.46      | 123.84   |
| 14  | cA    | 3122 | CL7  | O2D-CGD-CBD | 7.34  | 124.31      | 111.27   |
| 14  | bA    | 3125 | CL7  | O2D-CGD-O1D | -7.31 | 109.54      | 123.84   |
| 12  | cA    | 3101 | G9R  | CMB-C2B-C1B | 7.25  | 136.41      | 125.37   |
| 12  | aA    | 3101 | G9R  | C1C-C2C-C3C | -7.22 | 99.37       | 106.96   |
| 12  | bA    | 3101 | G9R  | CMB-C2B-C1B | 7.20  | 136.34      | 125.37   |
| 14  | aA    | 3124 | CL7  | O2D-CGD-CBD | 7.16  | 124.00      | 111.27   |
| 14  | bA    | 3123 | CL7  | O2D-CGD-CBD | 7.06  | 123.81      | 111.27   |
| 14  | bB    | 820  | CL7  | O2D-CGD-CBD | 7.01  | 123.73      | 111.27   |
| 14  | aA    | 3123 | CL7  | O2D-CGD-CBD | 6.99  | 123.69      | 111.27   |
| 14  | bA    | 3122 | CL7  | O2D-CGD-CBD | 6.99  | 123.69      | 111.27   |
| 14  | bL    | 204  | CL7  | O2D-CGD-CBD | 6.88  | 123.49      | 111.27   |
| 14  | aB    | 3019 | CL7  | O2D-CGD-CBD | 6.85  | 123.45      | 111.27   |
| 13  | aA    | 3102 | PHO  | C1C-C2C-C3C | -6.75 | 103.00      | 108.61   |
| 13  | bB    | 805  | PHO  | C1C-C2C-C3C | -6.74 | 103.01      | 108.61   |
| 13  | aB    | 3004 | PHO  | C1C-C2C-C3C | -6.73 | 103.01      | 108.61   |
| 14  | bB    | 827  | CL7  | O2D-CGD-O1D | -6.73 | 110.68      | 123.84   |
| 14  | aB    | 3002 | CL7  | O2D-CGD-CBD | 6.72  | 123.21      | 111.27   |
| 14  | cB    | 820  | CL7  | O2D-CGD-CBD | 6.70  | 123.18      | 111.27   |
| 13  | cB    | 805  | PHO  | C1C-C2C-C3C | -6.70 | 103.04      | 108.61   |
| 13  | cB    | 801  | PHO  | C4D-CHA-CBD | -6.61 | 105.53      | 108.52   |
| 14  | cA    | 3102 | CL7  | CHC-C1C-NC  | -6.57 | 118.42      | 124.45   |
| 12  | cA    | 3101 | G9R  | C1C-C2C-C3C | -6.52 | 100.10      | 106.96   |
| 12  | aA    | 3101 | G9R  | C2D-C1D-ND  | 6.45  | 114.86      | 110.10   |
| 14  | bA    | 3124 | CL7  | CHB-C1B-NB  | -6.44 | 117.44      | 124.26   |
| 14  | aA    | 3125 | CL7  | CHB-C1B-NB  | -6.41 | 117.47      | 124.26   |
| 14  | cA    | 3124 | CL7  | CHB-C1B-NB  | -6.38 | 117.51      | 124.26   |
| 14  | cB    | 819  | CL7  | O2D-CGD-CBD | 6.36  | 122.58      | 111.27   |
| 14  | cB    | 803  | CL7  | O2D-CGD-O1D | -6.36 | 111.40      | 123.84   |
| 14  | cA    | 3124 | CL7  | C1-C2-C3    | -6.36 | 115.05      | 126.04   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | aA    | 3103 | CL7  | O2D-CGD-CBD | 6.35  | 122.55      | 111.27   |
| 14  | cA    | 3142 | CL7  | O2D-CGD-CBD | 6.31  | 122.48      | 111.27   |
| 14  | bA    | 3102 | CL7  | CHC-C1C-NC  | -6.29 | 118.67      | 124.45   |
| 12  | cA    | 3101 | G9R  | C2B-C1B-NB  | 6.28  | 114.44      | 110.23   |
| 13  | bB    | 801  | PHO  | C1C-C2C-C3C | -6.27 | 103.39      | 108.61   |
| 14  | aA    | 3103 | CL7  | CHC-C1C-NC  | -6.20 | 118.75      | 124.45   |
| 12  | bA    | 3101 | G9R  | C2B-C1B-NB  | 6.20  | 114.39      | 110.23   |
| 13  | cB    | 801  | PHO  | C1C-C2C-C3C | -6.16 | 103.49      | 108.61   |
| 13  | bB    | 801  | PHO  | C4D-CHA-CBD | -6.16 | 105.73      | 108.52   |
| 14  | aA    | 3130 | CL7  | CHC-C4B-NB  | 6.15  | 130.76      | 124.26   |
| 13  | cB    | 801  | PHO  | CBC-CAC-C3C | -6.12 | 103.93      | 112.88   |
| 14  | aB    | 3018 | CL7  | O2D-CGD-CBD | 6.11  | 122.13      | 111.27   |
| 12  | bA    | 3101 | G9R  | C1C-C2C-C3C | -6.11 | 100.53      | 106.96   |
| 17  | bA    | 3143 | PQN  | C14-C13-C15 | 6.11  | 125.55      | 115.27   |
| 14  | bA    | 3142 | CL7  | O2D-CGD-CBD | 6.11  | 122.12      | 111.27   |
| 13  | aA    | 3102 | PHO  | C4D-CHA-CBD | -6.09 | 105.76      | 108.52   |
| 14  | cB    | 822  | CL7  | O2D-CGD-O1D | -6.09 | 111.92      | 123.84   |
| 14  | bB    | 819  | CL7  | O2D-CGD-CBD | 6.09  | 122.09      | 111.27   |
| 14  | bB    | 816  | CL7  | C1-C2-C3    | -6.09 | 116.90      | 126.75   |
| 14  | bB    | 816  | CL7  | O2D-CGD-CBD | 6.07  | 122.05      | 111.27   |
| 14  | cA    | 3123 | CL7  | C4-C3-C5    | -6.06 | 109.05      | 115.98   |
| 12  | aA    | 3101 | G9R  | CMB-C2B-C1B | 6.06  | 134.60      | 125.37   |
| 14  | bL    | 204  | CL7  | O2D-CGD-O1D | -6.06 | 111.99      | 123.84   |
| 12  | cA    | 3101 | G9R  | C2D-C1D-ND  | 6.02  | 114.54      | 110.10   |
| 14  | cB    | 832  | CL7  | O2D-CGD-CBD | 6.01  | 121.95      | 111.27   |
| 14  | cB    | 811  | CL7  | O2D-CGD-CBD | 6.01  | 121.95      | 111.27   |
| 14  | bA    | 3125 | CL7  | C1-C2-C3    | -5.99 | 115.68      | 126.04   |
| 14  | bA    | 3121 | CL7  | CAA-C2A-C3A | -5.96 | 102.19      | 116.10   |
| 14  | aB    | 3026 | CL7  | O2D-CGD-O1D | -5.96 | 112.19      | 123.84   |
| 17  | cA    | 3143 | PQN  | C14-C13-C15 | 5.93  | 125.25      | 115.27   |
| 14  | bB    | 832  | CL7  | O2D-CGD-CBD | 5.93  | 121.80      | 111.27   |
| 14  | cA    | 3110 | CL7  | O2D-CGD-CBD | 5.92  | 121.78      | 111.27   |
| 12  | bA    | 3101 | G9R  | C3B-C2B-C1B | -5.91 | 100.03      | 107.16   |
| 14  | aA    | 3122 | CL7  | CAA-C2A-C3A | -5.89 | 102.35      | 116.10   |
| 12  | aA    | 3101 | G9R  | C2B-C1B-NB  | 5.87  | 114.17      | 110.23   |
| 14  | cB    | 808  | CL7  | O2D-CGD-O1D | -5.86 | 112.39      | 123.84   |
| 14  | aB    | 3015 | CL7  | O2D-CGD-CBD | 5.85  | 121.66      | 111.27   |
| 14  | cL    | 204  | CL7  | O2D-CGD-O1D | -5.84 | 112.41      | 123.84   |
| 14  | cA    | 3125 | CL7  | C1-C2-C3    | -5.84 | 115.94      | 126.04   |
| 14  | cA    | 3121 | CL7  | CAA-C2A-C3A | -5.83 | 102.50      | 116.10   |
| 14  | aA    | 3146 | CL7  | O2D-CGD-CBD | 5.82  | 121.62      | 111.27   |
| 17  | bB    | 828  | PQN  | C16-C15-C13 | -5.82 | 98.20       | 113.45   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | bA    | 3129 | CL7  | CHC-C4B-NB  | 5.80  | 130.39      | 124.26   |
| 17  | cB    | 828  | PQN  | C16-C15-C13 | -5.79 | 98.27       | 113.45   |
| 14  | bB    | 803  | CL7  | O2D-CGD-O1D | -5.77 | 112.56      | 123.84   |
| 14  | cA    | 3123 | CL7  | C1-C2-C3    | -5.73 | 116.12      | 126.04   |
| 14  | cL    | 204  | CL7  | O2D-CGD-CBD | 5.73  | 121.45      | 111.27   |
| 14  | bB    | 808  | CL7  | O2D-CGD-O1D | -5.72 | 112.65      | 123.84   |
| 14  | aL    | 203  | CL7  | O2D-CGD-O1D | -5.71 | 112.67      | 123.84   |
| 14  | cB    | 822  | CL7  | CHB-C1B-NB  | -5.71 | 118.21      | 124.26   |
| 14  | cB    | 810  | CL7  | O2D-CGD-CBD | 5.70  | 121.40      | 111.27   |
| 14  | bB    | 818  | CL7  | O2D-CGD-CBD | 5.69  | 121.39      | 111.27   |
| 14  | aB    | 3017 | CL7  | O2D-CGD-CBD | 5.67  | 121.35      | 111.27   |
| 14  | bB    | 822  | CL7  | CHB-C1B-NB  | -5.67 | 118.26      | 124.26   |
| 14  | cB    | 827  | CL7  | O2D-CGD-O1D | -5.65 | 112.80      | 123.84   |
| 14  | aB    | 3031 | CL7  | O2D-CGD-CBD | 5.61  | 121.23      | 111.27   |
| 14  | aL    | 203  | CL7  | O2D-CGD-CBD | 5.60  | 121.22      | 111.27   |
| 12  | cA    | 3101 | G9R  | CHD-C1D-ND  | -5.59 | 119.31      | 124.45   |
| 14  | bL    | 203  | CL7  | O1D-CGD-CBD | -5.58 | 113.06      | 124.48   |
| 14  | bA    | 3120 | CL7  | O2D-CGD-CBD | 5.57  | 121.16      | 111.27   |
| 14  | cA    | 3140 | CL7  | O2D-CGD-CBD | 5.56  | 121.14      | 111.27   |
| 14  | aA    | 3132 | CL7  | O2D-CGD-CBD | 5.55  | 121.13      | 111.27   |
| 14  | cA    | 3129 | CL7  | CHC-C4B-NB  | 5.54  | 130.12      | 124.26   |
| 14  | cA    | 3126 | CL7  | O2D-CGD-CBD | 5.54  | 121.10      | 111.27   |
| 14  | cA    | 3141 | CL7  | O2D-CGD-CBD | 5.52  | 121.08      | 111.27   |
| 14  | bA    | 3102 | CL7  | O2D-CGD-CBD | 5.51  | 121.06      | 111.27   |
| 13  | bB    | 801  | PHO  | CBC-CAC-C3C | -5.50 | 104.83      | 112.88   |
| 14  | aA    | 3142 | CL7  | O2D-CGD-CBD | 5.49  | 121.02      | 111.27   |
| 13  | aA    | 3102 | PHO  | CBC-CAC-C3C | -5.48 | 104.85      | 112.88   |
| 14  | bA    | 3124 | CL7  | CMB-C2B-C1B | 5.48  | 133.72      | 125.37   |
| 14  | cB    | 816  | CL7  | O2D-CGD-CBD | 5.47  | 120.99      | 111.27   |
| 14  | bA    | 3140 | CL7  | O2D-CGD-CBD | 5.47  | 120.98      | 111.27   |
| 14  | cB    | 826  | CL7  | C3B-C4B-NB  | -5.45 | 105.46      | 110.52   |
| 14  | aA    | 3141 | CL7  | O2D-CGD-CBD | 5.44  | 120.94      | 111.27   |
| 14  | bA    | 3102 | CL7  | C6-C5-C3    | -5.43 | 99.22       | 113.45   |
| 14  | aB    | 3021 | CL7  | CHB-C1B-NB  | -5.43 | 118.51      | 124.26   |
| 14  | aA    | 3121 | CL7  | C3B-C4B-NB  | -5.40 | 105.50      | 110.52   |
| 14  | aL    | 202  | CL7  | O1D-CGD-CBD | -5.40 | 113.43      | 124.48   |
| 14  | bB    | 826  | CL7  | C3B-C4B-NB  | -5.39 | 105.52      | 110.52   |
| 12  | cA    | 3101 | G9R  | C3B-C2B-C1B | -5.36 | 100.69      | 107.16   |
| 14  | aA    | 3143 | CL7  | O2D-CGD-CBD | 5.36  | 120.79      | 111.27   |
| 14  | cA    | 3102 | CL7  | O2D-CGD-CBD | 5.33  | 120.73      | 111.27   |
| 14  | bB    | 804  | CL7  | C3B-C4B-NB  | -5.31 | 105.58      | 110.52   |
| 12  | bA    | 3101 | G9R  | O2A-CGA-O1A | -5.31 | 110.19      | 123.59   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | bA    | 3139 | CL7  | O2D-CGD-CBD | 5.29  | 120.67      | 111.27   |
| 14  | aB    | 3007 | CL7  | O2D-CGD-O1D | -5.28 | 113.51      | 123.84   |
| 14  | cA    | 3129 | CL7  | C3B-C4B-NB  | -5.28 | 105.62      | 110.52   |
| 17  | aB    | 3027 | PQN  | C16-C15-C13 | -5.27 | 99.63       | 113.45   |
| 14  | cA    | 3120 | CL7  | O2D-CGD-CBD | 5.27  | 120.63      | 111.27   |
| 14  | aA    | 3125 | CL7  | C1-C2-C3    | -5.26 | 116.95      | 126.04   |
| 14  | bA    | 3119 | CL7  | C3B-C4B-NB  | -5.25 | 105.64      | 110.52   |
| 12  | bA    | 3101 | G9R  | O2A-CGA-CBA | 5.24  | 128.36      | 111.91   |
| 14  | cB    | 808  | CL7  | O2D-CGD-CBD | 5.24  | 120.58      | 111.27   |
| 14  | cA    | 3122 | CL7  | O1D-CGD-CBD | -5.23 | 113.79      | 124.48   |
| 14  | bA    | 3141 | CL7  | O2D-CGD-CBD | 5.22  | 120.54      | 111.27   |
| 14  | bB    | 833  | CL7  | O2D-CGD-CBD | 5.18  | 120.47      | 111.27   |
| 14  | cA    | 3116 | CL7  | O1D-CGD-CBD | -5.18 | 113.89      | 124.48   |
| 14  | bB    | 823  | CL7  | O2D-CGD-CBD | 5.17  | 120.46      | 111.27   |
| 14  | bA    | 3125 | CL7  | O1D-CGD-CBD | -5.17 | 113.91      | 124.48   |
| 14  | bA    | 3114 | CL7  | C1-C2-C3    | -5.16 | 117.12      | 126.04   |
| 14  | cB    | 823  | CL7  | O2D-CGD-CBD | 5.16  | 120.43      | 111.27   |
| 14  | bA    | 3132 | CL7  | C3B-C4B-NB  | -5.15 | 105.74      | 110.52   |
| 14  | aA    | 3140 | CL7  | O2D-CGD-CBD | 5.15  | 120.42      | 111.27   |
| 14  | cA    | 3119 | CL7  | C3B-C4B-NB  | -5.15 | 105.74      | 110.52   |
| 14  | bA    | 3122 | CL7  | C1-C2-C3    | -5.14 | 118.44      | 126.75   |
| 12  | aA    | 3101 | G9R  | O2A-CGA-O1A | -5.14 | 110.62      | 123.59   |
| 14  | aB    | 3007 | CL7  | O2D-CGD-CBD | 5.14  | 120.39      | 111.27   |
| 14  | bB    | 804  | CL7  | O2D-CGD-CBD | 5.13  | 120.39      | 111.27   |
| 12  | aA    | 3101 | G9R  | C3C-C4C-NC  | 5.12  | 116.32      | 110.57   |
| 14  | bA    | 3121 | CL7  | O2D-CGD-CBD | 5.12  | 120.37      | 111.27   |
| 12  | aA    | 3101 | G9R  | C1-C2-C3    | -5.12 | 117.19      | 126.04   |
| 14  | aB    | 3016 | CL7  | O2D-CGD-CBD | 5.11  | 120.36      | 111.27   |
| 13  | aB    | 3004 | PHO  | CMB-C2B-C3B | 5.11  | 134.24      | 124.68   |
| 14  | bB    | 822  | CL7  | O2D-CGD-CBD | 5.10  | 120.34      | 111.27   |
| 14  | aB    | 3021 | CL7  | O2D-CGD-CBD | 5.10  | 120.33      | 111.27   |
| 14  | aA    | 3123 | CL7  | O1D-CGD-CBD | -5.10 | 114.05      | 124.48   |
| 14  | cA    | 3132 | CL7  | C1A-NA-C4A  | -5.10 | 103.22      | 106.30   |
| 14  | aL    | 203  | CL7  | O2A-CGA-O1A | -5.09 | 110.74      | 123.59   |
| 13  | bB    | 801  | PHO  | C1-C2-C3    | -5.09 | 117.24      | 126.04   |
| 14  | bA    | 3102 | CL7  | C1-C2-C3    | -5.09 | 117.24      | 126.04   |
| 14  | cA    | 3124 | CL7  | CMB-C2B-C1B | 5.09  | 133.12      | 125.37   |
| 14  | cB    | 804  | CL7  | C3B-C4B-NB  | -5.08 | 105.80      | 110.52   |
| 14  | cA    | 3125 | CL7  | O2D-CGD-CBD | 5.05  | 120.24      | 111.27   |
| 14  | bB    | 804  | CL7  | C1-C2-C3    | -5.04 | 117.33      | 126.04   |
| 14  | aA    | 3122 | CL7  | O2D-CGD-CBD | 5.04  | 120.22      | 111.27   |
| 14  | cA    | 3140 | CL7  | O2D-CGD-O1D | -5.02 | 114.02      | 123.84   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | aB    | 3030 | CL7  | O2D-CGD-CBD | 5.02  | 120.18      | 111.27   |
| 14  | cA    | 3105 | CL7  | CAA-C2A-C3A | -5.01 | 104.41      | 116.10   |
| 13  | cB    | 805  | PHO  | CMB-C2B-C3B | 5.00  | 134.04      | 124.68   |
| 14  | bA    | 3129 | CL7  | C3B-C4B-NB  | -5.00 | 105.87      | 110.52   |
| 14  | cA    | 3132 | CL7  | C3B-C4B-NB  | -4.99 | 105.89      | 110.52   |
| 14  | cA    | 3129 | CL7  | CAA-C2A-C3A | -4.97 | 104.50      | 116.10   |
| 14  | aB    | 3032 | CL7  | O2D-CGD-CBD | 4.97  | 120.10      | 111.27   |
| 12  | cA    | 3101 | G9R  | O2A-CGA-O1A | -4.97 | 111.05      | 123.59   |
| 13  | aB    | 3004 | PHO  | O2D-CGD-CBD | 4.96  | 117.28      | 111.00   |
| 14  | aA    | 3133 | CL7  | C1A-NA-C4A  | -4.95 | 103.31      | 106.30   |
| 14  | cA    | 3131 | CL7  | O2D-CGD-CBD | 4.95  | 120.06      | 111.27   |
| 14  | bA    | 3105 | CL7  | CAA-C2A-C3A | -4.95 | 104.55      | 116.10   |
| 14  | aB    | 3031 | CL7  | O2D-CGD-O1D | -4.94 | 114.18      | 123.84   |
| 12  | aA    | 3101 | G9R  | C2C-C1C-NC  | 4.94  | 114.60      | 109.97   |
| 14  | cB    | 822  | CL7  | O2D-CGD-CBD | 4.94  | 120.04      | 111.27   |
| 12  | bA    | 3101 | G9R  | C3D-C2D-C1D | -4.94 | 99.10       | 105.83   |
| 14  | cL    | 205  | CL7  | O2D-CGD-CBD | 4.93  | 120.03      | 111.27   |
| 14  | bL    | 204  | CL7  | O2A-CGA-O1A | -4.92 | 111.17      | 123.59   |
| 14  | cL    | 203  | CL7  | O1D-CGD-CBD | -4.92 | 114.42      | 124.48   |
| 14  | cA    | 3127 | CL7  | O2D-CGD-CBD | 4.92  | 120.01      | 111.27   |
| 14  | bB    | 817  | CL7  | O2D-CGD-CBD | 4.91  | 119.99      | 111.27   |
| 14  | aB    | 3022 | CL7  | O2D-CGD-CBD | 4.90  | 119.98      | 111.27   |
| 13  | cB    | 805  | PHO  | O2D-CGD-CBD | 4.90  | 117.21      | 111.00   |
| 14  | bA    | 3122 | CL7  | O1D-CGD-CBD | -4.90 | 114.45      | 124.48   |
| 13  | aA    | 3102 | PHO  | C1-C2-C3    | -4.90 | 117.57      | 126.04   |
| 14  | bA    | 3131 | CL7  | O2D-CGD-CBD | 4.89  | 119.95      | 111.27   |
| 14  | bA    | 3133 | CL7  | C3A-C4A-CHB | -4.88 | 116.45      | 123.70   |
| 14  | aB    | 3010 | CL7  | O2D-CGD-CBD | 4.88  | 119.94      | 111.27   |
| 14  | aA    | 3119 | CL7  | C1D-ND-C4D  | -4.87 | 102.88      | 106.33   |
| 14  | cB    | 818  | CL7  | O2D-CGD-CBD | 4.87  | 119.92      | 111.27   |
| 14  | cA    | 3118 | CL7  | C1D-ND-C4D  | -4.86 | 102.88      | 106.33   |
| 14  | bA    | 3123 | CL7  | C3B-C4B-NB  | -4.86 | 106.00      | 110.52   |
| 14  | cB    | 804  | CL7  | O2D-CGD-CBD | 4.86  | 119.90      | 111.27   |
| 14  | bA    | 3127 | CL7  | O2D-CGD-CBD | 4.85  | 119.89      | 111.27   |
| 12  | bA    | 3101 | G9R  | C1D-CHD-C4C | -4.85 | 115.60      | 126.06   |
| 14  | aB    | 3025 | CL7  | C4-C3-C2    | -4.84 | 111.25      | 123.68   |
| 14  | cB    | 803  | CL7  | C3B-C4B-NB  | -4.84 | 106.02      | 110.52   |
| 14  | aA    | 3133 | CL7  | C3B-C4B-NB  | -4.84 | 106.03      | 110.52   |
| 14  | aB    | 3009 | CL7  | O2D-CGD-CBD | 4.83  | 119.86      | 111.27   |
| 12  | aA    | 3101 | G9R  | CHD-C1D-ND  | -4.83 | 120.02      | 124.45   |
| 14  | cA    | 3116 | CL7  | C1-C2-C3    | -4.83 | 117.69      | 126.04   |
| 14  | aB    | 3003 | CL7  | O2D-CGD-CBD | 4.83  | 119.85      | 111.27   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | aA    | 3109 | CL7  | O2D-CGD-CBD | 4.83  | 119.84      | 111.27   |
| 17  | aA    | 3144 | PQN  | C14-C13-C15 | 4.82  | 123.39      | 115.27   |
| 14  | aB    | 3025 | CL7  | C3B-C4B-NB  | -4.82 | 106.04      | 110.52   |
| 14  | bA    | 3125 | CL7  | O2D-CGD-CBD | 4.82  | 119.84      | 111.27   |
| 12  | aA    | 3101 | G9R  | C3D-C2D-C1D | -4.82 | 99.25       | 105.83   |
| 14  | bB    | 808  | CL7  | O2D-CGD-CBD | 4.82  | 119.83      | 111.27   |
| 14  | cA    | 3116 | CL7  | C1D-ND-C4D  | -4.80 | 102.92      | 106.33   |
| 13  | cB    | 801  | PHO  | C4A-C3A-C2A | -4.80 | 98.27       | 102.84   |
| 14  | aA    | 3111 | CL7  | O2D-CGD-CBD | 4.80  | 119.80      | 111.27   |
| 14  | aA    | 3103 | CL7  | C6-C5-C3    | -4.80 | 100.86      | 113.45   |
| 14  | bA    | 3110 | CL7  | O2D-CGD-CBD | 4.80  | 119.80      | 111.27   |
| 14  | cA    | 3121 | CL7  | O2D-CGD-CBD | 4.80  | 119.79      | 111.27   |
| 14  | aA    | 3117 | CL7  | C1D-ND-C4D  | -4.80 | 102.93      | 106.33   |
| 12  | aA    | 3101 | G9R  | C3B-C2B-C1B | -4.78 | 101.39      | 107.16   |
| 14  | cA    | 3139 | CL7  | O2D-CGD-CBD | 4.78  | 119.75      | 111.27   |
| 13  | cB    | 805  | PHO  | C4A-C3A-C2A | -4.78 | 98.30       | 102.84   |
| 14  | aA    | 3126 | CL7  | O2D-CGD-O1D | -4.77 | 114.51      | 123.84   |
| 14  | bB    | 809  | CL7  | O2D-CGD-CBD | 4.77  | 119.74      | 111.27   |
| 13  | bB    | 805  | PHO  | CMB-C2B-C3B | 4.77  | 133.60      | 124.68   |
| 14  | aA    | 3129 | CL7  | CAC-C3C-C2C | -4.76 | 119.38      | 127.53   |
| 14  | bA    | 3108 | CL7  | O2D-CGD-CBD | 4.76  | 119.73      | 111.27   |
| 14  | bB    | 811  | CL7  | O2D-CGD-CBD | 4.75  | 119.72      | 111.27   |
| 14  | cB    | 833  | CL7  | O2D-CGD-CBD | 4.75  | 119.70      | 111.27   |
| 14  | aA    | 3130 | CL7  | C3B-C4B-NB  | -4.74 | 106.12      | 110.52   |
| 14  | aB    | 3003 | CL7  | C1-C2-C3    | -4.73 | 117.86      | 126.04   |
| 14  | cL    | 203  | CL7  | O2D-CGD-O1D | -4.73 | 114.59      | 123.84   |
| 14  | aA    | 3121 | CL7  | C3A-C4A-CHB | -4.73 | 116.68      | 123.70   |
| 14  | bA    | 3133 | CL7  | CAA-C2A-C3A | -4.73 | 105.07      | 116.10   |
| 14  | cB    | 804  | CL7  | C1-C2-C3    | -4.72 | 117.88      | 126.04   |
| 14  | aA    | 3128 | CL7  | O2D-CGD-CBD | 4.71  | 119.64      | 111.27   |
| 13  | cB    | 801  | PHO  | C1-C2-C3    | -4.71 | 117.90      | 126.04   |
| 12  | cA    | 3101 | G9R  | C3C-C4C-NC  | 4.70  | 115.85      | 110.57   |
| 14  | bA    | 3128 | CL7  | CAC-C3C-C2C | -4.70 | 119.48      | 127.53   |
| 14  | bA    | 3116 | CL7  | C1D-ND-C4D  | -4.70 | 103.00      | 106.33   |
| 14  | cA    | 3123 | CL7  | O2D-CGD-O1D | -4.70 | 114.66      | 123.84   |
| 14  | cA    | 3129 | CL7  | O2D-CGD-O1D | -4.69 | 114.66      | 123.84   |
| 14  | cA    | 3104 | CL7  | O2D-CGD-CBD | 4.69  | 119.60      | 111.27   |
| 14  | bB    | 803  | CL7  | C3A-C4A-CHB | -4.68 | 116.76      | 123.70   |
| 14  | bA    | 3129 | CL7  | O2D-CGD-O1D | -4.67 | 114.70      | 123.84   |
| 14  | aA    | 3105 | CL7  | O2D-CGD-CBD | 4.66  | 119.55      | 111.27   |
| 14  | cA    | 3127 | CL7  | O1D-CGD-CBD | -4.66 | 114.96      | 124.48   |
| 14  | cA    | 3113 | CL7  | CMB-C2B-C1B | 4.65  | 132.46      | 125.37   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | bB    | 804  | CL7  | CHC-C1C-NC  | -4.65 | 120.18      | 124.45   |
| 14  | aA    | 3123 | CL7  | O2D-CGD-O1D | -4.65 | 114.75      | 123.84   |
| 14  | aB    | 3008 | CL7  | O2D-CGD-CBD | 4.65  | 119.52      | 111.27   |
| 14  | cB    | 809  | CL7  | O2D-CGD-CBD | 4.64  | 119.52      | 111.27   |
| 12  | aA    | 3101 | G9R  | O2A-CGA-CBA | 4.64  | 126.47      | 111.91   |
| 14  | cA    | 3114 | CL7  | C1-C2-C3    | -4.63 | 118.03      | 126.04   |
| 14  | cA    | 3102 | CL7  | C2D-C1D-ND  | -4.63 | 107.13      | 110.23   |
| 14  | cA    | 3102 | CL7  | C6-C5-C3    | -4.63 | 101.31      | 113.45   |
| 14  | aB    | 3030 | CL7  | CHB-C1B-NB  | -4.63 | 119.36      | 124.26   |
| 14  | bB    | 803  | CL7  | C3B-C4B-NB  | -4.62 | 106.23      | 110.52   |
| 14  | cB    | 827  | CL7  | CHC-C4B-NB  | 4.62  | 129.15      | 124.26   |
| 14  | cB    | 817  | CL7  | O2D-CGD-CBD | 4.61  | 119.46      | 111.27   |
| 14  | aB    | 3015 | CL7  | C3A-C4A-CHB | -4.61 | 116.86      | 123.70   |
| 14  | cL    | 204  | CL7  | O2A-CGA-O1A | -4.61 | 111.96      | 123.59   |
| 14  | aA    | 3126 | CL7  | O2D-CGD-CBD | 4.61  | 119.45      | 111.27   |
| 14  | bB    | 824  | CL7  | O2D-CGD-CBD | 4.60  | 119.45      | 111.27   |
| 14  | cB    | 824  | CL7  | CMB-C2B-C1B | 4.60  | 132.38      | 125.37   |
| 14  | bA    | 3127 | CL7  | O1D-CGD-CBD | -4.60 | 115.08      | 124.48   |
| 14  | aA    | 3106 | CL7  | CAA-C2A-C3A | -4.60 | 105.37      | 116.10   |
| 14  | bL    | 203  | CL7  | C3B-C4B-NB  | -4.59 | 106.25      | 110.52   |
| 14  | cA    | 3102 | CL7  | O2D-CGD-O1D | -4.59 | 114.87      | 123.84   |
| 14  | cA    | 3129 | CL7  | CMB-C2B-C1B | 4.58  | 132.34      | 125.37   |
| 14  | cA    | 3133 | CL7  | CAA-C2A-C3A | -4.57 | 105.44      | 116.10   |
| 14  | bA    | 3107 | CL7  | O2D-CGD-CBD | 4.57  | 119.38      | 111.27   |
| 14  | bA    | 3116 | CL7  | O1D-CGD-CBD | -4.56 | 115.15      | 124.48   |
| 14  | cA    | 3105 | CL7  | C3B-C4B-NB  | -4.56 | 106.28      | 110.52   |
| 14  | bA    | 3132 | CL7  | C6-C5-C3    | -4.56 | 101.51      | 113.45   |
| 14  | bA    | 3145 | CL7  | O2D-CGD-CBD | 4.55  | 119.36      | 111.27   |
| 14  | bA    | 3123 | CL7  | O2D-CGD-O1D | -4.54 | 114.95      | 123.84   |
| 14  | cA    | 3125 | CL7  | C7-C6-C5    | -4.54 | 101.02      | 113.36   |
| 14  | bB    | 824  | CL7  | CMB-C2B-C1B | 4.54  | 132.29      | 125.37   |
| 14  | bA    | 3124 | CL7  | C1-C2-C3    | -4.54 | 118.20      | 126.04   |
| 13  | aA    | 3102 | PHO  | C4A-C3A-C2A | -4.53 | 98.53       | 102.84   |
| 12  | cA    | 3101 | G9R  | C1D-CHD-C4C | -4.53 | 116.29      | 126.06   |
| 12  | aA    | 3101 | G9R  | C1D-CHD-C4C | -4.52 | 116.30      | 126.06   |
| 14  | cA    | 3132 | CL7  | O1A-CGA-CBA | -4.52 | 106.09      | 123.73   |
| 14  | bA    | 3129 | CL7  | CMB-C2B-C1B | 4.52  | 132.26      | 125.37   |
| 14  | bA    | 3104 | CL7  | O2D-CGD-CBD | 4.52  | 119.30      | 111.27   |
| 14  | bA    | 3122 | CL7  | O2D-CGD-O1D | -4.52 | 115.01      | 123.84   |
| 14  | aA    | 3133 | CL7  | O1A-CGA-CBA | -4.51 | 106.14      | 123.73   |
| 14  | aA    | 3128 | CL7  | O1D-CGD-CBD | -4.51 | 115.26      | 124.48   |
| 14  | cB    | 803  | CL7  | CHC-C1C-NC  | -4.51 | 120.31      | 124.45   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 19  | cB    | 830  | LMG  | C1-O6-C5    | -4.50 | 104.85      | 113.69   |
| 14  | bA    | 3140 | CL7  | C6-C5-C3    | -4.50 | 101.65      | 113.45   |
| 14  | aA    | 3120 | CL7  | C3B-C4B-NB  | -4.50 | 106.34      | 110.52   |
| 14  | cA    | 3132 | CL7  | C6-C5-C3    | -4.50 | 101.66      | 113.45   |
| 12  | bA    | 3101 | G9R  | O2D-CGD-O1D | -4.50 | 115.05      | 123.84   |
| 14  | aB    | 3003 | CL7  | CHC-C1C-NC  | -4.50 | 120.32      | 124.45   |
| 14  | bB    | 803  | CL7  | CHC-C1C-NC  | -4.50 | 120.32      | 124.45   |
| 14  | cA    | 3122 | CL7  | O2D-CGD-O1D | -4.49 | 115.06      | 123.84   |
| 14  | bA    | 3132 | CL7  | O1A-CGA-CBA | -4.49 | 106.22      | 123.73   |
| 14  | cB    | 824  | CL7  | O2D-CGD-CBD | 4.49  | 119.24      | 111.27   |
| 14  | cA    | 3139 | CL7  | O2D-CGD-O1D | -4.48 | 115.07      | 123.84   |
| 14  | cA    | 3128 | CL7  | CAC-C3C-C2C | -4.48 | 119.87      | 127.53   |
| 14  | bA    | 3105 | CL7  | C3B-C4B-NB  | -4.48 | 106.36      | 110.52   |
| 13  | bB    | 801  | PHO  | C4A-C3A-C2A | -4.47 | 98.59       | 102.84   |
| 14  | cB    | 808  | CL7  | C3B-C4B-NB  | -4.47 | 106.37      | 110.52   |
| 14  | aB    | 3025 | CL7  | C4D-C3D-C2D | -4.46 | 101.48      | 107.30   |
| 14  | cB    | 815  | CL7  | O2D-CGD-CBD | 4.46  | 119.19      | 111.27   |
| 12  | bA    | 3101 | G9R  | C2A-C3A-C4A | -4.46 | 94.67       | 101.87   |
| 14  | bB    | 808  | CL7  | O1D-CGD-CBD | -4.45 | 115.38      | 124.48   |
| 14  | cB    | 808  | CL7  | O1D-CGD-CBD | -4.45 | 115.39      | 124.48   |
| 14  | aB    | 3007 | CL7  | C3A-C4A-CHB | -4.44 | 117.10      | 123.70   |
| 14  | bB    | 831  | CL7  | O2D-CGD-CBD | 4.44  | 119.16      | 111.27   |
| 12  | cA    | 3101 | G9R  | CAA-C2A-C3A | -4.44 | 100.62      | 112.78   |
| 14  | aL    | 202  | CL7  | O2D-CGD-O1D | -4.44 | 115.16      | 123.84   |
| 14  | cB    | 832  | CL7  | O2D-CGD-O1D | -4.44 | 115.17      | 123.84   |
| 14  | bB    | 831  | CL7  | CHB-C1B-NB  | -4.43 | 119.56      | 124.26   |
| 14  | cB    | 831  | CL7  | CHB-C1B-NB  | -4.43 | 119.56      | 124.26   |
| 14  | cA    | 3106 | CL7  | C1-C2-C3    | -4.43 | 118.39      | 126.04   |
| 14  | bL    | 203  | CL7  | O2D-CGD-O1D | -4.43 | 115.18      | 123.84   |
| 14  | bB    | 810  | CL7  | C1A-NA-C4A  | -4.42 | 103.62      | 106.30   |
| 14  | cA    | 3108 | CL7  | O2D-CGD-CBD | 4.42  | 119.13      | 111.27   |
| 14  | cA    | 3132 | CL7  | O2D-CGD-CBD | 4.42  | 119.13      | 111.27   |
| 13  | cB    | 805  | PHO  | C2D-C1D-ND  | 4.42  | 112.58      | 109.53   |
| 14  | aB    | 3015 | CL7  | O1D-CGD-CBD | -4.42 | 115.44      | 124.48   |
| 17  | cA    | 3143 | PQN  | C11-C12-C13 | -4.42 | 119.44      | 126.79   |
| 14  | aA    | 3125 | CL7  | CMB-C2B-C1B | 4.42  | 132.10      | 125.37   |
| 13  | aB    | 3004 | PHO  | C1-C2-C3    | -4.41 | 118.42      | 126.04   |
| 14  | cB    | 804  | CL7  | CHC-C1C-NC  | -4.40 | 120.41      | 124.45   |
| 14  | cB    | 808  | CL7  | C1D-ND-C4D  | -4.40 | 103.21      | 106.33   |
| 14  | bB    | 810  | CL7  | C3B-C4B-NB  | -4.40 | 106.44      | 110.52   |
| 14  | bA    | 3123 | CL7  | O2A-CGA-O1A | -4.39 | 112.50      | 123.59   |
| 13  | bB    | 805  | PHO  | C2D-C1D-ND  | 4.39  | 112.56      | 109.53   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | cA    | 3126 | CL7  | C1D-ND-C4D  | -4.39 | 103.22      | 106.33   |
| 14  | cB    | 810  | CL7  | C3B-C4B-NB  | -4.39 | 106.44      | 110.52   |
| 12  | bA    | 3101 | G9R  | C2C-C1C-NC  | 4.38  | 114.08      | 109.97   |
| 14  | aA    | 3115 | CL7  | C1-C2-C3    | -4.38 | 118.46      | 126.04   |
| 14  | cL    | 204  | CL7  | CMB-C2B-C1B | 4.38  | 132.04      | 125.37   |
| 17  | bA    | 3143 | PQN  | C11-C12-C13 | -4.38 | 119.51      | 126.79   |
| 14  | aB    | 3006 | CL7  | O2D-CGD-CBD | 4.37  | 119.03      | 111.27   |
| 14  | aB    | 3014 | CL7  | O2D-CGD-CBD | 4.37  | 119.03      | 111.27   |
| 14  | cB    | 803  | CL7  | CHC-C4B-NB  | 4.36  | 128.88      | 124.26   |
| 14  | bA    | 3132 | CL7  | C1A-NA-C4A  | -4.36 | 103.66      | 106.30   |
| 14  | bB    | 803  | CL7  | CHC-C4B-NB  | 4.35  | 128.87      | 124.26   |
| 14  | aB    | 3023 | CL7  | CMB-C2B-C1B | 4.35  | 132.00      | 125.37   |
| 14  | aB    | 3023 | CL7  | O2D-CGD-CBD | 4.35  | 119.00      | 111.27   |
| 14  | bB    | 815  | CL7  | O2D-CGD-CBD | 4.35  | 118.99      | 111.27   |
| 14  | bB    | 820  | CL7  | C3A-C4A-CHB | -4.35 | 117.25      | 123.70   |
| 12  | cA    | 3101 | G9R  | C3D-C4D-ND  | 4.35  | 117.27      | 110.24   |
| 14  | cA    | 3127 | CL7  | C3A-C2A-C1A | 4.34  | 107.84      | 101.34   |
| 14  | cA    | 3111 | CL7  | CMB-C2B-C1B | 4.34  | 131.98      | 125.37   |
| 14  | bA    | 3125 | CL7  | C3B-C4B-NB  | -4.33 | 106.49      | 110.52   |
| 14  | aA    | 3121 | CL7  | C1-C2-C3    | -4.33 | 118.56      | 126.04   |
| 14  | cA    | 3114 | CL7  | C1A-NA-C4A  | -4.32 | 103.69      | 106.30   |
| 14  | aA    | 3103 | CL7  | C1-C2-C3    | -4.32 | 118.57      | 126.04   |
| 14  | cA    | 3119 | CL7  | O2D-CGD-CBD | 4.32  | 118.95      | 111.27   |
| 14  | aB    | 3003 | CL7  | C3B-C4B-NB  | -4.32 | 106.51      | 110.52   |
| 12  | cA    | 3101 | G9R  | C3D-C2D-C1D | -4.31 | 99.95       | 105.83   |
| 14  | aA    | 3129 | CL7  | O2D-CGD-O1D | -4.31 | 115.41      | 123.84   |
| 14  | bA    | 3106 | CL7  | C1-C2-C3    | -4.31 | 118.58      | 126.04   |
| 14  | aB    | 3026 | CL7  | C1D-ND-C4D  | -4.31 | 103.27      | 106.33   |
| 14  | bA    | 3139 | CL7  | O2D-CGD-O1D | -4.31 | 115.42      | 123.84   |
| 14  | aA    | 3121 | CL7  | O2D-CGD-CBD | 4.31  | 118.92      | 111.27   |
| 14  | bB    | 822  | CL7  | O2D-CGD-O1D | -4.29 | 115.45      | 123.84   |
| 14  | bL    | 205  | CL7  | C3B-C4B-NB  | -4.29 | 106.54      | 110.52   |
| 14  | cF    | 201  | CL7  | CHB-C1B-NB  | -4.29 | 119.72      | 124.26   |
| 14  | bA    | 3106 | CL7  | C3A-C4A-CHB | -4.29 | 117.34      | 123.70   |
| 14  | aB    | 3018 | CL7  | C4D-C3D-CAD | -4.28 | 104.54      | 107.42   |
| 14  | cB    | 806  | CL7  | O2D-CGD-CBD | 4.28  | 118.87      | 111.27   |
| 14  | aB    | 3021 | CL7  | O2D-CGD-O1D | -4.27 | 115.48      | 123.84   |
| 14  | bB    | 814  | CL7  | O2D-CGD-CBD | 4.27  | 118.86      | 111.27   |
| 14  | bB    | 827  | CL7  | O2D-CGD-CBD | 4.26  | 118.85      | 111.27   |
| 14  | bB    | 809  | CL7  | C3B-C4B-NB  | -4.26 | 106.56      | 110.52   |
| 13  | aB    | 3004 | PHO  | CMC-C2C-C3C | 4.26  | 137.68      | 126.12   |
| 14  | bA    | 3118 | CL7  | C3A-C4A-CHB | -4.26 | 117.38      | 123.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | aB    | 3006 | CL7  | O2D-CGD-O1D | -4.26 | 115.52      | 123.84   |
| 12  | bA    | 3101 | G9R  | CAA-C2A-C3A | -4.26 | 101.12      | 112.78   |
| 14  | aA    | 3130 | CL7  | CMC-C2C-C1C | -4.25 | 117.21      | 124.71   |
| 14  | aB    | 3013 | CL7  | O2D-CGD-CBD | 4.25  | 118.83      | 111.27   |
| 14  | bB    | 826  | CL7  | C4D-C3D-CAD | 4.25  | 110.29      | 107.42   |
| 14  | cA    | 3125 | CL7  | C3B-C4B-NB  | -4.25 | 106.57      | 110.52   |
| 14  | bB    | 826  | CL7  | C4-C3-C2    | -4.25 | 112.78      | 123.68   |
| 14  | aA    | 3120 | CL7  | O2D-CGD-CBD | 4.25  | 118.81      | 111.27   |
| 14  | aB    | 3025 | CL7  | C2D-C1D-ND  | -4.25 | 107.39      | 110.23   |
| 14  | bA    | 3124 | CL7  | O2D-CGD-CBD | 4.24  | 118.81      | 111.27   |
| 14  | aB    | 3021 | CL7  | CMB-C2B-C1B | 4.24  | 131.83      | 125.37   |
| 14  | aA    | 3108 | CL7  | O2D-CGD-CBD | 4.24  | 118.80      | 111.27   |
| 14  | aB    | 3009 | CL7  | C3B-C4B-NB  | -4.24 | 106.59      | 110.52   |
| 14  | cB    | 823  | CL7  | O1D-CGD-CBD | -4.23 | 115.82      | 124.48   |
| 12  | cA    | 3101 | G9R  | O2A-CGA-CBA | 4.23  | 125.19      | 111.91   |
| 13  | bB    | 805  | PHO  | CMD-C2D-C3D | 4.23  | 132.59      | 124.68   |
| 14  | cB    | 814  | CL7  | O2D-CGD-CBD | 4.22  | 118.76      | 111.27   |
| 14  | aL    | 204  | CL7  | O2D-CGD-CBD | 4.22  | 118.76      | 111.27   |
| 14  | bA    | 3142 | CL7  | O2D-CGD-O1D | -4.22 | 115.60      | 123.84   |
| 14  | aA    | 3117 | CL7  | O1D-CGD-CBD | -4.21 | 115.86      | 124.48   |
| 14  | aB    | 3016 | CL7  | C3A-C4A-CHB | -4.21 | 117.45      | 123.70   |
| 12  | bA    | 3101 | G9R  | CHD-C1D-ND  | -4.21 | 120.59      | 124.45   |
| 14  | cB    | 827  | CL7  | C3B-C4B-NB  | -4.21 | 106.61      | 110.52   |
| 14  | bB    | 832  | CL7  | C1A-NA-C4A  | -4.20 | 103.76      | 106.30   |
| 14  | bA    | 3118 | CL7  | CAA-C2A-C3A | -4.20 | 106.30      | 116.10   |
| 14  | bA    | 3103 | CL7  | CMB-C2B-C1B | 4.20  | 131.76      | 125.37   |
| 14  | bA    | 3133 | CL7  | O2D-CGD-CBD | 4.19  | 118.72      | 111.27   |
| 14  | bA    | 3126 | CL7  | C1D-ND-C4D  | -4.19 | 103.36      | 106.33   |
| 14  | bB    | 827  | CL7  | C2C-C1C-NC  | 4.18  | 113.19      | 110.10   |
| 14  | aA    | 3115 | CL7  | C1A-NA-C4A  | -4.18 | 103.77      | 106.30   |
| 14  | cB    | 831  | CL7  | O2D-CGD-CBD | 4.18  | 118.70      | 111.27   |
| 14  | bB    | 808  | CL7  | O2A-CGA-O1A | -4.18 | 113.04      | 123.59   |
| 14  | cA    | 3113 | CL7  | CHC-C1C-NC  | -4.18 | 120.62      | 124.45   |
| 14  | aB    | 3007 | CL7  | O1D-CGD-CBD | -4.17 | 115.94      | 124.48   |
| 13  | aA    | 3102 | PHO  | C2D-C1D-ND  | 4.17  | 112.41      | 109.53   |
| 14  | bA    | 3111 | CL7  | CMB-C2B-C1B | 4.17  | 131.72      | 125.37   |
| 14  | bA    | 3112 | CL7  | O2D-CGD-CBD | 4.17  | 118.68      | 111.27   |
| 14  | aA    | 3120 | CL7  | CHB-C1B-NB  | -4.17 | 119.84      | 124.26   |
| 14  | bB    | 827  | CL7  | CHC-C4B-NB  | 4.16  | 128.66      | 124.26   |
| 14  | bA    | 3125 | CL7  | C7-C6-C5    | -4.16 | 102.06      | 113.36   |
| 14  | cB    | 808  | CL7  | O2A-CGA-O1A | -4.16 | 113.09      | 123.59   |
| 14  | cA    | 3133 | CL7  | C3A-C4A-CHB | -4.16 | 117.53      | 123.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12  | bA    | 3101 | G9R  | C3C-C4C-NC  | 4.16  | 115.23      | 110.57   |
| 14  | cL    | 203  | CL7  | O2D-CGD-CBD | 4.15  | 118.65      | 111.27   |
| 14  | aA    | 3115 | CL7  | CMB-C2B-C1B | 4.15  | 131.69      | 125.37   |
| 13  | cB    | 805  | PHO  | CMD-C2D-C3D | 4.15  | 132.45      | 124.68   |
| 14  | cA    | 3140 | CL7  | CHB-C1B-NB  | -4.15 | 119.86      | 124.26   |
| 14  | aB    | 3002 | CL7  | CHC-C1C-NC  | -4.15 | 120.64      | 124.45   |
| 14  | cA    | 3112 | CL7  | C3A-C4A-CHB | -4.15 | 117.54      | 123.70   |
| 14  | bA    | 3124 | CL7  | C1-O2A-CGA  | -4.14 | 105.57      | 116.44   |
| 14  | cA    | 3108 | CL7  | CMB-C2B-C1B | 4.14  | 131.68      | 125.37   |
| 14  | aB    | 3025 | CL7  | C5-C3-C2    | -4.14 | 112.73      | 121.12   |
| 14  | cA    | 3114 | CL7  | O1D-CGD-CBD | -4.14 | 116.01      | 124.48   |
| 14  | aA    | 3134 | CL7  | C3A-C4A-CHB | -4.14 | 117.56      | 123.70   |
| 14  | aL    | 203  | CL7  | C1-C2-C3    | -4.13 | 118.89      | 126.04   |
| 14  | cA    | 3102 | CL7  | C3A-C4A-CHB | -4.13 | 117.57      | 123.70   |
| 12  | cA    | 3101 | G9R  | C2A-C3A-C4A | -4.13 | 95.20       | 101.87   |
| 14  | bA    | 3132 | CL7  | O2D-CGD-CBD | 4.13  | 118.61      | 111.27   |
| 13  | aB    | 3004 | PHO  | CMD-C2D-C3D | 4.13  | 132.40      | 124.68   |
| 14  | aA    | 3127 | CL7  | C1D-ND-C4D  | -4.13 | 103.40      | 106.33   |
| 14  | bK    | 101  | CL7  | C1A-NA-C4A  | -4.13 | 103.80      | 106.30   |
| 14  | bF    | 201  | CL7  | CAA-C2A-C3A | -4.12 | 106.49      | 116.10   |
| 14  | bB    | 810  | CL7  | O2D-CGD-CBD | 4.12  | 118.59      | 111.27   |
| 14  | aF    | 201  | CL7  | C3A-C4A-CHB | -4.12 | 117.59      | 123.70   |
| 19  | bB    | 830  | LMG  | C1-O6-C5    | -4.12 | 105.61      | 113.69   |
| 14  | bA    | 3120 | CL7  | C3B-C4B-NB  | -4.12 | 106.70      | 110.52   |
| 14  | cA    | 3129 | CL7  | CMC-C2C-C1C | -4.12 | 117.46      | 124.71   |
| 14  | aA    | 3114 | CL7  | CMB-C2B-C1B | 4.12  | 131.64      | 125.37   |
| 14  | bB    | 807  | CL7  | O2D-CGD-O1D | -4.11 | 115.79      | 123.84   |
| 13  | aB    | 3004 | PHO  | C2D-C1D-ND  | 4.11  | 112.36      | 109.53   |
| 14  | aB    | 3022 | CL7  | O1D-CGD-CBD | -4.10 | 116.09      | 124.48   |
| 14  | cB    | 826  | CL7  | C4-C3-C2    | -4.10 | 113.16      | 123.68   |
| 14  | aA    | 3117 | CL7  | C1-C2-C3    | -4.10 | 118.95      | 126.04   |
| 14  | cF    | 201  | CL7  | C3A-C4A-CHB | -4.10 | 117.62      | 123.70   |
| 14  | bL    | 205  | CL7  | O2D-CGD-CBD | 4.10  | 118.55      | 111.27   |
| 14  | bB    | 817  | CL7  | C3A-C4A-CHB | -4.09 | 117.62      | 123.70   |
| 14  | bB    | 804  | CL7  | CHC-C4B-NB  | 4.09  | 128.59      | 124.26   |
| 14  | cA    | 3123 | CL7  | O1A-CGA-CBA | -4.09 | 107.79      | 123.73   |
| 14  | aF    | 201  | CL7  | CAA-C2A-C3A | -4.08 | 106.58      | 116.10   |
| 14  | aA    | 3113 | CL7  | C3A-C4A-CHB | -4.08 | 117.65      | 123.70   |
| 14  | bA    | 3102 | CL7  | O2D-CGD-O1D | -4.08 | 115.86      | 123.84   |
| 14  | cA    | 3144 | CL7  | O2D-CGD-CBD | 4.08  | 118.52      | 111.27   |
| 14  | bA    | 3105 | CL7  | C3A-C4A-CHB | -4.08 | 117.65      | 123.70   |
| 13  | cB    | 805  | PHO  | C1-C2-C3    | -4.08 | 119.00      | 126.04   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | bA    | 3123 | CL7  | C1-C2-C3    | -4.07 | 119.00      | 126.04   |
| 14  | aA    | 3132 | CL7  | CAA-C2A-C3A | -4.07 | 106.59      | 116.10   |
| 14  | aA    | 3124 | CL7  | C3A-C2A-C1A | 4.07  | 107.44      | 101.34   |
| 14  | cA    | 3108 | CL7  | C3A-C4A-CHB | -4.07 | 117.66      | 123.70   |
| 14  | cB    | 826  | CL7  | C4D-C3D-CAD | 4.07  | 110.17      | 107.42   |
| 14  | aB    | 3002 | CL7  | C3B-C4B-NB  | -4.07 | 106.74      | 110.52   |
| 14  | aL    | 202  | CL7  | C3B-C4B-NB  | -4.07 | 106.74      | 110.52   |
| 14  | cA    | 3127 | CL7  | CBA-CAA-C2A | -4.06 | 101.88      | 113.86   |
| 14  | cA    | 3133 | CL7  | O2D-CGD-CBD | 4.06  | 118.47      | 111.27   |
| 14  | aA    | 3124 | CL7  | O2D-CGD-O1D | -4.05 | 115.91      | 123.84   |
| 14  | aA    | 3131 | CL7  | O2D-CGD-CBD | 4.05  | 118.47      | 111.27   |
| 14  | aA    | 3113 | CL7  | O2D-CGD-CBD | 4.05  | 118.47      | 111.27   |
| 14  | cB    | 819  | CL7  | O2A-CGA-O1A | -4.05 | 113.37      | 123.59   |
| 14  | bA    | 3129 | CL7  | O2D-CGD-CBD | 4.05  | 118.46      | 111.27   |
| 14  | bA    | 3119 | CL7  | O2D-CGD-CBD | 4.05  | 118.46      | 111.27   |
| 14  | bB    | 827  | CL7  | O2A-CGA-O1A | -4.04 | 113.39      | 123.59   |
| 14  | cA    | 3130 | CL7  | O2D-CGD-CBD | 4.04  | 118.45      | 111.27   |
| 14  | cA    | 3102 | CL7  | C1-C2-C3    | -4.04 | 119.06      | 126.04   |
| 14  | bL    | 203  | CL7  | CHC-C4B-NB  | 4.03  | 128.53      | 124.26   |
| 14  | bL    | 203  | CL7  | C3A-C4A-CHB | -4.03 | 117.72      | 123.70   |
| 14  | aB    | 3009 | CL7  | O1D-CGD-CBD | -4.03 | 116.24      | 124.48   |
| 14  | aA    | 3126 | CL7  | C3B-C4B-NB  | -4.02 | 106.78      | 110.52   |
| 14  | cL    | 205  | CL7  | C3B-C4B-NB  | -4.02 | 106.78      | 110.52   |
| 14  | aA    | 3134 | CL7  | O2D-CGD-CBD | 4.02  | 118.41      | 111.27   |
| 14  | aF    | 201  | CL7  | CHB-C1B-NB  | -4.02 | 120.00      | 124.26   |
| 14  | cB    | 810  | CL7  | C1A-NA-C4A  | -4.02 | 103.87      | 106.30   |
| 14  | bA    | 3113 | CL7  | CMB-C2B-C1B | 4.02  | 131.49      | 125.37   |
| 14  | cA    | 3141 | CL7  | C3A-C4A-CHB | -4.02 | 117.74      | 123.70   |
| 14  | cB    | 823  | CL7  | O2D-CGD-O1D | -4.02 | 115.99      | 123.84   |
| 14  | bB    | 817  | CL7  | CHB-C1B-NB  | -4.01 | 120.01      | 124.26   |
| 14  | cA    | 3117 | CL7  | C3A-C4A-CHB | -4.01 | 117.74      | 123.70   |
| 14  | cA    | 3125 | CL7  | O1D-CGD-CBD | -4.01 | 116.28      | 124.48   |
| 14  | bK    | 101  | CL7  | C1D-ND-C4D  | -4.01 | 103.49      | 106.33   |
| 14  | cA    | 3106 | CL7  | C3A-C4A-CHB | -4.01 | 117.75      | 123.70   |
| 14  | aA    | 3141 | CL7  | CHB-C1B-NB  | -4.01 | 120.02      | 124.26   |
| 14  | bA    | 3112 | CL7  | C3A-C4A-CHB | -4.00 | 117.76      | 123.70   |
| 14  | bA    | 3128 | CL7  | C6-C5-C3    | -4.00 | 102.96      | 113.45   |
| 14  | cB    | 817  | CL7  | CHB-C1B-NB  | -4.00 | 120.02      | 124.26   |
| 14  | cA    | 3113 | CL7  | C3B-C4B-NB  | -4.00 | 106.81      | 110.52   |
| 14  | bA    | 3130 | CL7  | O2D-CGD-CBD | 4.00  | 118.37      | 111.27   |
| 14  | aB    | 3018 | CL7  | C3B-C4B-NB  | -4.00 | 106.81      | 110.52   |
| 14  | bB    | 823  | CL7  | O1D-CGD-CBD | -4.00 | 116.31      | 124.48   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | cA    | 3122 | CL7  | OBD-CAD-C3D | -3.99 | 118.91      | 128.52   |
| 14  | cB    | 822  | CL7  | CAA-C2A-C3A | -3.99 | 106.78      | 116.10   |
| 14  | bA    | 3140 | CL7  | CHB-C1B-NB  | -3.99 | 120.03      | 124.26   |
| 14  | aA    | 3124 | CL7  | C3A-C4A-CHB | -3.99 | 117.78      | 123.70   |
| 14  | bA    | 3120 | CL7  | C1-C2-C3    | -3.99 | 119.14      | 126.04   |
| 14  | aB    | 3019 | CL7  | C1-C2-C3    | -3.99 | 119.14      | 126.04   |
| 14  | cB    | 820  | CL7  | C1-C2-C3    | -3.99 | 119.15      | 126.04   |
| 14  | bA    | 3118 | CL7  | C1D-ND-C4D  | -3.99 | 103.50      | 106.33   |
| 14  | aL    | 202  | CL7  | O2D-CGD-CBD | 3.98  | 118.34      | 111.27   |
| 14  | cB    | 826  | CL7  | C4D-C3D-C2D | -3.98 | 102.12      | 107.30   |
| 14  | bB    | 823  | CL7  | O2D-CGD-O1D | -3.98 | 116.07      | 123.84   |
| 14  | aK    | 101  | CL7  | C1D-ND-C4D  | -3.97 | 103.51      | 106.33   |
| 14  | aA    | 3119 | CL7  | C3A-C4A-CHB | -3.97 | 117.80      | 123.70   |
| 13  | bB    | 801  | PHO  | C2D-C1D-ND  | 3.97  | 112.27      | 109.53   |
| 14  | cA    | 3142 | CL7  | C3A-C4A-CHB | -3.97 | 117.81      | 123.70   |
| 14  | cA    | 3122 | CL7  | C1-C2-C3    | -3.97 | 120.33      | 126.75   |
| 14  | bA    | 3107 | CL7  | C3B-C4B-NB  | -3.97 | 106.83      | 110.52   |
| 14  | cB    | 808  | CL7  | C3A-C4A-CHB | -3.97 | 117.81      | 123.70   |
| 14  | aB    | 3002 | CL7  | CHC-C4B-NB  | 3.96  | 128.45      | 124.26   |
| 14  | bA    | 3113 | CL7  | CHC-C1C-NC  | -3.96 | 120.81      | 124.45   |
| 14  | aB    | 3007 | CL7  | CMB-C2B-C1B | 3.96  | 131.40      | 125.37   |
| 14  | aB    | 3002 | CL7  | O1D-CGD-CBD | -3.96 | 116.38      | 124.48   |
| 14  | bA    | 3114 | CL7  | CMB-C2B-C1B | 3.96  | 131.40      | 125.37   |
| 14  | aA    | 3117 | CL7  | O2D-CGD-CBD | 3.96  | 118.30      | 111.27   |
| 12  | bA    | 3101 | G9R  | C1-C2-C3    | -3.95 | 119.20      | 126.04   |
| 14  | cB    | 808  | CL7  | CMB-C2B-C1B | 3.95  | 131.38      | 125.37   |
| 14  | cB    | 816  | CL7  | C1-C2-C3    | -3.95 | 120.36      | 126.75   |
| 14  | aB    | 3010 | CL7  | C3A-C4A-CHB | -3.95 | 117.84      | 123.70   |
| 14  | bA    | 3128 | CL7  | CMB-C2B-C1B | 3.95  | 131.38      | 125.37   |
| 14  | cA    | 3107 | CL7  | C3B-C4B-NB  | -3.95 | 106.85      | 110.52   |
| 14  | bA    | 3117 | CL7  | C3A-C4A-CHB | -3.95 | 117.84      | 123.70   |
| 14  | bB    | 810  | CL7  | O1D-CGD-CBD | -3.94 | 116.42      | 124.48   |
| 14  | cB    | 809  | CL7  | C3B-C4B-NB  | -3.94 | 106.86      | 110.52   |
| 14  | bB    | 820  | CL7  | O1D-CGD-CBD | -3.94 | 116.42      | 124.48   |
| 14  | bA    | 3106 | CL7  | CAA-C2A-C3A | -3.94 | 101.99      | 112.78   |
| 14  | aA    | 3133 | CL7  | C6-C5-C3    | -3.94 | 103.13      | 113.45   |
| 14  | cA    | 3140 | CL7  | O2A-CGA-O1A | -3.94 | 113.66      | 123.59   |
| 14  | aB    | 3026 | CL7  | O2A-CGA-O1A | -3.93 | 113.66      | 123.59   |
| 12  | cA    | 3101 | G9R  | C2A-C1A-CHA | -3.93 | 116.98      | 123.86   |
| 14  | cB    | 827  | CL7  | CAC-C3C-C2C | -3.93 | 120.81      | 127.53   |
| 14  | bB    | 819  | CL7  | O2A-CGA-O1A | -3.93 | 113.68      | 123.59   |
| 14  | aB    | 3018 | CL7  | O2A-CGA-O1A | -3.93 | 113.68      | 123.59   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | aL    | 203  | CL7  | CMB-C2B-C1B | 3.92  | 131.35      | 125.37   |
| 14  | cA    | 3128 | CL7  | O2D-CGD-CBD | 3.92  | 118.24      | 111.27   |
| 13  | bB    | 805  | PHO  | CMC-C2C-C3C | 3.92  | 136.76      | 126.12   |
| 14  | aA    | 3133 | CL7  | O2D-CGD-CBD | 3.92  | 118.23      | 111.27   |
| 14  | bB    | 832  | CL7  | O2A-CGA-O1A | -3.92 | 113.70      | 123.59   |
| 14  | bB    | 823  | CL7  | CMB-C2B-C1B | 3.92  | 131.34      | 125.37   |
| 14  | aA    | 3126 | CL7  | C1-C2-C3    | -3.92 | 119.27      | 126.04   |
| 14  | bB    | 814  | CL7  | C1D-ND-C4D  | -3.92 | 103.55      | 106.33   |
| 14  | cA    | 3118 | CL7  | C3A-C4A-CHB | -3.92 | 117.89      | 123.70   |
| 14  | aB    | 3025 | CL7  | C6-C7-C8    | -3.92 | 103.26      | 115.92   |
| 14  | cB    | 803  | CL7  | C3A-C4A-CHB | -3.92 | 117.89      | 123.70   |
| 14  | aB    | 3018 | CL7  | C6-C5-C3    | -3.92 | 103.19      | 113.45   |
| 14  | aB    | 3016 | CL7  | CHB-C1B-NB  | -3.92 | 120.11      | 124.26   |
| 14  | cK    | 101  | CL7  | C1D-ND-C4D  | -3.91 | 103.55      | 106.33   |
| 12  | bA    | 3101 | G9R  | C2A-C1A-CHA | -3.91 | 117.02      | 123.86   |
| 14  | cF    | 201  | CL7  | CAA-C2A-C3A | -3.91 | 106.97      | 116.10   |
| 14  | aB    | 3023 | CL7  | O2A-CGA-O1A | -3.91 | 113.72      | 123.59   |
| 14  | aA    | 3107 | CL7  | C3A-C4A-CHB | -3.91 | 117.90      | 123.70   |
| 14  | cA    | 3124 | CL7  | C1D-ND-C4D  | -3.90 | 103.56      | 106.33   |
| 13  | aA    | 3102 | PHO  | CMD-C2D-C3D | 3.90  | 131.97      | 124.68   |
| 14  | bA    | 3116 | CL7  | O2D-CGD-CBD | 3.89  | 118.19      | 111.27   |
| 14  | cA    | 3105 | CL7  | C3A-C4A-CHB | -3.89 | 117.92      | 123.70   |
| 14  | aB    | 3003 | CL7  | CHC-C4B-NB  | 3.89  | 128.38      | 124.26   |
| 13  | bB    | 805  | PHO  | O2D-CGD-CBD | 3.89  | 115.93      | 111.00   |
| 14  | bA    | 3114 | CL7  | C1-O2A-CGA  | -3.89 | 106.23      | 116.44   |
| 14  | aB    | 3019 | CL7  | C3A-C4A-CHB | -3.89 | 117.92      | 123.70   |
| 14  | cA    | 3126 | CL7  | CBD-CHA-C4D | -3.89 | 99.83       | 109.14   |
| 14  | aL    | 204  | CL7  | C3B-C4B-NB  | -3.89 | 106.91      | 110.52   |
| 14  | aA    | 3109 | CL7  | C1A-NA-C4A  | -3.89 | 103.95      | 106.30   |
| 14  | cA    | 3120 | CL7  | C3B-C4B-NB  | -3.89 | 106.91      | 110.52   |
| 14  | bB    | 807  | CL7  | O2D-CGD-CBD | 3.89  | 118.17      | 111.27   |
| 13  | cB    | 801  | PHO  | C2D-C1D-ND  | 3.89  | 112.21      | 109.53   |
| 14  | aB    | 3007 | CL7  | C1D-ND-C4D  | -3.89 | 103.58      | 106.33   |
| 14  | cA    | 3116 | CL7  | C3A-C4A-CHB | -3.88 | 117.94      | 123.70   |
| 14  | bB    | 823  | CL7  | C1D-ND-C4D  | -3.88 | 103.58      | 106.33   |
| 12  | bA    | 3101 | G9R  | OBB-CAB-C3B | -3.88 | 116.91      | 125.69   |
| 14  | bF    | 201  | CL7  | CHB-C1B-NB  | -3.88 | 120.15      | 124.26   |
| 14  | aB    | 3026 | CL7  | CHC-C4B-NB  | 3.87  | 128.36      | 124.26   |
| 14  | aA    | 3130 | CL7  | CHB-C1B-NB  | -3.87 | 120.16      | 124.26   |
| 14  | bA    | 3129 | CL7  | CAA-C2A-C3A | -3.87 | 107.07      | 116.10   |
| 14  | aB    | 3022 | CL7  | CMB-C2B-C1B | 3.87  | 131.26      | 125.37   |
| 14  | cB    | 827  | CL7  | O1D-CGD-CBD | -3.87 | 116.57      | 124.48   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | bB    | 811  | CL7  | O2D-CGD-O1D | -3.87 | 116.27      | 123.84   |
| 14  | cA    | 3106 | CL7  | O2D-CGD-CBD | 3.87  | 118.14      | 111.27   |
| 14  | bB    | 803  | CL7  | O1D-CGD-CBD | -3.87 | 116.57      | 124.48   |
| 14  | aB    | 3005 | CL7  | O2D-CGD-CBD | 3.86  | 118.14      | 111.27   |
| 14  | aB    | 3031 | CL7  | C1A-NA-C4A  | -3.86 | 103.96      | 106.30   |
| 14  | cB    | 827  | CL7  | O2D-CGD-CBD | 3.86  | 118.13      | 111.27   |
| 14  | cB    | 823  | CL7  | CHB-C1B-NB  | -3.86 | 120.17      | 124.26   |
| 14  | aA    | 3124 | CL7  | C3B-C4B-NB  | -3.86 | 106.93      | 110.52   |
| 14  | cB    | 806  | CL7  | C3A-C4A-CHB | -3.86 | 117.97      | 123.70   |
| 14  | aA    | 3130 | CL7  | CMA-C3A-C2A | -3.86 | 107.09      | 116.10   |
| 14  | aB    | 3026 | CL7  | CAC-C3C-C2C | -3.86 | 120.93      | 127.53   |
| 14  | bA    | 3128 | CL7  | CHC-C4B-NB  | 3.85  | 128.34      | 124.26   |
| 14  | cA    | 3120 | CL7  | C1-C2-C3    | -3.85 | 119.38      | 126.04   |
| 14  | bA    | 3121 | CL7  | C3A-C4A-CHB | -3.85 | 117.98      | 123.70   |
| 12  | aA    | 3101 | G9R  | CAA-C2A-C3A | -3.85 | 102.23      | 112.78   |
| 14  | aB    | 3022 | CL7  | C1D-ND-C4D  | -3.85 | 103.60      | 106.33   |
| 14  | cA    | 3120 | CL7  | O2A-CGA-O1A | -3.85 | 113.87      | 123.59   |
| 14  | bA    | 3133 | CL7  | C1D-ND-C4D  | -3.85 | 103.60      | 106.33   |
| 14  | aA    | 3134 | CL7  | C1D-ND-C4D  | -3.85 | 103.60      | 106.33   |
| 14  | cA    | 3139 | CL7  | C3B-C4B-NB  | -3.85 | 106.94      | 110.52   |
| 14  | aA    | 3112 | CL7  | CHB-C1B-NB  | -3.85 | 120.18      | 124.26   |
| 14  | aB    | 3002 | CL7  | O2D-CGD-O1D | -3.85 | 116.31      | 123.84   |
| 14  | aA    | 3140 | CL7  | O2D-CGD-O1D | -3.85 | 116.32      | 123.84   |
| 14  | bF    | 201  | CL7  | C3A-C4A-CHB | -3.85 | 117.99      | 123.70   |
| 14  | cA    | 3123 | CL7  | C3A-C2A-C1A | 3.85  | 107.10      | 101.34   |
| 14  | aB    | 3015 | CL7  | O2D-CGD-O1D | -3.84 | 116.32      | 123.84   |
| 14  | cB    | 824  | CL7  | O2A-CGA-O1A | -3.84 | 113.89      | 123.59   |
| 14  | cA    | 3108 | CL7  | CHB-C1B-NB  | -3.84 | 120.19      | 124.26   |
| 14  | cA    | 3104 | CL7  | CHB-C1B-NB  | -3.84 | 120.19      | 124.26   |
| 14  | aB    | 3007 | CL7  | C3B-C4B-NB  | -3.84 | 106.95      | 110.52   |
| 14  | aA    | 3122 | CL7  | C3A-C4A-CHB | -3.84 | 118.00      | 123.70   |
| 14  | aA    | 3130 | CL7  | C4D-C3D-C2D | -3.84 | 102.30      | 107.30   |
| 14  | cB    | 819  | CL7  | O1D-CGD-CBD | -3.84 | 116.64      | 124.48   |
| 13  | cB    | 801  | PHO  | CMD-C2D-C3D | 3.84  | 131.85      | 124.68   |
| 14  | bA    | 3128 | CL7  | C4D-C3D-C2D | -3.83 | 102.30      | 107.30   |
| 14  | cB    | 814  | CL7  | C1D-ND-C4D  | -3.83 | 103.61      | 106.33   |
| 14  | aA    | 3111 | CL7  | CAA-C2A-C3A | -3.83 | 107.17      | 116.10   |
| 14  | cA    | 3107 | CL7  | O1D-CGD-CBD | -3.83 | 116.66      | 124.48   |
| 14  | bA    | 3113 | CL7  | C3B-C4B-NB  | -3.83 | 106.97      | 110.52   |
| 14  | cB    | 806  | CL7  | C3B-C4B-NB  | -3.82 | 106.97      | 110.52   |
| 14  | cA    | 3121 | CL7  | C1D-ND-C4D  | -3.82 | 103.62      | 106.33   |
| 14  | bB    | 808  | CL7  | C3A-C4A-CHB | -3.82 | 118.03      | 123.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | aA    | 3143 | CL7  | C3A-C4A-CHB | -3.82 | 118.03      | 123.70   |
| 14  | bA    | 3114 | CL7  | O2D-CGD-O1D | -3.82 | 116.37      | 123.84   |
| 14  | aB    | 3007 | CL7  | O2A-CGA-O1A | -3.82 | 113.96      | 123.59   |
| 14  | cA    | 3128 | CL7  | C6-C7-C8    | -3.81 | 103.59      | 115.92   |
| 14  | bA    | 3103 | CL7  | O2D-CGD-CBD | 3.81  | 118.04      | 111.27   |
| 14  | bB    | 823  | CL7  | CHB-C1B-NB  | -3.81 | 120.22      | 124.26   |
| 14  | aB    | 3009 | CL7  | C1A-NA-C4A  | -3.81 | 104.00      | 106.30   |
| 14  | cA    | 3139 | CL7  | C1D-ND-C4D  | -3.81 | 103.63      | 106.33   |
| 14  | aB    | 3022 | CL7  | CHB-C1B-NB  | -3.81 | 120.23      | 124.26   |
| 14  | bA    | 3141 | CL7  | O2D-CGD-O1D | -3.81 | 116.39      | 123.84   |
| 14  | cA    | 3112 | CL7  | O2D-CGD-CBD | 3.81  | 118.03      | 111.27   |
| 14  | cA    | 3133 | CL7  | C1D-ND-C4D  | -3.80 | 103.63      | 106.33   |
| 14  | aA    | 3117 | CL7  | C3A-C4A-CHB | -3.80 | 118.06      | 123.70   |
| 14  | aB    | 3021 | CL7  | C3B-C4B-NB  | -3.80 | 106.99      | 110.52   |
| 14  | cB    | 817  | CL7  | C1D-ND-C4D  | -3.80 | 103.64      | 106.33   |
| 14  | bA    | 3108 | CL7  | C2A-C1A-CHA | -3.80 | 118.77      | 126.36   |
| 14  | cA    | 3107 | CL7  | O2D-CGD-CBD | 3.80  | 118.01      | 111.27   |
| 14  | aA    | 3114 | CL7  | C3B-C4B-NB  | -3.79 | 107.00      | 110.52   |
| 14  | bB    | 804  | CL7  | CBD-CHA-C4D | -3.79 | 100.07      | 109.14   |
| 14  | bB    | 824  | CL7  | O2A-CGA-O1A | -3.79 | 114.02      | 123.59   |
| 14  | bA    | 3107 | CL7  | O1D-CGD-CBD | -3.79 | 116.73      | 124.48   |
| 14  | cB    | 823  | CL7  | CMB-C2B-C1B | 3.79  | 131.14      | 125.37   |
| 14  | cB    | 817  | CL7  | C3A-C4A-CHB | -3.79 | 118.08      | 123.70   |
| 14  | aA    | 3114 | CL7  | CHC-C1C-NC  | -3.79 | 120.97      | 124.45   |
| 14  | aB    | 3019 | CL7  | O1D-CGD-CBD | -3.79 | 116.74      | 124.48   |
| 14  | cA    | 3106 | CL7  | CAA-C2A-C3A | -3.79 | 102.41      | 112.78   |
| 14  | bB    | 808  | CL7  | C1D-ND-C4D  | -3.79 | 103.65      | 106.33   |
| 14  | cA    | 3124 | CL7  | C1-O2A-CGA  | -3.78 | 106.52      | 116.44   |
| 14  | aA    | 3108 | CL7  | O1D-CGD-CBD | -3.78 | 116.75      | 124.48   |
| 14  | bA    | 3129 | CL7  | CMC-C2C-C1C | -3.77 | 118.06      | 124.71   |
| 14  | aB    | 3031 | CL7  | O2A-CGA-O1A | -3.77 | 114.07      | 123.59   |
| 14  | cA    | 3128 | CL7  | C3B-C4B-NB  | -3.77 | 107.02      | 110.52   |
| 14  | bA    | 3142 | CL7  | C3A-C4A-CHB | -3.77 | 118.10      | 123.70   |
| 13  | bB    | 801  | PHO  | CMD-C2D-C3D | 3.77  | 131.73      | 124.68   |
| 14  | cA    | 3123 | CL7  | O2A-C1-C2   | 3.77  | 118.53      | 108.64   |
| 14  | bA    | 3124 | CL7  | O2A-CGA-O1A | -3.76 | 114.09      | 123.59   |
| 14  | bB    | 827  | CL7  | CAC-C3C-C2C | -3.76 | 121.09      | 127.53   |
| 14  | bA    | 3120 | CL7  | O2A-CGA-O1A | -3.76 | 114.11      | 123.59   |
| 14  | aB    | 3002 | CL7  | C3A-C4A-CHB | -3.76 | 118.12      | 123.70   |
| 14  | aA    | 3130 | CL7  | O2D-CGD-CBD | 3.76  | 117.94      | 111.27   |
| 14  | aA    | 3107 | CL7  | C1-C2-C3    | -3.76 | 119.55      | 126.04   |
| 14  | cA    | 3114 | CL7  | C4D-C3D-C2D | -3.76 | 102.41      | 107.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | aB    | 3013 | CL7  | C1D-ND-C4D  | -3.75 | 103.67      | 106.33   |
| 14  | cA    | 3141 | CL7  | O2A-CGA-O1A | -3.75 | 114.13      | 123.59   |
| 14  | aA    | 3113 | CL7  | C1D-ND-C4D  | -3.75 | 103.67      | 106.33   |
| 14  | bB    | 819  | CL7  | C3B-C4B-NB  | -3.75 | 107.04      | 110.52   |
| 13  | cB    | 801  | PHO  | CMB-C2B-C3B | 3.75  | 131.69      | 124.68   |
| 14  | bA    | 3121 | CL7  | C1D-ND-C4D  | -3.74 | 103.67      | 106.33   |
| 14  | bB    | 832  | CL7  | C1-C2-C3    | -3.74 | 119.57      | 126.04   |
| 13  | aB    | 3004 | PHO  | O2D-CGD-O1D | -3.74 | 116.52      | 123.84   |
| 14  | aA    | 3134 | CL7  | CAA-C2A-C3A | -3.74 | 107.36      | 116.10   |
| 14  | bB    | 806  | CL7  | C3B-C4B-NB  | -3.74 | 107.05      | 110.52   |
| 14  | cB    | 823  | CL7  | C1D-ND-C4D  | -3.74 | 103.68      | 106.33   |
| 14  | cA    | 3107 | CL7  | C1-C2-C3    | -3.74 | 119.58      | 126.04   |
| 14  | cB    | 807  | CL7  | O1D-CGD-CBD | -3.74 | 116.84      | 124.48   |
| 13  | bB    | 805  | PHO  | C4A-C3A-C2A | -3.74 | 99.28       | 102.84   |
| 14  | cB    | 807  | CL7  | O2D-CGD-CBD | 3.74  | 117.91      | 111.27   |
| 14  | aB    | 3026 | CL7  | O2D-CGD-CBD | 3.73  | 117.90      | 111.27   |
| 14  | aA    | 3130 | CL7  | CMB-C2B-C1B | 3.73  | 131.05      | 125.37   |
| 14  | cB    | 804  | CL7  | CBD-CHA-C4D | -3.73 | 100.22      | 109.14   |
| 14  | bB    | 823  | CL7  | CAA-C2A-C3A | -3.73 | 107.40      | 116.10   |
| 14  | bB    | 816  | CL7  | C1-O2A-CGA  | -3.73 | 106.67      | 116.44   |
| 14  | bB    | 818  | CL7  | CAA-C2A-C3A | -3.72 | 107.41      | 116.10   |
| 14  | aA    | 3110 | CL7  | C1D-ND-C4D  | -3.72 | 103.69      | 106.33   |
| 14  | bA    | 3114 | CL7  | C4D-C3D-C2D | -3.72 | 102.45      | 107.30   |
| 14  | cB    | 817  | CL7  | C4D-C3D-C2D | -3.72 | 102.45      | 107.30   |
| 14  | bA    | 3129 | CL7  | CMA-C3A-C2A | -3.72 | 107.42      | 116.10   |
| 14  | cA    | 3141 | CL7  | CBD-CHA-C4D | -3.72 | 100.25      | 109.14   |
| 14  | aB    | 3031 | CL7  | C1D-ND-C4D  | -3.72 | 103.69      | 106.33   |
| 14  | aB    | 3016 | CL7  | C4D-C3D-C2D | -3.71 | 102.46      | 107.30   |
| 14  | bA    | 3104 | CL7  | CAA-C2A-C3A | -3.71 | 107.43      | 116.10   |
| 14  | cA    | 3142 | CL7  | CMB-C2B-C1B | 3.71  | 131.03      | 125.37   |
| 14  | bA    | 3109 | CL7  | O2D-CGD-CBD | 3.71  | 117.87      | 111.27   |
| 14  | aB    | 3003 | CL7  | C1D-ND-C4D  | -3.71 | 103.70      | 106.33   |
| 14  | bA    | 3127 | CL7  | O2D-CGD-O1D | -3.71 | 116.58      | 123.84   |
| 14  | bB    | 810  | CL7  | C1-C2-C3    | -3.70 | 119.64      | 126.04   |
| 14  | aB    | 3009 | CL7  | C1-C2-C3    | -3.70 | 119.64      | 126.04   |
| 14  | bB    | 807  | CL7  | C1-C2-C3    | -3.70 | 119.64      | 126.04   |
| 14  | bA    | 3140 | CL7  | O2D-CGD-O1D | -3.70 | 116.60      | 123.84   |
| 13  | aB    | 3004 | PHO  | CBA-CAA-C2A | -3.70 | 103.00      | 113.81   |
| 14  | bB    | 826  | CL7  | C4D-C3D-C2D | -3.70 | 102.48      | 107.30   |
| 14  | cA    | 3142 | CL7  | O2D-CGD-O1D | -3.70 | 116.60      | 123.84   |
| 13  | cB    | 805  | PHO  | CMC-C2C-C3C | 3.70  | 136.16      | 126.12   |
| 14  | cB    | 816  | CL7  | C3A-C4A-CHB | -3.70 | 118.21      | 123.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | aA    | 3125 | CL7  | O2D-CGD-CBD | 3.70  | 117.84      | 111.27   |
| 14  | aA    | 3123 | CL7  | O2A-CGA-O1A | -3.70 | 114.26      | 123.59   |
| 14  | cA    | 3112 | CL7  | C1D-ND-C4D  | -3.70 | 103.71      | 106.33   |
| 14  | cB    | 807  | CL7  | O2D-CGD-O1D | -3.70 | 116.61      | 123.84   |
| 14  | aB    | 3005 | CL7  | C3B-C4B-NB  | -3.70 | 107.09      | 110.52   |
| 14  | aB    | 3032 | CL7  | C3B-C4B-NB  | -3.70 | 107.09      | 110.52   |
| 14  | bL    | 204  | CL7  | C3B-C4B-NB  | -3.70 | 107.09      | 110.52   |
| 14  | bL    | 204  | CL7  | C1-C2-C3    | -3.69 | 119.66      | 126.04   |
| 14  | cA    | 3116 | CL7  | O2D-CGD-CBD | 3.69  | 117.83      | 111.27   |
| 14  | cB    | 804  | CL7  | CHC-C4B-NB  | 3.69  | 128.16      | 124.26   |
| 14  | bA    | 3127 | CL7  | C3A-C2A-C1A | 3.69  | 106.87      | 101.34   |
| 14  | bJ    | 101  | CL7  | C3A-C4A-CHB | -3.69 | 118.22      | 123.70   |
| 14  | aA    | 3110 | CL7  | CMB-C2B-C1B | 3.69  | 130.99      | 125.37   |
| 14  | bB    | 823  | CL7  | C3A-C4A-CHB | -3.69 | 118.23      | 123.70   |
| 14  | cB    | 817  | CL7  | CAA-C2A-C3A | -3.69 | 107.49      | 116.10   |
| 13  | bB    | 805  | PHO  | C1-C2-C3    | -3.68 | 119.67      | 126.04   |
| 14  | aB    | 3022 | CL7  | O2D-CGD-O1D | -3.68 | 116.63      | 123.84   |
| 14  | bA    | 3109 | CL7  | C1D-ND-C4D  | -3.68 | 103.72      | 106.33   |
| 14  | cA    | 3132 | CL7  | C4D-C3D-C2D | -3.68 | 102.50      | 107.30   |
| 14  | bB    | 817  | CL7  | C1D-ND-C4D  | -3.68 | 103.72      | 106.33   |
| 14  | cA    | 3104 | CL7  | O1D-CGD-CBD | -3.68 | 116.96      | 124.48   |
| 14  | bA    | 3112 | CL7  | C1D-ND-C4D  | -3.68 | 103.72      | 106.33   |
| 14  | bB    | 806  | CL7  | O2D-CGD-CBD | 3.68  | 117.80      | 111.27   |
| 14  | bB    | 820  | CL7  | C1-C2-C3    | -3.68 | 119.69      | 126.04   |
| 14  | cA    | 3126 | CL7  | O2A-CGA-O1A | -3.68 | 114.32      | 123.59   |
| 14  | cA    | 3116 | CL7  | C3C-C4C-NC  | 3.67  | 112.84      | 110.18   |
| 14  | cL    | 203  | CL7  | C3B-C4B-NB  | -3.67 | 107.11      | 110.52   |
| 19  | aB    | 3029 | LMG  | C1-O6-C5    | -3.67 | 106.49      | 113.69   |
| 14  | aA    | 3120 | CL7  | C4D-C3D-C2D | -3.67 | 102.52      | 107.30   |
| 14  | cA    | 3109 | CL7  | C1D-ND-C4D  | -3.67 | 103.73      | 106.33   |
| 14  | cL    | 204  | CL7  | CHC-C4B-NB  | 3.67  | 128.14      | 124.26   |
| 14  | aB    | 3022 | CL7  | CAA-C2A-C3A | -3.67 | 107.54      | 116.10   |
| 14  | cA    | 3103 | CL7  | O2D-CGD-CBD | 3.67  | 117.78      | 111.27   |
| 14  | bA    | 3104 | CL7  | CHB-C1B-NB  | -3.66 | 120.38      | 124.26   |
| 14  | aB    | 3008 | CL7  | C3B-C4B-NB  | -3.66 | 107.12      | 110.52   |
| 14  | bA    | 3122 | CL7  | OBD-CAD-C3D | -3.66 | 119.72      | 128.52   |
| 14  | bB    | 832  | CL7  | C1D-ND-C4D  | -3.66 | 103.74      | 106.33   |
| 14  | cA    | 3111 | CL7  | CHB-C1B-NB  | -3.66 | 120.38      | 124.26   |
| 14  | aA    | 3113 | CL7  | CHB-C1B-NB  | -3.66 | 120.39      | 124.26   |
| 14  | bB    | 806  | CL7  | C1D-ND-C4D  | -3.66 | 103.74      | 106.33   |
| 14  | cA    | 3118 | CL7  | C4D-C3D-C2D | -3.66 | 102.54      | 107.30   |
| 14  | cA    | 3131 | CL7  | C1D-ND-C4D  | -3.65 | 103.74      | 106.33   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | bL    | 204  | CL7  | CHC-C4B-NB  | 3.65  | 128.12      | 124.26   |
| 14  | bA    | 3140 | CL7  | O2A-CGA-O1A | -3.65 | 114.38      | 123.59   |
| 14  | aA    | 3146 | CL7  | C1D-ND-C4D  | -3.65 | 103.74      | 106.33   |
| 14  | aA    | 3106 | CL7  | C4D-C3D-C2D | -3.65 | 102.54      | 107.30   |
| 12  | cA    | 3101 | G9R  | O2D-CGD-O1D | -3.65 | 116.70      | 123.84   |
| 14  | bB    | 817  | CL7  | CAA-C2A-C3A | -3.65 | 107.59      | 116.10   |
| 14  | aA    | 3104 | CL7  | CAA-C2A-C3A | -3.64 | 107.59      | 116.10   |
| 13  | aB    | 3004 | PHO  | C4A-C3A-C2A | -3.64 | 99.37       | 102.84   |
| 14  | aA    | 3132 | CL7  | C1D-ND-C4D  | -3.64 | 103.75      | 106.33   |
| 14  | aA    | 3129 | CL7  | C4D-C3D-C2D | -3.64 | 102.56      | 107.30   |
| 14  | bB    | 819  | CL7  | C4D-C3D-CAD | -3.64 | 104.97      | 107.42   |
| 14  | bA    | 3141 | CL7  | O2A-CGA-O1A | -3.64 | 114.41      | 123.59   |
| 14  | aA    | 3123 | CL7  | C1-C2-C3    | -3.63 | 120.87      | 126.75   |
| 14  | aA    | 3125 | CL7  | C1D-ND-C4D  | -3.63 | 103.75      | 106.33   |
| 12  | bA    | 3101 | G9R  | O2A-C1-C2   | -3.63 | 99.08       | 108.64   |
| 14  | bA    | 3126 | CL7  | C3A-C4A-CHB | -3.63 | 118.63      | 124.02   |
| 14  | cB    | 822  | CL7  | O1D-CGD-CBD | -3.63 | 117.05      | 124.48   |
| 14  | aA    | 3115 | CL7  | C4D-C3D-C2D | -3.63 | 102.57      | 107.30   |
| 14  | aA    | 3104 | CL7  | O2D-CGD-CBD | 3.63  | 117.72      | 111.27   |
| 14  | aB    | 3020 | CL7  | C1D-ND-C4D  | -3.63 | 103.76      | 106.33   |
| 14  | aB    | 3016 | CL7  | CAA-C2A-C3A | -3.63 | 107.63      | 116.10   |
| 12  | aA    | 3101 | G9R  | C2A-C1A-CHA | -3.63 | 117.52      | 123.86   |
| 14  | bB    | 809  | CL7  | C1A-NA-C4A  | -3.63 | 104.11      | 106.30   |
| 14  | bB    | 804  | CL7  | C6-C5-C3    | -3.62 | 103.95      | 113.45   |
| 14  | bA    | 3128 | CL7  | C3B-C4B-NB  | -3.62 | 107.15      | 110.52   |
| 14  | aA    | 3119 | CL7  | C4D-C3D-C2D | -3.62 | 102.58      | 107.30   |
| 14  | bA    | 3122 | CL7  | C3B-C4B-NB  | -3.62 | 107.16      | 110.52   |
| 14  | cA    | 3129 | CL7  | CMA-C3A-C2A | -3.62 | 107.65      | 116.10   |
| 14  | aB    | 3017 | CL7  | C1D-ND-C4D  | -3.62 | 103.76      | 106.33   |
| 14  | cL    | 203  | CL7  | C3A-C4A-CHB | -3.62 | 118.33      | 123.70   |
| 14  | bA    | 3131 | CL7  | C1D-ND-C4D  | -3.62 | 103.77      | 106.33   |
| 14  | bB    | 821  | CL7  | C1D-ND-C4D  | -3.61 | 103.77      | 106.33   |
| 14  | aA    | 3107 | CL7  | C6-C7-C8    | -3.61 | 104.24      | 115.92   |
| 12  | bA    | 3101 | G9R  | C3D-C4D-ND  | 3.61  | 116.08      | 110.24   |
| 14  | bA    | 3114 | CL7  | O1D-CGD-CBD | -3.61 | 117.09      | 124.48   |
| 14  | cB    | 821  | CL7  | C1D-ND-C4D  | -3.61 | 103.77      | 106.33   |
| 14  | bB    | 808  | CL7  | C3B-C4B-NB  | -3.61 | 107.17      | 110.52   |
| 14  | aA    | 3111 | CL7  | C1D-ND-C4D  | -3.61 | 103.77      | 106.33   |
| 14  | bA    | 3106 | CL7  | O2D-CGD-CBD | 3.61  | 117.68      | 111.27   |
| 14  | bA    | 3116 | CL7  | C3A-C4A-CHB | -3.61 | 118.34      | 123.70   |
| 14  | bB    | 816  | CL7  | O2A-CGA-O1A | -3.61 | 114.49      | 123.59   |
| 14  | aB    | 3031 | CL7  | C3A-C4A-CHB | -3.61 | 118.35      | 123.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | aA    | 3106 | CL7  | C3B-C4B-NB  | -3.60 | 107.17      | 110.52   |
| 14  | bA    | 3123 | CL7  | O1D-CGD-CBD | -3.60 | 117.12      | 124.48   |
| 14  | cA    | 3110 | CL7  | C1D-ND-C4D  | -3.60 | 103.78      | 106.33   |
| 14  | bL    | 205  | CL7  | O2D-CGD-O1D | -3.60 | 116.81      | 123.84   |
| 14  | cL    | 205  | CL7  | O2D-CGD-O1D | -3.60 | 116.81      | 123.84   |
| 14  | cB    | 823  | CL7  | CAA-C2A-C3A | -3.60 | 107.71      | 116.10   |
| 14  | aA    | 3122 | CL7  | C1D-ND-C4D  | -3.60 | 103.78      | 106.33   |
| 14  | aA    | 3130 | CL7  | C1D-ND-C4D  | -3.60 | 103.78      | 106.33   |
| 14  | cA    | 3129 | CL7  | C1D-ND-C4D  | -3.59 | 103.78      | 106.33   |
| 14  | aA    | 3109 | CL7  | C1D-ND-C4D  | -3.59 | 103.78      | 106.33   |
| 14  | bA    | 3129 | CL7  | C1D-ND-C4D  | -3.59 | 103.78      | 106.33   |
| 14  | aB    | 3017 | CL7  | CHB-C1B-NB  | -3.59 | 120.45      | 124.26   |
| 14  | bA    | 3140 | CL7  | C1-C2-C3    | -3.59 | 119.83      | 126.04   |
| 14  | bB    | 809  | CL7  | C1-C2-C3    | -3.59 | 120.94      | 126.75   |
| 14  | aB    | 3018 | CL7  | C1-C2-C3    | -3.59 | 119.84      | 126.04   |
| 14  | cA    | 3114 | CL7  | O2D-CGD-O1D | -3.58 | 116.83      | 123.84   |
| 14  | cA    | 3112 | CL7  | CHB-C1B-NB  | -3.58 | 120.47      | 124.26   |
| 14  | aA    | 3105 | CL7  | CAA-C2A-C3A | -3.58 | 107.74      | 116.10   |
| 14  | aA    | 3143 | CL7  | CMB-C2B-C1B | 3.58  | 130.82      | 125.37   |
| 14  | cB    | 833  | CL7  | O2D-CGD-O1D | -3.58 | 116.84      | 123.84   |
| 14  | aB    | 3031 | CL7  | C1-C2-C3    | -3.58 | 119.85      | 126.04   |
| 14  | aB    | 3016 | CL7  | C1D-ND-C4D  | -3.58 | 103.79      | 106.33   |
| 14  | aA    | 3146 | CL7  | O2D-CGD-O1D | -3.58 | 116.85      | 123.84   |
| 17  | aB    | 3027 | PQN  | C24-C23-C22 | -3.57 | 98.35       | 111.29   |
| 14  | bB    | 825  | CL7  | CAA-C2A-C3A | -3.57 | 107.76      | 116.10   |
| 14  | bA    | 3103 | CL7  | CAA-C2A-C3A | -3.57 | 107.76      | 116.10   |
| 14  | bB    | 827  | CL7  | C3B-C4B-NB  | -3.57 | 107.20      | 110.52   |
| 14  | aB    | 3003 | CL7  | CBD-CHA-C4D | -3.57 | 100.60      | 109.14   |
| 14  | cA    | 3129 | CL7  | C3A-C4A-CHB | -3.57 | 118.40      | 123.70   |
| 14  | cA    | 3144 | CL7  | C1D-ND-C4D  | -3.57 | 103.80      | 106.33   |
| 14  | bA    | 3128 | CL7  | O2D-CGD-CBD | 3.57  | 117.61      | 111.27   |
| 12  | cA    | 3101 | G9R  | C4C-C3C-C2C | -3.57 | 101.70      | 106.90   |
| 14  | aB    | 3014 | CL7  | CAA-C2A-C3A | -3.57 | 107.78      | 116.10   |
| 14  | bB    | 803  | CL7  | C6-C5-C3    | -3.57 | 104.10      | 113.45   |
| 14  | bA    | 3112 | CL7  | CHB-C1B-NB  | -3.57 | 120.48      | 124.26   |
| 14  | aB    | 3032 | CL7  | O2D-CGD-O1D | -3.56 | 116.87      | 123.84   |
| 13  | aB    | 3004 | PHO  | CBC-CAC-C3C | -3.56 | 107.66      | 112.88   |
| 14  | bB    | 817  | CL7  | C4D-C3D-C2D | -3.56 | 102.66      | 107.30   |
| 14  | bB    | 806  | CL7  | C3A-C4A-CHB | -3.56 | 118.41      | 123.70   |
| 14  | bA    | 3114 | CL7  | C1A-NA-C4A  | -3.56 | 104.15      | 106.30   |
| 14  | bA    | 3145 | CL7  | C1D-ND-C4D  | -3.56 | 103.81      | 106.33   |
| 14  | cB    | 803  | CL7  | O2A-CGA-O1A | -3.56 | 114.61      | 123.59   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | cB    | 819  | CL7  | C6-C5-C3    | -3.56 | 104.12      | 113.45   |
| 14  | aB    | 3006 | CL7  | O1D-CGD-CBD | -3.56 | 117.20      | 124.48   |
| 13  | bB    | 805  | PHO  | C4-C3-C5    | 3.56  | 121.25      | 115.27   |
| 14  | aA    | 3105 | CL7  | C1D-ND-C4D  | -3.56 | 103.81      | 106.33   |
| 14  | bA    | 3120 | CL7  | C1D-ND-C4D  | -3.55 | 103.81      | 106.33   |
| 14  | cB    | 816  | CL7  | C3B-C4B-NB  | -3.55 | 107.22      | 110.52   |
| 14  | cA    | 3114 | CL7  | CMB-C2B-C1B | 3.55  | 130.78      | 125.37   |
| 14  | bA    | 3116 | CL7  | C1-C2-C3    | -3.55 | 119.90      | 126.04   |
| 14  | bB    | 812  | CL7  | CHB-C1B-NB  | -3.55 | 120.50      | 124.26   |
| 14  | aA    | 3123 | CL7  | C3B-C4B-NB  | -3.55 | 107.22      | 110.52   |
| 14  | cA    | 3144 | CL7  | CAA-C2A-C3A | -3.55 | 107.81      | 116.10   |
| 14  | cA    | 3128 | CL7  | O2A-CGA-O1A | -3.55 | 114.64      | 123.59   |
| 14  | cB    | 811  | CL7  | C3A-C4A-CHB | -3.55 | 118.44      | 123.70   |
| 14  | aB    | 3009 | CL7  | C1D-ND-C4D  | -3.55 | 103.81      | 106.33   |
| 14  | bA    | 3128 | CL7  | C6-C7-C8    | -3.54 | 104.47      | 115.92   |
| 14  | aA    | 3121 | CL7  | O2A-CGA-O1A | -3.54 | 114.65      | 123.59   |
| 14  | aB    | 3017 | CL7  | CAA-C2A-C3A | -3.54 | 107.84      | 116.10   |
| 14  | aB    | 3002 | CL7  | CMB-C2B-C1B | 3.54  | 130.76      | 125.37   |
| 14  | bK    | 101  | CL7  | CAD-CBD-CHA | -3.54 | 101.15      | 105.14   |
| 14  | bA    | 3140 | CL7  | C1D-ND-C4D  | -3.54 | 103.82      | 106.33   |
| 14  | cB    | 831  | CL7  | C3B-C4B-NB  | -3.53 | 107.24      | 110.52   |
| 12  | aA    | 3101 | G9R  | O2D-CGD-O1D | -3.53 | 116.94      | 123.84   |
| 13  | cB    | 805  | PHO  | C4-C3-C5    | 3.53  | 121.21      | 115.27   |
| 14  | cA    | 3127 | CL7  | O2D-CGD-O1D | -3.53 | 116.94      | 123.84   |
| 14  | cB    | 825  | CL7  | C4D-C3D-C2D | -3.53 | 102.70      | 107.30   |
| 14  | cB    | 807  | CL7  | C3A-C4A-CHB | -3.53 | 118.47      | 123.70   |
| 14  | bA    | 3104 | CL7  | O1D-CGD-CBD | -3.53 | 117.27      | 124.48   |
| 14  | bA    | 3127 | CL7  | CBA-CAA-C2A | -3.53 | 103.45      | 113.86   |
| 14  | aA    | 3130 | CL7  | CAA-C2A-C3A | -3.53 | 107.87      | 116.10   |
| 14  | aB    | 3006 | CL7  | CAC-C3C-C2C | -3.52 | 121.50      | 127.53   |
| 14  | aA    | 3128 | CL7  | C3A-C2A-C1A | 3.52  | 106.62      | 101.34   |
| 14  | cB    | 818  | CL7  | C1D-ND-C4D  | -3.52 | 103.83      | 106.33   |
| 14  | bA    | 3131 | CL7  | CAA-C2A-C3A | -3.52 | 107.88      | 116.10   |
| 14  | bA    | 3116 | CL7  | C3C-C4C-NC  | 3.52  | 112.73      | 110.18   |
| 14  | cB    | 818  | CL7  | CAA-C2A-C3A | -3.52 | 107.88      | 116.10   |
| 14  | bL    | 204  | CL7  | CMB-C2B-C1B | 3.52  | 130.73      | 125.37   |
| 14  | aL    | 202  | CL7  | C3A-C4A-CHB | -3.52 | 118.47      | 123.70   |
| 14  | bB    | 825  | CL7  | C1D-ND-C4D  | -3.52 | 103.83      | 106.33   |
| 14  | aB    | 3011 | CL7  | CHB-C1B-NB  | -3.52 | 120.53      | 124.26   |
| 12  | cA    | 3101 | G9R  | O2D-CGD-CBD | 3.52  | 117.52      | 111.27   |
| 14  | cB    | 816  | CL7  | O2A-CGA-O1A | -3.52 | 114.71      | 123.59   |
| 13  | bB    | 801  | PHO  | CMB-C2B-C3B | 3.52  | 131.26      | 124.68   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | aA    | 3118 | CL7  | C1D-ND-C4D  | -3.51 | 103.84      | 106.33   |
| 14  | aA    | 3126 | CL7  | CHA-C1A-NA  | -3.51 | 117.66      | 125.98   |
| 14  | aA    | 3124 | CL7  | O2A-CGA-O1A | -3.51 | 114.72      | 123.59   |
| 14  | cA    | 3115 | CL7  | CHB-C1B-NB  | -3.51 | 120.54      | 124.26   |
| 14  | aA    | 3110 | CL7  | O2D-CGD-CBD | 3.51  | 117.51      | 111.27   |
| 14  | cB    | 807  | CL7  | C1-C2-C3    | -3.51 | 119.97      | 126.04   |
| 14  | bB    | 816  | CL7  | C3A-C4A-CHB | -3.51 | 118.49      | 123.70   |
| 14  | bA    | 3125 | CL7  | CHA-C1A-NA  | -3.51 | 117.67      | 125.98   |
| 14  | cA    | 3104 | CL7  | C1D-ND-C4D  | -3.51 | 103.84      | 106.33   |
| 14  | aA    | 3106 | CL7  | CMA-C3A-C2A | -3.51 | 107.92      | 116.10   |
| 14  | aA    | 3116 | CL7  | CHB-C1B-NB  | -3.50 | 120.55      | 124.26   |
| 14  | cB    | 827  | CL7  | C2C-C1C-NC  | 3.50  | 112.68      | 110.10   |
| 14  | cA    | 3125 | CL7  | CHA-C1A-NA  | -3.50 | 117.69      | 125.98   |
| 14  | aA    | 3116 | CL7  | C4D-C3D-C2D | -3.50 | 102.74      | 107.30   |
| 14  | bA    | 3111 | CL7  | CHB-C1B-NB  | -3.50 | 120.56      | 124.26   |
| 14  | aA    | 3114 | CL7  | C1D-ND-C4D  | -3.50 | 103.85      | 106.33   |
| 14  | aA    | 3143 | CL7  | C1D-ND-C4D  | -3.49 | 103.85      | 106.33   |
| 14  | aB    | 3030 | CL7  | C1D-ND-C4D  | -3.49 | 103.85      | 106.33   |
| 14  | cB    | 812  | CL7  | CHB-C1B-NB  | -3.49 | 120.56      | 124.26   |
| 14  | bA    | 3109 | CL7  | CMB-C2B-C1B | 3.49  | 130.69      | 125.37   |
| 14  | cA    | 3128 | CL7  | CHC-C4B-NB  | 3.49  | 127.95      | 124.26   |
| 14  | bB    | 804  | CL7  | O2A-CGA-O1A | -3.49 | 114.78      | 123.59   |
| 14  | bB    | 811  | CL7  | CAA-C2A-C3A | -3.49 | 107.95      | 116.10   |
| 14  | cA    | 3103 | CL7  | CAA-C2A-C3A | -3.49 | 107.96      | 116.10   |
| 14  | aL    | 202  | CL7  | CHC-C4B-NB  | 3.49  | 127.95      | 124.26   |
| 14  | cB    | 804  | CL7  | C1D-ND-C4D  | -3.49 | 103.86      | 106.33   |
| 14  | cA    | 3103 | CL7  | CMB-C2B-C1B | 3.49  | 130.68      | 125.37   |
| 14  | aA    | 3141 | CL7  | C1D-ND-C4D  | -3.49 | 103.86      | 106.33   |
| 14  | bA    | 3117 | CL7  | C1D-ND-C4D  | -3.49 | 103.86      | 106.33   |
| 14  | bA    | 3115 | CL7  | CHB-C1B-NB  | -3.48 | 120.57      | 124.26   |
| 14  | bB    | 832  | CL7  | C3A-C4A-CHB | -3.48 | 118.53      | 123.70   |
| 14  | cB    | 826  | CL7  | C2D-C1D-ND  | -3.48 | 107.90      | 110.23   |
| 14  | cA    | 3102 | CL7  | O2A-CGA-O1A | -3.48 | 114.81      | 123.59   |
| 14  | aB    | 3008 | CL7  | CMB-C2B-C1B | 3.48  | 130.67      | 125.37   |
| 14  | bA    | 3145 | CL7  | CAA-C2A-C3A | -3.48 | 107.98      | 116.10   |
| 14  | aA    | 3140 | CL7  | C1D-ND-C4D  | -3.48 | 103.87      | 106.33   |
| 14  | bA    | 3114 | CL7  | C6-C7-C8    | -3.48 | 104.69      | 115.92   |
| 14  | cA    | 3122 | CL7  | C3B-C4B-NB  | -3.47 | 107.29      | 110.52   |
| 14  | cA    | 3123 | CL7  | C3B-C4B-NB  | -3.47 | 107.30      | 110.52   |
| 14  | cB    | 819  | CL7  | C1-C2-C3    | -3.47 | 120.04      | 126.04   |
| 14  | cA    | 3104 | CL7  | CAA-C2A-C3A | -3.47 | 108.00      | 116.10   |
| 14  | bA    | 3115 | CL7  | C4D-C3D-C2D | -3.47 | 102.78      | 107.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | bA    | 3102 | CL7  | C3A-C4A-CHB | -3.47 | 118.55      | 123.70   |
| 14  | bA    | 3109 | CL7  | CED-O2D-CGD | 3.47  | 123.78      | 115.94   |
| 14  | cB    | 819  | CL7  | CHC-C4B-NB  | 3.47  | 127.93      | 124.26   |
| 14  | cA    | 3115 | CL7  | C4D-C3D-C2D | -3.47 | 102.78      | 107.30   |
| 14  | cA    | 3109 | CL7  | CMB-C2B-C1B | 3.46  | 130.65      | 125.37   |
| 14  | cB    | 820  | CL7  | C3B-C4B-NB  | -3.46 | 107.30      | 110.52   |
| 14  | aA    | 3118 | CL7  | CAA-C2A-C3A | -3.46 | 108.02      | 116.10   |
| 14  | aA    | 3127 | CL7  | C3A-C4A-CHB | -3.46 | 118.88      | 124.02   |
| 14  | aA    | 3105 | CL7  | CHB-C1B-NB  | -3.46 | 120.59      | 124.26   |
| 14  | bA    | 3107 | CL7  | C1-C2-C3    | -3.46 | 120.06      | 126.04   |
| 14  | cB    | 833  | CL7  | C3A-C4A-CHB | -3.46 | 118.56      | 123.70   |
| 14  | cA    | 3106 | CL7  | O1D-CGD-CBD | -3.46 | 117.41      | 124.48   |
| 14  | bB    | 822  | CL7  | CMB-C2B-C1B | 3.46  | 130.64      | 125.37   |
| 14  | aA    | 3146 | CL7  | CAA-C2A-C3A | -3.46 | 108.03      | 116.10   |
| 14  | aB    | 3015 | CL7  | C3B-C4B-NB  | -3.46 | 107.31      | 110.52   |
| 14  | cB    | 824  | CL7  | C4D-C3D-C2D | -3.46 | 102.80      | 107.30   |
| 14  | bA    | 3104 | CL7  | C1D-ND-C4D  | -3.46 | 103.88      | 106.33   |
| 14  | cA    | 3121 | CL7  | C3B-C4B-NB  | -3.46 | 107.31      | 110.52   |
| 14  | cA    | 3128 | CL7  | C1D-ND-C4D  | -3.45 | 103.88      | 106.33   |
| 14  | cB    | 832  | CL7  | O2A-CGA-O1A | -3.45 | 114.88      | 123.59   |
| 14  | cJ    | 101  | CL7  | C3A-C4A-CHB | -3.45 | 118.58      | 123.70   |
| 14  | cA    | 3102 | CL7  | C4-C3-C5    | -3.45 | 109.46      | 115.27   |
| 14  | cA    | 3117 | CL7  | C1D-ND-C4D  | -3.45 | 103.88      | 106.33   |
| 14  | aA    | 3126 | CL7  | C7-C6-C5    | -3.45 | 103.99      | 113.36   |
| 12  | cA    | 3101 | G9R  | CHC-C1C-C2C | -3.45 | 117.15      | 126.73   |
| 14  | cA    | 3121 | CL7  | C3A-C4A-CHB | -3.45 | 118.58      | 123.70   |
| 14  | cA    | 3105 | CL7  | O2D-CGD-CBD | 3.45  | 117.39      | 111.27   |
| 14  | bA    | 3109 | CL7  | C1A-NA-C4A  | -3.45 | 104.22      | 106.30   |
| 14  | cB    | 833  | CL7  | C3B-C4B-NB  | -3.45 | 107.32      | 110.52   |
| 14  | aA    | 3113 | CL7  | C4D-C3D-C2D | -3.44 | 102.81      | 107.30   |
| 14  | bA    | 3117 | CL7  | C4D-C3D-C2D | -3.44 | 102.81      | 107.30   |
| 14  | cA    | 3103 | CL7  | C3A-C4A-CHB | -3.44 | 118.59      | 123.70   |
| 14  | bA    | 3110 | CL7  | C1D-ND-C4D  | -3.44 | 103.89      | 106.33   |
| 14  | aJ    | 101  | CL7  | C3A-C4A-CHB | -3.44 | 118.59      | 123.70   |
| 14  | bB    | 831  | CL7  | C3B-C4B-NB  | -3.44 | 107.32      | 110.52   |
| 14  | cA    | 3106 | CL7  | C3A-C2A-C1A | 3.44  | 106.49      | 101.34   |
| 14  | cB    | 804  | CL7  | O2A-CGA-O1A | -3.44 | 114.91      | 123.59   |
| 14  | aB    | 3010 | CL7  | CAA-C2A-C3A | -3.44 | 108.07      | 116.10   |
| 14  | bA    | 3116 | CL7  | O2D-CGD-O1D | -3.44 | 117.11      | 123.84   |
| 14  | cB    | 809  | CL7  | C1A-NA-C4A  | -3.44 | 104.22      | 106.30   |
| 14  | bA    | 3141 | CL7  | C3A-C4A-CHB | -3.44 | 118.60      | 123.70   |
| 14  | bA    | 3111 | CL7  | C1D-ND-C4D  | -3.44 | 103.89      | 106.33   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12  | bA    | 3101 | G9R  | CMD-C2D-C1D | 3.44  | 130.77      | 124.71   |
| 14  | cA    | 3105 | CL7  | C4D-C3D-C2D | -3.44 | 102.82      | 107.30   |
| 14  | aA    | 3133 | CL7  | C4D-C3D-C2D | -3.44 | 102.82      | 107.30   |
| 14  | cA    | 3128 | CL7  | OBb-CAB-C3B | -3.44 | 117.92      | 125.69   |
| 14  | aA    | 3115 | CL7  | CHB-C1B-NB  | -3.43 | 120.62      | 124.26   |
| 14  | cB    | 832  | CL7  | C1-C2-C3    | -3.43 | 120.11      | 126.04   |
| 14  | cA    | 3117 | CL7  | CAA-C2A-C3A | -3.43 | 108.09      | 116.10   |
| 14  | cA    | 3119 | CL7  | CMB-C2B-C1B | 3.43  | 130.59      | 125.37   |
| 14  | cA    | 3109 | CL7  | C1A-NA-C4A  | -3.43 | 104.23      | 106.30   |
| 14  | cB    | 825  | CL7  | C3B-C4B-NB  | -3.43 | 107.33      | 110.52   |
| 14  | aB    | 3025 | CL7  | C4D-C3D-CAD | 3.43  | 109.73      | 107.42   |
| 14  | aB    | 3030 | CL7  | C3B-C4B-NB  | -3.43 | 107.33      | 110.52   |
| 14  | bA    | 3117 | CL7  | CAA-C2A-C3A | -3.43 | 108.10      | 116.10   |
| 14  | bA    | 3108 | CL7  | CHB-C1B-NB  | -3.43 | 120.63      | 124.26   |
| 14  | aB    | 3008 | CL7  | C3A-C2A-C1A | 3.43  | 106.47      | 101.34   |
| 14  | cA    | 3129 | CL7  | O2D-CGD-CBD | 3.43  | 117.36      | 111.27   |
| 14  | bA    | 3121 | CL7  | C3B-C4B-NB  | -3.43 | 107.34      | 110.52   |
| 14  | aB    | 3031 | CL7  | O1D-CGD-CBD | -3.43 | 117.47      | 124.48   |
| 14  | bA    | 3118 | CL7  | C4D-C3D-C2D | -3.42 | 102.84      | 107.30   |
| 14  | bA    | 3105 | CL7  | O2D-CGD-CBD | 3.42  | 117.35      | 111.27   |
| 14  | bB    | 809  | CL7  | C3A-C2A-C1A | 3.42  | 106.47      | 101.34   |
| 14  | cB    | 813  | CL7  | CHB-C1B-NB  | -3.42 | 120.63      | 124.26   |
| 14  | aA    | 3105 | CL7  | O1D-CGD-CBD | -3.42 | 117.48      | 124.48   |
| 14  | aA    | 3114 | CL7  | O2D-CGD-CBD | 3.42  | 117.34      | 111.27   |
| 12  | aA    | 3101 | G9R  | C2A-C3A-C4A | -3.42 | 96.35       | 101.87   |
| 14  | bA    | 3105 | CL7  | CMA-C3A-C2A | -3.42 | 108.12      | 116.10   |
| 14  | aB    | 3024 | CL7  | C4D-C3D-C2D | -3.42 | 102.85      | 107.30   |
| 14  | cB    | 808  | CL7  | CHC-C1C-NC  | -3.42 | 121.31      | 124.45   |
| 14  | aA    | 3107 | CL7  | O2D-CGD-CBD | 3.42  | 117.34      | 111.27   |
| 14  | bB    | 818  | CL7  | CHB-C1B-NB  | -3.41 | 120.64      | 124.26   |
| 14  | cA    | 3102 | CL7  | C4C-C3C-C2C | 3.41  | 111.57      | 107.13   |
| 14  | aA    | 3105 | CL7  | C4D-C3D-C2D | -3.41 | 102.86      | 107.30   |
| 14  | bA    | 3119 | CL7  | C4D-C3D-C2D | -3.41 | 102.86      | 107.30   |
| 14  | aA    | 3115 | CL7  | C1D-ND-C4D  | -3.41 | 103.92      | 106.33   |
| 14  | cB    | 820  | CL7  | O1D-CGD-CBD | -3.41 | 117.52      | 124.48   |
| 13  | bB    | 805  | PHO  | CBA-CAA-C2A | -3.41 | 103.86      | 113.81   |
| 14  | cA    | 3126 | CL7  | C3B-C4B-NB  | -3.40 | 107.36      | 110.52   |
| 14  | bA    | 3102 | CL7  | OBb-CAB-C3B | 3.40  | 133.38      | 125.69   |
| 14  | bB    | 822  | CL7  | C3B-C4B-NB  | -3.40 | 107.36      | 110.52   |
| 14  | aK    | 101  | CL7  | C1A-NA-C4A  | -3.40 | 104.24      | 106.30   |
| 14  | cA    | 3131 | CL7  | CAA-C2A-C3A | -3.40 | 108.17      | 116.10   |
| 14  | aB    | 3005 | CL7  | C1D-ND-C4D  | -3.40 | 103.92      | 106.33   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 13  | aA    | 3102 | PHO  | O2D-CGD-CBD | 3.40  | 115.30      | 111.00   |
| 14  | aA    | 3112 | CL7  | C1D-ND-C4D  | -3.40 | 103.92      | 106.33   |
| 12  | cA    | 3101 | G9R  | OBb-CAB-C3B | -3.39 | 118.01      | 125.69   |
| 14  | cK    | 101  | CL7  | CAA-C2A-C3A | -3.39 | 108.18      | 116.10   |
| 14  | aB    | 3016 | CL7  | O2D-CGD-O1D | -3.39 | 117.21      | 123.84   |
| 14  | bB    | 809  | CL7  | O2D-CGD-O1D | -3.39 | 117.21      | 123.84   |
| 14  | bL    | 204  | CL7  | CHC-C1C-NC  | -3.39 | 121.34      | 124.45   |
| 14  | aA    | 3103 | CL7  | C3A-C4A-CHB | -3.39 | 118.67      | 123.70   |
| 14  | aB    | 3023 | CL7  | C4D-C3D-C2D | -3.39 | 102.88      | 107.30   |
| 14  | bB    | 816  | CL7  | CMB-C2B-C1B | 3.39  | 130.53      | 125.37   |
| 14  | aB    | 3031 | CL7  | C16-C15-C13 | -3.39 | 104.98      | 115.92   |
| 14  | aK    | 101  | CL7  | CAA-C2A-C3A | -3.39 | 108.20      | 116.10   |
| 14  | aA    | 3110 | CL7  | CHB-C1B-NB  | -3.38 | 120.67      | 124.26   |
| 14  | cL    | 203  | CL7  | CED-O2D-CGD | 3.38  | 123.59      | 115.94   |
| 14  | cA    | 3124 | CL7  | C2A-C1A-CHA | -3.38 | 119.60      | 126.36   |
| 14  | aA    | 3129 | CL7  | C1D-ND-C4D  | -3.38 | 103.93      | 106.33   |
| 14  | cA    | 3109 | CL7  | O2D-CGD-CBD | 3.38  | 117.27      | 111.27   |
| 14  | aA    | 3104 | CL7  | C3B-C4B-NB  | -3.38 | 107.38      | 110.52   |
| 14  | cA    | 3129 | CL7  | C3A-C2A-C1A | 3.38  | 105.68      | 101.64   |
| 14  | bB    | 809  | CL7  | C1D-ND-C4D  | -3.38 | 103.94      | 106.33   |
| 14  | bA    | 3119 | CL7  | CHB-C1B-NB  | -3.38 | 120.68      | 124.26   |
| 14  | aL    | 204  | CL7  | O2D-CGD-O1D | -3.38 | 117.23      | 123.84   |
| 14  | bB    | 808  | CL7  | CMB-C2B-C1B | 3.38  | 130.51      | 125.37   |
| 12  | aA    | 3101 | G9R  | C3D-C4D-ND  | 3.37  | 115.69      | 110.24   |
| 14  | cA    | 3111 | CL7  | C1D-ND-C4D  | -3.37 | 103.94      | 106.33   |
| 14  | cB    | 811  | CL7  | O1D-CGD-CBD | -3.37 | 117.58      | 124.48   |
| 14  | bA    | 3119 | CL7  | CMB-C2B-C1B | 3.37  | 130.50      | 125.37   |
| 14  | bA    | 3104 | CL7  | C3A-C4A-CHB | -3.37 | 118.70      | 123.70   |
| 14  | bA    | 3110 | CL7  | CAA-C2A-C3A | -3.37 | 108.23      | 116.10   |
| 14  | bA    | 3113 | CL7  | O2D-CGD-CBD | 3.37  | 117.26      | 111.27   |
| 14  | bB    | 806  | CL7  | C6-C7-C8    | -3.37 | 105.03      | 115.92   |
| 14  | bB    | 818  | CL7  | C1D-ND-C4D  | -3.37 | 103.94      | 106.33   |
| 14  | aA    | 3125 | CL7  | C1-O2A-CGA  | -3.37 | 107.61      | 116.44   |
| 14  | bB    | 833  | CL7  | C3B-C4B-NB  | -3.37 | 107.39      | 110.52   |
| 14  | bB    | 808  | CL7  | C1-O2A-CGA  | -3.36 | 107.62      | 116.44   |
| 14  | aA    | 3104 | CL7  | CMB-C2B-C1B | 3.36  | 130.49      | 125.37   |
| 14  | aB    | 3007 | CL7  | CHC-C1C-NC  | -3.36 | 121.36      | 124.45   |
| 14  | aA    | 3115 | CL7  | O2D-CGD-CBD | 3.36  | 117.24      | 111.27   |
| 14  | cA    | 3128 | CL7  | C4D-C3D-C2D | -3.36 | 102.92      | 107.30   |
| 14  | bB    | 807  | CL7  | CAC-C3C-C2C | -3.36 | 121.78      | 127.53   |
| 14  | aB    | 3006 | CL7  | C4D-C3D-C2D | -3.36 | 102.92      | 107.30   |
| 14  | cB    | 816  | CL7  | CMB-C2B-C1B | 3.36  | 130.49      | 125.37   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | aA    | 3110 | CL7  | C4D-C3D-C2D | -3.36 | 102.92      | 107.30   |
| 13  | aB    | 3004 | PHO  | C4-C3-C5    | 3.36  | 120.92      | 115.27   |
| 14  | bB    | 819  | CL7  | O1D-CGD-CBD | -3.36 | 117.62      | 124.48   |
| 14  | bA    | 3132 | CL7  | CMB-C2B-C1B | 3.36  | 130.48      | 125.37   |
| 14  | bA    | 3105 | CL7  | C4D-C3D-C2D | -3.36 | 102.93      | 107.30   |
| 14  | aA    | 3129 | CL7  | CHB-C1B-NB  | -3.36 | 120.70      | 124.26   |
| 14  | aA    | 3128 | CL7  | O2A-CGA-O1A | -3.36 | 115.12      | 123.59   |
| 14  | aB    | 3012 | CL7  | C4D-C3D-C2D | -3.35 | 102.93      | 107.30   |
| 14  | cB    | 807  | CL7  | CAC-C3C-C2C | -3.35 | 121.79      | 127.53   |
| 14  | bA    | 3108 | CL7  | C3A-C4A-CHB | -3.35 | 118.72      | 123.70   |
| 14  | cB    | 832  | CL7  | O1D-CGD-CBD | -3.35 | 117.62      | 124.48   |
| 14  | aA    | 3104 | CL7  | O1D-CGD-CBD | -3.35 | 117.62      | 124.48   |
| 14  | cA    | 3117 | CL7  | C4D-C3D-C2D | -3.35 | 102.93      | 107.30   |
| 14  | bB    | 821  | CL7  | CAA-C2A-C3A | -3.35 | 108.28      | 116.10   |
| 14  | bA    | 3107 | CL7  | CMB-C2B-C1B | 3.35  | 130.47      | 125.37   |
| 14  | aB    | 3006 | CL7  | C1-C2-C3    | -3.35 | 120.25      | 126.04   |
| 14  | aA    | 3112 | CL7  | CAA-C2A-C3A | -3.35 | 108.29      | 116.10   |
| 14  | aA    | 3118 | CL7  | C4D-C3D-C2D | -3.35 | 102.94      | 107.30   |
| 14  | cB    | 825  | CL7  | CAA-C2A-C3A | -3.35 | 108.29      | 116.10   |
| 14  | cB    | 803  | CL7  | CMB-C2B-C1B | 3.35  | 130.46      | 125.37   |
| 14  | aA    | 3129 | CL7  | CHC-C4B-NB  | 3.34  | 127.80      | 124.26   |
| 14  | cA    | 3113 | CL7  | O2D-CGD-CBD | 3.34  | 117.21      | 111.27   |
| 14  | cB    | 807  | CL7  | CMB-C2B-C1B | 3.34  | 130.46      | 125.37   |
| 17  | bA    | 3143 | PQN  | C15-C13-C12 | -3.34 | 114.35      | 121.12   |
| 14  | aA    | 3108 | CL7  | C1-C2-C3    | -3.34 | 120.26      | 126.04   |
| 14  | cB    | 817  | CL7  | O2D-CGD-O1D | -3.34 | 117.30      | 123.84   |
| 14  | cK    | 101  | CL7  | CHB-C1B-NB  | -3.34 | 120.72      | 124.26   |
| 14  | aA    | 3123 | CL7  | OBD-CAD-C3D | -3.34 | 120.48      | 128.52   |
| 14  | cA    | 3111 | CL7  | CAA-C2A-C3A | -3.34 | 108.30      | 116.10   |
| 17  | bB    | 828  | PQN  | C11-C12-C13 | -3.34 | 121.23      | 126.79   |
| 14  | cB    | 804  | CL7  | CMB-C2B-C1B | 3.34  | 130.45      | 125.37   |
| 14  | bB    | 814  | CL7  | C4D-C3D-C2D | -3.34 | 102.95      | 107.30   |
| 13  | aA    | 3102 | PHO  | CMB-C2B-C3B | 3.34  | 130.92      | 124.68   |
| 14  | cB    | 827  | CL7  | O2A-CGA-O1A | -3.34 | 115.17      | 123.59   |
| 14  | cA    | 3144 | CL7  | C4D-C3D-C2D | -3.34 | 102.95      | 107.30   |
| 14  | bB    | 804  | CL7  | C1D-ND-C4D  | -3.34 | 103.96      | 106.33   |
| 14  | bL    | 205  | CL7  | CMB-C2B-C1B | 3.34  | 130.45      | 125.37   |
| 14  | bB    | 813  | CL7  | CHB-C1B-NB  | -3.34 | 120.72      | 124.26   |
| 14  | aA    | 3115 | CL7  | O1D-CGD-CBD | -3.33 | 117.66      | 124.48   |
| 14  | cA    | 3109 | CL7  | CHB-C1B-NB  | -3.33 | 120.73      | 124.26   |
| 14  | cB    | 809  | CL7  | C1-C2-C3    | -3.33 | 121.36      | 126.75   |
| 14  | aB    | 3024 | CL7  | CAA-C2A-C3A | -3.33 | 108.32      | 116.10   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | bA    | 3112 | CL7  | C4D-C3D-C2D | -3.33 | 102.96      | 107.30   |
| 14  | aA    | 3114 | CL7  | CAA-C2A-C3A | -3.33 | 108.32      | 116.10   |
| 14  | aA    | 3126 | CL7  | CHB-C1B-NB  | -3.33 | 120.73      | 124.26   |
| 14  | aA    | 3131 | CL7  | O2D-CGD-O1D | -3.33 | 117.33      | 123.84   |
| 14  | cA    | 3119 | CL7  | C4D-C3D-C2D | -3.33 | 102.96      | 107.30   |
| 14  | aA    | 3142 | CL7  | O2A-CGA-O1A | -3.33 | 115.19      | 123.59   |
| 14  | aA    | 3142 | CL7  | CBD-CHA-C4D | -3.33 | 101.18      | 109.14   |
| 14  | bA    | 3103 | CL7  | C3A-C4A-CHB | -3.33 | 118.76      | 123.70   |
| 14  | aB    | 3013 | CL7  | CAA-C2A-C3A | -3.33 | 108.33      | 116.10   |
| 14  | aA    | 3107 | CL7  | CAA-C2A-C3A | -3.33 | 103.67      | 112.78   |
| 14  | aB    | 3010 | CL7  | C1D-ND-C4D  | -3.33 | 103.97      | 106.33   |
| 14  | bA    | 3111 | CL7  | C4D-C3D-C2D | -3.33 | 102.97      | 107.30   |
| 14  | bA    | 3114 | CL7  | CHB-C1B-NB  | -3.32 | 120.74      | 124.26   |
| 14  | cB    | 832  | CL7  | CHB-C1B-NB  | -3.32 | 120.74      | 124.26   |
| 13  | cB    | 805  | PHO  | O2D-CGD-O1D | -3.32 | 117.34      | 123.84   |
| 14  | aB    | 3030 | CL7  | CBD-CHA-C4D | -3.32 | 101.20      | 109.14   |
| 14  | aB    | 3006 | CL7  | C3A-C4A-CHB | -3.32 | 118.77      | 123.70   |
| 14  | aA    | 3103 | CL7  | C6-C7-C8    | -3.32 | 105.19      | 115.92   |
| 14  | bA    | 3126 | CL7  | C3B-C4B-NB  | -3.32 | 107.44      | 110.52   |
| 14  | aA    | 3108 | CL7  | CHB-C1B-NB  | -3.32 | 120.74      | 124.26   |
| 14  | bA    | 3111 | CL7  | CAA-C2A-C3A | -3.32 | 108.35      | 116.10   |
| 14  | cB    | 809  | CL7  | CMB-C2B-C1B | 3.32  | 130.42      | 125.37   |
| 14  | bA    | 3128 | CL7  | C4-C3-C5    | -3.32 | 109.69      | 115.27   |
| 14  | aA    | 3115 | CL7  | O2D-CGD-O1D | -3.32 | 117.35      | 123.84   |
| 12  | cA    | 3101 | G9R  | CMD-C2D-C1D | 3.32  | 130.56      | 124.71   |
| 14  | cA    | 3141 | CL7  | C6-C5-C3    | -3.32 | 104.76      | 113.45   |
| 14  | bB    | 810  | CL7  | CHC-C4B-NB  | 3.32  | 127.77      | 124.26   |
| 14  | cA    | 3122 | CL7  | C1D-ND-C4D  | -3.32 | 103.98      | 106.33   |
| 14  | bB    | 807  | CL7  | C1A-NA-C4A  | -3.31 | 104.30      | 106.30   |
| 14  | cB    | 804  | CL7  | C7-C6-C5    | -3.31 | 104.36      | 113.36   |
| 14  | aA    | 3108 | CL7  | C3B-C4B-NB  | -3.31 | 107.44      | 110.52   |
| 14  | aB    | 3013 | CL7  | C3A-C4A-CHB | -3.31 | 118.78      | 123.70   |
| 14  | bB    | 814  | CL7  | C3A-C4A-CHB | -3.31 | 118.79      | 123.70   |
| 14  | aA    | 3127 | CL7  | C4D-C3D-C2D | -3.31 | 102.98      | 107.30   |
| 14  | bA    | 3131 | CL7  | CHB-C1B-NB  | -3.31 | 120.75      | 124.26   |
| 14  | aB    | 3012 | CL7  | C3B-C4B-NB  | -3.31 | 107.44      | 110.52   |
| 14  | bA    | 3102 | CL7  | C3B-C4B-NB  | -3.31 | 107.44      | 110.52   |
| 14  | cB    | 803  | CL7  | O1D-CGD-CBD | -3.31 | 117.71      | 124.48   |
| 14  | aB    | 3005 | CL7  | C6-C7-C8    | -3.31 | 105.23      | 115.92   |
| 14  | cA    | 3109 | CL7  | C4D-C3D-C2D | -3.31 | 102.99      | 107.30   |
| 14  | cA    | 3111 | CL7  | C4D-C3D-C2D | -3.31 | 102.99      | 107.30   |
| 14  | aA    | 3146 | CL7  | C4D-C3D-C2D | -3.30 | 102.99      | 107.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | cB    | 814  | CL7  | C4D-C3D-C2D | -3.30 | 103.00      | 107.30   |
| 14  | cB    | 809  | CL7  | C3A-C2A-C1A | 3.30  | 106.29      | 101.34   |
| 14  | bB    | 813  | CL7  | C3B-C4B-NB  | -3.30 | 107.45      | 110.52   |
| 14  | bA    | 3106 | CL7  | O1D-CGD-CBD | -3.30 | 117.73      | 124.48   |
| 13  | bB    | 805  | PHO  | CBC-CAC-C3C | -3.30 | 108.05      | 112.88   |
| 14  | cA    | 3105 | CL7  | CMA-C3A-C2A | -3.30 | 108.40      | 116.10   |
| 14  | aB    | 3019 | CL7  | C3B-C4B-NB  | -3.30 | 107.45      | 110.52   |
| 14  | cA    | 3140 | CL7  | O1D-CGD-CBD | -3.30 | 117.74      | 124.48   |
| 14  | cA    | 3112 | CL7  | C4D-C3D-C2D | -3.29 | 103.01      | 107.30   |
| 14  | aA    | 3105 | CL7  | O2D-CGD-O1D | -3.29 | 117.40      | 123.84   |
| 14  | aB    | 3026 | CL7  | C2C-C1C-NC  | 3.29  | 112.53      | 110.10   |
| 14  | cA    | 3140 | CL7  | C6-C5-C3    | -3.29 | 104.83      | 113.45   |
| 14  | aA    | 3103 | CL7  | O2A-CGA-O1A | -3.29 | 115.29      | 123.59   |
| 14  | cB    | 813  | CL7  | C3B-C4B-NB  | -3.29 | 107.46      | 110.52   |
| 14  | bJ    | 101  | CL7  | CHB-C1B-NB  | -3.29 | 120.78      | 124.26   |
| 14  | bA    | 3145 | CL7  | C4D-C3D-C2D | -3.29 | 103.02      | 107.30   |
| 14  | bB    | 817  | CL7  | O2D-CGD-O1D | -3.29 | 117.41      | 123.84   |
| 14  | bB    | 813  | CL7  | C4D-C3D-C2D | -3.29 | 103.02      | 107.30   |
| 14  | cB    | 806  | CL7  | C1D-ND-C4D  | -3.29 | 104.00      | 106.33   |
| 14  | cB    | 806  | CL7  | O2A-CGA-O1A | -3.29 | 115.30      | 123.59   |
| 14  | bA    | 3122 | CL7  | CMB-C2B-C1B | 3.28  | 130.37      | 125.37   |
| 14  | bB    | 812  | CL7  | C3A-C2A-C1A | -3.28 | 97.72       | 101.64   |
| 14  | aA    | 3129 | CL7  | C6-C7-C8    | -3.28 | 105.31      | 115.92   |
| 14  | aB    | 3018 | CL7  | O1D-CGD-CBD | -3.28 | 117.77      | 124.48   |
| 14  | aA    | 3106 | CL7  | C3A-C4A-CHB | -3.28 | 118.83      | 123.70   |
| 14  | bL    | 203  | CL7  | O2D-CGD-CBD | 3.28  | 117.10      | 111.27   |
| 14  | aB    | 3005 | CL7  | C3A-C4A-CHB | -3.28 | 118.83      | 123.70   |
| 14  | aB    | 3031 | CL7  | C7-C6-C5    | -3.28 | 104.46      | 113.36   |
| 14  | bB    | 812  | CL7  | C4D-C3D-C2D | -3.28 | 103.03      | 107.30   |
| 14  | aA    | 3106 | CL7  | O2D-CGD-CBD | 3.28  | 117.09      | 111.27   |
| 14  | cA    | 3128 | CL7  | C6-C5-C3    | -3.28 | 104.87      | 113.45   |
| 14  | aA    | 3130 | CL7  | CAD-C3D-C2D | 3.27  | 151.51      | 144.44   |
| 14  | cB    | 815  | CL7  | CAA-C2A-C3A | -3.27 | 108.46      | 116.10   |
| 14  | bA    | 3106 | CL7  | C3A-C2A-C1A | 3.27  | 106.24      | 101.34   |
| 14  | bA    | 3126 | CL7  | C4D-C3D-C2D | -3.27 | 103.04      | 107.30   |
| 14  | cA    | 3129 | CL7  | OBD-CAD-C3D | -3.27 | 120.65      | 128.52   |
| 14  | aB    | 3013 | CL7  | C4D-C3D-C2D | -3.27 | 103.04      | 107.30   |
| 14  | aB    | 3022 | CL7  | C4D-C3D-C2D | -3.27 | 103.04      | 107.30   |
| 14  | cB    | 812  | CL7  | C4D-C3D-C2D | -3.27 | 103.04      | 107.30   |
| 14  | bB    | 825  | CL7  | C4D-C3D-C2D | -3.27 | 103.04      | 107.30   |
| 14  | cA    | 3104 | CL7  | C3A-C4A-CHB | -3.27 | 118.85      | 123.70   |
| 14  | bA    | 3109 | CL7  | CHB-C1B-NB  | -3.27 | 120.80      | 124.26   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | aB    | 3003 | CL7  | CMB-C2B-C1B | 3.27  | 130.34      | 125.37   |
| 14  | cA    | 3104 | CL7  | C4D-C3D-C2D | -3.26 | 103.05      | 107.30   |
| 14  | cA    | 3110 | CL7  | CAA-C2A-C3A | -3.26 | 108.48      | 116.10   |
| 14  | bA    | 3114 | CL7  | C1D-ND-C4D  | -3.26 | 104.02      | 106.33   |
| 14  | cA    | 3140 | CL7  | C1D-ND-C4D  | -3.26 | 104.02      | 106.33   |
| 14  | cA    | 3121 | CL7  | CMB-C2B-C1B | 3.26  | 130.34      | 125.37   |
| 14  | bB    | 822  | CL7  | CAA-C2A-C3A | -3.26 | 108.49      | 116.10   |
| 14  | cB    | 819  | CL7  | C3B-C4B-NB  | -3.26 | 107.49      | 110.52   |
| 14  | cB    | 832  | CL7  | C1D-ND-C4D  | -3.26 | 104.02      | 106.33   |
| 14  | cB    | 812  | CL7  | C3A-C2A-C1A | -3.25 | 97.75       | 101.64   |
| 14  | bA    | 3139 | CL7  | CHC-C4B-NB  | 3.25  | 127.70      | 124.26   |
| 14  | cA    | 3114 | CL7  | O2D-CGD-CBD | 3.25  | 117.05      | 111.27   |
| 14  | aA    | 3108 | CL7  | O2A-CGA-O1A | -3.25 | 115.38      | 123.59   |
| 14  | cB    | 821  | CL7  | CAA-C2A-C3A | -3.25 | 108.51      | 116.10   |
| 14  | aB    | 3008 | CL7  | C1A-NA-C4A  | -3.25 | 104.33      | 106.30   |
| 14  | cA    | 3118 | CL7  | C1A-NA-C4A  | -3.25 | 104.33      | 106.30   |
| 14  | cB    | 821  | CL7  | CMB-C2B-C1B | 3.25  | 130.32      | 125.37   |
| 13  | cB    | 801  | PHO  | O2D-CGD-CBD | 3.25  | 115.11      | 111.00   |
| 14  | bA    | 3123 | CL7  | OBb-CAB-C3B | -3.25 | 118.34      | 125.69   |
| 14  | aL    | 202  | CL7  | CED-O2D-CGD | 3.25  | 123.29      | 115.94   |
| 14  | aB    | 3021 | CL7  | C3A-C4A-CHB | -3.25 | 118.88      | 123.70   |
| 14  | cB    | 825  | CL7  | C1D-ND-C4D  | -3.25 | 104.03      | 106.33   |
| 14  | cB    | 821  | CL7  | CHB-C1B-NB  | -3.25 | 120.82      | 124.26   |
| 14  | bA    | 3127 | CL7  | CHC-C1C-NC  | -3.25 | 121.47      | 124.45   |
| 14  | cB    | 813  | CL7  | C4D-C3D-C2D | -3.25 | 103.07      | 107.30   |
| 14  | aB    | 3018 | CL7  | CHC-C4B-NB  | 3.25  | 127.69      | 124.26   |
| 14  | bA    | 3139 | CL7  | C1D-ND-C4D  | -3.25 | 104.03      | 106.33   |
| 14  | cB    | 816  | CL7  | O1D-CGD-CBD | -3.25 | 117.84      | 124.48   |
| 12  | aA    | 3101 | G9R  | C4C-C3C-C2C | -3.25 | 102.17      | 106.90   |
| 14  | aB    | 3009 | CL7  | CAA-C2A-C3A | -3.25 | 103.89      | 112.78   |
| 14  | cB    | 812  | CL7  | CMB-C2B-C1B | 3.25  | 130.31      | 125.37   |
| 14  | bA    | 3128 | CL7  | C3A-C4A-CHB | -3.24 | 118.89      | 123.70   |
| 14  | aL    | 203  | CL7  | O1D-CGD-CBD | -3.24 | 117.85      | 124.48   |
| 14  | cB    | 833  | CL7  | C3A-C2A-C1A | 3.24  | 106.20      | 101.34   |
| 14  | aB    | 3010 | CL7  | O2D-CGD-O1D | -3.24 | 117.50      | 123.84   |
| 14  | bA    | 3142 | CL7  | C3B-C4B-NB  | -3.24 | 107.51      | 110.52   |
| 14  | aB    | 3009 | CL7  | CMB-C2B-C1B | 3.24  | 130.30      | 125.37   |
| 14  | cB    | 814  | CL7  | C3A-C4A-CHB | -3.24 | 118.89      | 123.70   |
| 14  | aB    | 3020 | CL7  | CHB-C1B-NB  | -3.24 | 120.83      | 124.26   |
| 14  | bB    | 807  | CL7  | C4D-C3D-C2D | -3.24 | 103.08      | 107.30   |
| 14  | aA    | 3112 | CL7  | C4D-C3D-C2D | -3.24 | 103.08      | 107.30   |
| 14  | aA    | 3120 | CL7  | CMB-C2B-C1B | 3.24  | 130.30      | 125.37   |

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| Mol | Chain | Res  | Type | Atoms        | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------------|-------|-------------|----------|
| 13  | bB    | 805  | PHO  | OBD-CAD-CBD  | -3.23 | 121.08      | 125.82   |
| 14  | aB    | 3022 | CL7  | C3A-C4A-CHB  | -3.23 | 118.91      | 123.70   |
| 14  | bB    | 824  | CL7  | C4D-C3D-C2D  | -3.23 | 103.09      | 107.30   |
| 14  | bB    | 807  | CL7  | O1D-CGD-CBD  | -3.23 | 117.88      | 124.48   |
| 14  | aA    | 3103 | CL7  | C3B-C4B-NB   | -3.23 | 107.52      | 110.52   |
| 14  | cA    | 3103 | CL7  | O1D-CGD-CBD  | -3.23 | 117.88      | 124.48   |
| 14  | cA    | 3102 | CL7  | C6-C7-C8     | -3.23 | 105.48      | 115.92   |
| 14  | bB    | 811  | CL7  | O1D-CGD-CBD  | -3.23 | 117.88      | 124.48   |
| 14  | bB    | 827  | CL7  | C1D-ND-C4D   | -3.23 | 104.04      | 106.33   |
| 14  | cA    | 3141 | CL7  | O2D-CGD-O1D  | -3.23 | 117.53      | 123.84   |
| 14  | bA    | 3130 | CL7  | CHB-C1B-NB   | -3.22 | 120.84      | 124.26   |
| 14  | cA    | 3114 | CL7  | CHB-C1B-NB   | -3.22 | 120.84      | 124.26   |
| 14  | aA    | 3125 | CL7  | O1D-CGD-CBD  | -3.22 | 117.89      | 124.48   |
| 14  | bA    | 3105 | CL7  | CHC-C4B-NB   | 3.22  | 127.67      | 124.26   |
| 14  | aA    | 3143 | CL7  | O2D-CGD-O1D  | -3.22 | 117.54      | 123.84   |
| 14  | bA    | 3109 | CL7  | C4D-C3D-C2D  | -3.22 | 103.10      | 107.30   |
| 14  | aA    | 3110 | CL7  | C3A-C4A-CHB  | -3.22 | 118.92      | 123.70   |
| 14  | bA    | 3103 | CL7  | O1D-CGD-CBD  | -3.22 | 117.90      | 124.48   |
| 14  | bB    | 811  | CL7  | C1D-ND-C4D   | -3.22 | 104.05      | 106.33   |
| 14  | aA    | 3129 | CL7  | C6-C5-C3     | -3.22 | 105.02      | 113.45   |
| 14  | bA    | 3128 | CL7  | OB B-CAB-C3B | -3.22 | 118.42      | 125.69   |
| 14  | cB    | 827  | CL7  | C2B-C1B-NB   | -3.21 | 108.08      | 110.23   |
| 14  | aB    | 3026 | CL7  | C3B-C4B-NB   | -3.21 | 107.53      | 110.52   |
| 14  | cA    | 3103 | CL7  | C3B-C4B-NB   | -3.21 | 107.53      | 110.52   |
| 13  | cB    | 805  | PHO  | OBD-CAD-CBD  | -3.21 | 121.11      | 125.82   |
| 14  | cA    | 3107 | CL7  | CMB-C2B-C1B  | 3.21  | 130.26      | 125.37   |
| 14  | cB    | 813  | CL7  | CAA-C2A-C3A  | -3.21 | 108.60      | 116.10   |
| 14  | bK    | 101  | CL7  | CAA-C2A-C3A  | -3.21 | 108.61      | 116.10   |
| 14  | bA    | 3103 | CL7  | C3B-C4B-NB   | -3.21 | 107.54      | 110.52   |
| 14  | cB    | 816  | CL7  | CMC-C2C-C1C  | -3.21 | 119.05      | 124.71   |
| 14  | aB    | 3020 | CL7  | CAA-C2A-C3A  | -3.21 | 108.61      | 116.10   |
| 14  | bA    | 3107 | CL7  | O2A-CGA-O1A  | -3.21 | 115.49      | 123.59   |
| 17  | cA    | 3143 | PQN  | C15-C13-C12  | -3.21 | 114.62      | 121.12   |
| 14  | bB    | 807  | CL7  | C1D-ND-C4D   | -3.21 | 104.06      | 106.33   |
| 14  | aA    | 3118 | CL7  | CMB-C2B-C1B  | 3.21  | 130.25      | 125.37   |
| 14  | aJ    | 101  | CL7  | C1D-ND-C4D   | -3.20 | 104.06      | 106.33   |
| 14  | cA    | 3107 | CL7  | C1A-NA-C4A   | -3.20 | 104.36      | 106.30   |
| 14  | bB    | 811  | CL7  | C3A-C4A-CHB  | -3.20 | 118.95      | 123.70   |
| 14  | cA    | 3102 | CL7  | C4D-C3D-C2D  | -3.20 | 103.13      | 107.30   |
| 14  | cA    | 3119 | CL7  | C3A-C4A-CHB  | -3.20 | 118.95      | 123.70   |
| 14  | bB    | 806  | CL7  | C11-C12-C13  | -3.20 | 105.58      | 115.92   |
| 14  | cB    | 808  | CL7  | C6-C5-C3     | -3.20 | 105.07      | 113.45   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | aB    | 3012 | CL7  | CAA-C2A-C3A | -3.20 | 108.64      | 116.10   |
| 14  | cA    | 3113 | CL7  | CAA-C2A-C3A | -3.20 | 108.64      | 116.10   |
| 14  | bA    | 3142 | CL7  | C4D-C3D-C2D | -3.20 | 103.14      | 107.30   |
| 14  | bL    | 205  | CL7  | CHC-C4B-NB  | 3.19  | 127.64      | 124.26   |
| 14  | bB    | 813  | CL7  | CMB-C2B-C1B | 3.19  | 130.23      | 125.37   |
| 14  | cB    | 813  | CL7  | CMB-C2B-C1B | 3.19  | 130.23      | 125.37   |
| 14  | bA    | 3124 | CL7  | C3B-C4B-NB  | -3.19 | 107.55      | 110.52   |
| 14  | cB    | 819  | CL7  | C4D-C3D-CAD | -3.19 | 105.27      | 107.42   |
| 14  | aB    | 3024 | CL7  | C1D-ND-C4D  | -3.19 | 104.07      | 106.33   |
| 14  | aA    | 3117 | CL7  | C4D-C3D-C2D | -3.19 | 103.14      | 107.30   |
| 14  | cA    | 3144 | CL7  | O1D-CGD-CBD | -3.19 | 117.95      | 124.48   |
| 14  | cB    | 816  | CL7  | C1-O2A-CGA  | -3.19 | 108.08      | 116.44   |
| 14  | cA    | 3102 | CL7  | CHC-C4B-NB  | 3.19  | 127.63      | 124.26   |
| 14  | aB    | 3011 | CL7  | C4D-C3D-C2D | -3.19 | 103.14      | 107.30   |
| 14  | bB    | 809  | CL7  | C3A-C4A-CHB | -3.19 | 118.97      | 123.70   |
| 14  | cA    | 3106 | CL7  | O2A-CGA-O1A | -3.19 | 115.55      | 123.59   |
| 14  | bA    | 3124 | CL7  | CAC-C3C-C2C | -3.19 | 122.08      | 127.53   |
| 14  | bA    | 3145 | CL7  | O1D-CGD-CBD | -3.19 | 117.96      | 124.48   |
| 14  | cA    | 3111 | CL7  | C3B-C4B-NB  | -3.19 | 107.56      | 110.52   |
| 14  | bB    | 823  | CL7  | C4D-C3D-C2D | -3.19 | 103.15      | 107.30   |
| 14  | aB    | 3006 | CL7  | C1A-NA-C4A  | -3.19 | 104.37      | 106.30   |
| 14  | bA    | 3113 | CL7  | CHB-C1B-NB  | -3.19 | 120.89      | 124.26   |
| 14  | cA    | 3114 | CL7  | C6-C7-C8    | -3.18 | 105.63      | 115.92   |
| 14  | cA    | 3133 | CL7  | C4D-C3D-C2D | -3.18 | 103.15      | 107.30   |
| 14  | aA    | 3119 | CL7  | C1A-NA-C4A  | -3.18 | 104.38      | 106.30   |
| 14  | bA    | 3123 | CL7  | O1A-CGA-CBA | -3.18 | 111.33      | 123.73   |
| 14  | cB    | 814  | CL7  | CAA-C2A-C3A | -3.18 | 108.68      | 116.10   |
| 14  | cA    | 3126 | CL7  | CAD-C3D-C2D | 3.18  | 151.30      | 144.44   |
| 14  | cA    | 3116 | CL7  | O2D-CGD-O1D | -3.17 | 117.63      | 123.84   |
| 14  | cA    | 3112 | CL7  | O1D-CGD-CBD | -3.17 | 117.99      | 124.48   |
| 14  | aA    | 3107 | CL7  | C3A-C2A-C1A | 3.17  | 106.09      | 101.34   |
| 14  | aB    | 3015 | CL7  | C1-O2A-CGA  | -3.17 | 108.12      | 116.44   |
| 14  | aB    | 3012 | CL7  | C1D-ND-C4D  | -3.17 | 104.08      | 106.33   |
| 14  | aA    | 3124 | CL7  | C4D-C3D-C2D | -3.17 | 103.17      | 107.30   |
| 14  | bB    | 813  | CL7  | CAA-C2A-C3A | -3.17 | 108.70      | 116.10   |
| 14  | cA    | 3118 | CL7  | CAA-C2A-C3A | -3.17 | 108.70      | 116.10   |
| 14  | bB    | 809  | CL7  | CMB-C2B-C1B | 3.17  | 130.20      | 125.37   |
| 14  | cA    | 3124 | CL7  | O2D-CGD-CBD | 3.17  | 116.90      | 111.27   |
| 14  | cA    | 3132 | CL7  | C3A-C2A-C1A | 3.17  | 106.08      | 101.34   |
| 14  | bA    | 3121 | CL7  | CMB-C2B-C1B | 3.17  | 130.19      | 125.37   |
| 14  | cB    | 807  | CL7  | C4D-C3D-C2D | -3.17 | 103.17      | 107.30   |
| 14  | cK    | 101  | CL7  | C4D-C3D-C2D | -3.17 | 103.17      | 107.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | bB    | 821  | CL7  | CHB-C1B-NB  | -3.17 | 120.90      | 124.26   |
| 14  | bA    | 3133 | CL7  | C4D-C3D-C2D | -3.17 | 103.17      | 107.30   |
| 14  | bA    | 3123 | CL7  | C4-C3-C5    | -3.16 | 112.36      | 115.98   |
| 14  | cA    | 3140 | CL7  | C16-C15-C13 | -3.16 | 105.69      | 115.92   |
| 14  | aA    | 3107 | CL7  | O1D-CGD-CBD | -3.16 | 118.01      | 124.48   |
| 14  | aA    | 3130 | CL7  | O1D-CGD-CBD | -3.16 | 118.01      | 124.48   |
| 14  | aJ    | 101  | CL7  | C4D-C3D-C2D | -3.16 | 103.18      | 107.30   |
| 14  | aA    | 3134 | CL7  | O1D-CGD-CBD | -3.16 | 118.01      | 124.48   |
| 14  | bB    | 815  | CL7  | CAA-C2A-C3A | -3.16 | 108.72      | 116.10   |
| 14  | cL    | 204  | CL7  | C11-C10-C8  | -3.16 | 105.70      | 115.92   |
| 14  | bA    | 3107 | CL7  | C3A-C4A-CHB | -3.16 | 119.01      | 123.70   |
| 14  | bB    | 819  | CL7  | C1-C2-C3    | -3.16 | 120.58      | 126.04   |
| 14  | bB    | 810  | CL7  | C1D-ND-C4D  | -3.16 | 104.09      | 106.33   |
| 14  | bB    | 819  | CL7  | CHC-C4B-NB  | 3.16  | 127.60      | 124.26   |
| 14  | bA    | 3113 | CL7  | C1D-ND-C4D  | -3.16 | 104.09      | 106.33   |
| 12  | cA    | 3101 | G9R  | C4D-C3D-CAD | -3.16 | 104.37      | 108.10   |
| 14  | aA    | 3134 | CL7  | C4D-C3D-C2D | -3.16 | 103.19      | 107.30   |
| 13  | cB    | 805  | PHO  | CBA-CAA-C2A | -3.16 | 104.59      | 113.81   |
| 14  | aB    | 3020 | CL7  | C4D-C3D-C2D | -3.15 | 103.19      | 107.30   |
| 14  | aA    | 3119 | CL7  | CAA-C2A-C3A | -3.15 | 108.74      | 116.10   |
| 14  | aB    | 3003 | CL7  | O2A-CGA-O1A | -3.15 | 115.64      | 123.59   |
| 14  | bA    | 3123 | CL7  | C4D-C3D-C2D | -3.15 | 103.20      | 107.30   |
| 14  | aA    | 3106 | CL7  | CHC-C4B-NB  | 3.15  | 127.59      | 124.26   |
| 14  | bA    | 3103 | CL7  | C4D-C3D-C2D | -3.15 | 103.20      | 107.30   |
| 14  | cJ    | 101  | CL7  | C4D-C3D-C2D | -3.15 | 103.20      | 107.30   |
| 14  | aA    | 3107 | CL7  | O2A-CGA-O1A | -3.15 | 115.65      | 123.59   |
| 14  | aB    | 3026 | CL7  | O1D-CGD-CBD | -3.15 | 118.05      | 124.48   |
| 14  | cA    | 3114 | CL7  | O2A-CGA-O1A | -3.15 | 115.65      | 123.59   |
| 14  | aB    | 3017 | CL7  | CBD-CHA-C4D | -3.15 | 101.61      | 109.14   |
| 14  | cB    | 827  | CL7  | CAA-C2A-C3A | -3.15 | 104.16      | 112.78   |
| 14  | cA    | 3110 | CL7  | C4D-C3D-C2D | -3.15 | 103.20      | 107.30   |
| 14  | cB    | 810  | CL7  | CMB-C2B-C1B | 3.15  | 130.16      | 125.37   |
| 14  | aA    | 3104 | CL7  | C1D-ND-C4D  | -3.14 | 104.10      | 106.33   |
| 14  | aA    | 3133 | CL7  | CAC-C3C-C2C | -3.14 | 122.15      | 127.53   |
| 17  | bB    | 828  | PQN  | C24-C23-C22 | -3.14 | 99.91       | 111.29   |
| 14  | bA    | 3110 | CL7  | CBD-CHA-C4D | -3.14 | 101.62      | 109.14   |
| 14  | bB    | 803  | CL7  | CMB-C2B-C1B | 3.14  | 130.16      | 125.37   |
| 14  | cA    | 3114 | CL7  | C1D-ND-C4D  | -3.14 | 104.10      | 106.33   |
| 14  | cB    | 818  | CL7  | CHB-C1B-NB  | -3.14 | 120.93      | 124.26   |
| 14  | bJ    | 101  | CL7  | C4D-C3D-C2D | -3.14 | 103.21      | 107.30   |
| 14  | aA    | 3123 | CL7  | C1D-ND-C4D  | -3.14 | 104.10      | 106.33   |
| 14  | cA    | 3126 | CL7  | O2D-CGD-O1D | -3.14 | 117.70      | 123.84   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | aB    | 3015 | CL7  | CMB-C2B-C1B | 3.14  | 130.15      | 125.37   |
| 14  | cA    | 3108 | CL7  | C2A-C1A-CHA | -3.14 | 120.09      | 126.36   |
| 14  | cA    | 3124 | CL7  | O2A-CGA-O1A | -3.13 | 115.68      | 123.59   |
| 14  | bA    | 3106 | CL7  | O2A-CGA-O1A | -3.13 | 115.68      | 123.59   |
| 14  | bA    | 3128 | CL7  | C1-O2A-CGA  | -3.13 | 108.22      | 116.44   |
| 14  | cA    | 3125 | CL7  | C2D-C1D-ND  | -3.13 | 108.13      | 110.23   |
| 14  | aA    | 3130 | CL7  | O2D-CGD-O1D | -3.13 | 117.71      | 123.84   |
| 14  | cA    | 3110 | CL7  | C3B-C4B-NB  | -3.13 | 107.61      | 110.52   |
| 14  | aA    | 3108 | CL7  | O2D-CGD-O1D | -3.13 | 117.71      | 123.84   |
| 14  | bB    | 809  | CL7  | CAA-C2A-C3A | -3.13 | 104.20      | 112.78   |
| 14  | cA    | 3108 | CL7  | C2C-C1C-NC  | 3.13  | 112.41      | 110.10   |
| 14  | aB    | 3012 | CL7  | CHB-C1B-NB  | -3.13 | 120.94      | 124.26   |
| 14  | aB    | 3024 | CL7  | C3A-C4A-CHB | -3.13 | 119.05      | 123.70   |
| 14  | bA    | 3114 | CL7  | O2D-CGD-CBD | 3.13  | 116.83      | 111.27   |
| 14  | aA    | 3127 | CL7  | C3B-C4B-NB  | -3.13 | 107.61      | 110.52   |
| 12  | cA    | 3101 | G9R  | CGD-CBD-CAD | -3.13 | 100.60      | 110.73   |
| 14  | bA    | 3127 | CL7  | O2A-CGA-O1A | -3.13 | 115.70      | 123.59   |
| 14  | cB    | 813  | CL7  | C1D-ND-C4D  | -3.13 | 104.11      | 106.33   |
| 12  | aA    | 3101 | G9R  | CHD-C4C-NC  | 3.13  | 129.13      | 124.20   |
| 14  | cB    | 804  | CL7  | C6-C5-C3    | -3.13 | 105.25      | 113.45   |
| 14  | bB    | 832  | CL7  | C3B-C4B-NB  | -3.13 | 107.61      | 110.52   |
| 14  | cA    | 3108 | CL7  | CAC-C3C-C2C | -3.13 | 122.18      | 127.53   |
| 14  | bA    | 3123 | CL7  | C3A-C4A-CHB | -3.13 | 119.06      | 123.70   |
| 14  | bA    | 3116 | CL7  | C1A-NA-C4A  | -3.13 | 104.41      | 106.30   |
| 14  | aA    | 3107 | CL7  | C4D-C3D-C2D | -3.13 | 103.23      | 107.30   |
| 14  | aB    | 3005 | CL7  | O2A-CGA-O1A | -3.13 | 115.70      | 123.59   |
| 14  | cA    | 3117 | CL7  | CMB-C2B-C1B | 3.12  | 130.13      | 125.37   |
| 14  | cB    | 822  | CL7  | CMB-C2B-C1B | 3.12  | 130.13      | 125.37   |
| 14  | aK    | 101  | CL7  | C4D-C3D-C2D | -3.12 | 103.23      | 107.30   |
| 14  | aA    | 3121 | CL7  | CHC-C1C-NC  | -3.12 | 121.59      | 124.45   |
| 14  | bB    | 812  | CL7  | CMB-C2B-C1B | 3.12  | 130.12      | 125.37   |
| 14  | aA    | 3110 | CL7  | CAA-C2A-C3A | -3.12 | 108.82      | 116.10   |
| 14  | aA    | 3140 | CL7  | CHB-C1B-NB  | -3.12 | 120.95      | 124.26   |
| 12  | aA    | 3101 | G9R  | CMD-C2D-C1D | 3.12  | 130.21      | 124.71   |
| 14  | bA    | 3102 | CL7  | C2D-C1D-ND  | -3.12 | 108.14      | 110.23   |
| 14  | bA    | 3125 | CL7  | C2D-C1D-ND  | -3.12 | 108.14      | 110.23   |
| 14  | cA    | 3107 | CL7  | O2A-CGA-O1A | -3.12 | 115.72      | 123.59   |
| 14  | bA    | 3107 | CL7  | O2D-CGD-O1D | -3.12 | 117.74      | 123.84   |
| 14  | cB    | 809  | CL7  | CAA-C2A-C3A | -3.12 | 104.24      | 112.78   |
| 14  | bB    | 833  | CL7  | O2D-CGD-O1D | -3.12 | 117.74      | 123.84   |
| 13  | aB    | 3004 | PHO  | C6-C7-C8    | -3.12 | 105.84      | 115.92   |
| 14  | cA    | 3131 | CL7  | CMB-C2B-C1B | 3.12  | 130.12      | 125.37   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | bK    | 101  | CL7  | C4D-C3D-C2D | -3.12 | 103.24      | 107.30   |
| 14  | cA    | 3128 | CL7  | CMB-C2B-C1B | 3.12  | 130.11      | 125.37   |
| 14  | aA    | 3111 | CL7  | C4D-C3D-C2D | -3.11 | 103.24      | 107.30   |
| 14  | aA    | 3126 | CL7  | C6-C7-C8    | -3.11 | 105.85      | 115.92   |
| 14  | aA    | 3122 | CL7  | CMB-C2B-C1B | 3.11  | 130.11      | 125.37   |
| 14  | bB    | 814  | CL7  | CAA-C2A-C3A | -3.11 | 108.84      | 116.10   |
| 14  | bA    | 3127 | CL7  | C1D-ND-C4D  | -3.11 | 104.12      | 106.33   |
| 14  | cA    | 3105 | CL7  | CHC-C4B-NB  | 3.11  | 127.55      | 124.26   |
| 14  | cB    | 822  | CL7  | C3A-C4A-CHB | -3.11 | 119.09      | 123.70   |
| 14  | aA    | 3129 | CL7  | CMB-C2B-C1B | 3.11  | 130.10      | 125.37   |
| 14  | cL    | 205  | CL7  | CHC-C4B-NB  | 3.11  | 127.55      | 124.26   |
| 14  | aB    | 3031 | CL7  | C4D-C3D-C2D | -3.11 | 103.25      | 107.30   |
| 14  | bB    | 813  | CL7  | C1D-ND-C4D  | -3.11 | 104.13      | 106.33   |
| 14  | cA    | 3107 | CL7  | C4D-C3D-C2D | -3.11 | 103.25      | 107.30   |
| 14  | cA    | 3144 | CL7  | CHB-C1B-NB  | -3.11 | 120.97      | 124.26   |
| 14  | cB    | 814  | CL7  | O1D-CGD-CBD | -3.11 | 118.13      | 124.48   |
| 14  | bA    | 3145 | CL7  | CHB-C1B-NB  | -3.10 | 120.97      | 124.26   |
| 14  | bA    | 3111 | CL7  | C3B-C4B-NB  | -3.10 | 107.64      | 110.52   |
| 14  | cA    | 3113 | CL7  | CHB-C1B-NB  | -3.10 | 120.97      | 124.26   |
| 14  | aB    | 3008 | CL7  | CAA-C2A-C3A | -3.10 | 104.28      | 112.78   |
| 14  | aA    | 3128 | CL7  | CHC-C1C-NC  | -3.10 | 121.60      | 124.45   |
| 14  | aA    | 3129 | CL7  | CAC-C3C-C4C | 3.10  | 129.56      | 124.68   |
| 14  | bA    | 3114 | CL7  | C4-C3-C5    | -3.10 | 110.05      | 115.27   |
| 14  | cA    | 3130 | CL7  | CAA-C2A-C3A | -3.10 | 108.86      | 116.10   |
| 14  | bB    | 832  | CL7  | C4D-C3D-C2D | -3.10 | 103.26      | 107.30   |
| 14  | bB    | 816  | CL7  | C3B-C4B-NB  | -3.10 | 107.64      | 110.52   |
| 14  | bL    | 203  | CL7  | C6-C5-C3    | -3.10 | 105.33      | 113.45   |
| 14  | cA    | 3130 | CL7  | O2D-CGD-O1D | -3.10 | 117.78      | 123.84   |
| 14  | cA    | 3131 | CL7  | CHB-C1B-NB  | -3.10 | 120.98      | 124.26   |
| 14  | bB    | 807  | CL7  | C3A-C4A-CHB | -3.10 | 119.11      | 123.70   |
| 14  | aA    | 3108 | CL7  | C3A-C4A-CHB | -3.09 | 119.11      | 123.70   |
| 14  | cB    | 823  | CL7  | C4D-C3D-C2D | -3.09 | 103.27      | 107.30   |
| 14  | aB    | 3002 | CL7  | O2A-CGA-O1A | -3.09 | 115.79      | 123.59   |
| 14  | bB    | 808  | CL7  | C4D-C3D-C2D | -3.09 | 103.27      | 107.30   |
| 14  | cA    | 3127 | CL7  | CHC-C1C-NC  | -3.09 | 121.61      | 124.45   |
| 14  | bJ    | 101  | CL7  | C1D-ND-C4D  | -3.09 | 104.14      | 106.33   |
| 14  | bA    | 3142 | CL7  | CMB-C2B-C1B | 3.09  | 130.08      | 125.37   |
| 14  | aA    | 3121 | CL7  | C3A-C2A-C1A | 3.09  | 105.97      | 101.34   |
| 14  | cB    | 823  | CL7  | C3A-C4A-CHB | -3.09 | 119.11      | 123.70   |
| 17  | cB    | 828  | PQN  | C24-C23-C22 | -3.09 | 100.10      | 111.29   |
| 14  | cF    | 201  | CL7  | C4D-C3D-C2D | -3.09 | 103.27      | 107.30   |
| 12  | cA    | 3101 | G9R  | CMA-C3A-C2A | -3.09 | 101.37      | 113.83   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | bA    | 3103 | CL7  | C1D-ND-C4D  | -3.09 | 104.14      | 106.33   |
| 14  | bB    | 806  | CL7  | O2A-CGA-O1A | -3.09 | 115.80      | 123.59   |
| 14  | bA    | 3104 | CL7  | C4D-C3D-C2D | -3.09 | 103.28      | 107.30   |
| 14  | bA    | 3132 | CL7  | C4D-C3D-C2D | -3.09 | 103.28      | 107.30   |
| 14  | bB    | 821  | CL7  | C4D-C3D-C2D | -3.09 | 103.28      | 107.30   |
| 14  | cA    | 3118 | CL7  | CHC-C1C-NC  | -3.09 | 121.62      | 124.45   |
| 14  | bA    | 3124 | CL7  | C2A-C1A-CHA | -3.09 | 120.19      | 126.36   |
| 14  | aL    | 204  | CL7  | CHC-C4B-NB  | 3.09  | 127.52      | 124.26   |
| 14  | aB    | 3007 | CL7  | C6-C5-C3    | -3.08 | 105.37      | 113.45   |
| 14  | cA    | 3114 | CL7  | C1-O2A-CGA  | -3.08 | 108.35      | 116.44   |
| 14  | bA    | 3119 | CL7  | C3A-C4A-CHB | -3.08 | 119.12      | 123.70   |
| 14  | cB    | 821  | CL7  | C4D-C3D-C2D | -3.08 | 103.28      | 107.30   |
| 14  | aA    | 3129 | CL7  | O2A-CGA-O1A | -3.08 | 115.81      | 123.59   |
| 14  | cA    | 3103 | CL7  | C4D-C3D-C2D | -3.08 | 103.28      | 107.30   |
| 14  | aB    | 3026 | CL7  | CHB-C1B-NB  | -3.08 | 121.00      | 124.26   |
| 14  | bF    | 201  | CL7  | C4D-C3D-C2D | -3.08 | 103.28      | 107.30   |
| 14  | bB    | 820  | CL7  | C3B-C4B-NB  | -3.08 | 107.66      | 110.52   |
| 14  | bA    | 3125 | CL7  | CHB-C1B-NB  | -3.08 | 121.00      | 124.26   |
| 14  | aA    | 3141 | CL7  | O2A-CGA-O1A | -3.08 | 115.82      | 123.59   |
| 14  | aB    | 3020 | CL7  | CMB-C2B-C1B | 3.08  | 130.06      | 125.37   |
| 14  | cB    | 820  | CL7  | CAA-C2A-C3A | -3.08 | 104.35      | 112.78   |
| 14  | cA    | 3130 | CL7  | CHB-C1B-NB  | -3.08 | 121.00      | 124.26   |
| 14  | bB    | 811  | CL7  | C4D-C3D-C2D | -3.08 | 103.29      | 107.30   |
| 14  | bA    | 3128 | CL7  | CAC-C3C-C4C | 3.08  | 129.52      | 124.68   |
| 14  | aB    | 3013 | CL7  | O1D-CGD-CBD | -3.07 | 118.20      | 124.48   |
| 14  | aB    | 3011 | CL7  | CMB-C2B-C1B | 3.07  | 130.05      | 125.37   |
| 12  | aA    | 3101 | G9R  | CGD-CBD-CAD | -3.07 | 100.78      | 110.73   |
| 14  | cJ    | 101  | CL7  | C1D-ND-C4D  | -3.07 | 104.15      | 106.33   |
| 14  | bA    | 3130 | CL7  | CAA-C2A-C3A | -3.07 | 108.93      | 116.10   |
| 14  | bA    | 3114 | CL7  | C5-C3-C2    | -3.07 | 114.90      | 121.12   |
| 14  | bA    | 3106 | CL7  | C4D-C3D-C2D | -3.07 | 103.30      | 107.30   |
| 14  | bA    | 3109 | CL7  | C3A-C4A-CHB | -3.07 | 119.14      | 123.70   |
| 12  | aA    | 3101 | G9R  | O2D-CGD-CBD | 3.07  | 116.72      | 111.27   |
| 14  | bA    | 3102 | CL7  | C5-C3-C2    | -3.07 | 114.91      | 121.12   |
| 14  | cA    | 3132 | CL7  | CAC-C3C-C2C | -3.07 | 122.28      | 127.53   |
| 14  | aA    | 3122 | CL7  | O1D-CGD-CBD | -3.07 | 118.21      | 124.48   |
| 14  | cB    | 806  | CL7  | C6-C7-C8    | -3.07 | 106.01      | 115.92   |
| 14  | aB    | 3024 | CL7  | C3B-C4B-NB  | -3.07 | 107.67      | 110.52   |
| 12  | aA    | 3101 | G9R  | C4D-C3D-CAD | -3.07 | 104.48      | 108.10   |
| 14  | cA    | 3126 | CL7  | C4D-C3D-C2D | -3.07 | 103.31      | 107.30   |
| 14  | bA    | 3120 | CL7  | O2D-CGD-O1D | -3.06 | 117.85      | 123.84   |
| 14  | bB    | 818  | CL7  | O2D-CGD-O1D | -3.06 | 117.85      | 123.84   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | bA    | 3142 | CL7  | C1D-ND-C4D  | -3.06 | 104.16      | 106.33   |
| 14  | cA    | 3103 | CL7  | C1D-ND-C4D  | -3.06 | 104.16      | 106.33   |
| 14  | bA    | 3117 | CL7  | CMB-C2B-C1B | 3.06  | 130.03      | 125.37   |
| 14  | cB    | 808  | CL7  | C4D-C3D-C2D | -3.06 | 103.31      | 107.30   |
| 14  | bB    | 814  | CL7  | CHB-C1B-NB  | -3.06 | 121.02      | 124.26   |
| 14  | cB    | 826  | CL7  | CHB-C1B-NB  | -3.06 | 121.02      | 124.26   |
| 14  | bB    | 822  | CL7  | C3A-C4A-CHB | -3.06 | 119.16      | 123.70   |
| 14  | bA    | 3124 | CL7  | C1D-ND-C4D  | -3.06 | 104.16      | 106.33   |
| 14  | cB    | 824  | CL7  | C1A-NA-C4A  | 3.06  | 108.15      | 106.30   |
| 14  | bB    | 824  | CL7  | C3B-C4B-NB  | -3.06 | 107.68      | 110.52   |
| 14  | bA    | 3128 | CL7  | CHB-C1B-NB  | -3.06 | 121.02      | 124.26   |
| 14  | bA    | 3119 | CL7  | CAD-C3D-C2D | 3.06  | 151.04      | 144.44   |
| 14  | bJ    | 101  | CL7  | O2A-CGA-O1A | -3.05 | 115.69      | 123.30   |
| 14  | bA    | 3129 | CL7  | C4D-C3D-CAD | -3.05 | 105.37      | 107.42   |
| 14  | aL    | 203  | CL7  | CHC-C1C-NC  | -3.05 | 121.65      | 124.45   |
| 14  | bB    | 816  | CL7  | O2D-CGD-O1D | -3.05 | 117.87      | 123.84   |
| 14  | bA    | 3114 | CL7  | O2A-CGA-O1A | -3.05 | 115.89      | 123.59   |
| 14  | aA    | 3146 | CL7  | CHB-C1B-NB  | -3.05 | 121.03      | 124.26   |
| 13  | aA    | 3102 | PHO  | C3D-C4D-ND  | 3.05  | 111.88      | 107.72   |
| 14  | cA    | 3133 | CL7  | O1D-CGD-CBD | -3.05 | 118.25      | 124.48   |
| 14  | bA    | 3102 | CL7  | C6-C7-C8    | -3.05 | 106.07      | 115.92   |
| 14  | bK    | 101  | CL7  | CHB-C1B-NB  | -3.05 | 121.03      | 124.26   |
| 14  | aB    | 3010 | CL7  | O1D-CGD-CBD | -3.05 | 118.25      | 124.48   |
| 14  | bA    | 3131 | CL7  | C4D-C3D-C2D | -3.05 | 103.33      | 107.30   |
| 14  | bA    | 3122 | CL7  | O2A-CGA-O1A | -3.05 | 115.91      | 123.59   |
| 14  | cB    | 810  | CL7  | CHC-C4B-NB  | 3.05  | 127.48      | 124.26   |
| 14  | cA    | 3109 | CL7  | CED-O2D-CGD | 3.05  | 122.83      | 115.94   |
| 14  | aB    | 3002 | CL7  | C6-C5-C3    | -3.05 | 105.47      | 113.45   |
| 14  | aB    | 3010 | CL7  | C4D-C3D-C2D | -3.04 | 103.33      | 107.30   |
| 14  | aA    | 3143 | CL7  | CHB-C1B-NB  | -3.04 | 121.03      | 124.26   |
| 14  | aB    | 3021 | CL7  | CAA-C2A-C3A | -3.04 | 109.00      | 116.10   |
| 14  | cA    | 3112 | CL7  | CAA-C2A-C3A | -3.04 | 109.00      | 116.10   |
| 14  | cB    | 815  | CL7  | C1D-ND-C4D  | -3.04 | 104.17      | 106.33   |
| 14  | cB    | 811  | CL7  | C4D-C3D-C2D | -3.04 | 103.34      | 107.30   |
| 14  | cB    | 822  | CL7  | C3B-C4B-NB  | -3.04 | 107.69      | 110.52   |
| 14  | aF    | 201  | CL7  | C4D-C3D-C2D | -3.04 | 103.34      | 107.30   |
| 14  | aA    | 3142 | CL7  | O2D-CGD-O1D | -3.04 | 117.89      | 123.84   |
| 14  | cB    | 832  | CL7  | C4D-C3D-C2D | -3.04 | 103.34      | 107.30   |
| 14  | bB    | 817  | CL7  | CHC-C1C-NC  | -3.04 | 121.66      | 124.45   |
| 13  | bB    | 805  | PHO  | O2D-CGD-O1D | -3.04 | 117.90      | 123.84   |
| 14  | bA    | 3113 | CL7  | CAA-C2A-C3A | -3.04 | 109.01      | 116.10   |
| 12  | cA    | 3101 | G9R  | C2C-C1C-NC  | 3.04  | 112.82      | 109.97   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | cA    | 3108 | CL7  | CBD-CHA-C4D | -3.04 | 101.88      | 109.14   |
| 14  | bB    | 826  | CL7  | CMB-C2B-C1B | 3.03  | 129.99      | 125.37   |
| 14  | aA    | 3103 | CL7  | O2D-CGD-O1D | -3.03 | 117.91      | 123.84   |
| 14  | aB    | 3023 | CL7  | C3B-C4B-NB  | -3.03 | 107.70      | 110.52   |
| 14  | bB    | 826  | CL7  | C2D-C1D-ND  | -3.03 | 108.20      | 110.23   |
| 14  | bA    | 3110 | CL7  | C3B-C4B-NB  | -3.03 | 107.70      | 110.52   |
| 12  | bA    | 3101 | G9R  | CHD-C4C-NC  | 3.03  | 128.98      | 124.20   |
| 14  | bA    | 3112 | CL7  | O1D-CGD-CBD | -3.03 | 118.28      | 124.48   |
| 14  | bB    | 832  | CL7  | C7-C6-C5    | -3.03 | 105.13      | 113.36   |
| 14  | bA    | 3129 | CL7  | O1D-CGD-CBD | -3.03 | 118.29      | 124.48   |
| 14  | cA    | 3126 | CL7  | C4D-C3D-CAD | -3.03 | 105.38      | 107.42   |
| 14  | cB    | 807  | CL7  | C4-C3-C5    | -3.03 | 110.18      | 115.27   |
| 14  | cB    | 811  | CL7  | C1D-ND-C4D  | -3.03 | 104.18      | 106.33   |
| 14  | aA    | 3104 | CL7  | C4D-C3D-C2D | -3.03 | 103.35      | 107.30   |
| 14  | cA    | 3106 | CL7  | C4D-C3D-C2D | -3.03 | 103.35      | 107.30   |
| 14  | aA    | 3108 | CL7  | C4D-C3D-C2D | -3.03 | 103.36      | 107.30   |
| 14  | bB    | 818  | CL7  | O1D-CGD-CBD | -3.03 | 118.29      | 124.48   |
| 14  | cA    | 3139 | CL7  | C4D-C3D-C2D | -3.02 | 103.36      | 107.30   |
| 14  | cB    | 810  | CL7  | C4D-C3D-C2D | -3.02 | 103.36      | 107.30   |
| 14  | aA    | 3118 | CL7  | C3A-C4A-CHB | -3.02 | 119.21      | 123.70   |
| 14  | aA    | 3129 | CL7  | OBb-CAB-C3B | -3.02 | 118.86      | 125.69   |
| 14  | aA    | 3132 | CL7  | C4D-C3D-C2D | -3.02 | 103.36      | 107.30   |
| 14  | cA    | 3102 | CL7  | OBb-CAB-C3B | 3.02  | 132.51      | 125.69   |
| 14  | cB    | 809  | CL7  | C3A-C4A-CHB | -3.02 | 119.22      | 123.70   |
| 14  | cA    | 3133 | CL7  | CBD-CHA-C4D | -3.02 | 101.92      | 109.14   |
| 14  | bA    | 3133 | CL7  | CBD-CHA-C4D | -3.02 | 101.93      | 109.14   |
| 14  | cA    | 3120 | CL7  | CHC-C1C-NC  | -3.02 | 121.68      | 124.45   |
| 14  | aB    | 3009 | CL7  | CHC-C4B-NB  | 3.02  | 127.45      | 124.26   |
| 14  | cB    | 809  | CL7  | C1D-ND-C4D  | -3.01 | 104.19      | 106.33   |
| 14  | bA    | 3128 | CL7  | O1D-CGD-CBD | -3.01 | 118.32      | 124.48   |
| 14  | aB    | 3006 | CL7  | CMB-C2B-C1B | 3.01  | 129.96      | 125.37   |
| 14  | aB    | 3017 | CL7  | O1D-CGD-CBD | -3.01 | 118.32      | 124.48   |
| 14  | bA    | 3110 | CL7  | O1D-CGD-CBD | -3.01 | 118.32      | 124.48   |
| 14  | aB    | 3009 | CL7  | C6-C7-C8    | -3.01 | 106.19      | 115.92   |
| 14  | aB    | 3015 | CL7  | C4-C3-C5    | -3.01 | 107.95      | 114.60   |
| 14  | aB    | 3021 | CL7  | O1D-CGD-CBD | -3.01 | 118.33      | 124.48   |
| 12  | bA    | 3101 | G9R  | CMA-C3A-C2A | -3.01 | 101.69      | 113.83   |
| 14  | bA    | 3141 | CL7  | CBD-CHA-C4D | -3.01 | 101.94      | 109.14   |
| 14  | aB    | 3012 | CL7  | CMB-C2B-C1B | 3.01  | 129.95      | 125.37   |
| 14  | cB    | 810  | CL7  | C6-C7-C8    | -3.01 | 106.20      | 115.92   |
| 14  | bB    | 812  | CL7  | C1D-ND-C4D  | -3.01 | 104.20      | 106.33   |
| 14  | cB    | 812  | CL7  | C1D-ND-C4D  | -3.01 | 104.20      | 106.33   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | bA    | 3139 | CL7  | CHB-C1B-NB  | -3.00 | 121.08      | 124.26   |
| 14  | cA    | 3106 | CL7  | C6-C7-C8    | -3.00 | 106.22      | 115.92   |
| 14  | bA    | 3122 | CL7  | C3A-C2A-C1A | 3.00  | 105.83      | 101.34   |
| 14  | aA    | 3131 | CL7  | CAA-C2A-C3A | -3.00 | 109.10      | 116.10   |
| 14  | aB    | 3011 | CL7  | C1D-ND-C4D  | -3.00 | 104.20      | 106.33   |
| 14  | aA    | 3124 | CL7  | O1A-CGA-CBA | -3.00 | 112.04      | 123.73   |
| 14  | aA    | 3117 | CL7  | O2D-CGD-O1D | -3.00 | 117.98      | 123.84   |
| 14  | cB    | 827  | CL7  | C1D-ND-C4D  | -3.00 | 104.21      | 106.33   |
| 14  | aB    | 3017 | CL7  | O2D-CGD-O1D | -3.00 | 117.98      | 123.84   |
| 14  | aA    | 3128 | CL7  | C1-C2-C3    | -3.00 | 120.86      | 126.04   |
| 14  | aA    | 3107 | CL7  | CBD-CHA-C4D | -3.00 | 101.98      | 109.14   |
| 14  | bA    | 3128 | CL7  | C1-C2-C3    | -2.99 | 120.86      | 126.04   |
| 14  | bB    | 811  | CL7  | CHB-C1B-NB  | -2.99 | 121.09      | 124.26   |
| 14  | cB    | 810  | CL7  | O1D-CGD-CBD | -2.99 | 118.36      | 124.48   |
| 14  | aJ    | 101  | CL7  | CHB-C1B-NB  | -2.99 | 121.09      | 124.26   |
| 14  | bJ    | 101  | CL7  | CMB-C2B-C1B | 2.99  | 129.92      | 125.37   |
| 14  | cB    | 820  | CL7  | CHC-C1C-NC  | -2.99 | 121.71      | 124.45   |
| 14  | cA    | 3122 | CL7  | C2A-C1A-CHA | -2.99 | 120.39      | 126.36   |
| 14  | cA    | 3114 | CL7  | C2A-C1A-CHA | -2.99 | 120.39      | 126.36   |
| 14  | bA    | 3139 | CL7  | C6-C5-C3    | -2.99 | 105.63      | 113.45   |
| 14  | aA    | 3121 | CL7  | O1D-CGD-CBD | -2.99 | 118.38      | 124.48   |
| 14  | bA    | 3130 | CL7  | O2D-CGD-O1D | -2.98 | 118.00      | 123.84   |
| 14  | bB    | 804  | CL7  | CMB-C2B-C1B | 2.98  | 129.91      | 125.37   |
| 12  | cA    | 3101 | G9R  | CHD-C4C-NC  | 2.98  | 128.90      | 124.20   |
| 14  | bB    | 814  | CL7  | O1D-CGD-CBD | -2.98 | 118.38      | 124.48   |
| 14  | aL    | 202  | CL7  | C6-C5-C3    | -2.98 | 105.64      | 113.45   |
| 14  | cB    | 820  | CL7  | O2A-CGA-O1A | -2.98 | 116.07      | 123.59   |
| 14  | aA    | 3146 | CL7  | O1D-CGD-CBD | -2.98 | 118.39      | 124.48   |
| 14  | cA    | 3113 | CL7  | CBD-CHA-C4D | -2.98 | 102.01      | 109.14   |
| 14  | bA    | 3140 | CL7  | C3A-C2A-C1A | 2.98  | 105.80      | 101.34   |
| 14  | bB    | 833  | CL7  | C3A-C4A-CHB | -2.97 | 119.29      | 123.70   |
| 14  | cL    | 204  | CL7  | O1D-CGD-CBD | -2.97 | 118.40      | 124.48   |
| 14  | cB    | 822  | CL7  | C4D-C3D-C2D | -2.97 | 103.42      | 107.30   |
| 14  | cA    | 3109 | CL7  | C3A-C4A-CHB | -2.97 | 119.29      | 123.70   |
| 14  | bA    | 3128 | CL7  | C1D-ND-C4D  | -2.97 | 104.22      | 106.33   |
| 14  | cK    | 101  | CL7  | CHC-C1C-NC  | -2.97 | 121.72      | 124.45   |
| 14  | cA    | 3139 | CL7  | C6-C5-C3    | -2.97 | 105.66      | 113.45   |
| 14  | aA    | 3107 | CL7  | C16-C15-C13 | -2.97 | 106.31      | 115.92   |
| 14  | aB    | 3019 | CL7  | CMB-C2B-C1B | 2.97  | 129.89      | 125.37   |
| 14  | aA    | 3123 | CL7  | C3A-C4A-CHB | -2.97 | 119.29      | 123.70   |
| 13  | bB    | 801  | PHO  | C3D-C4D-ND  | 2.97  | 111.77      | 107.72   |
| 14  | bA    | 3123 | CL7  | C1D-ND-C4D  | -2.97 | 104.23      | 106.33   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | aA    | 3143 | CL7  | C4D-C3D-C2D | -2.97 | 103.43      | 107.30   |
| 14  | cB    | 827  | CL7  | CAC-C3C-C4C | 2.97  | 129.35      | 124.68   |
| 14  | cL    | 204  | CL7  | CHC-C1C-NC  | -2.97 | 121.73      | 124.45   |
| 14  | bA    | 3127 | CL7  | C1-C2-C3    | -2.97 | 120.91      | 126.04   |
| 14  | cB    | 817  | CL7  | CHC-C1C-NC  | -2.97 | 121.73      | 124.45   |
| 14  | bB    | 821  | CL7  | CMB-C2B-C1B | 2.97  | 129.89      | 125.37   |
| 14  | aB    | 3011 | CL7  | C3A-C2A-C1A | -2.97 | 98.10       | 101.64   |
| 14  | bA    | 3140 | CL7  | C6-C7-C8    | -2.97 | 106.33      | 115.92   |
| 14  | aA    | 3113 | CL7  | CAA-C2A-C3A | -2.97 | 109.18      | 116.10   |
| 14  | cB    | 833  | CL7  | CBD-CHA-C4D | -2.97 | 102.05      | 109.14   |
| 14  | cL    | 203  | CL7  | CBD-CHA-C4D | -2.97 | 102.05      | 109.14   |
| 14  | bB    | 803  | CL7  | O2A-CGA-O1A | -2.97 | 116.11      | 123.59   |
| 12  | cA    | 3101 | G9R  | C1-C2-C3    | -2.97 | 120.91      | 126.04   |
| 14  | cB    | 806  | CL7  | C5-C3-C2    | -2.97 | 115.11      | 121.12   |
| 14  | aB    | 3013 | CL7  | CHB-C1B-NB  | -2.97 | 121.12      | 124.26   |
| 14  | cJ    | 101  | CL7  | CHB-C1B-NB  | -2.96 | 121.12      | 124.26   |
| 14  | cB    | 832  | CL7  | C7-C6-C5    | -2.96 | 105.31      | 113.36   |
| 14  | aA    | 3131 | CL7  | C3B-C4B-NB  | -2.96 | 107.77      | 110.52   |
| 14  | cB    | 832  | CL7  | C3B-C4B-NB  | -2.96 | 107.77      | 110.52   |
| 14  | cA    | 3110 | CL7  | O1D-CGD-CBD | -2.96 | 118.43      | 124.48   |
| 14  | bB    | 818  | CL7  | C4D-C3D-C2D | -2.96 | 103.44      | 107.30   |
| 14  | bB    | 820  | CL7  | C4D-C3D-C2D | -2.96 | 103.44      | 107.30   |
| 14  | cB    | 818  | CL7  | C4D-C3D-C2D | -2.96 | 103.44      | 107.30   |
| 14  | bA    | 3121 | CL7  | O1D-CGD-CBD | -2.96 | 118.43      | 124.48   |
| 14  | cA    | 3124 | CL7  | C4D-C3D-C2D | -2.96 | 103.44      | 107.30   |
| 14  | aA    | 3120 | CL7  | CAD-C3D-C2D | 2.96  | 150.82      | 144.44   |
| 14  | cB    | 806  | CL7  | OBD-CAD-C3D | -2.96 | 121.41      | 128.52   |
| 14  | cA    | 3107 | CL7  | C3A-C4A-CHB | -2.96 | 119.31      | 123.70   |
| 14  | cA    | 3116 | CL7  | O2A-CGA-O1A | -2.96 | 116.13      | 123.59   |
| 14  | aL    | 203  | CL7  | C1-O2A-CGA  | -2.96 | 108.69      | 116.44   |
| 13  | cB    | 801  | PHO  | C3D-C4D-ND  | 2.95  | 111.75      | 107.72   |
| 12  | bA    | 3101 | G9R  | CHB-C1B-C2B | -2.95 | 118.90      | 127.24   |
| 14  | cB    | 815  | CL7  | C4D-C3D-C2D | -2.95 | 103.45      | 107.30   |
| 14  | aA    | 3132 | CL7  | CMB-C2B-C1B | 2.95  | 129.86      | 125.37   |
| 14  | bA    | 3139 | CL7  | O2A-CGA-O1A | -2.95 | 116.15      | 123.59   |
| 14  | aA    | 3118 | CL7  | CHB-C1B-NB  | -2.95 | 121.14      | 124.26   |
| 14  | cA    | 3102 | CL7  | O2A-CGA-CBA | 2.95  | 121.16      | 111.91   |
| 14  | cA    | 3122 | CL7  | CMB-C2B-C1B | 2.95  | 129.86      | 125.37   |
| 12  | aA    | 3101 | G9R  | CHC-C1C-C2C | -2.95 | 118.54      | 126.73   |
| 14  | aB    | 3031 | CL7  | C3B-C4B-NB  | -2.95 | 107.78      | 110.52   |
| 14  | aA    | 3109 | CL7  | C4D-C3D-C2D | -2.95 | 103.46      | 107.30   |
| 14  | cA    | 3113 | CL7  | OBD-CAD-C3D | -2.94 | 121.44      | 128.52   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | cL    | 204  | CL7  | O2A-C1-C2   | -2.94 | 100.90      | 108.64   |
| 14  | bB    | 811  | CL7  | C3B-C4B-NB  | -2.94 | 107.78      | 110.52   |
| 14  | cA    | 3109 | CL7  | CAA-C2A-C3A | -2.94 | 109.23      | 116.10   |
| 14  | bA    | 3123 | CL7  | CMB-C2B-C1B | 2.94  | 129.85      | 125.37   |
| 14  | cA    | 3131 | CL7  | C4D-C3D-C2D | -2.94 | 103.47      | 107.30   |
| 14  | aJ    | 101  | CL7  | O2A-CGA-O1A | -2.94 | 115.97      | 123.30   |
| 14  | cA    | 3132 | CL7  | CMB-C2B-C1B | 2.94  | 129.85      | 125.37   |
| 14  | cA    | 3132 | CL7  | CED-O2D-CGD | 2.94  | 122.59      | 115.94   |
| 14  | cA    | 3117 | CL7  | CHC-C1C-NC  | -2.94 | 121.75      | 124.45   |
| 14  | cA    | 3126 | CL7  | C3D-C4D-ND  | 2.94  | 114.38      | 110.17   |
| 14  | bA    | 3112 | CL7  | CAA-C2A-C3A | -2.94 | 109.24      | 116.10   |
| 14  | bA    | 3129 | CL7  | CAD-C3D-C2D | 2.94  | 150.79      | 144.44   |
| 14  | aA    | 3113 | CL7  | O1D-CGD-CBD | -2.94 | 118.47      | 124.48   |
| 12  | cA    | 3101 | G9R  | O2A-C1-C2   | -2.94 | 100.91      | 108.64   |
| 14  | aA    | 3142 | CL7  | CHB-C1B-NB  | -2.94 | 121.15      | 124.26   |
| 14  | bA    | 3114 | CL7  | C2A-C1A-CHA | -2.94 | 120.49      | 126.36   |
| 14  | cJ    | 101  | CL7  | C3B-C4B-NB  | -2.94 | 107.79      | 110.52   |
| 14  | aA    | 3103 | CL7  | C2D-C1D-ND  | -2.94 | 108.26      | 110.23   |
| 14  | bB    | 815  | CL7  | C4D-C3D-C2D | -2.94 | 103.47      | 107.30   |
| 14  | bJ    | 101  | CL7  | C3B-C4B-NB  | -2.94 | 107.79      | 110.52   |
| 13  | aA    | 3102 | PHO  | CAA-CBA-CGA | -2.94 | 104.67      | 113.25   |
| 14  | bL    | 203  | CL7  | CED-O2D-CGD | 2.94  | 122.58      | 115.94   |
| 14  | aJ    | 101  | CL7  | CMB-C2B-C1B | 2.93  | 129.84      | 125.37   |
| 14  | cB    | 825  | CL7  | CMB-C2B-C1B | 2.93  | 129.84      | 125.37   |
| 14  | bA    | 3112 | CL7  | C3B-C4B-NB  | -2.93 | 107.79      | 110.52   |
| 14  | cA    | 3105 | CL7  | O1D-CGD-CBD | -2.93 | 118.48      | 124.48   |
| 17  | cA    | 3143 | PQN  | C16-C17-C18 | -2.93 | 106.44      | 115.92   |
| 14  | aA    | 3128 | CL7  | CHB-C1B-NB  | -2.93 | 121.16      | 124.26   |
| 14  | aA    | 3110 | CL7  | C3B-C4B-NB  | -2.93 | 107.80      | 110.52   |
| 14  | aB    | 3032 | CL7  | C1-C2-C3    | -2.93 | 120.98      | 126.04   |
| 14  | aA    | 3128 | CL7  | C1D-ND-C4D  | -2.93 | 104.25      | 106.33   |
| 14  | cL    | 203  | CL7  | C6-C5-C3    | -2.93 | 105.78      | 113.45   |
| 14  | cB    | 818  | CL7  | C3B-C4B-NB  | -2.93 | 107.80      | 110.52   |
| 14  | bA    | 3124 | CL7  | C4D-C3D-C2D | -2.93 | 103.49      | 107.30   |
| 14  | bB    | 808  | CL7  | C6-C5-C3    | -2.93 | 105.78      | 113.45   |
| 14  | aA    | 3132 | CL7  | O2D-CGD-O1D | -2.93 | 118.12      | 123.84   |
| 14  | aA    | 3115 | CL7  | O2A-CGA-O1A | -2.93 | 116.21      | 123.59   |
| 14  | aA    | 3133 | CL7  | C1-C2-C3    | -2.92 | 120.98      | 126.04   |
| 14  | cA    | 3113 | CL7  | C1D-ND-C4D  | -2.92 | 104.26      | 106.33   |
| 14  | cL    | 203  | CL7  | O2A-CGA-O1A | -2.92 | 116.22      | 123.59   |
| 14  | cJ    | 101  | CL7  | CMB-C2B-C1B | 2.92  | 129.82      | 125.37   |
| 14  | cJ    | 101  | CL7  | O2A-CGA-O1A | -2.92 | 116.02      | 123.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | cA    | 3128 | CL7  | C1-C2-C3    | -2.92 | 120.99      | 126.04   |
| 14  | cB    | 815  | CL7  | O2D-CGD-O1D | -2.92 | 118.12      | 123.84   |
| 14  | bA    | 3116 | CL7  | C4D-C3D-C2D | -2.92 | 103.49      | 107.30   |
| 14  | aB    | 3016 | CL7  | CHC-C1C-NC  | -2.92 | 121.77      | 124.45   |
| 14  | bB    | 808  | CL7  | CHC-C1C-NC  | -2.92 | 121.77      | 124.45   |
| 14  | bA    | 3106 | CL7  | CBD-CHA-C4D | -2.92 | 102.15      | 109.14   |
| 14  | aA    | 3146 | CL7  | CMB-C2B-C1B | 2.92  | 129.82      | 125.37   |
| 14  | aA    | 3119 | CL7  | CHC-C1C-NC  | -2.92 | 121.77      | 124.45   |
| 14  | cA    | 3104 | CL7  | O2D-CGD-O1D | -2.92 | 118.13      | 123.84   |
| 14  | aL    | 202  | CL7  | CHC-C1C-NC  | -2.92 | 121.77      | 124.45   |
| 14  | bA    | 3108 | CL7  | O2D-CGD-O1D | -2.92 | 118.14      | 123.84   |
| 14  | bB    | 822  | CL7  | O1D-CGD-CBD | -2.92 | 118.52      | 124.48   |
| 14  | cA    | 3114 | CL7  | C4-C3-C5    | -2.91 | 110.37      | 115.27   |
| 14  | aB    | 3018 | CL7  | C3A-C4A-CHB | -2.91 | 119.38      | 123.70   |
| 14  | aA    | 3131 | CL7  | CHB-C1B-NB  | -2.91 | 121.17      | 124.26   |
| 14  | aB    | 3025 | CL7  | CHB-C1B-NB  | -2.91 | 121.17      | 124.26   |
| 14  | aA    | 3129 | CL7  | C4C-C3C-C2C | 2.91  | 110.92      | 107.13   |
| 14  | cB    | 824  | CL7  | C3B-C4B-NB  | -2.91 | 107.81      | 110.52   |
| 14  | bA    | 3113 | CL7  | CBD-CHA-C4D | -2.91 | 102.18      | 109.14   |
| 14  | bA    | 3113 | CL7  | OBD-CAD-C3D | -2.91 | 121.52      | 128.52   |
| 14  | cB    | 823  | CL7  | C3B-C4B-NB  | -2.91 | 107.82      | 110.52   |
| 14  | bA    | 3108 | CL7  | CBD-CHA-C4D | -2.91 | 102.19      | 109.14   |
| 14  | cA    | 3130 | CL7  | C3B-C4B-NB  | -2.91 | 107.82      | 110.52   |
| 14  | aA    | 3108 | CL7  | CMB-C2B-C1B | 2.91  | 129.80      | 125.37   |
| 14  | cA    | 3141 | CL7  | C6-C7-C8    | -2.91 | 106.52      | 115.92   |
| 14  | cA    | 3122 | CL7  | CHB-C1B-NB  | -2.91 | 121.18      | 124.26   |
| 14  | aA    | 3140 | CL7  | CHC-C4B-NB  | 2.91  | 127.33      | 124.26   |
| 14  | aA    | 3123 | CL7  | CHC-C1C-NC  | -2.91 | 121.78      | 124.45   |
| 14  | cB    | 806  | CL7  | C1-C2-C3    | -2.91 | 121.02      | 126.04   |
| 14  | aB    | 3019 | CL7  | CHC-C1C-NC  | -2.91 | 121.78      | 124.45   |
| 14  | bB    | 820  | CL7  | C2A-C1A-CHA | -2.90 | 120.55      | 126.36   |
| 14  | bB    | 816  | CL7  | C1A-NA-C4A  | -2.90 | 104.54      | 106.30   |
| 14  | bK    | 101  | CL7  | CMB-C2B-C1B | 2.90  | 129.79      | 125.37   |
| 14  | aA    | 3120 | CL7  | OBD-CAD-C3D | -2.90 | 121.53      | 128.52   |
| 14  | bB    | 827  | CL7  | O1D-CGD-CBD | -2.90 | 118.54      | 124.48   |
| 14  | bA    | 3109 | CL7  | C3B-C4B-NB  | -2.90 | 107.82      | 110.52   |
| 14  | aA    | 3130 | CL7  | C1C-C2C-C3C | 2.90  | 111.18      | 106.94   |
| 14  | bA    | 3110 | CL7  | C4D-C3D-C2D | -2.90 | 103.52      | 107.30   |
| 14  | cL    | 203  | CL7  | CHC-C4B-NB  | 2.90  | 127.33      | 124.26   |
| 14  | bB    | 818  | CL7  | C3B-C4B-NB  | -2.90 | 107.82      | 110.52   |
| 14  | aA    | 3110 | CL7  | C1A-NA-C4A  | -2.90 | 104.55      | 106.30   |
| 14  | bB    | 826  | CL7  | CHB-C1B-NB  | -2.90 | 121.19      | 124.26   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | aA    | 3120 | CL7  | C2A-C1A-CHA | -2.90 | 120.56      | 126.36   |
| 14  | bB    | 807  | CL7  | O2A-CGA-O1A | -2.90 | 116.27      | 123.59   |
| 14  | aA    | 3141 | CL7  | O1D-CGD-CBD | -2.90 | 118.55      | 124.48   |
| 14  | bB    | 815  | CL7  | C1D-ND-C4D  | -2.90 | 104.28      | 106.33   |
| 17  | bA    | 3143 | PQN  | C16-C17-C18 | -2.90 | 106.55      | 115.92   |
| 14  | aB    | 3023 | CL7  | C6-C5-C3    | -2.90 | 105.85      | 113.45   |
| 14  | aA    | 3111 | CL7  | O1D-CGD-CBD | -2.90 | 118.55      | 124.48   |
| 14  | aA    | 3133 | CL7  | O2A-CGA-O1A | -2.90 | 116.28      | 123.59   |
| 13  | cB    | 801  | PHO  | CAA-CBA-CGA | -2.90 | 104.78      | 113.25   |
| 14  | aB    | 3007 | CL7  | C4D-C3D-C2D | -2.90 | 103.52      | 107.30   |
| 14  | aA    | 3109 | CL7  | CHB-C1B-NB  | -2.90 | 121.19      | 124.26   |
| 14  | bB    | 815  | CL7  | C3B-C4B-NB  | -2.89 | 107.83      | 110.52   |
| 14  | cA    | 3142 | CL7  | C3B-C4B-NB  | -2.89 | 107.83      | 110.52   |
| 14  | cA    | 3142 | CL7  | C4D-C3D-C2D | -2.89 | 103.53      | 107.30   |
| 14  | bA    | 3109 | CL7  | CAA-C2A-C3A | -2.89 | 109.34      | 116.10   |
| 14  | cA    | 3119 | CL7  | C2A-C1A-CHA | -2.89 | 120.58      | 126.36   |
| 14  | cA    | 3128 | CL7  | C4C-C3C-C2C | 2.89  | 110.90      | 107.13   |
| 14  | bA    | 3132 | CL7  | CAC-C3C-C2C | -2.89 | 122.58      | 127.53   |
| 14  | bA    | 3140 | CL7  | O1D-CGD-CBD | -2.89 | 118.57      | 124.48   |
| 14  | aA    | 3125 | CL7  | C4D-C3D-C2D | -2.89 | 103.53      | 107.30   |
| 14  | cA    | 3122 | CL7  | O2A-CGA-O1A | -2.89 | 116.30      | 123.59   |
| 14  | cA    | 3106 | CL7  | CBD-CHA-C4D | -2.89 | 102.23      | 109.14   |
| 14  | aB    | 3009 | CL7  | C4D-C3D-C2D | -2.89 | 103.54      | 107.30   |
| 14  | aA    | 3104 | CL7  | C3A-C4A-CHB | -2.89 | 119.42      | 123.70   |
| 14  | aB    | 3032 | CL7  | CHC-C1C-NC  | -2.88 | 121.80      | 124.45   |
| 14  | bA    | 3130 | CL7  | C3B-C4B-NB  | -2.88 | 107.84      | 110.52   |
| 14  | bB    | 833  | CL7  | C1D-ND-C4D  | -2.88 | 104.29      | 106.33   |
| 14  | aA    | 3143 | CL7  | C1-C2-C3    | -2.88 | 121.06      | 126.04   |
| 14  | bK    | 101  | CL7  | OBD-CAD-C3D | -2.88 | 123.97      | 128.74   |
| 14  | bB    | 810  | CL7  | CAA-C2A-C3A | -2.88 | 104.89      | 112.78   |
| 14  | bB    | 816  | CL7  | C4D-C3D-C2D | -2.88 | 103.55      | 107.30   |
| 14  | aB    | 3017 | CL7  | C4D-C3D-C2D | -2.88 | 103.55      | 107.30   |
| 14  | aL    | 204  | CL7  | C1D-ND-C4D  | -2.88 | 104.29      | 106.33   |
| 14  | bB    | 833  | CL7  | O1D-CGD-CBD | -2.88 | 118.59      | 124.48   |
| 14  | aA    | 3143 | CL7  | C3A-C2A-C1A | 2.88  | 105.65      | 101.34   |
| 14  | aA    | 3118 | CL7  | CHC-C1C-NC  | -2.88 | 121.81      | 124.45   |
| 14  | aA    | 3132 | CL7  | C3B-C4B-NB  | -2.88 | 107.84      | 110.52   |
| 14  | aA    | 3133 | CL7  | CMB-C2B-C1B | 2.88  | 129.75      | 125.37   |
| 14  | cB    | 824  | CL7  | O2D-CGD-O1D | -2.88 | 118.21      | 123.84   |
| 14  | bA    | 3132 | CL7  | C1-C2-C3    | -2.88 | 121.07      | 126.04   |
| 14  | aB    | 3014 | CL7  | CHB-C1B-NB  | -2.88 | 121.21      | 124.26   |
| 13  | aB    | 3004 | PHO  | CMC-C2C-C1C | -2.88 | 119.30      | 124.73   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | bA    | 3106 | CL7  | C6-C7-C8    | -2.87 | 106.63      | 115.92   |
| 14  | aA    | 3129 | CL7  | C3D-C4D-ND  | 2.87  | 114.29      | 110.17   |
| 17  | aB    | 3027 | PQN  | C2M-C2-C1   | -2.87 | 111.51      | 116.27   |
| 14  | aA    | 3140 | CL7  | C4D-C3D-C2D | -2.87 | 103.56      | 107.30   |
| 14  | cK    | 101  | CL7  | CAD-CBD-CHA | -2.87 | 101.90      | 105.14   |
| 14  | bB    | 807  | CL7  | C3B-C4B-NB  | -2.87 | 107.85      | 110.52   |
| 14  | bB    | 831  | CL7  | O2D-CGD-O1D | -2.87 | 118.22      | 123.84   |
| 14  | aA    | 3109 | CL7  | CAC-C3C-C2C | -2.87 | 122.62      | 127.53   |
| 14  | cA    | 3119 | CL7  | CAD-C3D-C2D | 2.87  | 150.64      | 144.44   |
| 14  | bA    | 3141 | CL7  | CMB-C2B-C1B | 2.87  | 129.74      | 125.37   |
| 14  | cA    | 3142 | CL7  | C1D-ND-C4D  | -2.87 | 104.30      | 106.33   |
| 14  | cL    | 205  | CL7  | C3A-C4A-CHB | -2.87 | 119.44      | 123.70   |
| 14  | aA    | 3129 | CL7  | O2D-CGD-CBD | 2.87  | 116.37      | 111.27   |
| 17  | cB    | 828  | PQN  | C2M-C2-C1   | -2.87 | 111.51      | 116.27   |
| 14  | cA    | 3122 | CL7  | C3A-C2A-C1A | 2.87  | 105.64      | 101.34   |
| 14  | aA    | 3105 | CL7  | C3A-C4A-CHB | -2.87 | 119.44      | 123.70   |
| 14  | cA    | 3118 | CL7  | C3D-C4D-ND  | 2.87  | 114.28      | 110.17   |
| 14  | aA    | 3121 | CL7  | C4D-C3D-C2D | -2.87 | 103.56      | 107.30   |
| 14  | aB    | 3009 | CL7  | C3A-C4A-CHB | -2.87 | 119.44      | 123.70   |
| 14  | bB    | 833  | CL7  | CBD-CHA-C4D | -2.87 | 102.28      | 109.14   |
| 14  | cB    | 824  | CL7  | C6-C5-C3    | -2.87 | 105.94      | 113.45   |
| 14  | aK    | 101  | CL7  | CHC-C1C-NC  | -2.87 | 121.82      | 124.45   |
| 14  | bL    | 203  | CL7  | CHC-C1C-NC  | -2.87 | 121.82      | 124.45   |
| 14  | bA    | 3128 | CL7  | O2A-CGA-O1A | -2.86 | 116.36      | 123.59   |
| 14  | cB    | 820  | CL7  | C3A-C4A-CHB | -2.86 | 119.45      | 123.70   |
| 14  | bA    | 3127 | CL7  | C2A-C1A-CHA | -2.86 | 120.64      | 126.36   |
| 14  | aA    | 3115 | CL7  | C1-O2A-CGA  | -2.86 | 108.93      | 116.44   |
| 14  | cB    | 831  | CL7  | O2D-CGD-O1D | -2.86 | 118.24      | 123.84   |
| 14  | aA    | 3132 | CL7  | CHB-C1B-NB  | -2.86 | 121.23      | 124.26   |
| 14  | cA    | 3116 | CL7  | CHB-C1B-NB  | -2.86 | 121.23      | 124.26   |
| 14  | bA    | 3139 | CL7  | C4D-C3D-C2D | -2.86 | 103.57      | 107.30   |
| 12  | cA    | 3101 | G9R  | CHB-C1B-C2B | -2.86 | 119.16      | 127.24   |
| 14  | bA    | 3104 | CL7  | O2D-CGD-O1D | -2.86 | 118.25      | 123.84   |
| 14  | cA    | 3105 | CL7  | C4C-C3C-C2C | 2.86  | 110.85      | 107.13   |
| 14  | aB    | 3014 | CL7  | C4D-C3D-C2D | -2.86 | 103.58      | 107.30   |
| 14  | cA    | 3109 | CL7  | C3B-C4B-NB  | -2.86 | 107.86      | 110.52   |
| 14  | aA    | 3106 | CL7  | O1D-CGD-CBD | -2.86 | 118.64      | 124.48   |
| 14  | aB    | 3025 | CL7  | C2A-C1A-CHA | -2.86 | 120.65      | 126.36   |
| 14  | cA    | 3128 | CL7  | C3A-C4A-CHB | -2.86 | 119.46      | 123.70   |
| 14  | aA    | 3143 | CL7  | C3B-C4B-NB  | -2.86 | 107.86      | 110.52   |
| 14  | aK    | 101  | CL7  | CHB-C1B-NB  | -2.86 | 121.23      | 124.26   |
| 14  | cA    | 3139 | CL7  | CMB-C2B-C1B | 2.85  | 129.72      | 125.37   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | aA    | 3110 | CL7  | CED-O2D-CGD | 2.85  | 122.39      | 115.94   |
| 14  | bA    | 3132 | CL7  | C3A-C2A-C1A | 2.85  | 105.61      | 101.34   |
| 14  | bB    | 807  | CL7  | C4-C3-C5    | -2.85 | 110.47      | 115.27   |
| 14  | aB    | 3008 | CL7  | C3A-C4A-CHB | -2.85 | 119.47      | 123.70   |
| 14  | bB    | 832  | CL7  | O1D-CGD-CBD | -2.85 | 118.65      | 124.48   |
| 14  | aB    | 3007 | CL7  | C1-O2A-CGA  | -2.85 | 108.96      | 116.44   |
| 14  | aB    | 3032 | CL7  | C1D-ND-C4D  | -2.85 | 104.31      | 106.33   |
| 14  | cA    | 3106 | CL7  | C16-C15-C13 | -2.85 | 106.70      | 115.92   |
| 14  | cB    | 814  | CL7  | CHB-C1B-NB  | -2.85 | 121.24      | 124.26   |
| 14  | aB    | 3017 | CL7  | C3B-C4B-NB  | -2.85 | 107.87      | 110.52   |
| 14  | cA    | 3116 | CL7  | C4D-C3D-C2D | -2.85 | 103.58      | 107.30   |
| 14  | bB    | 825  | CL7  | C3B-C4B-NB  | -2.85 | 107.87      | 110.52   |
| 13  | aB    | 3004 | PHO  | OBD-CAD-CBD | -2.85 | 121.64      | 125.82   |
| 14  | bB    | 832  | CL7  | CAC-C3C-C2C | -2.85 | 122.66      | 127.53   |
| 14  | cA    | 3109 | CL7  | O1D-CGD-CBD | -2.85 | 118.66      | 124.48   |
| 14  | bA    | 3132 | CL7  | CED-O2D-CGD | 2.85  | 122.38      | 115.94   |
| 12  | bA    | 3101 | G9R  | CGD-CBD-CAD | -2.85 | 101.52      | 110.73   |
| 14  | aB    | 3019 | CL7  | O2A-CGA-O1A | -2.85 | 116.41      | 123.59   |
| 14  | aA    | 3119 | CL7  | C3D-C4D-ND  | 2.85  | 114.25      | 110.17   |
| 14  | bA    | 3122 | CL7  | CHA-C1A-NA  | -2.84 | 119.25      | 125.98   |
| 14  | bB    | 819  | CL7  | C6-C7-C8    | -2.84 | 106.73      | 115.92   |
| 14  | bB    | 804  | CL7  | CHB-C1B-NB  | -2.84 | 121.25      | 124.26   |
| 14  | aB    | 3009 | CL7  | C4-C3-C5    | -2.84 | 110.49      | 115.27   |
| 14  | bA    | 3124 | CL7  | CMB-C2B-C3B | -2.84 | 119.70      | 126.59   |
| 14  | aA    | 3123 | CL7  | CMB-C2B-C1B | 2.84  | 129.69      | 125.37   |
| 14  | aL    | 203  | CL7  | C11-C12-C13 | -2.84 | 106.74      | 115.92   |
| 14  | aA    | 3111 | CL7  | C3B-C4B-NB  | -2.84 | 107.88      | 110.52   |
| 14  | cA    | 3119 | CL7  | OBD-CAD-C3D | -2.84 | 121.69      | 128.52   |
| 14  | cA    | 3120 | CL7  | C1D-ND-C4D  | -2.84 | 104.32      | 106.33   |
| 14  | aA    | 3141 | CL7  | C4D-C3D-C2D | -2.84 | 103.60      | 107.30   |
| 14  | aB    | 3025 | CL7  | C3D-C4D-ND  | 2.84  | 114.24      | 110.17   |
| 14  | bA    | 3132 | CL7  | O1D-CGD-CBD | -2.84 | 118.68      | 124.48   |
| 14  | aB    | 3022 | CL7  | C3B-C4B-NB  | -2.83 | 107.89      | 110.52   |
| 14  | bA    | 3131 | CL7  | CMB-C2B-C1B | 2.83  | 129.68      | 125.37   |
| 14  | cB    | 809  | CL7  | O2D-CGD-O1D | -2.83 | 118.30      | 123.84   |
| 14  | cB    | 826  | CL7  | CMB-C2B-C1B | 2.83  | 129.68      | 125.37   |
| 14  | aB    | 3016 | CL7  | C3B-C4B-NB  | -2.83 | 107.89      | 110.52   |
| 14  | bA    | 3140 | CL7  | CHC-C1C-NC  | -2.83 | 121.85      | 124.45   |
| 14  | cB    | 824  | CL7  | CAD-C3D-C2D | 2.83  | 150.55      | 144.44   |
| 14  | aF    | 201  | CL7  | CAD-C3D-C2D | 2.83  | 150.55      | 144.44   |
| 14  | aA    | 3103 | CL7  | C2B-C1B-NB  | -2.83 | 108.33      | 110.23   |
| 17  | cB    | 828  | PQN  | O4-C4-C5    | -2.83 | 116.98      | 121.56   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | bA    | 3105 | CL7  | C4C-C3C-C2C | 2.83  | 110.81      | 107.13   |
| 14  | aB    | 3002 | CL7  | OBD-CAD-C3D | -2.83 | 121.72      | 128.52   |
| 14  | aJ    | 101  | CL7  | C3B-C4B-NB  | -2.83 | 107.89      | 110.52   |
| 14  | aA    | 3119 | CL7  | CHB-C1B-NB  | -2.82 | 121.27      | 124.26   |
| 14  | aL    | 203  | CL7  | CHC-C4B-NB  | 2.82  | 127.25      | 124.26   |
| 14  | cA    | 3141 | CL7  | O1D-CGD-CBD | -2.82 | 118.71      | 124.48   |
| 14  | cA    | 3127 | CL7  | C2A-C1A-CHA | -2.82 | 120.72      | 126.36   |
| 14  | bA    | 3120 | CL7  | CHC-C1C-NC  | -2.82 | 121.86      | 124.45   |
| 14  | cA    | 3107 | CL7  | O2D-CGD-O1D | -2.82 | 118.32      | 123.84   |
| 14  | aA    | 3111 | CL7  | CMB-C2B-C1B | 2.82  | 129.66      | 125.37   |
| 14  | bL    | 203  | CL7  | CMB-C2B-C1B | 2.82  | 129.66      | 125.37   |
| 14  | bB    | 827  | CL7  | C2B-C1B-NB  | -2.82 | 108.34      | 110.23   |
| 14  | cA    | 3116 | CL7  | C1A-NA-C4A  | -2.82 | 104.60      | 106.30   |
| 14  | cB    | 826  | CL7  | CHC-C4B-NB  | 2.82  | 127.24      | 124.26   |
| 14  | bA    | 3116 | CL7  | O2A-CGA-O1A | -2.82 | 116.48      | 123.59   |
| 14  | bA    | 3119 | CL7  | C2A-C1A-CHA | -2.82 | 120.73      | 126.36   |
| 14  | bA    | 3110 | CL7  | CHB-C1B-NB  | -2.81 | 121.28      | 124.26   |
| 14  | bA    | 3110 | CL7  | CED-O2D-CGD | 2.81  | 122.30      | 115.94   |
| 14  | aA    | 3134 | CL7  | CBD-CHA-C4D | -2.81 | 102.41      | 109.14   |
| 14  | aA    | 3125 | CL7  | C7-C6-C5    | -2.81 | 105.72      | 113.36   |
| 14  | cA    | 3119 | CL7  | CHB-C1B-NB  | -2.81 | 121.28      | 124.26   |
| 14  | bB    | 833  | CL7  | OBD-CAD-C3D | -2.81 | 121.75      | 128.52   |
| 14  | aA    | 3129 | CL7  | C3B-C4B-NB  | -2.81 | 107.91      | 110.52   |
| 17  | bB    | 828  | PQN  | C2M-C2-C1   | -2.81 | 111.61      | 116.27   |
| 14  | bA    | 3102 | CL7  | C4C-C3C-C2C | 2.81  | 110.79      | 107.13   |
| 14  | bB    | 832  | CL7  | CHB-C1B-NB  | -2.81 | 121.29      | 124.26   |
| 14  | aA    | 3128 | CL7  | C3A-C4A-CHB | -2.81 | 119.54      | 123.70   |
| 14  | aB    | 3002 | CL7  | CHB-C1B-NB  | -2.80 | 121.29      | 124.26   |
| 14  | bA    | 3117 | CL7  | CHB-C1B-NB  | -2.80 | 121.29      | 124.26   |
| 17  | aB    | 3027 | PQN  | C11-C12-C13 | -2.80 | 122.13      | 126.79   |
| 14  | cA    | 3105 | CL7  | OBB-CAB-C3B | -2.80 | 119.35      | 125.69   |
| 14  | aA    | 3142 | CL7  | C3A-C4A-CHB | -2.80 | 119.54      | 123.70   |
| 14  | bA    | 3117 | CL7  | CHC-C1C-NC  | -2.80 | 121.88      | 124.45   |
| 14  | cA    | 3108 | CL7  | O2D-CGD-O1D | -2.80 | 118.36      | 123.84   |
| 14  | aA    | 3140 | CL7  | C6-C5-C3    | -2.80 | 106.11      | 113.45   |
| 14  | bB    | 808  | CL7  | C1-C2-C3    | -2.80 | 121.20      | 126.04   |
| 14  | bA    | 3116 | CL7  | C3B-C4B-NB  | -2.80 | 107.92      | 110.52   |
| 14  | cA    | 3125 | CL7  | C3A-C2A-C1A | 2.80  | 105.53      | 101.34   |
| 14  | cA    | 3139 | CL7  | C3A-C4A-CHB | -2.80 | 119.55      | 123.70   |
| 14  | cA    | 3144 | CL7  | C3B-C4B-NB  | -2.80 | 107.92      | 110.52   |
| 14  | bA    | 3110 | CL7  | C3A-C4A-CHB | -2.80 | 119.55      | 123.70   |
| 14  | cA    | 3144 | CL7  | C3D-C4D-ND  | 2.80  | 114.18      | 110.17   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 13  | cB    | 805  | PHO  | CBC-CAC-C3C | -2.80 | 108.78      | 112.88   |
| 14  | bB    | 810  | CL7  | C6-C7-C8    | -2.80 | 106.88      | 115.92   |
| 14  | cB    | 825  | CL7  | C3A-C4A-CHB | -2.80 | 119.55      | 123.70   |
| 14  | cB    | 816  | CL7  | C1A-NA-C4A  | -2.80 | 104.61      | 106.30   |
| 12  | aA    | 3101 | G9R  | CMA-C3A-C2A | -2.80 | 102.55      | 113.83   |
| 14  | bB    | 818  | CL7  | CBD-CHA-C4D | -2.80 | 102.45      | 109.14   |
| 14  | bL    | 203  | CL7  | CBD-CHA-C4D | -2.79 | 102.46      | 109.14   |
| 14  | cA    | 3142 | CL7  | CHB-C1B-NB  | -2.79 | 121.30      | 124.26   |
| 14  | cB    | 831  | CL7  | CMB-C2B-C1B | 2.79  | 129.62      | 125.37   |
| 14  | bA    | 3106 | CL7  | C16-C15-C13 | -2.79 | 106.89      | 115.92   |
| 14  | cA    | 3128 | CL7  | C3D-C4D-ND  | 2.79  | 114.17      | 110.17   |
| 14  | bA    | 3103 | CL7  | CHB-C1B-NB  | -2.79 | 121.30      | 124.26   |
| 14  | bB    | 822  | CL7  | C4D-C3D-C2D | -2.79 | 103.66      | 107.30   |
| 14  | cB    | 807  | CL7  | C3B-C4B-NB  | -2.79 | 107.92      | 110.52   |
| 14  | cB    | 807  | CL7  | CBC-CAC-C3C | 2.79  | 120.13      | 112.43   |
| 13  | aA    | 3102 | PHO  | C2B-C1B-NB  | -2.79 | 107.60      | 109.53   |
| 14  | aA    | 3122 | CL7  | CGD-CBD-CAD | -2.79 | 101.69      | 110.73   |
| 14  | aB    | 3006 | CL7  | O2A-CGA-O1A | -2.79 | 116.55      | 123.59   |
| 14  | cA    | 3128 | CL7  | CAC-C3C-C4C | 2.79  | 129.07      | 124.68   |
| 14  | aB    | 3023 | CL7  | CHB-C1B-NB  | -2.79 | 121.30      | 124.26   |
| 14  | cB    | 824  | CL7  | CHB-C1B-NB  | -2.79 | 121.30      | 124.26   |
| 14  | aA    | 3128 | CL7  | C4D-C3D-C2D | -2.79 | 103.67      | 107.30   |
| 14  | aA    | 3123 | CL7  | C3A-C2A-C1A | 2.79  | 105.52      | 101.34   |
| 14  | aB    | 3031 | CL7  | CAA-C2A-C3A | -2.79 | 105.14      | 112.78   |
| 14  | aB    | 3032 | CL7  | CBD-CHA-C4D | -2.79 | 102.47      | 109.14   |
| 14  | cB    | 816  | CL7  | CMC-C2C-C3C | 2.79  | 133.68      | 126.12   |
| 14  | bA    | 3126 | CL7  | C3D-C4D-ND  | 2.79  | 114.17      | 110.17   |
| 14  | aB    | 3003 | CL7  | C6-C5-C3    | -2.79 | 106.15      | 113.45   |
| 14  | aA    | 3109 | CL7  | C3B-C4B-NB  | -2.79 | 107.93      | 110.52   |
| 14  | bA    | 3128 | CL7  | C4C-C3C-C2C | 2.78  | 110.75      | 107.13   |
| 14  | aA    | 3146 | CL7  | C3D-C4D-ND  | 2.78  | 114.16      | 110.17   |
| 14  | bB    | 804  | CL7  | C7-C6-C5    | -2.78 | 105.81      | 113.36   |
| 14  | bB    | 810  | CL7  | C4D-C3D-C2D | -2.78 | 103.68      | 107.30   |
| 14  | cA    | 3124 | CL7  | C3B-C4B-NB  | -2.78 | 107.94      | 110.52   |
| 14  | cA    | 3127 | CL7  | C4D-C3D-C2D | -2.78 | 103.68      | 107.30   |
| 14  | aL    | 203  | CL7  | CHA-C1A-NA  | -2.78 | 119.41      | 125.98   |
| 14  | bA    | 3133 | CL7  | O1D-CGD-CBD | -2.78 | 118.80      | 124.48   |
| 14  | cB    | 816  | CL7  | CHC-C4B-NB  | 2.78  | 127.20      | 124.26   |
| 14  | cA    | 3110 | CL7  | CBD-CHA-C4D | -2.78 | 102.50      | 109.14   |
| 14  | cL    | 204  | CL7  | C3B-C4B-NB  | -2.78 | 107.94      | 110.52   |
| 14  | aA    | 3127 | CL7  | C3D-C4D-ND  | 2.77  | 114.15      | 110.17   |
| 14  | aA    | 3125 | CL7  | CAC-C3C-C2C | -2.77 | 122.78      | 127.53   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | bB    | 833  | CL7  | C3A-C2A-C1A | 2.77  | 105.49      | 101.34   |
| 14  | cA    | 3142 | CL7  | C3A-C2A-C1A | 2.77  | 105.49      | 101.34   |
| 14  | cA    | 3123 | CL7  | C4C-C3C-C2C | 2.77  | 110.74      | 107.13   |
| 14  | cB    | 832  | CL7  | C1A-NA-C4A  | -2.77 | 104.62      | 106.30   |
| 14  | cB    | 803  | CL7  | C4D-C3D-C2D | -2.77 | 103.69      | 107.30   |
| 14  | aA    | 3122 | CL7  | C3B-C4B-NB  | -2.77 | 107.94      | 110.52   |
| 14  | aA    | 3142 | CL7  | O1D-CGD-CBD | -2.77 | 118.81      | 124.48   |
| 14  | bA    | 3107 | CL7  | C4D-C3D-C2D | -2.77 | 103.69      | 107.30   |
| 14  | aB    | 3014 | CL7  | C1D-ND-C4D  | -2.77 | 104.37      | 106.33   |
| 14  | cB    | 833  | CL7  | OBD-CAD-C3D | -2.77 | 121.85      | 128.52   |
| 14  | aB    | 3005 | CL7  | C1-C2-C3    | -2.77 | 121.25      | 126.04   |
| 14  | cA    | 3116 | CL7  | C6-C5-C3    | -2.77 | 106.19      | 113.45   |
| 14  | bA    | 3102 | CL7  | CBD-CHA-C4D | -2.77 | 102.52      | 109.14   |
| 14  | bB    | 825  | CL7  | C3A-C4A-CHB | -2.77 | 119.59      | 123.70   |
| 14  | cA    | 3120 | CL7  | CMB-C2B-C1B | 2.77  | 129.58      | 125.37   |
| 14  | bL    | 203  | CL7  | O2A-CGA-O1A | -2.77 | 116.61      | 123.59   |
| 14  | bA    | 3130 | CL7  | CMB-C2B-C1B | 2.77  | 129.58      | 125.37   |
| 14  | aA    | 3121 | CL7  | CAA-C2A-C3A | -2.77 | 105.20      | 112.78   |
| 14  | aA    | 3142 | CL7  | C4D-C3D-C2D | -2.77 | 103.69      | 107.30   |
| 14  | bA    | 3117 | CL7  | C3D-C4D-ND  | 2.77  | 114.14      | 110.17   |
| 14  | cA    | 3119 | CL7  | O2A-CGA-O1A | -2.76 | 114.48      | 123.14   |
| 14  | cB    | 812  | CL7  | C3B-C4B-NB  | -2.76 | 107.95      | 110.52   |
| 14  | aA    | 3111 | CL7  | CBD-CHA-C4D | -2.76 | 102.53      | 109.14   |
| 14  | aA    | 3131 | CL7  | CMB-C2B-C1B | 2.76  | 129.57      | 125.37   |
| 14  | aA    | 3133 | CL7  | CED-O2D-CGD | 2.76  | 122.18      | 115.94   |
| 14  | cB    | 816  | CL7  | O2D-CGD-O1D | -2.76 | 118.44      | 123.84   |
| 14  | aA    | 3108 | CL7  | C4C-C3C-C2C | 2.76  | 110.72      | 107.13   |
| 14  | cL    | 204  | CL7  | C3A-C4A-CHB | -2.76 | 119.60      | 123.70   |
| 14  | cA    | 3129 | CL7  | CAA-C2A-C1A | -2.76 | 104.91      | 112.08   |
| 14  | aB    | 3031 | CL7  | CAC-C3C-C2C | -2.76 | 122.81      | 127.53   |
| 12  | bA    | 3101 | G9R  | C4C-C3C-C2C | -2.76 | 102.88      | 106.90   |
| 14  | aA    | 3105 | CL7  | C3B-C4B-NB  | -2.76 | 107.95      | 110.52   |
| 14  | aA    | 3113 | CL7  | C3B-C4B-NB  | -2.76 | 107.95      | 110.52   |
| 14  | aL    | 202  | CL7  | CBD-CHA-C4D | -2.76 | 102.54      | 109.14   |
| 14  | cB    | 818  | CL7  | CBD-CHA-C4D | -2.76 | 102.54      | 109.14   |
| 14  | aA    | 3114 | CL7  | CBD-CHA-C4D | -2.76 | 102.54      | 109.14   |
| 14  | bB    | 831  | CL7  | C1D-ND-C4D  | -2.76 | 104.38      | 106.33   |
| 14  | bA    | 3129 | CL7  | C4D-C3D-C2D | -2.76 | 103.71      | 107.30   |
| 14  | cA    | 3140 | CL7  | CHC-C4B-NB  | 2.76  | 127.18      | 124.26   |
| 14  | aB    | 3019 | CL7  | CBD-CHA-C4D | -2.76 | 102.55      | 109.14   |
| 14  | bB    | 832  | CL7  | CHC-C4B-NB  | 2.76  | 127.17      | 124.26   |
| 14  | aB    | 3032 | CL7  | OBD-CAD-C3D | -2.76 | 121.89      | 128.52   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 13  | bB    | 801  | PHO  | CAA-CBA-CGA | -2.76 | 105.20      | 113.25   |
| 14  | aL    | 202  | CL7  | C4D-C3D-C2D | -2.76 | 103.71      | 107.30   |
| 14  | bA    | 3120 | CL7  | C3A-C4A-CHB | -2.75 | 119.61      | 123.70   |
| 14  | bB    | 812  | CL7  | C3B-C4B-NB  | -2.75 | 107.96      | 110.52   |
| 14  | cB    | 827  | CL7  | CMD-C2D-C1D | -2.75 | 121.18      | 125.37   |
| 14  | bB    | 824  | CL7  | CAD-C3D-C2D | 2.75  | 150.38      | 144.44   |
| 14  | cA    | 3116 | CL7  | CBD-CHA-C4D | -2.75 | 102.56      | 109.14   |
| 14  | aB    | 3018 | CL7  | CMB-C2B-C1B | 2.75  | 129.56      | 125.37   |
| 14  | cA    | 3112 | CL7  | C3B-C4B-NB  | -2.75 | 107.96      | 110.52   |
| 14  | aB    | 3019 | CL7  | CAA-C2A-C3A | -2.75 | 105.25      | 112.78   |
| 14  | bA    | 3128 | CL7  | C3D-C4D-ND  | 2.75  | 114.11      | 110.17   |
| 14  | bA    | 3129 | CL7  | C1C-C2C-C3C | 2.75  | 110.96      | 106.94   |
| 14  | bA    | 3124 | CL7  | OBD-CAD-C3D | -2.75 | 121.91      | 128.52   |
| 14  | cA    | 3102 | CL7  | C5-C3-C2    | -2.75 | 115.56      | 121.12   |
| 14  | bA    | 3121 | CL7  | CGD-CBD-CAD | -2.75 | 101.84      | 110.73   |
| 14  | aB    | 3023 | CL7  | CAD-C3D-C2D | 2.74  | 150.37      | 144.44   |
| 14  | cA    | 3117 | CL7  | CHB-C1B-NB  | -2.74 | 121.35      | 124.26   |
| 14  | cA    | 3106 | CL7  | CHC-C4B-NB  | 2.74  | 127.16      | 124.26   |
| 19  | bB    | 830  | LMG  | O6-C5-C4    | -2.74 | 104.71      | 109.69   |
| 14  | bA    | 3145 | CL7  | C3D-C4D-ND  | 2.74  | 114.10      | 110.17   |
| 14  | cB    | 816  | CL7  | C4D-C3D-C2D | -2.74 | 103.73      | 107.30   |
| 14  | cA    | 3128 | CL7  | C4-C3-C5    | -2.74 | 110.66      | 115.27   |
| 14  | bB    | 826  | CL7  | CHC-C1C-NC  | -2.74 | 121.94      | 124.45   |
| 14  | cB    | 807  | CL7  | C1A-NA-C4A  | -2.74 | 104.64      | 106.30   |
| 14  | aA    | 3121 | CL7  | CMB-C2B-C1B | 2.74  | 129.54      | 125.37   |
| 14  | bB    | 824  | CL7  | CHB-C1B-NB  | -2.74 | 121.36      | 124.26   |
| 14  | aA    | 3129 | CL7  | O1D-CGD-CBD | -2.74 | 118.88      | 124.48   |
| 14  | bB    | 817  | CL7  | C3B-C4B-NB  | -2.74 | 107.97      | 110.52   |
| 14  | cA    | 3115 | CL7  | C3B-C4B-NB  | -2.74 | 107.97      | 110.52   |
| 14  | cA    | 3122 | CL7  | CHA-C1A-NA  | -2.74 | 119.50      | 125.98   |
| 14  | cB    | 803  | CL7  | C11-C10-C8  | -2.74 | 107.07      | 115.92   |
| 14  | cA    | 3125 | CL7  | OBD-CAD-C3D | -2.74 | 121.93      | 128.52   |
| 14  | cB    | 832  | CL7  | CAC-C3C-C2C | -2.74 | 122.85      | 127.53   |
| 12  | bA    | 3101 | G9R  | OBD-CAD-C3D | -2.74 | 121.94      | 128.52   |
| 14  | aB    | 3014 | CL7  | C3B-C4B-NB  | -2.73 | 107.98      | 110.52   |
| 14  | bB    | 823  | CL7  | C3B-C4B-NB  | -2.73 | 107.98      | 110.52   |
| 14  | bB    | 816  | CL7  | CHC-C4B-NB  | 2.73  | 127.15      | 124.26   |
| 14  | aA    | 3129 | CL7  | C3A-C4A-CHB | -2.73 | 119.64      | 123.70   |
| 14  | aB    | 3006 | CL7  | CAC-C3C-C4C | 2.73  | 128.98      | 124.68   |
| 14  | aA    | 3111 | CL7  | CHB-C1B-NB  | -2.73 | 121.36      | 124.26   |
| 14  | bA    | 3129 | CL7  | C3A-C2A-C1A | 2.73  | 104.91      | 101.64   |
| 14  | aB    | 3006 | CL7  | C4-C3-C5    | -2.73 | 110.68      | 115.27   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | aA    | 3124 | CL7  | C1D-ND-C4D  | -2.73 | 104.39      | 106.33   |
| 14  | bA    | 3119 | CL7  | OBD-CAD-C3D | -2.73 | 121.95      | 128.52   |
| 13  | bB    | 801  | PHO  | O2D-CGD-CBD | 2.73  | 114.45      | 111.00   |
| 14  | cB    | 820  | CL7  | C6-C5-C3    | -2.73 | 106.30      | 113.45   |
| 14  | aA    | 3125 | CL7  | C3B-C4B-NB  | -2.73 | 107.98      | 110.52   |
| 14  | cB    | 827  | CL7  | CHA-C1A-NA  | -2.73 | 119.53      | 125.98   |
| 14  | bA    | 3145 | CL7  | C3B-C4B-NB  | -2.73 | 107.98      | 110.52   |
| 14  | bB    | 806  | CL7  | CBD-CHA-C4D | -2.73 | 102.62      | 109.14   |
| 14  | aB    | 3011 | CL7  | C3B-C4B-NB  | -2.73 | 107.99      | 110.52   |
| 14  | cB    | 832  | CL7  | CAA-C2A-C3A | -2.73 | 105.31      | 112.78   |
| 14  | aA    | 3134 | CL7  | CHB-C1B-NB  | -2.72 | 121.37      | 124.26   |
| 14  | bA    | 3105 | CL7  | OBB-CAB-C3B | -2.72 | 119.53      | 125.69   |
| 14  | bA    | 3111 | CL7  | CAD-C3D-C2D | 2.72  | 150.32      | 144.44   |
| 19  | aB    | 3029 | LMG  | O2-C2-C3    | -2.72 | 104.05      | 110.35   |
| 14  | aB    | 3005 | CL7  | C16-C15-C13 | -2.72 | 107.12      | 115.92   |
| 13  | aA    | 3102 | PHO  | C4D-ND-C1D  | -2.72 | 106.06      | 108.83   |
| 14  | cB    | 826  | CL7  | C2A-C1A-CHA | -2.72 | 120.92      | 126.36   |
| 14  | aA    | 3128 | CL7  | O2D-CGD-O1D | -2.72 | 118.52      | 123.84   |
| 14  | bA    | 3105 | CL7  | O1D-CGD-CBD | -2.72 | 118.92      | 124.48   |
| 14  | bB    | 831  | CL7  | CHC-C1C-NC  | -2.72 | 121.95      | 124.45   |
| 14  | bB    | 826  | CL7  | C3D-C4D-ND  | 2.72  | 114.07      | 110.17   |
| 14  | aB    | 3005 | CL7  | O1D-CGD-CBD | -2.72 | 118.92      | 124.48   |
| 14  | cB    | 817  | CL7  | C3B-C4B-NB  | -2.72 | 107.99      | 110.52   |
| 14  | aA    | 3107 | CL7  | C1D-ND-C4D  | -2.72 | 104.40      | 106.33   |
| 14  | aA    | 3121 | CL7  | C1D-ND-C4D  | -2.72 | 104.40      | 106.33   |
| 14  | bA    | 3108 | CL7  | C1D-ND-C4D  | -2.72 | 104.40      | 106.33   |
| 14  | aA    | 3115 | CL7  | C6-C7-C8    | -2.72 | 107.13      | 115.92   |
| 14  | aA    | 3106 | CL7  | CAC-C3C-C2C | -2.72 | 122.88      | 127.53   |
| 14  | bB    | 816  | CL7  | O1D-CGD-CBD | -2.72 | 118.93      | 124.48   |
| 14  | bL    | 204  | CL7  | C11-C10-C8  | -2.72 | 107.14      | 115.92   |
| 14  | cB    | 808  | CL7  | C1-C2-C3    | -2.72 | 121.35      | 126.04   |
| 14  | cA    | 3114 | CL7  | CAC-C3C-C2C | -2.72 | 122.88      | 127.53   |
| 17  | aA    | 3144 | PQN  | C16-C17-C18 | -2.72 | 107.14      | 115.92   |
| 14  | cB    | 810  | CL7  | CBD-CHA-C4D | -2.71 | 102.65      | 109.14   |
| 14  | aB    | 3026 | CL7  | CAC-C3C-C4C | 2.71  | 128.95      | 124.68   |
| 14  | bA    | 3111 | CL7  | C3D-C4D-ND  | 2.71  | 114.06      | 110.17   |
| 14  | cB    | 826  | CL7  | C3D-C4D-ND  | 2.71  | 114.06      | 110.17   |
| 12  | cA    | 3101 | G9R  | C4D-CHA-C1A | -2.71 | 117.95      | 121.25   |
| 14  | aA    | 3118 | CL7  | C3D-C4D-ND  | 2.71  | 114.06      | 110.17   |
| 14  | aB    | 3025 | CL7  | CMB-C2B-C1B | 2.71  | 129.50      | 125.37   |
| 14  | cF    | 201  | CL7  | CAD-C3D-C2D | 2.71  | 150.30      | 144.44   |
| 14  | bA    | 3139 | CL7  | C3B-C4B-NB  | -2.71 | 108.00      | 110.52   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | aA    | 3109 | CL7  | C2B-C1B-NB  | -2.71 | 108.41      | 110.23   |
| 14  | cA    | 3124 | CL7  | CMB-C2B-C3B | -2.71 | 120.02      | 126.59   |
| 12  | aA    | 3101 | G9R  | OBD-CAD-C3D | -2.71 | 122.00      | 128.52   |
| 14  | cA    | 3127 | CL7  | C1D-ND-C4D  | -2.71 | 104.41      | 106.33   |
| 14  | bL    | 204  | CL7  | O1D-CGD-CBD | -2.71 | 118.94      | 124.48   |
| 14  | cB    | 808  | CL7  | CBD-CHA-C4D | -2.71 | 102.66      | 109.14   |
| 14  | cA    | 3116 | CL7  | CHC-C1C-NC  | -2.71 | 121.97      | 124.45   |
| 14  | bA    | 3128 | CL7  | CAD-C3D-C2D | 2.71  | 150.29      | 144.44   |
| 14  | cA    | 3105 | CL7  | CAC-C3C-C2C | -2.71 | 122.90      | 127.53   |
| 14  | bB    | 820  | CL7  | CBD-CHA-C4D | -2.71 | 102.67      | 109.14   |
| 14  | aB    | 3007 | CL7  | C1-C2-C3    | -2.71 | 121.36      | 126.04   |
| 14  | bB    | 827  | CL7  | CMD-C2D-C1D | -2.71 | 121.25      | 125.37   |
| 14  | cA    | 3111 | CL7  | C3D-C4D-ND  | 2.71  | 114.05      | 110.17   |
| 14  | cB    | 807  | CL7  | CAC-C3C-C4C | 2.71  | 128.94      | 124.68   |
| 14  | cA    | 3126 | CL7  | C1-C2-C3    | -2.71 | 121.36      | 126.04   |
| 14  | bB    | 810  | CL7  | CHC-C1C-NC  | -2.70 | 121.97      | 124.45   |
| 14  | bA    | 3141 | CL7  | C4D-C3D-C2D | -2.70 | 103.78      | 107.30   |
| 14  | aA    | 3110 | CL7  | CBD-CHA-C4D | -2.70 | 102.67      | 109.14   |
| 14  | aA    | 3140 | CL7  | C3B-C4B-NB  | -2.70 | 108.01      | 110.52   |
| 14  | aB    | 3021 | CL7  | CBD-CHA-C4D | -2.70 | 102.68      | 109.14   |
| 14  | aA    | 3133 | CL7  | O1D-CGD-CBD | -2.70 | 118.96      | 124.48   |
| 14  | bA    | 3105 | CL7  | CAC-C3C-C2C | -2.70 | 122.91      | 127.53   |
| 14  | bL    | 205  | CL7  | C1D-ND-C4D  | -2.70 | 104.42      | 106.33   |
| 14  | aB    | 3024 | CL7  | CAD-C3D-C2D | 2.70  | 150.27      | 144.44   |
| 14  | bA    | 3132 | CL7  | CHA-C1A-NA  | -2.70 | 119.59      | 125.98   |
| 14  | aA    | 3140 | CL7  | CBD-CHA-C4D | -2.70 | 102.69      | 109.14   |
| 14  | aA    | 3133 | CL7  | CHA-C1A-NA  | -2.70 | 119.60      | 125.98   |
| 14  | aA    | 3112 | CL7  | CAD-C3D-C2D | 2.70  | 150.26      | 144.44   |
| 14  | aA    | 3107 | CL7  | CHC-C1C-NC  | -2.70 | 121.98      | 124.45   |
| 14  | aA    | 3124 | CL7  | C1A-NA-C4A  | 2.70  | 107.93      | 106.30   |
| 14  | aB    | 3006 | CL7  | C6-C5-C3    | -2.70 | 106.39      | 113.45   |
| 14  | bB    | 810  | CL7  | CBD-CHA-C4D | -2.69 | 102.70      | 109.14   |
| 14  | bB    | 815  | CL7  | O2D-CGD-O1D | -2.69 | 118.57      | 123.84   |
| 14  | aB    | 3021 | CL7  | C4D-C3D-C2D | -2.69 | 103.79      | 107.30   |
| 14  | cA    | 3114 | CL7  | C6-C5-C3    | -2.69 | 106.39      | 113.45   |
| 14  | bL    | 204  | CL7  | CHA-C1A-NA  | -2.69 | 119.61      | 125.98   |
| 14  | bF    | 201  | CL7  | CAD-C3D-C2D | 2.69  | 150.25      | 144.44   |
| 14  | cB    | 833  | CL7  | C1-C2-C3    | -2.69 | 121.39      | 126.04   |
| 17  | aA    | 3144 | PQN  | C15-C13-C12 | -2.69 | 115.67      | 121.12   |
| 14  | aB    | 3018 | CL7  | C1-O2A-CGA  | -2.69 | 109.39      | 116.44   |
| 14  | aA    | 3106 | CL7  | C4C-C3C-C2C | 2.69  | 110.63      | 107.13   |
| 14  | bA    | 3123 | CL7  | C4C-C3C-C2C | 2.69  | 110.63      | 107.13   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | cA    | 3105 | CL7  | CMB-C2B-C1B | 2.69  | 129.47      | 125.37   |
| 14  | bA    | 3139 | CL7  | CAA-C2A-C3A | -2.69 | 105.41      | 112.78   |
| 16  | cA    | 3138 | LHG  | O4-P-O5     | 2.69  | 125.54      | 112.24   |
| 14  | cA    | 3110 | CL7  | CHB-C1B-NB  | -2.69 | 121.41      | 124.26   |
| 14  | cB    | 807  | CL7  | CBD-CHA-C4D | -2.69 | 102.71      | 109.14   |
| 14  | cB    | 804  | CL7  | O2D-CGD-O1D | -2.69 | 118.58      | 123.84   |
| 14  | bA    | 3115 | CL7  | C3A-C4A-CHB | -2.69 | 119.71      | 123.70   |
| 17  | bA    | 3143 | PQN  | C17-C16-C15 | -2.69 | 106.06      | 113.36   |
| 14  | aB    | 3025 | CL7  | O2D-CGD-CBD | 2.69  | 116.04      | 111.27   |
| 14  | cA    | 3111 | CL7  | CAD-C3D-C2D | 2.69  | 150.24      | 144.44   |
| 14  | cA    | 3107 | CL7  | C4C-C3C-C2C | 2.69  | 110.63      | 107.13   |
| 14  | cB    | 831  | CL7  | O2A-CGA-O1A | -2.69 | 116.81      | 123.59   |
| 14  | cB    | 831  | CL7  | CAA-C2A-C3A | -2.69 | 105.42      | 112.78   |
| 14  | aA    | 3142 | CL7  | C7-C6-C5    | -2.68 | 106.07      | 113.36   |
| 14  | bA    | 3127 | CL7  | C3A-C4A-CHB | -2.68 | 119.72      | 123.70   |
| 14  | cB    | 807  | CL7  | C6-C5-C3    | -2.68 | 106.42      | 113.45   |
| 14  | cB    | 815  | CL7  | C3B-C4B-NB  | -2.68 | 108.03      | 110.52   |
| 14  | cB    | 833  | CL7  | O1D-CGD-CBD | -2.68 | 119.00      | 124.48   |
| 14  | bB    | 807  | CL7  | CAC-C3C-C4C | 2.68  | 128.90      | 124.68   |
| 14  | cA    | 3116 | CL7  | C3B-C4B-NB  | -2.68 | 108.03      | 110.52   |
| 14  | bA    | 3145 | CL7  | CMB-C2B-C1B | 2.67  | 129.44      | 125.37   |
| 14  | aA    | 3116 | CL7  | C3D-C4D-ND  | 2.67  | 114.00      | 110.17   |
| 14  | bB    | 824  | CL7  | C6-C5-C3    | -2.67 | 106.44      | 113.45   |
| 19  | cB    | 830  | LMG  | O2-C2-C3    | -2.67 | 104.17      | 110.35   |
| 14  | cB    | 810  | CL7  | C1-C2-C3    | -2.67 | 121.42      | 126.04   |
| 14  | bA    | 3128 | CL7  | CBA-CAA-C2A | 2.67  | 121.75      | 113.86   |
| 14  | aB    | 3010 | CL7  | C3B-C4B-NB  | -2.67 | 108.03      | 110.52   |
| 14  | bA    | 3124 | CL7  | C7-C6-C5    | -2.67 | 106.10      | 113.36   |
| 14  | aA    | 3111 | CL7  | O2D-CGD-O1D | -2.67 | 118.61      | 123.84   |
| 14  | aA    | 3126 | CL7  | C2D-C1D-ND  | -2.67 | 108.44      | 110.23   |
| 14  | aA    | 3124 | CL7  | C4-C3-C5    | -2.67 | 112.93      | 115.98   |
| 14  | bL    | 204  | CL7  | C4D-C3D-C2D | -2.67 | 103.82      | 107.30   |
| 14  | bB    | 827  | CL7  | CMA-C3A-C2A | -2.67 | 103.06      | 113.83   |
| 14  | cA    | 3131 | CL7  | C3B-C4B-NB  | -2.67 | 108.04      | 110.52   |
| 14  | cA    | 3132 | CL7  | CHA-C1A-NA  | -2.67 | 119.66      | 125.98   |
| 14  | cK    | 101  | CL7  | CMB-C2B-C1B | 2.67  | 129.43      | 125.37   |
| 14  | bA    | 3104 | CL7  | C3B-C4B-NB  | -2.67 | 108.04      | 110.52   |
| 14  | bB    | 807  | CL7  | CBC-CAC-C3C | 2.67  | 119.78      | 112.43   |
| 14  | cA    | 3110 | CL7  | O2D-CGD-O1D | -2.66 | 118.63      | 123.84   |
| 14  | cA    | 3107 | CL7  | CHB-C1B-NB  | -2.66 | 121.44      | 124.26   |
| 14  | bA    | 3120 | CL7  | CMB-C2B-C1B | 2.66  | 129.43      | 125.37   |
| 14  | bA    | 3127 | CL7  | C4D-C3D-C2D | -2.66 | 103.83      | 107.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | bA    | 3108 | CL7  | CMB-C2B-C1B | 2.66  | 129.43      | 125.37   |
| 14  | cB    | 810  | CL7  | C1D-ND-C4D  | -2.66 | 104.44      | 106.33   |
| 14  | cA    | 3140 | CL7  | C4D-C3D-C2D | -2.66 | 103.83      | 107.30   |
| 14  | bB    | 833  | CL7  | CHC-C1C-NC  | -2.66 | 122.01      | 124.45   |
| 14  | bK    | 101  | CL7  | C3B-C4B-NB  | -2.66 | 108.05      | 110.52   |
| 14  | bA    | 3126 | CL7  | O2D-CGD-CBD | 2.66  | 116.00      | 111.27   |
| 14  | aA    | 3107 | CL7  | CHB-C1B-NB  | -2.66 | 121.44      | 124.26   |
| 17  | cB    | 828  | PQN  | C11-C12-C13 | -2.66 | 122.37      | 126.79   |
| 14  | cA    | 3114 | CL7  | C3D-C4D-ND  | 2.66  | 113.98      | 110.17   |
| 14  | aB    | 3026 | CL7  | C2B-C1B-NB  | -2.66 | 108.45      | 110.23   |
| 14  | bA    | 3102 | CL7  | C2B-C1B-NB  | -2.66 | 108.45      | 110.23   |
| 14  | cA    | 3127 | CL7  | C3A-C4A-CHB | -2.66 | 119.76      | 123.70   |
| 14  | aA    | 3108 | CL7  | C1D-ND-C4D  | -2.66 | 104.45      | 106.33   |
| 14  | bA    | 3140 | CL7  | CHC-C4B-NB  | 2.66  | 127.07      | 124.26   |
| 14  | aA    | 3119 | CL7  | C4D-C3D-CAD | 2.66  | 109.21      | 107.42   |
| 14  | aA    | 3117 | CL7  | C3C-C4C-NC  | 2.66  | 112.10      | 110.18   |
| 13  | cB    | 801  | PHO  | C4D-ND-C1D  | -2.66 | 106.13      | 108.83   |
| 14  | aA    | 3108 | CL7  | C6-C5-C3    | -2.66 | 106.49      | 113.45   |
| 14  | bB    | 832  | CL7  | CAA-C2A-C3A | -2.65 | 105.51      | 112.78   |
| 14  | bA    | 3113 | CL7  | C4D-C3D-C2D | -2.65 | 103.84      | 107.30   |
| 14  | aB    | 3031 | CL7  | CHB-C1B-NB  | -2.65 | 121.45      | 124.26   |
| 16  | bA    | 3138 | LHG  | O4-P-O5     | 2.65  | 125.35      | 112.24   |
| 14  | cB    | 820  | CL7  | CBD-CHA-C4D | -2.65 | 102.80      | 109.14   |
| 14  | cF    | 201  | CL7  | C1D-ND-C4D  | -2.65 | 104.45      | 106.33   |
| 14  | aB    | 3032 | CL7  | C4D-C3D-C2D | -2.65 | 103.85      | 107.30   |
| 14  | aB    | 3015 | CL7  | CBD-CHA-C4D | -2.65 | 102.80      | 109.14   |
| 14  | aB    | 3018 | CL7  | CAD-C3D-C2D | 2.65  | 150.16      | 144.44   |
| 14  | bA    | 3114 | CL7  | CAC-C3C-C2C | -2.65 | 123.00      | 127.53   |
| 14  | aA    | 3116 | CL7  | C3B-C4B-NB  | -2.65 | 108.06      | 110.52   |
| 14  | cA    | 3115 | CL7  | CMB-C2B-C1B | 2.65  | 129.40      | 125.37   |
| 14  | cA    | 3144 | CL7  | CMB-C2B-C1B | 2.65  | 129.40      | 125.37   |
| 14  | bA    | 3106 | CL7  | C1D-ND-C4D  | -2.65 | 104.45      | 106.33   |
| 14  | bB    | 814  | CL7  | C3D-C4D-ND  | 2.65  | 113.97      | 110.17   |
| 14  | bB    | 803  | CL7  | OBD-CAD-C3D | -2.65 | 122.15      | 128.52   |
| 14  | aA    | 3114 | CL7  | C4D-C3D-C2D | -2.65 | 103.85      | 107.30   |
| 16  | aA    | 3139 | LHG  | O4-P-O5     | 2.64  | 125.31      | 112.24   |
| 19  | cB    | 830  | LMG  | O6-C5-C4    | -2.64 | 104.89      | 109.69   |
| 14  | cL    | 203  | CL7  | CHC-C1C-NC  | -2.64 | 122.02      | 124.45   |
| 14  | cL    | 205  | CL7  | C1D-ND-C4D  | -2.64 | 104.46      | 106.33   |
| 14  | bB    | 831  | CL7  | CBD-CHA-C4D | -2.64 | 102.82      | 109.14   |
| 14  | bA    | 3115 | CL7  | C3B-C4B-NB  | -2.64 | 108.06      | 110.52   |
| 14  | bA    | 3129 | CL7  | CHB-C1B-NB  | -2.64 | 121.46      | 124.26   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | cB    | 832  | CL7  | C3A-C4A-CHB | -2.64 | 119.78      | 123.70   |
| 14  | cA    | 3140 | CL7  | CHC-C1C-NC  | -2.64 | 122.03      | 124.45   |
| 14  | aB    | 3025 | CL7  | O2A-CGA-O1A | -2.64 | 116.93      | 123.59   |
| 14  | aA    | 3117 | CL7  | CBD-CHA-C4D | -2.64 | 102.83      | 109.14   |
| 14  | cA    | 3117 | CL7  | C3D-C4D-ND  | 2.64  | 113.95      | 110.17   |
| 14  | cB    | 811  | CL7  | C3B-C4B-NB  | -2.64 | 108.07      | 110.52   |
| 14  | aA    | 3116 | CL7  | C3A-C4A-CHB | -2.64 | 119.78      | 123.70   |
| 14  | aA    | 3118 | CL7  | C3B-C4B-NB  | -2.64 | 108.07      | 110.52   |
| 14  | aB    | 3030 | CL7  | O1D-CGD-CBD | -2.64 | 119.08      | 124.48   |
| 14  | bA    | 3129 | CL7  | CAA-C2A-C1A | -2.64 | 105.23      | 112.08   |
| 12  | aA    | 3101 | G9R  | O2A-C1-C2   | -2.64 | 101.70      | 108.64   |
| 14  | aA    | 3146 | CL7  | C3B-C4B-NB  | -2.64 | 108.07      | 110.52   |
| 14  | cA    | 3124 | CL7  | OBD-CAD-C3D | -2.64 | 122.17      | 128.52   |
| 14  | aB    | 3008 | CL7  | O2D-CGD-O1D | -2.64 | 118.68      | 123.84   |
| 14  | aB    | 3008 | CL7  | CGD-CBD-CAD | -2.64 | 102.20      | 110.73   |
| 14  | aB    | 3030 | CL7  | O2A-CGA-O1A | -2.64 | 116.94      | 123.59   |
| 13  | bB    | 801  | PHO  | C4D-ND-C1D  | -2.63 | 106.15      | 108.83   |
| 14  | aA    | 3121 | CL7  | C4-C3-C5    | -2.63 | 112.97      | 115.98   |
| 14  | aA    | 3117 | CL7  | C3B-C4B-NB  | -2.63 | 108.07      | 110.52   |
| 14  | aA    | 3117 | CL7  | C3D-C4D-ND  | 2.63  | 113.94      | 110.17   |
| 14  | cB    | 806  | CL7  | C2A-C1A-CHA | -2.63 | 121.10      | 126.36   |
| 14  | cB    | 825  | CL7  | CAD-C3D-C2D | 2.63  | 150.12      | 144.44   |
| 14  | bA    | 3131 | CL7  | C3A-C2A-C1A | 2.63  | 104.79      | 101.64   |
| 14  | bB    | 806  | CL7  | C4D-C3D-C2D | -2.63 | 103.87      | 107.30   |
| 14  | aB    | 3026 | CL7  | CBC-CAC-C3C | 2.63  | 119.68      | 112.43   |
| 14  | aA    | 3112 | CL7  | CMB-C2B-C1B | 2.63  | 129.37      | 125.37   |
| 14  | aB    | 3005 | CL7  | CBD-CHA-C4D | -2.63 | 102.86      | 109.14   |
| 14  | cA    | 3119 | CL7  | O2D-CGD-O1D | -2.63 | 118.70      | 123.84   |
| 14  | aB    | 3032 | CL7  | C1-O2A-CGA  | -2.63 | 109.56      | 116.44   |
| 14  | bA    | 3133 | CL7  | C3B-C4B-NB  | -2.62 | 108.08      | 110.52   |
| 14  | cL    | 204  | CL7  | CHA-C1A-NA  | -2.62 | 119.77      | 125.98   |
| 14  | aB    | 3007 | CL7  | CHB-C1B-NB  | -2.62 | 121.48      | 124.26   |
| 14  | aL    | 203  | CL7  | C4D-C3D-C2D | -2.62 | 103.88      | 107.30   |
| 14  | bA    | 3102 | CL7  | O2A-CGA-O1A | -2.62 | 116.97      | 123.59   |
| 14  | aB    | 3006 | CL7  | CBC-CAC-C3C | 2.62  | 119.66      | 112.43   |
| 12  | bA    | 3101 | G9R  | C4B-CHC-C1C | -2.62 | 120.12      | 126.34   |
| 14  | aA    | 3115 | CL7  | C3B-C4B-NB  | -2.62 | 108.08      | 110.52   |
| 14  | aA    | 3113 | CL7  | C3D-C4D-ND  | 2.62  | 113.93      | 110.17   |
| 14  | cA    | 3118 | CL7  | C4D-C3D-CAD | 2.62  | 109.19      | 107.42   |
| 14  | bB    | 832  | CL7  | OBD-CAD-C3D | -2.62 | 122.22      | 128.52   |
| 14  | bA    | 3114 | CL7  | C3D-C4D-ND  | 2.62  | 113.93      | 110.17   |
| 14  | bA    | 3127 | CL7  | CAA-C2A-C3A | -2.62 | 105.60      | 112.78   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | aA    | 3141 | CL7  | C3A-C2A-C1A | 2.62  | 105.26      | 101.34   |
| 14  | bA    | 3124 | CL7  | C6-C5-C3    | -2.62 | 106.59      | 113.45   |
| 14  | aB    | 3008 | CL7  | CBD-CHA-C4D | -2.62 | 102.88      | 109.14   |
| 14  | aB    | 3030 | CL7  | C4D-C3D-C2D | -2.62 | 103.89      | 107.30   |
| 14  | cA    | 3128 | CL7  | CAD-C3D-C2D | 2.62  | 150.09      | 144.44   |
| 14  | aB    | 3019 | CL7  | C4D-C3D-C2D | -2.62 | 103.89      | 107.30   |
| 14  | cA    | 3115 | CL7  | C3A-C4A-CHB | -2.62 | 119.82      | 123.70   |
| 14  | cB    | 814  | CL7  | C3D-C4D-ND  | 2.62  | 113.92      | 110.17   |
| 14  | aB    | 3006 | CL7  | C1D-ND-C4D  | -2.62 | 104.48      | 106.33   |
| 14  | aA    | 3130 | CL7  | CAA-C2A-C1A | -2.62 | 105.29      | 112.08   |
| 14  | aB    | 3005 | CL7  | C4-C3-C5    | -2.62 | 110.87      | 115.27   |
| 14  | cA    | 3124 | CL7  | C7-C6-C5    | -2.61 | 106.26      | 113.36   |
| 14  | bA    | 3139 | CL7  | CBD-CHA-C4D | -2.61 | 102.89      | 109.14   |
| 14  | cB    | 807  | CL7  | C1D-ND-C4D  | -2.61 | 104.48      | 106.33   |
| 14  | cA    | 3104 | CL7  | C3B-C4B-NB  | -2.61 | 108.09      | 110.52   |
| 14  | bB    | 809  | CL7  | CGD-CBD-CAD | -2.61 | 102.28      | 110.73   |
| 14  | cA    | 3115 | CL7  | C3D-C4D-ND  | 2.61  | 113.91      | 110.17   |
| 14  | aA    | 3114 | CL7  | CHB-C1B-NB  | -2.61 | 121.49      | 124.26   |
| 14  | bB    | 822  | CL7  | CBD-CHA-C4D | -2.61 | 102.90      | 109.14   |
| 14  | bB    | 820  | CL7  | CHC-C1C-NC  | -2.61 | 122.06      | 124.45   |
| 14  | aA    | 3122 | CL7  | CHB-C1B-NB  | -2.61 | 121.50      | 124.26   |
| 14  | cB    | 807  | CL7  | O2A-CGA-O1A | -2.61 | 117.01      | 123.59   |
| 14  | cB    | 818  | CL7  | O1D-CGD-CBD | -2.61 | 119.15      | 124.48   |
| 14  | cA    | 3133 | CL7  | C3B-C4B-NB  | -2.61 | 108.10      | 110.52   |
| 14  | bA    | 3140 | CL7  | C4D-C3D-C2D | -2.60 | 103.91      | 107.30   |
| 14  | bA    | 3116 | CL7  | CHB-C1B-NB  | -2.60 | 121.50      | 124.26   |
| 14  | bB    | 808  | CL7  | CHB-C1B-NB  | -2.60 | 121.50      | 124.26   |
| 14  | bA    | 3126 | CL7  | O2A-CGA-O1A | -2.60 | 117.02      | 123.59   |
| 14  | bL    | 204  | CL7  | C6-C7-C8    | -2.60 | 107.50      | 115.92   |
| 14  | cB    | 833  | CL7  | O2A-CGA-O1A | -2.60 | 117.02      | 123.59   |
| 14  | cA    | 3106 | CL7  | C6-C5-C3    | -2.60 | 106.63      | 113.45   |
| 14  | cA    | 3120 | CL7  | C4D-C3D-C2D | -2.60 | 103.91      | 107.30   |
| 14  | cA    | 3141 | CL7  | C4D-C3D-C2D | -2.60 | 103.91      | 107.30   |
| 14  | cB    | 820  | CL7  | C4D-C3D-C2D | -2.60 | 103.91      | 107.30   |
| 14  | aB    | 3002 | CL7  | CBD-CHA-C4D | -2.60 | 102.92      | 109.14   |
| 14  | bB    | 826  | CL7  | O2D-CGD-CBD | 2.60  | 115.89      | 111.27   |
| 14  | bB    | 833  | CL7  | O2A-CGA-O1A | -2.60 | 117.03      | 123.59   |
| 14  | cA    | 3130 | CL7  | CMB-C2B-C1B | 2.60  | 129.33      | 125.37   |
| 14  | bB    | 814  | CL7  | CMB-C2B-C1B | 2.60  | 129.32      | 125.37   |
| 17  | aA    | 3144 | PQN  | C11-C12-C13 | -2.60 | 122.47      | 126.79   |
| 14  | bA    | 3129 | CL7  | OBD-CAD-C3D | -2.60 | 122.27      | 128.52   |
| 14  | cA    | 3132 | CL7  | C3D-C4D-ND  | 2.60  | 113.89      | 110.17   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | aL    | 203  | CL7  | C3B-C4B-NB  | -2.59 | 108.11      | 110.52   |
| 14  | aA    | 3121 | CL7  | CBD-CHA-C4D | -2.59 | 102.94      | 109.14   |
| 14  | bA    | 3107 | CL7  | C1D-ND-C4D  | -2.59 | 104.49      | 106.33   |
| 14  | bB    | 816  | CL7  | C1D-ND-C4D  | -2.59 | 104.49      | 106.33   |
| 14  | aB    | 3007 | CL7  | CBD-CHA-C4D | -2.59 | 102.94      | 109.14   |
| 14  | bA    | 3108 | CL7  | C3B-C4B-NB  | -2.59 | 108.11      | 110.52   |
| 14  | bB    | 824  | CL7  | O2D-CGD-O1D | -2.59 | 118.77      | 123.84   |
| 14  | aB    | 3005 | CL7  | C2A-C1A-CHA | -2.59 | 121.18      | 126.36   |
| 14  | aA    | 3134 | CL7  | C3A-C2A-C1A | 2.59  | 104.74      | 101.64   |
| 14  | bA    | 3112 | CL7  | C3D-C4D-ND  | 2.59  | 113.89      | 110.17   |
| 14  | aA    | 3128 | CL7  | CBA-CAA-C2A | -2.59 | 106.21      | 113.86   |
| 14  | bB    | 816  | CL7  | CHB-C1B-NB  | -2.59 | 121.51      | 124.26   |
| 14  | bA    | 3106 | CL7  | C6-C5-C3    | -2.59 | 106.66      | 113.45   |
| 14  | aA    | 3117 | CL7  | CHC-C1C-NC  | -2.59 | 122.07      | 124.45   |
| 14  | bA    | 3140 | CL7  | CBD-CHA-C4D | -2.59 | 102.94      | 109.14   |
| 14  | aA    | 3120 | CL7  | C3A-C4A-CHB | -2.59 | 119.86      | 123.70   |
| 14  | bB    | 826  | CL7  | O2A-CGA-O1A | -2.59 | 117.05      | 123.59   |
| 14  | bB    | 827  | CL7  | CAC-C3C-C4C | 2.59  | 128.75      | 124.68   |
| 14  | bA    | 3122 | CL7  | C2A-C1A-CHA | -2.59 | 121.18      | 126.36   |
| 14  | bA    | 3122 | CL7  | CHC-C1C-NC  | -2.59 | 122.07      | 124.45   |
| 14  | aB    | 3010 | CL7  | CAC-C3C-C2C | -2.59 | 123.10      | 127.53   |
| 14  | aA    | 3115 | CL7  | C14-C13-C12 | -2.59 | 101.92      | 111.29   |
| 14  | cB    | 803  | CL7  | OBD-CAD-C3D | -2.59 | 122.29      | 128.52   |
| 14  | cA    | 3108 | CL7  | C3A-C2A-C1A | 2.59  | 105.21      | 101.34   |
| 14  | bA    | 3115 | CL7  | C3D-C4D-ND  | 2.59  | 113.88      | 110.17   |
| 14  | cA    | 3128 | CL7  | CHC-C1C-NC  | 2.59  | 126.83      | 124.45   |
| 14  | bA    | 3108 | CL7  | CAA-C2A-C3A | -2.58 | 107.80      | 114.26   |
| 14  | bB    | 807  | CL7  | CMB-C2B-C1B | 2.58  | 129.31      | 125.37   |
| 14  | cA    | 3141 | CL7  | CMB-C2B-C1B | 2.58  | 129.30      | 125.37   |
| 14  | cA    | 3114 | CL7  | CAA-C2A-C1A | -2.58 | 103.69      | 112.19   |
| 14  | bA    | 3131 | CL7  | C3A-C4A-CHB | -2.58 | 119.87      | 123.70   |
| 14  | aB    | 3009 | CL7  | CBD-CHA-C4D | -2.58 | 102.96      | 109.14   |
| 14  | cA    | 3117 | CL7  | C3B-C4B-NB  | -2.58 | 108.12      | 110.52   |
| 14  | aA    | 3109 | CL7  | CBD-CHA-C4D | -2.58 | 102.97      | 109.14   |
| 14  | aB    | 3018 | CL7  | O2D-CGD-O1D | -2.58 | 118.79      | 123.84   |
| 14  | cK    | 101  | CL7  | C3D-C4D-ND  | 2.58  | 113.87      | 110.17   |
| 14  | cA    | 3114 | CL7  | C3B-C4B-NB  | -2.58 | 108.12      | 110.52   |
| 14  | cB    | 831  | CL7  | CHA-C1A-NA  | -2.58 | 119.88      | 125.98   |
| 14  | bB    | 808  | CL7  | CBC-CAC-C3C | -2.58 | 105.33      | 112.43   |
| 14  | cB    | 809  | CL7  | CMB-C2B-C3B | -2.58 | 120.34      | 126.59   |
| 14  | aA    | 3117 | CL7  | CHB-C1B-NB  | -2.57 | 121.53      | 124.26   |
| 13  | bB    | 805  | PHO  | C6-C7-C8    | -2.57 | 107.60      | 115.92   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | aA    | 3125 | CL7  | CBD-CHA-C4D | -2.57 | 102.98      | 109.14   |
| 14  | cA    | 3141 | CL7  | CHB-C1B-NB  | -2.57 | 121.53      | 124.26   |
| 14  | cB    | 819  | CL7  | C6-C7-C8    | -2.57 | 107.60      | 115.92   |
| 14  | aF    | 201  | CL7  | C1D-ND-C4D  | -2.57 | 104.51      | 106.33   |
| 14  | bA    | 3120 | CL7  | C4-C3-C2    | -2.57 | 117.08      | 123.68   |
| 14  | cA    | 3132 | CL7  | CAD-C3D-C2D | 2.57  | 149.99      | 144.44   |
| 14  | cB    | 806  | CL7  | C4D-C3D-C2D | -2.57 | 103.95      | 107.30   |
| 14  | cB    | 811  | CL7  | CAA-C2A-C3A | -2.57 | 110.10      | 116.10   |
| 14  | bA    | 3116 | CL7  | CBD-CHA-C4D | -2.57 | 103.00      | 109.14   |
| 14  | cA    | 3112 | CL7  | C3D-C4D-ND  | 2.57  | 113.85      | 110.17   |
| 14  | bA    | 3123 | CL7  | C2D-C1D-ND  | -2.57 | 108.51      | 110.23   |
| 14  | bA    | 3118 | CL7  | C3D-C4D-ND  | 2.57  | 113.85      | 110.17   |
| 14  | bB    | 831  | CL7  | CMB-C2B-C1B | 2.57  | 129.28      | 125.37   |
| 16  | aA    | 3139 | LHG  | P-O3-C3     | -2.57 | 106.63      | 121.68   |
| 14  | bA    | 3107 | CL7  | CHB-C1B-NB  | -2.57 | 121.54      | 124.26   |
| 14  | bA    | 3122 | CL7  | C1D-ND-C4D  | -2.57 | 104.51      | 106.33   |
| 14  | cB    | 810  | CL7  | CAA-C2A-C3A | -2.57 | 105.75      | 112.78   |
| 14  | cL    | 205  | CL7  | C3A-C2A-C1A | 2.57  | 105.18      | 101.34   |
| 14  | cA    | 3132 | CL7  | O2A-CGA-O1A | -2.57 | 117.12      | 123.59   |
| 14  | aA    | 3111 | CL7  | C3A-C4A-CHB | -2.56 | 119.89      | 123.70   |
| 14  | bA    | 3102 | CL7  | O2A-CGA-CBA | 2.56  | 119.95      | 111.91   |
| 14  | cA    | 3107 | CL7  | C6-C5-C3    | -2.56 | 106.74      | 113.45   |
| 14  | aK    | 101  | CL7  | OBD-CAD-C3D | -2.56 | 124.50      | 128.74   |
| 14  | bB    | 808  | CL7  | C7-C6-C5    | -2.56 | 106.41      | 113.36   |
| 14  | aA    | 3112 | CL7  | C3D-C4D-ND  | 2.56  | 113.84      | 110.17   |
| 14  | cB    | 819  | CL7  | O2D-CGD-O1D | -2.56 | 118.83      | 123.84   |
| 19  | bB    | 830  | LMG  | O2-C2-C3    | -2.56 | 104.44      | 110.35   |
| 14  | bA    | 3107 | CL7  | C1A-NA-C4A  | -2.56 | 104.75      | 106.30   |
| 14  | aB    | 3006 | CL7  | C7-C6-C5    | -2.56 | 106.42      | 113.36   |
| 14  | aA    | 3127 | CL7  | O2D-CGD-CBD | 2.56  | 115.81      | 111.27   |
| 14  | aL    | 203  | CL7  | C2C-C1C-NC  | 2.56  | 111.99      | 110.10   |
| 14  | aB    | 3014 | CL7  | CBD-CHA-C4D | -2.55 | 103.03      | 109.14   |
| 14  | cA    | 3144 | CL7  | CBD-CHA-C4D | -2.55 | 103.03      | 109.14   |
| 14  | aA    | 3116 | CL7  | CMB-C2B-C1B | 2.55  | 129.26      | 125.37   |
| 14  | aB    | 3011 | CL7  | CAA-C2A-C3A | -2.55 | 110.14      | 116.10   |
| 14  | cB    | 808  | CL7  | CBC-CAC-C3C | -2.55 | 105.39      | 112.43   |
| 14  | bB    | 815  | CL7  | OBD-CAD-C3D | -2.55 | 122.38      | 128.52   |
| 14  | bA    | 3102 | CL7  | C7-C6-C5    | -2.55 | 106.43      | 113.36   |
| 14  | aB    | 3008 | CL7  | C1D-ND-C4D  | -2.55 | 104.52      | 106.33   |
| 14  | aB    | 3030 | CL7  | CHC-C1C-NC  | -2.55 | 122.11      | 124.45   |
| 14  | aB    | 3025 | CL7  | CHA-C1A-NA  | -2.55 | 119.94      | 125.98   |
| 14  | bA    | 3116 | CL7  | C6-C5-C3    | -2.55 | 106.76      | 113.45   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | bA    | 3106 | CL7  | CHC-C4B-NB  | 2.55  | 126.96      | 124.26   |
| 14  | aK    | 101  | CL7  | C3D-C4D-ND  | 2.55  | 113.83      | 110.17   |
| 14  | bA    | 3125 | CL7  | OBD-CAD-C3D | -2.55 | 122.38      | 128.52   |
| 14  | cB    | 817  | CL7  | OBD-CAD-C3D | -2.55 | 122.38      | 128.52   |
| 14  | bL    | 203  | CL7  | C4D-C3D-C2D | -2.55 | 103.98      | 107.30   |
| 14  | bA    | 3117 | CL7  | C3B-C4B-NB  | -2.55 | 108.15      | 110.52   |
| 12  | aA    | 3101 | G9R  | C4D-CHA-C1A | -2.55 | 118.15      | 121.25   |
| 14  | bA    | 3132 | CL7  | CAD-C3D-C2D | 2.55  | 149.94      | 144.44   |
| 14  | aB    | 3023 | CL7  | O2D-CGD-O1D | -2.55 | 118.86      | 123.84   |
| 14  | aA    | 3123 | CL7  | C4D-C3D-C2D | -2.55 | 103.98      | 107.30   |
| 13  | cB    | 801  | PHO  | C2B-C1B-NB  | -2.55 | 107.77      | 109.53   |
| 14  | aA    | 3129 | CL7  | CHC-C1C-NC  | 2.55  | 126.80      | 124.45   |
| 14  | cB    | 833  | CL7  | CHC-C1C-NC  | -2.55 | 122.11      | 124.45   |
| 12  | bA    | 3101 | G9R  | CHC-C1C-C2C | -2.55 | 119.65      | 126.73   |
| 14  | bB    | 831  | CL7  | C4D-C3D-C2D | -2.55 | 103.98      | 107.30   |
| 14  | cA    | 3123 | CL7  | C4D-C3D-C2D | -2.55 | 103.98      | 107.30   |
| 14  | aB    | 3002 | CL7  | C4D-C3D-C2D | -2.55 | 103.98      | 107.30   |
| 14  | cB    | 816  | CL7  | C1D-ND-C4D  | -2.55 | 104.53      | 106.33   |
| 14  | bA    | 3102 | CL7  | C4D-C3D-C2D | -2.55 | 103.98      | 107.30   |
| 14  | cB    | 831  | CL7  | CBD-CHA-C4D | -2.54 | 103.06      | 109.14   |
| 14  | cA    | 3133 | CL7  | CHB-C1B-NB  | -2.54 | 121.56      | 124.26   |
| 14  | bB    | 806  | CL7  | C1-C2-C3    | -2.54 | 121.64      | 126.04   |
| 14  | bB    | 831  | CL7  | CAA-C2A-C3A | -2.54 | 105.81      | 112.78   |
| 14  | cB    | 806  | CL7  | CMB-C2B-C1B | 2.54  | 129.24      | 125.37   |
| 14  | bB    | 819  | CL7  | C6-C5-C3    | -2.54 | 106.79      | 113.45   |
| 14  | aB    | 3020 | CL7  | C3B-C4B-NB  | -2.54 | 108.16      | 110.52   |
| 14  | cL    | 203  | CL7  | C4D-C3D-C2D | -2.54 | 103.99      | 107.30   |
| 14  | aA    | 3123 | CL7  | C2A-C1A-CHA | -2.54 | 121.28      | 126.36   |
| 14  | bA    | 3109 | CL7  | CBD-CHA-C4D | -2.54 | 103.06      | 109.14   |
| 14  | cA    | 3121 | CL7  | O1D-CGD-CBD | -2.54 | 119.28      | 124.48   |
| 14  | bB    | 808  | CL7  | CBD-CHA-C4D | -2.54 | 103.06      | 109.14   |
| 14  | aL    | 202  | CL7  | C11-C10-C8  | -2.54 | 107.71      | 115.92   |
| 14  | aB    | 3025 | CL7  | C11-C10-C8  | -2.54 | 107.71      | 115.92   |
| 14  | aA    | 3110 | CL7  | C3D-C4D-ND  | 2.54  | 113.81      | 110.17   |
| 14  | cA    | 3120 | CL7  | C3A-C2A-C1A | 2.54  | 105.14      | 101.34   |
| 14  | cB    | 812  | CL7  | CAA-C2A-C3A | -2.54 | 110.17      | 116.10   |
| 14  | cB    | 819  | CL7  | C3A-C4A-CHB | -2.54 | 119.93      | 123.70   |
| 14  | aB    | 3006 | CL7  | C3B-C4B-NB  | -2.54 | 108.16      | 110.52   |
| 14  | bA    | 3145 | CL7  | CBD-CHA-C4D | -2.54 | 103.07      | 109.14   |
| 14  | bA    | 3123 | CL7  | O2A-CGA-CBA | 2.54  | 119.87      | 111.91   |
| 14  | aA    | 3115 | CL7  | C3D-C4D-ND  | 2.54  | 113.81      | 110.17   |
| 14  | cA    | 3109 | CL7  | C3D-C4D-ND  | 2.54  | 113.81      | 110.17   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | cB    | 831  | CL7  | C1D-ND-C4D  | -2.54 | 104.53      | 106.33   |
| 14  | aA    | 3110 | CL7  | CHC-C1C-NC  | -2.54 | 122.12      | 124.45   |
| 14  | bA    | 3119 | CL7  | O2A-CGA-O1A | -2.53 | 115.20      | 123.14   |
| 14  | cB    | 825  | CL7  | CHB-C1B-NB  | -2.53 | 121.57      | 124.26   |
| 14  | bA    | 3132 | CL7  | CHB-C1B-NB  | -2.53 | 121.58      | 124.26   |
| 14  | cB    | 810  | CL7  | CHC-C1C-NC  | -2.53 | 122.13      | 124.45   |
| 14  | bA    | 3105 | CL7  | OBD-CAD-C3D | -2.53 | 122.42      | 128.52   |
| 14  | bA    | 3141 | CL7  | O1D-CGD-CBD | -2.53 | 119.30      | 124.48   |
| 14  | cL    | 203  | CL7  | C3A-C2A-C1A | 2.53  | 105.13      | 101.34   |
| 14  | cA    | 3113 | CL7  | C4D-C3D-C2D | -2.53 | 104.00      | 107.30   |
| 14  | cA    | 3124 | CL7  | CAC-C3C-C2C | -2.53 | 123.20      | 127.53   |
| 14  | bA    | 3122 | CL7  | CAA-C2A-C3A | -2.53 | 105.85      | 112.78   |
| 14  | aK    | 101  | CL7  | CBD-CHA-C1A | 2.53  | 134.58      | 129.44   |
| 14  | aB    | 3013 | CL7  | C3D-C4D-ND  | 2.53  | 113.80      | 110.17   |
| 14  | cA    | 3139 | CL7  | CAA-C2A-C3A | -2.53 | 105.85      | 112.78   |
| 14  | bA    | 3106 | CL7  | CHB-C1B-NB  | -2.53 | 121.58      | 124.26   |
| 14  | bB    | 831  | CL7  | O1D-CGD-CBD | -2.53 | 119.31      | 124.48   |
| 14  | bA    | 3116 | CL7  | CHC-C1C-NC  | -2.53 | 122.13      | 124.45   |
| 14  | bB    | 823  | CL7  | C3A-C2A-C1A | 2.53  | 104.66      | 101.64   |
| 14  | cB    | 821  | CL7  | C3B-C4B-NB  | -2.53 | 108.17      | 110.52   |
| 14  | aB    | 3026 | CL7  | C4D-C3D-C2D | -2.53 | 104.01      | 107.30   |
| 14  | aA    | 3127 | CL7  | O2A-CGA-O1A | -2.53 | 117.22      | 123.59   |
| 14  | aA    | 3116 | CL7  | CAA-C2A-C3A | -2.53 | 110.20      | 116.10   |
| 14  | aB    | 3008 | CL7  | CMB-C2B-C3B | -2.52 | 120.47      | 126.59   |
| 17  | aB    | 3027 | PQN  | O4-C4-C5    | -2.52 | 117.47      | 121.56   |
| 14  | cA    | 3131 | CL7  | CMA-C3A-C2A | -2.52 | 110.21      | 116.10   |
| 14  | bF    | 201  | CL7  | C1D-ND-C4D  | -2.52 | 104.54      | 106.33   |
| 14  | aL    | 203  | CL7  | CHB-C1B-NB  | -2.52 | 121.59      | 124.26   |
| 14  | bA    | 3109 | CL7  | O1D-CGD-CBD | -2.52 | 119.33      | 124.48   |
| 14  | cB    | 804  | CL7  | C6-C7-C8    | -2.52 | 107.77      | 115.92   |
| 14  | cA    | 3106 | CL7  | C1D-ND-C4D  | -2.52 | 104.55      | 106.33   |
| 14  | bA    | 3120 | CL7  | C4D-C3D-C2D | -2.52 | 104.02      | 107.30   |
| 12  | bA    | 3101 | G9R  | CMB-C2B-C3B | -2.52 | 120.49      | 126.59   |
| 14  | cA    | 3126 | CL7  | CHC-C1C-NC  | -2.52 | 122.14      | 124.45   |
| 14  | bB    | 827  | CL7  | C4D-C3D-C2D | -2.52 | 104.02      | 107.30   |
| 14  | cB    | 807  | CL7  | CAA-C2A-C3A | -2.52 | 105.89      | 112.78   |
| 14  | aB    | 3020 | CL7  | C3D-C4D-ND  | 2.52  | 113.78      | 110.17   |
| 14  | bA    | 3145 | CL7  | CAD-C3D-C2D | 2.52  | 149.87      | 144.44   |
| 12  | aA    | 3101 | G9R  | C1-O2A-CGA  | 2.52  | 123.04      | 116.44   |
| 14  | cA    | 3102 | CL7  | CMB-C2B-C1B | 2.52  | 129.20      | 125.37   |
| 14  | bB    | 812  | CL7  | CAA-C2A-C3A | -2.51 | 110.23      | 116.10   |
| 14  | aA    | 3128 | CL7  | CBD-CHA-C4D | -2.51 | 103.13      | 109.14   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | cA    | 3109 | CL7  | CBD-CHA-C4D | -2.51 | 103.13      | 109.14   |
| 14  | cA    | 3105 | CL7  | O2D-CGD-O1D | -2.51 | 118.92      | 123.84   |
| 14  | bB    | 807  | CL7  | C7-C6-C5    | -2.51 | 106.53      | 113.36   |
| 14  | bA    | 3105 | CL7  | O2D-CGD-O1D | -2.51 | 118.92      | 123.84   |
| 14  | aK    | 101  | CL7  | CMB-C2B-C1B | 2.51  | 129.20      | 125.37   |
| 14  | bB    | 810  | CL7  | CMB-C2B-C1B | 2.51  | 129.19      | 125.37   |
| 14  | cL    | 204  | CL7  | C4D-C3D-C2D | -2.51 | 104.03      | 107.30   |
| 14  | cB    | 831  | CL7  | C4D-C3D-C2D | -2.51 | 104.03      | 107.30   |
| 14  | cA    | 3102 | CL7  | CBC-CAC-C3C | -2.51 | 105.51      | 112.43   |
| 14  | bK    | 101  | CL7  | C3D-C4D-ND  | 2.51  | 113.77      | 110.17   |
| 14  | cB    | 832  | CL7  | CHC-C4B-NB  | 2.51  | 126.92      | 124.26   |
| 14  | aB    | 3003 | CL7  | C6-C7-C8    | -2.51 | 107.80      | 115.92   |
| 14  | cA    | 3120 | CL7  | CHB-C1B-NB  | -2.51 | 121.60      | 124.26   |
| 14  | aA    | 3141 | CL7  | O2D-CGD-O1D | -2.51 | 118.93      | 123.84   |
| 14  | aA    | 3133 | CL7  | CHB-C1B-NB  | -2.51 | 121.60      | 124.26   |
| 14  | cA    | 3105 | CL7  | CHD-C1D-ND  | 2.51  | 126.91      | 124.26   |
| 14  | aA    | 3133 | CL7  | CAA-C2A-C3A | -2.51 | 105.91      | 112.78   |
| 14  | aA    | 3123 | CL7  | CBD-CHA-C4D | -2.51 | 103.14      | 109.14   |
| 14  | cA    | 3132 | CL7  | C1-C2-C3    | -2.51 | 121.70      | 126.04   |
| 14  | cA    | 3110 | CL7  | C3A-C4A-CHB | -2.51 | 119.98      | 123.70   |
| 14  | bA    | 3114 | CL7  | CAA-C2A-C1A | -2.51 | 103.94      | 112.19   |
| 14  | bB    | 814  | CL7  | C3B-C4B-NB  | -2.51 | 108.19      | 110.52   |
| 14  | aA    | 3126 | CL7  | C1D-ND-C4D  | -2.51 | 104.55      | 106.33   |
| 14  | cB    | 812  | CL7  | C3D-C4D-ND  | 2.51  | 113.76      | 110.17   |
| 14  | cB    | 831  | CL7  | OBD-CAD-C3D | -2.51 | 122.49      | 128.52   |
| 14  | cA    | 3121 | CL7  | CBD-CHA-C4D | -2.51 | 103.15      | 109.14   |
| 12  | aA    | 3101 | G9R  | CHB-C1B-C2B | -2.51 | 120.16      | 127.24   |
| 14  | bB    | 821  | CL7  | C3B-C4B-NB  | -2.51 | 108.19      | 110.52   |
| 14  | cB    | 806  | CL7  | C11-C12-C13 | -2.51 | 107.82      | 115.92   |
| 14  | aA    | 3131 | CL7  | C4D-C3D-C2D | -2.51 | 104.03      | 107.30   |
| 14  | aK    | 101  | CL7  | C3B-C4B-NB  | -2.51 | 108.19      | 110.52   |
| 14  | bA    | 3141 | CL7  | CHB-C1B-NB  | -2.51 | 121.61      | 124.26   |
| 14  | aB    | 3013 | CL7  | CHC-C1C-NC  | -2.50 | 122.15      | 124.45   |
| 14  | aB    | 3013 | CL7  | CMB-C2B-C1B | 2.50  | 129.18      | 125.37   |
| 14  | cB    | 826  | CL7  | CHA-C1A-NA  | -2.50 | 120.05      | 125.98   |
| 14  | aA    | 3141 | CL7  | CBD-CHA-C4D | -2.50 | 103.15      | 109.14   |
| 14  | aA    | 3103 | CL7  | CBD-CHA-C4D | -2.50 | 103.15      | 109.14   |
| 14  | aA    | 3116 | CL7  | CMC-C2C-C1C | -2.50 | 120.30      | 124.71   |
| 14  | aB    | 3003 | CL7  | C4C-C3C-C2C | 2.50  | 110.39      | 107.13   |
| 14  | aB    | 3008 | CL7  | C2D-C1D-ND  | -2.50 | 108.55      | 110.23   |
| 14  | cB    | 827  | CL7  | CBC-CAC-C3C | 2.50  | 119.33      | 112.43   |
| 14  | cA    | 3112 | CL7  | CMB-C2B-C1B | 2.50  | 129.18      | 125.37   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | aB    | 3003 | CL7  | C7-C6-C5    | -2.50 | 106.56      | 113.36   |
| 14  | aB    | 3007 | CL7  | C7-C6-C5    | -2.50 | 106.56      | 113.36   |
| 14  | cA    | 3129 | CL7  | CHB-C1B-NB  | -2.50 | 121.61      | 124.26   |
| 14  | aA    | 3130 | CL7  | CAC-C3C-C4C | 2.50  | 128.61      | 124.68   |
| 14  | cA    | 3132 | CL7  | C2A-C1A-CHA | -2.50 | 121.36      | 126.36   |
| 14  | aA    | 3126 | CL7  | OBD-CAD-C3D | -2.50 | 122.50      | 128.52   |
| 17  | bB    | 828  | PQN  | O4-C4-C5    | -2.50 | 117.52      | 121.56   |
| 14  | aB    | 3032 | CL7  | C2B-C1B-NB  | -2.50 | 108.56      | 110.23   |
| 14  | cA    | 3120 | CL7  | O1D-CGD-CBD | -2.50 | 119.37      | 124.48   |
| 19  | aB    | 3029 | LMG  | O6-C5-C4    | -2.50 | 105.16      | 109.69   |
| 14  | cL    | 204  | CL7  | CBD-CHA-C4D | -2.50 | 103.17      | 109.14   |
| 17  | bB    | 828  | PQN  | C19-C18-C20 | -2.50 | 102.25      | 111.29   |
| 14  | cA    | 3132 | CL7  | C2D-C1D-ND  | -2.50 | 108.56      | 110.23   |
| 14  | bA    | 3107 | CL7  | CBD-CHA-C4D | -2.50 | 103.17      | 109.14   |
| 14  | aA    | 3117 | CL7  | C1A-NA-C4A  | -2.50 | 104.79      | 106.30   |
| 14  | cA    | 3120 | CL7  | C3A-C4A-CHB | -2.50 | 120.00      | 123.70   |
| 14  | bB    | 809  | CL7  | CBD-CHA-C4D | -2.49 | 103.17      | 109.14   |
| 14  | cB    | 817  | CL7  | C3D-C4D-ND  | 2.49  | 113.75      | 110.17   |
| 14  | aA    | 3109 | CL7  | CAA-C2A-C3A | -2.49 | 108.03      | 114.26   |
| 14  | aB    | 3009 | CL7  | CHC-C1C-NC  | -2.49 | 122.16      | 124.45   |
| 14  | bB    | 807  | CL7  | CHC-C1C-NC  | -2.49 | 122.16      | 124.45   |
| 14  | aA    | 3104 | CL7  | CHB-C1B-NB  | -2.49 | 121.62      | 124.26   |
| 14  | cA    | 3144 | CL7  | CAD-C3D-C2D | 2.49  | 149.82      | 144.44   |
| 14  | bA    | 3105 | CL7  | CMB-C2B-C1B | 2.49  | 129.16      | 125.37   |
| 14  | bA    | 3127 | CL7  | C4-C3-C5    | -2.49 | 113.14      | 115.98   |
| 14  | bB    | 820  | CL7  | O2A-CGA-O1A | -2.49 | 117.31      | 123.59   |
| 14  | bB    | 803  | CL7  | C4D-C3D-C2D | -2.49 | 104.06      | 107.30   |
| 14  | aB    | 3020 | CL7  | CAD-C3D-C2D | 2.49  | 149.81      | 144.44   |
| 14  | aK    | 101  | CL7  | CAD-CBD-CHA | -2.49 | 102.34      | 105.14   |
| 14  | cA    | 3106 | CL7  | CHC-C1C-NC  | -2.49 | 122.17      | 124.45   |
| 13  | bB    | 801  | PHO  | C2B-C1B-NB  | -2.49 | 107.81      | 109.53   |
| 14  | aA    | 3127 | CL7  | CHC-C1C-NC  | -2.49 | 122.17      | 124.45   |
| 14  | aB    | 3015 | CL7  | CHC-C4B-NB  | 2.49  | 126.89      | 124.26   |
| 14  | bA    | 3139 | CL7  | C3A-C4A-CHB | -2.49 | 120.01      | 123.70   |
| 14  | aL    | 203  | CL7  | C1D-ND-C4D  | -2.48 | 104.57      | 106.33   |
| 14  | aA    | 3141 | CL7  | C3A-C4A-CHB | -2.48 | 120.02      | 123.70   |
| 14  | bA    | 3107 | CL7  | C6-C5-C3    | -2.48 | 106.95      | 113.45   |
| 14  | cA    | 3142 | CL7  | C1-C2-C3    | -2.48 | 121.75      | 126.04   |
| 14  | aB    | 3010 | CL7  | OBD-CAD-C3D | -2.48 | 122.55      | 128.52   |
| 14  | aA    | 3131 | CL7  | O1D-CGD-CBD | -2.48 | 119.41      | 124.48   |
| 14  | cA    | 3132 | CL7  | O1D-CGD-CBD | -2.48 | 119.41      | 124.48   |
| 14  | bA    | 3107 | CL7  | C4C-C3C-C2C | 2.48  | 110.36      | 107.13   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | aA    | 3123 | CL7  | CHA-C1A-NA  | -2.48 | 120.11      | 125.98   |
| 14  | cB    | 826  | CL7  | CHC-C1C-NC  | -2.48 | 122.17      | 124.45   |
| 13  | cB    | 805  | PHO  | C6-C7-C8    | -2.48 | 107.91      | 115.92   |
| 14  | aA    | 3142 | CL7  | C6-C7-C8    | -2.48 | 107.91      | 115.92   |
| 14  | cA    | 3131 | CL7  | CBD-CHA-C4D | -2.48 | 103.21      | 109.14   |
| 14  | bA    | 3109 | CL7  | C3D-C4D-ND  | 2.48  | 113.72      | 110.17   |
| 14  | bB    | 812  | CL7  | C3D-C4D-ND  | 2.48  | 113.72      | 110.17   |
| 14  | bA    | 3131 | CL7  | CBD-CHA-C4D | -2.48 | 103.22      | 109.14   |
| 14  | aA    | 3103 | CL7  | C4C-C3C-C2C | 2.48  | 110.36      | 107.13   |
| 14  | aB    | 3032 | CL7  | O1D-CGD-CBD | -2.48 | 119.42      | 124.48   |
| 14  | cB    | 821  | CL7  | C3D-C4D-ND  | 2.48  | 113.72      | 110.17   |
| 14  | bL    | 204  | CL7  | C9-C8-C7    | -2.48 | 102.32      | 111.29   |
| 14  | bK    | 101  | CL7  | CHC-C1C-NC  | -2.48 | 122.18      | 124.45   |
| 14  | aB    | 3023 | CL7  | C1D-ND-C4D  | -2.48 | 104.58      | 106.33   |
| 14  | bB    | 831  | CL7  | OBD-CAD-C3D | -2.47 | 122.57      | 128.52   |
| 14  | aB    | 3010 | CL7  | CHB-C1B-NB  | -2.47 | 121.64      | 124.26   |
| 14  | aA    | 3122 | CL7  | CBD-CHA-C4D | -2.47 | 103.23      | 109.14   |
| 14  | aA    | 3112 | CL7  | CHC-C4B-NB  | 2.47  | 126.88      | 124.26   |
| 13  | aA    | 3102 | PHO  | CMC-C2C-C1C | 2.47  | 129.40      | 124.73   |
| 14  | bA    | 3127 | CL7  | CGD-CBD-CAD | -2.47 | 102.73      | 110.73   |
| 14  | cA    | 3127 | CL7  | C1-C2-C3    | -2.47 | 121.77      | 126.04   |
| 14  | aA    | 3133 | CL7  | C3A-C2A-C1A | 2.47  | 105.04      | 101.34   |
| 14  | aA    | 3131 | CL7  | CHC-C1C-NC  | -2.47 | 122.19      | 124.45   |
| 14  | bA    | 3142 | CL7  | CHC-C4B-NB  | 2.47  | 126.87      | 124.26   |
| 14  | cB    | 811  | CL7  | CHB-C1B-NB  | -2.47 | 121.64      | 124.26   |
| 14  | cA    | 3121 | CL7  | CHB-C1B-NB  | -2.47 | 121.64      | 124.26   |
| 14  | bA    | 3133 | CL7  | C3A-C2A-C1A | 2.47  | 104.59      | 101.64   |
| 14  | cA    | 3123 | CL7  | O1D-CGD-CBD | -2.47 | 119.44      | 124.48   |
| 14  | cA    | 3131 | CL7  | C3A-C4A-CHB | -2.47 | 120.04      | 123.70   |
| 14  | cA    | 3128 | CL7  | O2D-CGD-O1D | -2.47 | 119.02      | 123.84   |
| 14  | cA    | 3139 | CL7  | CAD-C3D-C2D | 2.46  | 149.76      | 144.44   |
| 14  | bB    | 821  | CL7  | CAD-C3D-C2D | 2.46  | 149.76      | 144.44   |
| 14  | bA    | 3105 | CL7  | CHB-C1B-NB  | -2.46 | 121.65      | 124.26   |
| 14  | bB    | 827  | CL7  | C1-C2-C3    | -2.46 | 121.78      | 126.04   |
| 14  | aF    | 201  | CL7  | C3D-C4D-ND  | 2.46  | 113.70      | 110.17   |
| 14  | bA    | 3133 | CL7  | CMB-C2B-C1B | 2.46  | 129.12      | 125.37   |
| 14  | aA    | 3105 | CL7  | C3D-C4D-ND  | 2.46  | 113.70      | 110.17   |
| 14  | bB    | 806  | CL7  | OBD-CAD-C3D | -2.46 | 122.60      | 128.52   |
| 14  | bA    | 3126 | CL7  | CAD-C3D-C2D | 2.46  | 149.75      | 144.44   |
| 14  | aA    | 3103 | CL7  | C3A-C2A-C1A | 2.46  | 105.02      | 101.34   |
| 14  | cA    | 3129 | CL7  | CBC-CAC-C3C | -2.46 | 105.65      | 112.43   |
| 14  | cF    | 201  | CL7  | C3D-C4D-ND  | 2.46  | 113.69      | 110.17   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | cB    | 815  | CL7  | CBD-CHA-C4D | -2.46 | 103.26      | 109.14   |
| 14  | aB    | 3003 | CL7  | C4D-C3D-C2D | -2.46 | 104.10      | 107.30   |
| 14  | bA    | 3122 | CL7  | CBD-CHA-C4D | -2.46 | 103.26      | 109.14   |
| 14  | cB    | 831  | CL7  | CHC-C1C-NC  | -2.46 | 122.20      | 124.45   |
| 14  | cA    | 3142 | CL7  | CHD-C1D-ND  | 2.46  | 126.86      | 124.26   |
| 14  | cB    | 820  | CL7  | O2D-CGD-O1D | -2.46 | 119.03      | 123.84   |
| 14  | aB    | 3017 | CL7  | CMB-C2B-C1B | 2.46  | 129.11      | 125.37   |
| 14  | cA    | 3104 | CL7  | CMB-C2B-C1B | 2.46  | 129.11      | 125.37   |
| 14  | aB    | 3012 | CL7  | C3D-C4D-ND  | 2.45  | 113.69      | 110.17   |
| 14  | bB    | 821  | CL7  | C3D-C4D-ND  | 2.45  | 113.69      | 110.17   |
| 14  | aA    | 3141 | CL7  | CHC-C1C-NC  | -2.45 | 122.20      | 124.45   |
| 14  | bA    | 3129 | CL7  | C3A-C4A-CHB | -2.45 | 120.06      | 123.70   |
| 14  | bA    | 3123 | CL7  | C3A-C2A-C1A | 2.45  | 105.01      | 101.34   |
| 14  | aL    | 204  | CL7  | C3A-C4A-CHB | -2.45 | 120.06      | 123.70   |
| 14  | bA    | 3141 | CL7  | C3B-C4B-NB  | -2.45 | 108.24      | 110.52   |
| 14  | cB    | 809  | CL7  | CBD-CHA-C4D | -2.45 | 103.28      | 109.14   |
| 14  | cA    | 3115 | CL7  | CAA-C2A-C3A | -2.45 | 110.38      | 116.10   |
| 14  | aA    | 3127 | CL7  | CAD-C3D-C2D | 2.45  | 149.73      | 144.44   |
| 14  | cB    | 804  | CL7  | C4C-C3C-C2C | 2.45  | 110.32      | 107.13   |
| 14  | aB    | 3005 | CL7  | OBD-CAD-C3D | -2.45 | 122.62      | 128.52   |
| 14  | cB    | 826  | CL7  | CBD-CHA-C4D | -2.45 | 103.28      | 109.14   |
| 14  | aA    | 3116 | CL7  | C4D-C3D-CAD | 2.45  | 109.07      | 107.42   |
| 14  | bB    | 825  | CL7  | CAD-C3D-C2D | 2.45  | 149.73      | 144.44   |
| 14  | cB    | 809  | CL7  | CGD-CBD-CAD | -2.45 | 102.80      | 110.73   |
| 14  | cB    | 810  | CL7  | O2A-CGA-O1A | -2.45 | 117.41      | 123.59   |
| 14  | aA    | 3140 | CL7  | CAD-C3D-C2D | 2.45  | 149.73      | 144.44   |
| 14  | bB    | 815  | CL7  | CBD-CHA-C4D | -2.45 | 103.29      | 109.14   |
| 14  | cA    | 3127 | CL7  | O2A-CGA-O1A | -2.45 | 117.42      | 123.59   |
| 14  | cB    | 823  | CL7  | C3A-C2A-C1A | 2.45  | 104.57      | 101.64   |
| 14  | cB    | 819  | CL7  | CAD-C3D-C2D | 2.45  | 149.72      | 144.44   |
| 14  | aL    | 204  | CL7  | C4D-C3D-C2D | -2.45 | 104.11      | 107.30   |
| 14  | aA    | 3133 | CL7  | C3D-C4D-ND  | 2.44  | 113.67      | 110.17   |
| 14  | cA    | 3122 | CL7  | CBD-CHA-C4D | -2.44 | 103.29      | 109.14   |
| 14  | aA    | 3141 | CL7  | C3B-C4B-NB  | -2.44 | 108.25      | 110.52   |
| 14  | cA    | 3125 | CL7  | C6-C7-C8    | -2.44 | 108.03      | 115.92   |
| 14  | bA    | 3126 | CL7  | CBD-CHA-C4D | -2.44 | 103.31      | 109.14   |
| 14  | aB    | 3019 | CL7  | C1D-ND-C4D  | -2.44 | 104.60      | 106.33   |
| 14  | cB    | 814  | CL7  | C3B-C4B-NB  | -2.44 | 108.25      | 110.52   |
| 14  | aB    | 3012 | CL7  | CAD-C3D-C2D | 2.44  | 149.71      | 144.44   |
| 14  | cB    | 827  | CL7  | CHB-C1B-NB  | -2.44 | 121.67      | 124.26   |
| 14  | cB    | 833  | CL7  | C4D-C3D-C2D | -2.44 | 104.12      | 107.30   |
| 14  | cA    | 3102 | CL7  | C3B-C4B-NB  | -2.44 | 108.25      | 110.52   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | cA    | 3122 | CL7  | CHC-C1C-NC  | -2.44 | 122.21      | 124.45   |
| 14  | bB    | 827  | CL7  | C1-O2A-CGA  | -2.44 | 110.05      | 116.44   |
| 14  | cA    | 3131 | CL7  | O1D-CGD-CBD | -2.44 | 119.50      | 124.48   |
| 14  | cA    | 3129 | CL7  | CAD-C3D-C2D | 2.44  | 149.70      | 144.44   |
| 14  | bB    | 826  | CL7  | C2A-C1A-CHA | -2.44 | 121.49      | 126.36   |
| 14  | bL    | 205  | CL7  | C3A-C4A-CHB | -2.44 | 120.08      | 123.70   |
| 14  | aB    | 3013 | CL7  | C3B-C4B-NB  | -2.44 | 108.25      | 110.52   |
| 14  | cB    | 808  | CL7  | C7-C6-C5    | -2.44 | 106.74      | 113.36   |
| 14  | cB    | 811  | CL7  | O2D-CGD-O1D | -2.44 | 119.08      | 123.84   |
| 14  | bB    | 826  | CL7  | CHA-C1A-NA  | -2.44 | 120.22      | 125.98   |
| 19  | cB    | 830  | LMG  | C7-O1-C1    | -2.44 | 108.98      | 113.74   |
| 14  | cB    | 803  | CL7  | C1-C2-C3    | -2.43 | 121.83      | 126.04   |
| 14  | cB    | 813  | CL7  | OBD-CAD-C3D | -2.43 | 122.66      | 128.52   |
| 14  | aA    | 3133 | CL7  | OBB-CAB-C3B | -2.43 | 120.19      | 125.69   |
| 14  | aA    | 3110 | CL7  | CHC-C4B-NB  | 2.43  | 126.83      | 124.26   |
| 14  | bA    | 3115 | CL7  | CAA-C2A-C3A | -2.43 | 110.42      | 116.10   |
| 14  | bA    | 3126 | CL7  | CHC-C1C-NC  | -2.43 | 122.22      | 124.45   |
| 14  | bB    | 810  | CL7  | C3A-C4A-CHB | -2.43 | 120.09      | 123.70   |
| 14  | aA    | 3134 | CL7  | C3D-C4D-ND  | 2.43  | 113.66      | 110.17   |
| 14  | aA    | 3108 | CL7  | CBD-CHA-C4D | -2.43 | 103.32      | 109.14   |
| 14  | aA    | 3141 | CL7  | CHC-C4B-NB  | 2.43  | 126.83      | 124.26   |
| 14  | bA    | 3105 | CL7  | C1A-NA-C4A  | 2.43  | 107.77      | 106.30   |
| 14  | cA    | 3140 | CL7  | CBD-CHA-C4D | -2.43 | 103.33      | 109.14   |
| 14  | aB    | 3031 | CL7  | CBD-CHA-C4D | -2.43 | 103.33      | 109.14   |
| 14  | bA    | 3131 | CL7  | O1D-CGD-CBD | -2.43 | 119.51      | 124.48   |
| 14  | cA    | 3107 | CL7  | CBD-CHA-C4D | -2.43 | 103.33      | 109.14   |
| 14  | cB    | 824  | CL7  | C4C-C3C-C2C | 2.43  | 110.29      | 107.13   |
| 14  | aB    | 3022 | CL7  | C4D-C3D-CAD | 2.43  | 109.06      | 107.42   |
| 14  | cB    | 807  | CL7  | C7-C6-C5    | -2.43 | 106.76      | 113.36   |
| 14  | bF    | 201  | CL7  | C3D-C4D-ND  | 2.43  | 113.65      | 110.17   |
| 14  | cB    | 814  | CL7  | CHC-C1C-NC  | -2.43 | 122.22      | 124.45   |
| 14  | cA    | 3118 | CL7  | CHB-C1B-NB  | -2.43 | 121.69      | 124.26   |
| 14  | cL    | 204  | CL7  | C1-C2-C3    | -2.43 | 121.85      | 126.04   |
| 14  | aA    | 3127 | CL7  | CBD-CHA-C4D | -2.43 | 103.34      | 109.14   |
| 14  | bB    | 812  | CL7  | C4C-C3C-C2C | 2.43  | 110.29      | 107.13   |
| 14  | bA    | 3117 | CL7  | CAD-C3D-C2D | 2.42  | 149.68      | 144.44   |
| 14  | bA    | 3115 | CL7  | CMB-C2B-C1B | 2.42  | 129.06      | 125.37   |
| 14  | aA    | 3104 | CL7  | O2D-CGD-O1D | -2.42 | 119.10      | 123.84   |
| 14  | aA    | 3126 | CL7  | C3A-C2A-C1A | 2.42  | 104.97      | 101.34   |
| 14  | aB    | 3014 | CL7  | O2D-CGD-O1D | -2.42 | 119.10      | 123.84   |
| 14  | bB    | 826  | CL7  | CBD-CHA-C4D | -2.42 | 103.35      | 109.14   |
| 14  | cB    | 827  | CL7  | CGD-CBD-CAD | -2.42 | 102.89      | 110.73   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | aA    | 3116 | CL7  | C1D-ND-C4D  | -2.42 | 104.61      | 106.33   |
| 14  | aA    | 3126 | CL7  | CAC-C3C-C2C | -2.42 | 123.39      | 127.53   |
| 14  | bB    | 833  | CL7  | C7-C6-C5    | -2.42 | 106.78      | 113.36   |
| 14  | bB    | 819  | CL7  | C3A-C4A-CHB | -2.42 | 120.11      | 123.70   |
| 14  | aL    | 204  | CL7  | CHB-C1B-NB  | -2.42 | 121.69      | 124.26   |
| 14  | aB    | 3003 | CL7  | O1D-CGD-CBD | -2.42 | 119.53      | 124.48   |
| 14  | bB    | 827  | CL7  | CHB-C1B-NB  | -2.42 | 121.70      | 124.26   |
| 14  | cA    | 3114 | CL7  | CAD-C3D-C2D | 2.42  | 149.66      | 144.44   |
| 14  | bB    | 819  | CL7  | C1D-ND-C4D  | -2.42 | 104.62      | 106.33   |
| 14  | cA    | 3130 | CL7  | C4D-C3D-C2D | -2.42 | 104.15      | 107.30   |
| 14  | aA    | 3103 | CL7  | O1D-CGD-CBD | -2.42 | 119.54      | 124.48   |
| 14  | bA    | 3109 | CL7  | CHC-C4B-NB  | 2.42  | 126.82      | 124.26   |
| 14  | cA    | 3102 | CL7  | C3D-C4D-ND  | 2.42  | 113.64      | 110.17   |
| 14  | bB    | 809  | CL7  | CHB-C1B-NB  | -2.42 | 121.70      | 124.26   |
| 14  | aA    | 3109 | CL7  | CMB-C2B-C1B | 2.42  | 129.05      | 125.37   |
| 14  | aB    | 3030 | CL7  | CMB-C2B-C1B | 2.42  | 129.05      | 125.37   |
| 14  | bA    | 3115 | CL7  | CMC-C2C-C1C | -2.42 | 120.45      | 124.71   |
| 14  | cB    | 815  | CL7  | OBD-CAD-C3D | -2.42 | 122.71      | 128.52   |
| 14  | aB    | 3011 | CL7  | C3D-C4D-ND  | 2.42  | 113.63      | 110.17   |
| 14  | cL    | 204  | CL7  | CHB-C1B-NB  | -2.42 | 121.70      | 124.26   |
| 14  | bA    | 3142 | CL7  | CHB-C1B-NB  | -2.41 | 121.70      | 124.26   |
| 14  | cB    | 823  | CL7  | CHA-C1A-NA  | -2.41 | 120.27      | 125.98   |
| 14  | cK    | 101  | CL7  | CBD-CHA-C1A | 2.41  | 134.35      | 129.44   |
| 14  | cB    | 812  | CL7  | C4C-C3C-C2C | 2.41  | 110.27      | 107.13   |
| 14  | aB    | 3025 | CL7  | CBD-CHA-C4D | -2.41 | 103.37      | 109.14   |
| 14  | cA    | 3120 | CL7  | C4-C3-C2    | -2.41 | 117.49      | 123.68   |
| 14  | cA    | 3141 | CL7  | C3B-C4B-NB  | -2.41 | 108.28      | 110.52   |
| 14  | aA    | 3140 | CL7  | O2A-CGA-O1A | -2.41 | 117.51      | 123.59   |
| 14  | bA    | 3142 | CL7  | C6-C7-C8    | -2.41 | 108.13      | 115.92   |
| 14  | cL    | 204  | CL7  | CAA-C2A-C3A | -2.41 | 106.18      | 112.78   |
| 14  | bA    | 3103 | CL7  | O2D-CGD-O1D | -2.41 | 119.13      | 123.84   |
| 14  | bA    | 3120 | CL7  | C3A-C2A-C1A | 2.41  | 104.94      | 101.34   |
| 14  | aB    | 3023 | CL7  | C4C-C3C-C2C | 2.41  | 110.26      | 107.13   |
| 14  | aB    | 3006 | CL7  | CAD-C3D-C2D | 2.41  | 149.63      | 144.44   |
| 14  | bB    | 806  | CL7  | C2A-C1A-CHA | -2.41 | 121.55      | 126.36   |
| 14  | bA    | 3120 | CL7  | O1D-CGD-CBD | -2.41 | 119.56      | 124.48   |
| 12  | bA    | 3101 | G9R  | CBC-CAC-C3C | -2.40 | 105.80      | 112.43   |
| 14  | cA    | 3140 | CL7  | C4-C3-C5    | -2.40 | 111.23      | 115.27   |
| 14  | aA    | 3124 | CL7  | O1D-CGD-CBD | -2.40 | 119.57      | 124.48   |
| 14  | bB    | 818  | CL7  | CMB-C2B-C1B | 2.40  | 129.03      | 125.37   |
| 14  | bB    | 804  | CL7  | C4C-C3C-C2C | 2.40  | 110.25      | 107.13   |
| 14  | cB    | 826  | CL7  | C6-C7-C8    | -2.40 | 108.17      | 115.92   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | cB    | 819  | CL7  | C1D-ND-C4D  | -2.40 | 104.63      | 106.33   |
| 14  | bA    | 3133 | CL7  | CHB-C1B-NB  | -2.40 | 121.72      | 124.26   |
| 14  | bB    | 811  | CL7  | OBD-CAD-C3D | -2.40 | 122.75      | 128.52   |
| 14  | bB    | 807  | CL7  | C9-C8-C7    | -2.40 | 102.61      | 111.29   |
| 14  | cB    | 806  | CL7  | CBD-CHA-C4D | -2.40 | 103.41      | 109.14   |
| 14  | aA    | 3132 | CL7  | CBD-CHA-C4D | -2.40 | 103.41      | 109.14   |
| 14  | cA    | 3103 | CL7  | CHB-C1B-NB  | -2.40 | 121.72      | 124.26   |
| 14  | aB    | 3032 | CL7  | C3A-C2A-C1A | 2.40  | 104.93      | 101.34   |
| 14  | bA    | 3114 | CL7  | C3B-C4B-NB  | -2.40 | 108.29      | 110.52   |
| 14  | bL    | 205  | CL7  | CHB-C1B-NB  | -2.39 | 121.72      | 124.26   |
| 14  | bA    | 3126 | CL7  | CED-O2D-CGD | 2.39  | 121.35      | 115.94   |
| 14  | aB    | 3022 | CL7  | C3D-C4D-ND  | 2.39  | 113.60      | 110.17   |
| 14  | cB    | 816  | CL7  | OBD-CAD-C3D | -2.39 | 122.76      | 128.52   |
| 14  | bA    | 3120 | CL7  | C1-O2A-CGA  | -2.39 | 110.17      | 116.44   |
| 14  | bA    | 3131 | CL7  | C3B-C4B-NB  | -2.39 | 108.30      | 110.52   |
| 14  | cA    | 3122 | CL7  | CAA-C2A-C3A | -2.39 | 106.23      | 112.78   |
| 14  | bA    | 3130 | CL7  | C1D-ND-C4D  | -2.39 | 104.64      | 106.33   |
| 14  | cA    | 3139 | CL7  | CBD-CHA-C4D | -2.39 | 103.42      | 109.14   |
| 14  | bA    | 3140 | CL7  | C3A-C4A-CHB | -2.39 | 120.15      | 123.70   |
| 14  | bA    | 3131 | CL7  | CMA-C3A-C2A | -2.39 | 110.52      | 116.10   |
| 14  | bB    | 807  | CL7  | C6-C5-C3    | -2.39 | 107.19      | 113.45   |
| 14  | cA    | 3102 | CL7  | C3B-C2B-C1B | -2.39 | 104.28      | 107.16   |
| 14  | bB    | 807  | CL7  | CBD-CHA-C4D | -2.39 | 103.43      | 109.14   |
| 14  | bB    | 811  | CL7  | C3D-C4D-ND  | 2.39  | 113.59      | 110.17   |
| 14  | cA    | 3115 | CL7  | CMC-C2C-C1C | -2.39 | 120.50      | 124.71   |
| 14  | aL    | 203  | CL7  | C4C-C3C-C2C | 2.39  | 110.24      | 107.13   |
| 14  | aB    | 3016 | CL7  | C3D-C4D-ND  | 2.39  | 113.59      | 110.17   |
| 14  | bA    | 3114 | CL7  | C6-C5-C3    | -2.39 | 107.20      | 113.45   |
| 14  | bB    | 813  | CL7  | C3D-C4D-ND  | 2.39  | 113.59      | 110.17   |
| 14  | bB    | 820  | CL7  | C3A-C2A-C1A | 2.39  | 104.91      | 101.34   |
| 14  | aA    | 3141 | CL7  | C6-C5-C3    | -2.39 | 107.20      | 113.45   |
| 14  | aA    | 3146 | CL7  | CAD-C3D-C2D | 2.38  | 149.59      | 144.44   |
| 14  | bA    | 3122 | CL7  | CHB-C1B-NB  | -2.38 | 121.73      | 124.26   |
| 14  | cL    | 205  | CL7  | C4D-C3D-C2D | -2.38 | 104.19      | 107.30   |
| 13  | bB    | 805  | PHO  | CMC-C2C-C1C | -2.38 | 120.23      | 124.73   |
| 14  | aB    | 3008 | CL7  | O1D-CGD-CBD | -2.38 | 119.61      | 124.48   |
| 14  | cB    | 810  | CL7  | CAD-C3D-C2D | 2.38  | 149.59      | 144.44   |
| 14  | aB    | 3024 | CL7  | CHB-C1B-NB  | -2.38 | 121.73      | 124.26   |
| 14  | aA    | 3134 | CL7  | C3B-C4B-NB  | -2.38 | 108.31      | 110.52   |
| 14  | cB    | 831  | CL7  | O1D-CGD-CBD | -2.38 | 119.61      | 124.48   |
| 16  | aA    | 3138 | LHG  | O4-P-O5     | 2.38  | 124.01      | 112.24   |
| 14  | bL    | 203  | CL7  | C11-C10-C8  | -2.38 | 108.22      | 115.92   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | cB    | 818  | CL7  | CHA-C1A-NA  | -2.38 | 120.34      | 125.98   |
| 14  | aB    | 3026 | CL7  | C2A-C1A-CHA | -2.38 | 121.60      | 126.36   |
| 14  | cA    | 3115 | CL7  | C1D-ND-C4D  | -2.38 | 104.64      | 106.33   |
| 14  | aB    | 3010 | CL7  | C3A-C2A-C1A | 2.38  | 104.49      | 101.64   |
| 14  | aA    | 3113 | CL7  | CBD-CHA-C4D | -2.38 | 103.45      | 109.14   |
| 14  | bB    | 803  | CL7  | C6-C7-C8    | -2.38 | 108.23      | 115.92   |
| 14  | aB    | 3010 | CL7  | C3D-C4D-ND  | 2.38  | 113.58      | 110.17   |
| 14  | aB    | 3032 | CL7  | CHD-C1D-ND  | 2.38  | 126.78      | 124.26   |
| 14  | cA    | 3132 | CL7  | CHB-C1B-NB  | -2.38 | 121.74      | 124.26   |
| 14  | aA    | 3133 | CL7  | CBD-CHA-C4D | -2.38 | 103.45      | 109.14   |
| 14  | bA    | 3125 | CL7  | C9-C8-C7    | -2.38 | 102.68      | 111.29   |
| 14  | aA    | 3143 | CL7  | C6-C7-C8    | -2.38 | 108.24      | 115.92   |
| 14  | aA    | 3118 | CL7  | CAD-C3D-C2D | 2.38  | 149.57      | 144.44   |
| 14  | cB    | 825  | CL7  | CMA-C3A-C2A | -2.38 | 110.55      | 116.10   |
| 14  | bB    | 807  | CL7  | C3D-C4D-ND  | 2.38  | 113.58      | 110.17   |
| 14  | aA    | 3140 | CL7  | C3A-C4A-CHB | -2.38 | 120.18      | 123.70   |
| 14  | bA    | 3102 | CL7  | C2C-C1C-NC  | 2.37  | 111.85      | 110.10   |
| 14  | aB    | 3031 | CL7  | CAD-C3D-C2D | 2.37  | 149.57      | 144.44   |
| 14  | cB    | 807  | CL7  | C9-C8-C7    | -2.37 | 102.69      | 111.29   |
| 14  | cA    | 3108 | CL7  | CAA-C2A-C3A | -2.37 | 108.33      | 114.26   |
| 14  | bB    | 804  | CL7  | O2D-CGD-O1D | -2.37 | 119.20      | 123.84   |
| 14  | cA    | 3126 | CL7  | C3A-C4A-CHB | -2.37 | 120.50      | 124.02   |
| 14  | aJ    | 101  | CL7  | C3D-C4D-ND  | 2.37  | 113.57      | 110.17   |
| 14  | bB    | 813  | CL7  | CAD-C3D-C2D | 2.37  | 149.56      | 144.44   |
| 12  | bA    | 3101 | G9R  | O2D-CGD-CBD | 2.37  | 115.48      | 111.27   |
| 14  | aA    | 3106 | CL7  | OBB-CAB-C3B | -2.37 | 120.33      | 125.69   |
| 13  | bB    | 801  | PHO  | CMC-C2C-C1C | 2.37  | 129.21      | 124.73   |
| 14  | cA    | 3114 | CL7  | CHA-C1A-NA  | -2.37 | 120.37      | 125.98   |
| 14  | bA    | 3109 | CL7  | CHC-C1C-NC  | -2.37 | 122.28      | 124.45   |
| 14  | cA    | 3115 | CL7  | C4D-C3D-CAD | 2.37  | 109.02      | 107.42   |
| 14  | bA    | 3130 | CL7  | C4D-C3D-C2D | -2.37 | 104.21      | 107.30   |
| 14  | aA    | 3133 | CL7  | CAD-C3D-C2D | 2.37  | 149.55      | 144.44   |
| 14  | bL    | 203  | CL7  | CHB-C1B-NB  | -2.37 | 121.75      | 124.26   |
| 14  | cA    | 3133 | CL7  | C3A-C2A-C1A | 2.37  | 104.47      | 101.64   |
| 14  | bB    | 824  | CL7  | C1A-NA-C4A  | 2.37  | 107.73      | 106.30   |
| 14  | aA    | 3129 | CL7  | CAD-C3D-C2D | 2.37  | 149.55      | 144.44   |
| 14  | cB    | 813  | CL7  | CAD-C3D-C2D | 2.36  | 149.55      | 144.44   |
| 14  | aA    | 3115 | CL7  | CBD-CHA-C4D | -2.36 | 103.49      | 109.14   |
| 14  | bB    | 821  | CL7  | C3A-C4A-CHB | -2.36 | 120.19      | 123.70   |
| 14  | bB    | 806  | CL7  | CMB-C2B-C1B | 2.36  | 128.97      | 125.37   |
| 14  | cA    | 3123 | CL7  | C3A-C4A-CHB | -2.36 | 120.19      | 123.70   |
| 14  | bA    | 3125 | CL7  | C6-C7-C8    | -2.36 | 108.28      | 115.92   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 19  | cB    | 830  | LMG  | O3-C3-C4    | -2.36 | 104.89      | 110.35   |
| 14  | cA    | 3111 | CL7  | C3A-C4A-CHB | -2.36 | 120.20      | 123.70   |
| 14  | aB    | 3025 | CL7  | CHC-C1C-NC  | -2.36 | 122.28      | 124.45   |
| 14  | aB    | 3011 | CL7  | C4C-C3C-C2C | 2.36  | 110.20      | 107.13   |
| 14  | aB    | 3026 | CL7  | C1A-NA-C4A  | 2.36  | 107.73      | 106.30   |
| 14  | aB    | 3003 | CL7  | C3D-C4D-ND  | 2.36  | 113.55      | 110.17   |
| 14  | aB    | 3006 | CL7  | C9-C8-C7    | -2.36 | 102.75      | 111.29   |
| 14  | bK    | 101  | CL7  | CBD-CHA-C1A | 2.36  | 134.24      | 129.44   |
| 14  | cA    | 3126 | CL7  | CHB-C1B-NB  | -2.36 | 121.76      | 124.26   |
| 14  | bL    | 203  | CL7  | OBD-CAD-C3D | -2.36 | 122.84      | 128.52   |
| 14  | cA    | 3132 | CL7  | C4C-C3C-C2C | 2.36  | 110.20      | 107.13   |
| 14  | bB    | 817  | CL7  | C3D-C4D-ND  | 2.36  | 113.55      | 110.17   |
| 14  | bB    | 823  | CL7  | C4D-C3D-CAD | 2.36  | 109.01      | 107.42   |
| 14  | aA    | 3132 | CL7  | CMA-C3A-C2A | -2.36 | 110.60      | 116.10   |
| 14  | bB    | 832  | CL7  | CAC-C3C-C4C | 2.36  | 128.39      | 124.68   |
| 14  | bA    | 3116 | CL7  | C3D-C4D-ND  | 2.36  | 113.55      | 110.17   |
| 14  | aB    | 3002 | CL7  | C16-C15-C13 | -2.35 | 108.31      | 115.92   |
| 14  | bA    | 3115 | CL7  | C4D-C3D-CAD | 2.35  | 109.01      | 107.42   |
| 14  | aL    | 202  | CL7  | C1-C2-C3    | -2.35 | 121.97      | 126.04   |
| 14  | cA    | 3113 | CL7  | CMB-C2B-C3B | -2.35 | 120.89      | 126.59   |
| 14  | bA    | 3112 | CL7  | CBD-CHA-C4D | -2.35 | 103.51      | 109.14   |
| 14  | bA    | 3112 | CL7  | CMB-C2B-C1B | 2.35  | 128.95      | 125.37   |
| 14  | cA    | 3121 | CL7  | CGD-CBD-CAD | -2.35 | 103.11      | 110.73   |
| 14  | aL    | 202  | CL7  | C6-C7-C8    | -2.35 | 108.32      | 115.92   |
| 14  | cB    | 815  | CL7  | CHB-C1B-NB  | -2.35 | 121.77      | 124.26   |
| 14  | cA    | 3105 | CL7  | CGD-CBD-CAD | -2.35 | 103.12      | 110.73   |
| 14  | aA    | 3140 | CL7  | CMB-C2B-C1B | 2.35  | 128.95      | 125.37   |
| 14  | cB    | 822  | CL7  | CBD-CHA-C4D | -2.35 | 103.52      | 109.14   |
| 14  | bB    | 803  | CL7  | C4C-C3C-C2C | 2.35  | 110.19      | 107.13   |
| 14  | aB    | 3006 | CL7  | CBD-CHA-C4D | -2.35 | 103.52      | 109.14   |
| 14  | cA    | 3105 | CL7  | CHB-C1B-NB  | -2.35 | 121.77      | 124.26   |
| 16  | aA    | 3138 | LHG  | P-O6-C4     | -2.35 | 107.92      | 121.68   |
| 14  | bA    | 3130 | CL7  | CBD-CHA-C4D | -2.35 | 103.53      | 109.14   |
| 14  | aA    | 3134 | CL7  | O2D-CGD-O1D | -2.35 | 119.25      | 123.84   |
| 14  | cA    | 3109 | CL7  | CHC-C1C-NC  | -2.35 | 122.30      | 124.45   |
| 14  | bA    | 3139 | CL7  | CAD-C3D-C2D | 2.35  | 149.51      | 144.44   |
| 14  | bB    | 820  | CL7  | C4C-C3C-C2C | 2.35  | 110.18      | 107.13   |
| 14  | aA    | 3106 | CL7  | CBD-CHA-C4D | -2.34 | 103.53      | 109.14   |
| 14  | cA    | 3122 | CL7  | C4D-C3D-C2D | -2.34 | 104.25      | 107.30   |
| 14  | cA    | 3119 | CL7  | CHA-C1A-NA  | -2.34 | 120.44      | 125.98   |
| 14  | bA    | 3142 | CL7  | O2A-CGA-CBA | 2.34  | 119.26      | 111.91   |
| 14  | cB    | 823  | CL7  | CBD-CHA-C4D | -2.34 | 103.54      | 109.14   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | cA    | 3133 | CL7  | C3D-C4D-ND  | 2.34  | 113.53      | 110.17   |
| 14  | aA    | 3126 | CL7  | O1D-CGD-CBD | -2.34 | 119.69      | 124.48   |
| 14  | cL    | 204  | CL7  | C6-C7-C8    | -2.34 | 108.35      | 115.92   |
| 14  | bB    | 827  | CL7  | C6-C5-C3    | -2.34 | 107.31      | 113.45   |
| 14  | aB    | 3008 | CL7  | C1-C2-C3    | -2.34 | 122.96      | 126.75   |
| 14  | aA    | 3126 | CL7  | C3D-C4D-ND  | 2.34  | 113.53      | 110.17   |
| 14  | cA    | 3123 | CL7  | CAA-CBA-CGA | -2.34 | 106.42      | 113.25   |
| 14  | cA    | 3124 | CL7  | CAD-C3D-C2D | 2.34  | 149.49      | 144.44   |
| 14  | cB    | 810  | CL7  | C6-C5-C3    | -2.34 | 107.32      | 113.45   |
| 14  | cB    | 806  | CL7  | CGD-CBD-CAD | -2.34 | 103.16      | 110.73   |
| 14  | cB    | 814  | CL7  | CBD-CHA-C4D | -2.34 | 103.55      | 109.14   |
| 14  | cB    | 810  | CL7  | CED-O2D-CGD | 2.34  | 121.22      | 115.94   |
| 14  | bA    | 3133 | CL7  | C3D-C4D-ND  | 2.34  | 113.52      | 110.17   |
| 14  | bL    | 204  | CL7  | CBD-CHA-C4D | -2.34 | 103.55      | 109.14   |
| 14  | cA    | 3125 | CL7  | CAC-C3C-C2C | -2.34 | 123.53      | 127.53   |
| 14  | cA    | 3132 | CL7  | CAA-C2A-C3A | -2.34 | 106.38      | 112.78   |
| 14  | aB    | 3024 | CL7  | C3D-C4D-ND  | 2.34  | 113.52      | 110.17   |
| 14  | bA    | 3125 | CL7  | CAA-CBA-CGA | -2.34 | 106.43      | 113.25   |
| 14  | cA    | 3139 | CL7  | O2A-CGA-O1A | -2.33 | 117.70      | 123.59   |
| 14  | aA    | 3106 | CL7  | OBD-CAD-C3D | -2.33 | 122.90      | 128.52   |
| 14  | bL    | 204  | CL7  | C4C-C3C-C2C | 2.33  | 110.17      | 107.13   |
| 14  | cA    | 3130 | CL7  | CHC-C1C-NC  | -2.33 | 122.31      | 124.45   |
| 14  | aB    | 3013 | CL7  | CBD-CHA-C4D | -2.33 | 103.56      | 109.14   |
| 14  | bB    | 827  | CL7  | OBD-CAD-C3D | -2.33 | 122.90      | 128.52   |
| 14  | bB    | 819  | CL7  | C4-C3-C5    | -2.33 | 111.35      | 115.27   |
| 14  | aA    | 3126 | CL7  | C9-C8-C7    | -2.33 | 102.84      | 111.29   |
| 16  | cA    | 3137 | LHG  | O4-P-O5     | 2.33  | 123.77      | 112.24   |
| 16  | bA    | 3137 | LHG  | P-O6-C4     | -2.33 | 108.00      | 121.68   |
| 14  | cB    | 810  | CL7  | CHA-C1A-NA  | -2.33 | 120.47      | 125.98   |
| 14  | aA    | 3131 | CL7  | CBD-CHA-C4D | -2.33 | 103.57      | 109.14   |
| 14  | bA    | 3127 | CL7  | C1-O2A-CGA  | -2.33 | 110.33      | 116.44   |
| 14  | cB    | 813  | CL7  | C3D-C4D-ND  | 2.33  | 113.51      | 110.17   |
| 14  | cA    | 3125 | CL7  | C9-C8-C7    | -2.33 | 102.86      | 111.29   |
| 14  | cA    | 3109 | CL7  | CHC-C4B-NB  | 2.33  | 126.72      | 124.26   |
| 14  | bB    | 819  | CL7  | CAD-C3D-C2D | 2.33  | 149.47      | 144.44   |
| 14  | bB    | 824  | CL7  | C3A-C4A-CHB | -2.33 | 120.25      | 123.70   |
| 14  | cA    | 3104 | CL7  | C3D-C4D-ND  | 2.33  | 113.51      | 110.17   |
| 14  | cB    | 821  | CL7  | CAD-C3D-C2D | 2.33  | 149.47      | 144.44   |
| 14  | cA    | 3108 | CL7  | C4D-C3D-C2D | -2.33 | 104.27      | 107.30   |
| 14  | aA    | 3124 | CL7  | CAC-C3C-C2C | -2.33 | 123.55      | 127.53   |
| 14  | aA    | 3122 | CL7  | CHC-C4B-NB  | 2.33  | 126.72      | 124.26   |
| 14  | aA    | 3123 | CL7  | CHC-C4B-NB  | 2.33  | 126.72      | 124.26   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | aA    | 3128 | CL7  | CGD-CBD-CAD | -2.33 | 103.20      | 110.73   |
| 14  | bA    | 3142 | CL7  | C1D-CHD-C4C | -2.33 | 117.55      | 124.74   |
| 14  | bA    | 3122 | CL7  | C4D-C3D-C2D | -2.33 | 104.27      | 107.30   |
| 14  | aB    | 3006 | CL7  | CHC-C1C-NC  | -2.32 | 122.32      | 124.45   |
| 14  | bB    | 804  | CL7  | C3A-C2A-C1A | 2.32  | 104.82      | 101.34   |
| 14  | aB    | 3030 | CL7  | C6-C5-C3    | -2.32 | 107.36      | 113.45   |
| 14  | bB    | 831  | CL7  | CHA-C1A-NA  | -2.32 | 120.48      | 125.98   |
| 14  | aA    | 3125 | CL7  | CMB-C2B-C3B | -2.32 | 120.96      | 126.59   |
| 14  | aA    | 3125 | CL7  | C3A-C2A-C1A | 2.32  | 104.82      | 101.34   |
| 14  | bL    | 204  | CL7  | C1D-ND-C4D  | -2.32 | 104.69      | 106.33   |
| 14  | cA    | 3127 | CL7  | CHB-C1B-NB  | -2.32 | 121.80      | 124.26   |
| 14  | bA    | 3108 | CL7  | CMD-C2D-C1D | 2.32  | 128.90      | 125.37   |
| 14  | cB    | 827  | CL7  | C4D-C3D-C2D | -2.32 | 104.28      | 107.30   |
| 17  | cB    | 828  | PQN  | C19-C18-C20 | -2.32 | 102.89      | 111.29   |
| 14  | cL    | 203  | CL7  | C11-C10-C8  | -2.32 | 108.42      | 115.92   |
| 14  | cA    | 3114 | CL7  | CAC-C3C-C4C | 2.32  | 128.33      | 124.68   |
| 14  | cA    | 3105 | CL7  | C1D-CHD-C4C | -2.32 | 117.57      | 124.74   |
| 14  | cB    | 811  | CL7  | CBD-CHA-C4D | -2.32 | 103.60      | 109.14   |
| 14  | aA    | 3143 | CL7  | C4-C3-C2    | -2.32 | 117.73      | 123.68   |
| 14  | cA    | 3129 | CL7  | C4D-C3D-C2D | -2.32 | 104.28      | 107.30   |
| 14  | aL    | 202  | CL7  | CHB-C1B-NB  | -2.32 | 121.81      | 124.26   |
| 14  | cA    | 3128 | CL7  | CHB-C1B-NB  | -2.32 | 121.81      | 124.26   |
| 14  | aA    | 3124 | CL7  | C4C-C3C-C2C | 2.32  | 110.14      | 107.13   |
| 14  | bB    | 807  | CL7  | CAD-C3D-C2D | 2.32  | 149.44      | 144.44   |
| 14  | aB    | 3019 | CL7  | C4C-C3C-C2C | 2.32  | 110.14      | 107.13   |
| 14  | cA    | 3112 | CL7  | CBD-CHA-C4D | -2.31 | 103.61      | 109.14   |
| 14  | bB    | 806  | CL7  | CGD-CBD-CAD | -2.31 | 103.24      | 110.73   |
| 14  | aB    | 3032 | CL7  | C3A-C4A-CHB | -2.31 | 120.27      | 123.70   |
| 14  | cA    | 3117 | CL7  | CAD-C3D-C2D | 2.31  | 149.44      | 144.44   |
| 14  | bA    | 3132 | CL7  | O2A-CGA-O1A | -2.31 | 117.75      | 123.59   |
| 14  | bB    | 818  | CL7  | CHA-C1A-NA  | -2.31 | 120.51      | 125.98   |
| 14  | aA    | 3117 | CL7  | C6-C5-C3    | -2.31 | 107.39      | 113.45   |
| 14  | cB    | 814  | CL7  | CMB-C2B-C1B | 2.31  | 128.89      | 125.37   |
| 14  | aA    | 3114 | CL7  | OBD-CAD-C3D | -2.31 | 122.95      | 128.52   |
| 14  | bA    | 3121 | CL7  | CBD-CHA-C4D | -2.31 | 103.61      | 109.14   |
| 14  | bA    | 3108 | CL7  | CMC-C2C-C1C | -2.31 | 120.64      | 124.71   |
| 14  | cA    | 3140 | CL7  | C6-C7-C8    | -2.31 | 108.45      | 115.92   |
| 14  | aA    | 3146 | CL7  | CBD-CHA-C4D | -2.31 | 103.62      | 109.14   |
| 14  | cA    | 3130 | CL7  | CBD-CHA-C4D | -2.31 | 103.62      | 109.14   |
| 14  | aB    | 3009 | CL7  | C6-C5-C3    | -2.31 | 107.40      | 113.45   |
| 14  | cA    | 3107 | CL7  | C1D-ND-C4D  | -2.31 | 104.69      | 106.33   |
| 14  | cA    | 3142 | CL7  | C1D-CHD-C4C | -2.31 | 117.60      | 124.74   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | cA    | 3119 | CL7  | CHC-C1C-NC  | -2.31 | 122.33      | 124.45   |
| 14  | aL    | 203  | CL7  | C3A-C4A-CHB | -2.31 | 120.28      | 123.70   |
| 14  | aB    | 3023 | CL7  | C3D-C4D-ND  | 2.31  | 113.48      | 110.17   |
| 14  | aA    | 3106 | CL7  | O2D-CGD-O1D | -2.31 | 119.33      | 123.84   |
| 14  | cA    | 3110 | CL7  | CMB-C2B-C1B | 2.31  | 128.88      | 125.37   |
| 13  | bB    | 801  | PHO  | CBA-CAA-C2A | -2.31 | 107.08      | 113.81   |
| 14  | bB    | 820  | CL7  | CAA-C2A-C3A | -2.30 | 106.47      | 112.78   |
| 14  | bB    | 804  | CL7  | C9-C8-C7    | -2.30 | 102.94      | 111.29   |
| 14  | cB    | 824  | CL7  | O1D-CGD-CBD | -2.30 | 119.77      | 124.48   |
| 14  | cA    | 3125 | CL7  | CHB-C1B-NB  | -2.30 | 121.82      | 124.26   |
| 12  | bA    | 3101 | G9R  | C4D-CHA-C1A | -2.30 | 118.44      | 121.25   |
| 14  | cB    | 803  | CL7  | CBD-CHA-C4D | -2.30 | 103.64      | 109.14   |
| 14  | cA    | 3106 | CL7  | CHB-C1B-NB  | -2.30 | 121.82      | 124.26   |
| 14  | bB    | 809  | CL7  | CMB-C2B-C3B | -2.30 | 121.01      | 126.59   |
| 14  | cB    | 815  | CL7  | C3D-C4D-ND  | 2.30  | 113.47      | 110.17   |
| 14  | cA    | 3129 | CL7  | C4D-C3D-CAD | -2.30 | 105.87      | 107.42   |
| 14  | cA    | 3116 | CL7  | C3D-C4D-ND  | 2.30  | 113.47      | 110.17   |
| 14  | aA    | 3103 | CL7  | CHC-C4B-NB  | 2.30  | 126.69      | 124.26   |
| 14  | cA    | 3120 | CL7  | O2D-CGD-O1D | -2.30 | 119.34      | 123.84   |
| 14  | aB    | 3022 | CL7  | CHA-C1A-NA  | -2.30 | 120.54      | 125.98   |
| 14  | cA    | 3130 | CL7  | O1D-CGD-CBD | -2.30 | 119.78      | 124.48   |
| 14  | cA    | 3124 | CL7  | O1D-CGD-CBD | -2.30 | 119.78      | 124.48   |
| 14  | bA    | 3118 | CL7  | CHB-C1B-NB  | -2.30 | 121.83      | 124.26   |
| 14  | bB    | 804  | CL7  | C6-C7-C8    | -2.30 | 108.49      | 115.92   |
| 14  | aB    | 3022 | CL7  | CHC-C1C-NC  | -2.30 | 122.34      | 124.45   |
| 14  | aA    | 3110 | CL7  | O1D-CGD-CBD | -2.30 | 119.78      | 124.48   |
| 14  | cA    | 3127 | CL7  | CBD-CHA-C4D | -2.30 | 103.65      | 109.14   |
| 14  | aA    | 3124 | CL7  | C3D-C4D-ND  | 2.30  | 113.46      | 110.17   |
| 14  | bB    | 823  | CL7  | C3D-C4D-ND  | 2.30  | 113.46      | 110.17   |
| 14  | aB    | 3005 | CL7  | CMB-C2B-C1B | 2.30  | 128.87      | 125.37   |
| 14  | bB    | 815  | CL7  | CHB-C1B-NB  | -2.30 | 121.83      | 124.26   |
| 14  | cL    | 204  | CL7  | O1A-CGA-CBA | -2.30 | 114.78      | 123.73   |
| 14  | aB    | 3022 | CL7  | C3A-C2A-C1A | 2.29  | 104.39      | 101.64   |
| 14  | aA    | 3120 | CL7  | O2A-CGA-O1A | -2.29 | 115.95      | 123.14   |
| 14  | cA    | 3128 | CL7  | C16-C17-C18 | -2.29 | 105.17      | 115.98   |
| 14  | aB    | 3026 | CL7  | C1-O2A-CGA  | -2.29 | 110.43      | 116.44   |
| 14  | bB    | 820  | CL7  | C1D-ND-C4D  | -2.29 | 104.71      | 106.33   |
| 14  | bA    | 3125 | CL7  | CBD-CHA-C4D | -2.29 | 103.66      | 109.14   |
| 14  | bL    | 205  | CL7  | CAA-C2A-C3A | -2.29 | 108.53      | 114.26   |
| 14  | aA    | 3125 | CL7  | CGD-CBD-CAD | -2.29 | 103.31      | 110.73   |
| 14  | aA    | 3141 | CL7  | C6-C7-C8    | -2.29 | 108.51      | 115.92   |
| 14  | cL    | 203  | CL7  | C6-C7-C8    | -2.29 | 108.51      | 115.92   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | cA    | 3126 | CL7  | CMB-C2B-C1B | 2.29  | 128.86      | 125.37   |
| 14  | bB    | 809  | CL7  | C2B-C1B-NB  | -2.29 | 108.70      | 110.23   |
| 14  | aB    | 3023 | CL7  | CHC-C4B-NB  | 2.29  | 126.68      | 124.26   |
| 14  | cB    | 826  | CL7  | C16-C15-C13 | -2.29 | 108.52      | 115.92   |
| 14  | bA    | 3121 | CL7  | C4D-C3D-C2D | -2.29 | 104.32      | 107.30   |
| 13  | cB    | 801  | PHO  | CMC-C2C-C1C | 2.29  | 129.05      | 124.73   |
| 16  | bA    | 3138 | LHG  | P-O3-C3     | -2.29 | 108.26      | 121.68   |
| 14  | cB    | 818  | CL7  | CMB-C2B-C1B | 2.29  | 128.85      | 125.37   |
| 14  | aA    | 3117 | CL7  | C4-C3-C2    | -2.29 | 117.81      | 123.68   |
| 14  | cB    | 824  | CL7  | CMB-C2B-C3B | -2.29 | 121.05      | 126.59   |
| 14  | aB    | 3009 | CL7  | C4C-C3C-C2C | 2.29  | 110.11      | 107.13   |
| 14  | cA    | 3102 | CL7  | CBD-CHA-C4D | -2.29 | 103.67      | 109.14   |
| 14  | aA    | 3130 | CL7  | CAC-C3C-C2C | -2.28 | 123.62      | 127.53   |
| 14  | aJ    | 101  | CL7  | C1A-NA-C4A  | -2.28 | 104.92      | 106.30   |
| 14  | cA    | 3121 | CL7  | C4D-C3D-C2D | -2.28 | 104.32      | 107.30   |
| 14  | bA    | 3106 | CL7  | CHC-C1C-NC  | -2.28 | 122.36      | 124.45   |
| 14  | bA    | 3139 | CL7  | C16-C15-C13 | -2.28 | 108.54      | 115.92   |
| 14  | bB    | 813  | CL7  | OBD-CAD-C3D | -2.28 | 123.03      | 128.52   |
| 14  | cA    | 3121 | CL7  | CED-O2D-CGD | 2.28  | 121.10      | 115.94   |
| 14  | aA    | 3143 | CL7  | C1D-CHD-C4C | -2.28 | 117.69      | 124.74   |
| 14  | aB    | 3019 | CL7  | O2D-CGD-O1D | -2.28 | 119.38      | 123.84   |
| 14  | bA    | 3129 | CL7  | CMB-C2B-C3B | -2.28 | 121.06      | 126.59   |
| 14  | bB    | 814  | CL7  | CBD-CHA-C4D | -2.28 | 103.69      | 109.14   |
| 14  | aA    | 3119 | CL7  | OBD-CAD-C3D | -2.28 | 123.03      | 128.52   |
| 14  | cA    | 3121 | CL7  | CHC-C4B-NB  | 2.28  | 126.67      | 124.26   |
| 14  | cA    | 3106 | CL7  | CHA-C1A-NA  | -2.28 | 120.58      | 125.98   |
| 14  | aB    | 3015 | CL7  | C4D-C3D-C2D | -2.28 | 104.33      | 107.30   |
| 14  | cJ    | 101  | CL7  | C3D-C4D-ND  | 2.28  | 113.44      | 110.17   |
| 14  | cB    | 832  | CL7  | CAD-C3D-C2D | 2.28  | 149.36      | 144.44   |
| 14  | cB    | 803  | CL7  | C7-C6-C5    | -2.28 | 107.17      | 113.36   |
| 14  | bB    | 815  | CL7  | CHC-C1C-NC  | -2.28 | 122.36      | 124.45   |
| 14  | bA    | 3106 | CL7  | C1A-NA-C4A  | 2.28  | 107.68      | 106.30   |
| 14  | cK    | 101  | CL7  | C3B-C4B-NB  | -2.28 | 108.40      | 110.52   |
| 14  | aA    | 3128 | CL7  | C4D-C3D-CAD | 2.28  | 108.96      | 107.42   |
| 14  | aA    | 3126 | CL7  | C4D-C3D-C2D | -2.28 | 104.33      | 107.30   |
| 14  | cA    | 3118 | CL7  | OBD-CAD-C3D | -2.28 | 123.04      | 128.52   |
| 14  | aB    | 3019 | CL7  | C2A-C1A-CHA | -2.28 | 121.81      | 126.36   |
| 14  | aL    | 204  | CL7  | C3A-C2A-C1A | 2.28  | 104.75      | 101.34   |
| 14  | cA    | 3127 | CL7  | CAA-C2A-C3A | -2.27 | 106.55      | 112.78   |
| 14  | cA    | 3129 | CL7  | CMC-C2C-C3C | 2.27  | 132.29      | 126.12   |
| 14  | aB    | 3006 | CL7  | CHB-C1B-NB  | -2.27 | 121.85      | 124.26   |
| 14  | cB    | 823  | CL7  | C4D-C3D-CAD | 2.27  | 108.95      | 107.42   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | cB    | 827  | CL7  | C6-C5-C3    | -2.27 | 107.50      | 113.45   |
| 14  | aA    | 3111 | CL7  | C3D-C4D-ND  | 2.27  | 113.43      | 110.17   |
| 14  | cB    | 818  | CL7  | C3D-C4D-ND  | 2.27  | 113.43      | 110.17   |
| 14  | bB    | 824  | CL7  | CMB-C2B-C3B | -2.27 | 121.08      | 126.59   |
| 14  | aA    | 3109 | CL7  | O2D-CGD-O1D | -2.27 | 119.40      | 123.84   |
| 14  | cA    | 3131 | CL7  | C3A-C2A-C1A | 2.27  | 104.36      | 101.64   |
| 14  | bA    | 3107 | CL7  | CHC-C1C-NC  | -2.27 | 122.37      | 124.45   |
| 14  | aA    | 3143 | CL7  | CHD-C1D-ND  | 2.27  | 126.66      | 124.26   |
| 14  | cA    | 3114 | CL7  | C14-C13-C12 | -2.27 | 103.07      | 111.29   |
| 14  | aB    | 3018 | CL7  | C1D-ND-C4D  | -2.27 | 104.72      | 106.33   |
| 14  | aB    | 3018 | CL7  | C4-C3-C5    | -2.27 | 111.45      | 115.27   |
| 14  | cL    | 205  | CL7  | CAA-C2A-C3A | -2.27 | 108.59      | 114.26   |
| 19  | bB    | 830  | LMG  | C7-O1-C1    | -2.27 | 109.30      | 113.74   |
| 14  | bA    | 3132 | CL7  | C3D-C4D-ND  | 2.27  | 113.42      | 110.17   |
| 14  | bA    | 3114 | CL7  | CAD-C3D-C2D | 2.27  | 149.34      | 144.44   |
| 14  | cB    | 807  | CL7  | CAD-C3D-C2D | 2.27  | 149.34      | 144.44   |
| 14  | aB    | 3012 | CL7  | OBD-CAD-C3D | -2.27 | 123.06      | 128.52   |
| 14  | bB    | 817  | CL7  | OBD-CAD-C3D | -2.27 | 123.06      | 128.52   |
| 14  | cB    | 817  | CL7  | CMB-C2B-C1B | 2.27  | 128.82      | 125.37   |
| 14  | bB    | 833  | CL7  | C4D-C3D-C2D | -2.27 | 104.34      | 107.30   |
| 14  | bB    | 817  | CL7  | CMB-C2B-C1B | 2.27  | 128.82      | 125.37   |
| 14  | cB    | 818  | CL7  | CED-O2D-CGD | 2.27  | 121.06      | 115.94   |
| 14  | bB    | 823  | CL7  | CBD-CHA-C4D | -2.27 | 103.72      | 109.14   |
| 14  | cA    | 3123 | CL7  | CBD-CHA-C4D | -2.27 | 103.72      | 109.14   |
| 14  | bB    | 803  | CL7  | C1A-NA-C4A  | -2.27 | 104.93      | 106.30   |
| 14  | aB    | 3006 | CL7  | C3D-C4D-ND  | 2.26  | 113.42      | 110.17   |
| 14  | bA    | 3108 | CL7  | C2C-C1C-NC  | 2.26  | 111.77      | 110.10   |
| 14  | cA    | 3129 | CL7  | O1D-CGD-CBD | -2.26 | 119.85      | 124.48   |
| 16  | aA    | 3138 | LHG  | P-O3-C3     | -2.26 | 108.42      | 121.68   |
| 14  | aA    | 3129 | CL7  | C2B-C1B-NB  | 2.26  | 111.75      | 110.23   |
| 14  | cL    | 204  | CL7  | C9-C8-C7    | -2.26 | 103.10      | 111.29   |
| 14  | bL    | 204  | CL7  | C16-C15-C13 | -2.26 | 108.61      | 115.92   |
| 14  | bB    | 817  | CL7  | CBD-CHA-C4D | -2.26 | 103.73      | 109.14   |
| 14  | bA    | 3142 | CL7  | CHD-C1D-ND  | 2.26  | 126.65      | 124.26   |
| 14  | bB    | 818  | CL7  | CHC-C1C-NC  | -2.26 | 122.38      | 124.45   |
| 14  | bA    | 3118 | CL7  | CHC-C1C-NC  | -2.26 | 122.38      | 124.45   |
| 14  | bL    | 203  | CL7  | C1-C2-C3    | -2.26 | 122.14      | 126.04   |
| 14  | cA    | 3131 | CL7  | CHC-C4B-NB  | 2.26  | 126.65      | 124.26   |
| 14  | aA    | 3115 | CL7  | C7-C6-C5    | -2.26 | 107.23      | 113.36   |
| 14  | cA    | 3140 | CL7  | C3B-C4B-NB  | -2.26 | 108.42      | 110.52   |
| 14  | bB    | 819  | CL7  | CHA-C1A-NA  | -2.26 | 120.64      | 125.98   |
| 14  | aL    | 204  | CL7  | CMB-C2B-C1B | 2.26  | 128.81      | 125.37   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | bA    | 3105 | CL7  | CGD-CBD-CAD | -2.26 | 103.43      | 110.73   |
| 14  | cA    | 3124 | CL7  | C4C-C3C-C2C | 2.26  | 110.06      | 107.13   |
| 14  | cA    | 3117 | CL7  | CGD-CBD-CAD | -2.25 | 105.06      | 114.30   |
| 14  | aL    | 204  | CL7  | CAD-C3D-C2D | 2.25  | 149.31      | 144.44   |
| 16  | bA    | 3137 | LHG  | O4-P-O5     | 2.25  | 123.38      | 112.24   |
| 14  | bB    | 811  | CL7  | CBD-CHA-C4D | -2.25 | 103.75      | 109.14   |
| 14  | cB    | 832  | CL7  | CBD-CHA-C4D | -2.25 | 103.75      | 109.14   |
| 14  | bJ    | 101  | CL7  | C3D-C4D-ND  | 2.25  | 113.40      | 110.17   |
| 14  | bA    | 3129 | CL7  | C1D-CHD-C4C | -2.25 | 117.78      | 124.74   |
| 14  | aB    | 3003 | CL7  | CHB-C1B-NB  | -2.25 | 121.87      | 124.26   |
| 12  | bA    | 3101 | G9R  | CBA-CAA-C2A | -2.25 | 107.22      | 113.86   |
| 14  | aL    | 203  | CL7  | C7-C6-C5    | -2.25 | 107.24      | 113.36   |
| 14  | cB    | 823  | CL7  | C3D-C4D-ND  | 2.25  | 113.40      | 110.17   |
| 14  | bA    | 3105 | CL7  | CHD-C1D-ND  | 2.25  | 126.64      | 124.26   |
| 14  | aA    | 3103 | CL7  | OBD-CAD-C3D | -2.25 | 123.10      | 128.52   |
| 14  | aB    | 3022 | CL7  | CBD-CHA-C4D | -2.25 | 103.76      | 109.14   |
| 14  | cB    | 824  | CL7  | C3D-C4D-ND  | 2.25  | 113.40      | 110.17   |
| 14  | aB    | 3031 | CL7  | CHC-C4B-NB  | 2.25  | 126.64      | 124.26   |
| 14  | cA    | 3110 | CL7  | C3D-C4D-ND  | 2.25  | 113.39      | 110.17   |
| 14  | cA    | 3132 | CL7  | OBB-CAB-C3B | -2.25 | 120.60      | 125.69   |
| 14  | cB    | 811  | CL7  | CAC-C3C-C2C | -2.25 | 123.68      | 127.53   |
| 14  | aB    | 3005 | CL7  | C4D-C3D-C2D | -2.25 | 104.37      | 107.30   |
| 14  | aB    | 3005 | CL7  | CGD-CBD-CAD | -2.25 | 103.45      | 110.73   |
| 14  | aA    | 3129 | CL7  | C1A-NA-C4A  | 2.25  | 107.66      | 106.30   |
| 14  | cA    | 3124 | CL7  | C6-C5-C3    | -2.25 | 107.56      | 113.45   |
| 14  | bB    | 811  | CL7  | CMB-C2B-C1B | 2.25  | 128.79      | 125.37   |
| 14  | aA    | 3133 | CL7  | C4C-C3C-C2C | 2.25  | 110.05      | 107.13   |
| 14  | aA    | 3115 | CL7  | CHA-C1A-NA  | -2.25 | 120.66      | 125.98   |
| 14  | aA    | 3107 | CL7  | CHC-C4B-NB  | 2.25  | 126.64      | 124.26   |
| 14  | bA    | 3121 | CL7  | CHB-C1B-NB  | -2.25 | 121.88      | 124.26   |
| 14  | bB    | 806  | CL7  | C5-C3-C2    | -2.24 | 116.58      | 121.12   |
| 14  | cB    | 832  | CL7  | CAC-C3C-C4C | 2.24  | 128.21      | 124.68   |
| 14  | bB    | 810  | CL7  | C6-C5-C3    | -2.24 | 107.57      | 113.45   |
| 14  | bA    | 3140 | CL7  | C3B-C4B-NB  | -2.24 | 108.44      | 110.52   |
| 14  | bB    | 823  | CL7  | CHC-C1C-NC  | -2.24 | 122.39      | 124.45   |
| 19  | aB    | 3029 | LMG  | C7-O1-C1    | -2.24 | 109.36      | 113.74   |
| 14  | cA    | 3123 | CL7  | CAD-C3D-C2D | 2.24  | 149.28      | 144.44   |
| 14  | bA    | 3133 | CL7  | C4D-C3D-CAD | 2.24  | 108.93      | 107.42   |
| 14  | aA    | 3103 | CL7  | C4D-C3D-C2D | -2.24 | 104.38      | 107.30   |
| 14  | cB    | 823  | CL7  | CHC-C1C-NC  | -2.24 | 122.40      | 124.45   |
| 14  | bB    | 809  | CL7  | O2A-CGA-O1A | -2.24 | 117.94      | 123.59   |
| 14  | bA    | 3115 | CL7  | C1D-ND-C4D  | -2.24 | 104.75      | 106.33   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | aB    | 3018 | CL7  | C6-C7-C8    | -2.24 | 108.69      | 115.92   |
| 14  | cA    | 3140 | CL7  | C16-C17-C18 | -2.24 | 105.44      | 115.98   |
| 14  | cA    | 3114 | CL7  | C5-C3-C2    | -2.24 | 116.59      | 121.12   |
| 14  | aA    | 3142 | CL7  | CMB-C2B-C1B | 2.23  | 128.77      | 125.37   |
| 14  | bB    | 833  | CL7  | C1-C2-C3    | -2.23 | 122.18      | 126.04   |
| 14  | cB    | 817  | CL7  | C4D-C3D-CAD | 2.23  | 108.93      | 107.42   |
| 14  | cB    | 825  | CL7  | C3D-C4D-ND  | 2.23  | 113.37      | 110.17   |
| 14  | cA    | 3144 | CL7  | CED-O2D-CGD | 2.23  | 120.99      | 115.94   |
| 14  | bA    | 3119 | CL7  | O2D-CGD-O1D | -2.23 | 119.47      | 123.84   |
| 14  | bB    | 814  | CL7  | CHC-C1C-NC  | -2.23 | 122.40      | 124.45   |
| 14  | cA    | 3125 | CL7  | O2A-CGA-O1A | -2.23 | 117.96      | 123.59   |
| 14  | cA    | 3112 | CL7  | CAC-C3C-C2C | -2.23 | 123.71      | 127.53   |
| 14  | bB    | 810  | CL7  | O2A-CGA-O1A | -2.23 | 117.96      | 123.59   |
| 14  | bB    | 804  | CL7  | C3B-C2B-C1B | -2.23 | 104.47      | 107.16   |
| 16  | cA    | 3137 | LHG  | P-O6-C4     | -2.23 | 108.60      | 121.68   |
| 14  | bB    | 810  | CL7  | C2B-C1B-NB  | -2.23 | 108.74      | 110.23   |
| 14  | aA    | 3131 | CL7  | OBD-CAD-C3D | -2.23 | 123.15      | 128.52   |
| 14  | cA    | 3131 | CL7  | CHC-C1C-NC  | -2.23 | 122.41      | 124.45   |
| 14  | bA    | 3119 | CL7  | C4D-C3D-CAD | -2.23 | 105.92      | 107.42   |
| 14  | aB    | 3009 | CL7  | CAD-C3D-C2D | 2.23  | 149.25      | 144.44   |
| 14  | aA    | 3125 | CL7  | C2A-C1A-CHA | -2.23 | 121.91      | 126.36   |
| 14  | bA    | 3126 | CL7  | C6-C5-C3    | -2.23 | 107.61      | 113.45   |
| 14  | cB    | 827  | CL7  | C3A-C4A-CHB | -2.23 | 120.40      | 123.70   |
| 14  | bA    | 3108 | CL7  | CGD-CBD-CAD | -2.23 | 103.52      | 110.73   |
| 14  | cA    | 3125 | CL7  | C3A-C4A-CHB | -2.23 | 120.40      | 123.70   |
| 14  | aA    | 3120 | CL7  | CHA-C1A-NA  | -2.22 | 120.72      | 125.98   |
| 14  | cB    | 817  | CL7  | CBD-CHA-C4D | -2.22 | 103.82      | 109.14   |
| 14  | cA    | 3107 | CL7  | CAD-C3D-C2D | 2.22  | 149.24      | 144.44   |
| 14  | cL    | 205  | CL7  | CHB-C1B-NB  | -2.22 | 121.90      | 124.26   |
| 14  | bA    | 3128 | CL7  | C2B-C1B-NB  | 2.22  | 111.72      | 110.23   |
| 14  | bB    | 803  | CL7  | CAA-C2A-C3A | -2.22 | 106.69      | 112.78   |
| 19  | cB    | 830  | LMG  | C12-C11-C10 | -2.22 | 105.54      | 113.62   |
| 14  | bA    | 3113 | CL7  | CMA-C3A-C2A | -2.22 | 110.91      | 116.10   |
| 14  | aL    | 203  | CL7  | OBD-CAD-C3D | -2.22 | 123.18      | 128.52   |
| 14  | cA    | 3127 | CL7  | C1-O2A-CGA  | -2.22 | 110.62      | 116.44   |
| 14  | bB    | 827  | CL7  | CBC-CAC-C3C | 2.22  | 118.55      | 112.43   |
| 14  | aA    | 3121 | CL7  | O2D-CGD-O1D | -2.22 | 119.50      | 123.84   |
| 14  | cA    | 3129 | CL7  | C1C-C2C-C3C | 2.22  | 110.18      | 106.94   |
| 14  | bB    | 826  | CL7  | C16-C15-C13 | -2.22 | 108.75      | 115.92   |
| 14  | cA    | 3108 | CL7  | CAC-C3C-C4C | 2.22  | 128.17      | 124.68   |
| 14  | bB    | 824  | CL7  | CHC-C1C-NC  | -2.22 | 122.42      | 124.45   |
| 14  | cB    | 815  | CL7  | CHC-C1C-NC  | -2.22 | 122.42      | 124.45   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | bA    | 3104 | CL7  | C3D-C4D-ND  | 2.22  | 113.35      | 110.17   |
| 14  | cA    | 3139 | CL7  | C3D-C4D-ND  | 2.22  | 113.35      | 110.17   |
| 14  | bA    | 3129 | CL7  | C2C-C1C-NC  | -2.22 | 108.47      | 110.10   |
| 14  | aA    | 3105 | CL7  | CBD-CHA-C4D | -2.22 | 103.84      | 109.14   |
| 14  | cB    | 827  | CL7  | CBD-CHA-C4D | -2.21 | 103.84      | 109.14   |
| 14  | bA    | 3125 | CL7  | C3A-C2A-C1A | 2.21  | 104.66      | 101.34   |
| 14  | bB    | 825  | CL7  | C3D-C4D-ND  | 2.21  | 113.34      | 110.17   |
| 14  | aB    | 3031 | CL7  | CAC-C3C-C4C | 2.21  | 128.16      | 124.68   |
| 14  | bA    | 3114 | CL7  | CAC-C3C-C4C | 2.21  | 128.16      | 124.68   |
| 14  | aB    | 3026 | CL7  | OBD-CAD-C3D | -2.21 | 123.20      | 128.52   |
| 14  | aA    | 3107 | CL7  | CAD-C3D-C2D | 2.21  | 149.21      | 144.44   |
| 14  | cA    | 3106 | CL7  | C4C-C3C-C2C | 2.21  | 110.00      | 107.13   |
| 14  | aB    | 3005 | CL7  | C3A-C2A-C1A | 2.21  | 104.65      | 101.34   |
| 14  | bA    | 3120 | CL7  | CHB-C1B-NB  | -2.21 | 121.92      | 124.26   |
| 14  | cA    | 3139 | CL7  | CBA-CAA-C2A | -2.21 | 107.34      | 113.86   |
| 14  | aA    | 3115 | CL7  | CAD-C3D-C2D | 2.21  | 149.21      | 144.44   |
| 14  | aB    | 3002 | CL7  | C1A-NA-C4A  | -2.21 | 104.97      | 106.30   |
| 14  | cA    | 3113 | CL7  | CMA-C3A-C2A | -2.21 | 110.95      | 116.10   |
| 14  | bB    | 826  | CL7  | C6-C7-C8    | -2.21 | 108.79      | 115.92   |
| 14  | aA    | 3109 | CL7  | C3D-C4D-ND  | 2.21  | 113.33      | 110.17   |
| 14  | aA    | 3106 | CL7  | C1D-CHD-C4C | -2.21 | 117.92      | 124.74   |
| 14  | bA    | 3127 | CL7  | O2A-CGA-CBA | -2.21 | 104.98      | 111.91   |
| 14  | bA    | 3128 | CL7  | C16-C15-C13 | -2.21 | 108.79      | 115.92   |
| 14  | bA    | 3122 | CL7  | C3A-C4A-CHB | -2.21 | 120.43      | 123.70   |
| 14  | cB    | 824  | CL7  | C1D-ND-C4D  | -2.20 | 104.77      | 106.33   |
| 14  | cB    | 826  | CL7  | C6-C5-C3    | -2.20 | 107.68      | 113.45   |
| 14  | cB    | 818  | CL7  | CAD-C3D-C2D | 2.20  | 149.20      | 144.44   |
| 14  | cA    | 3125 | CL7  | C11-C10-C8  | -2.20 | 108.80      | 115.92   |
| 14  | cB    | 809  | CL7  | CHB-C1B-NB  | -2.20 | 121.92      | 124.26   |
| 14  | cA    | 3144 | CL7  | O2D-CGD-O1D | -2.20 | 119.53      | 123.84   |
| 14  | aB    | 3009 | CL7  | C3A-C2A-C1A | 2.20  | 104.64      | 101.34   |
| 14  | cB    | 816  | CL7  | CBD-CHA-C4D | -2.20 | 103.88      | 109.14   |
| 14  | aL    | 203  | CL7  | CBD-CHA-C4D | -2.20 | 103.88      | 109.14   |
| 14  | aL    | 204  | CL7  | CBD-CHA-C4D | -2.20 | 103.88      | 109.14   |
| 14  | bA    | 3105 | CL7  | C1D-CHD-C4C | -2.20 | 117.94      | 124.74   |
| 17  | cA    | 3143 | PQN  | O4-C4-C5    | -2.20 | 118.00      | 121.56   |
| 14  | aB    | 3026 | CL7  | CMA-C3A-C2A | -2.20 | 104.95      | 113.83   |
| 14  | aA    | 3133 | CL7  | C2D-C1D-ND  | -2.20 | 108.76      | 110.23   |
| 14  | aA    | 3120 | CL7  | C1D-ND-C4D  | -2.20 | 104.77      | 106.33   |
| 14  | aA    | 3103 | CL7  | CBC-CAC-C3C | -2.20 | 106.37      | 112.43   |
| 14  | bA    | 3108 | CL7  | C3A-C2A-C1A | 2.20  | 104.63      | 101.34   |
| 14  | cA    | 3131 | CL7  | O2D-CGD-O1D | -2.20 | 119.54      | 123.84   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | bB    | 826  | CL7  | C6-C5-C3    | -2.20 | 107.69      | 113.45   |
| 14  | cL    | 205  | CL7  | CBD-CHA-C4D | -2.20 | 103.88      | 109.14   |
| 14  | cA    | 3144 | CL7  | CHC-C4B-NB  | 2.20  | 126.58      | 124.26   |
| 14  | aA    | 3126 | CL7  | C4-C3-C2    | -2.20 | 118.04      | 123.68   |
| 14  | bA    | 3127 | CL7  | CBD-CHA-C4D | -2.20 | 103.88      | 109.14   |
| 14  | bA    | 3128 | CL7  | O2A-CGA-CBA | 2.20  | 118.81      | 111.91   |
| 14  | aA    | 3113 | CL7  | CAC-C3C-C2C | -2.20 | 123.77      | 127.53   |
| 14  | cB    | 833  | CL7  | C4C-C3C-C2C | 2.20  | 109.99      | 107.13   |
| 14  | bA    | 3124 | CL7  | CAD-C3D-C2D | 2.20  | 149.18      | 144.44   |
| 14  | bB    | 831  | CL7  | O2A-CGA-O1A | -2.20 | 118.05      | 123.59   |
| 14  | aB    | 3026 | CL7  | CGD-CBD-CAD | -2.20 | 103.62      | 110.73   |
| 16  | cA    | 3138 | LHG  | P-O3-C3     | -2.19 | 108.81      | 121.68   |
| 14  | cB    | 811  | CL7  | CAD-C3D-C2D | 2.19  | 149.18      | 144.44   |
| 14  | bB    | 832  | CL7  | O2D-CGD-O1D | -2.19 | 119.55      | 123.84   |
| 14  | cA    | 3103 | CL7  | O2D-CGD-O1D | -2.19 | 119.55      | 123.84   |
| 14  | bA    | 3145 | CL7  | CED-O2D-CGD | 2.19  | 120.90      | 115.94   |
| 14  | aA    | 3130 | CL7  | OBD-CAD-C3D | -2.19 | 123.24      | 128.52   |
| 14  | aB    | 3008 | CL7  | CHB-C1B-NB  | -2.19 | 121.94      | 124.26   |
| 14  | cB    | 811  | CL7  | C3D-C4D-ND  | 2.19  | 113.31      | 110.17   |
| 12  | cA    | 3101 | G9R  | OBD-CAD-C3D | -2.19 | 123.24      | 128.52   |
| 14  | bA    | 3142 | CL7  | C3A-C2A-C1A | 2.19  | 104.62      | 101.34   |
| 14  | bB    | 824  | CL7  | C1D-ND-C4D  | -2.19 | 104.78      | 106.33   |
| 14  | bB    | 833  | CL7  | C4C-C3C-C2C | 2.19  | 109.98      | 107.13   |
| 14  | cL    | 203  | CL7  | C4C-C3C-C2C | 2.19  | 109.98      | 107.13   |
| 14  | aA    | 3104 | CL7  | C3D-C4D-ND  | 2.19  | 113.31      | 110.17   |
| 14  | aL    | 203  | CL7  | C16-C15-C13 | -2.19 | 108.83      | 115.92   |
| 14  | cA    | 3109 | CL7  | C3A-C2A-C1A | -2.19 | 99.02       | 101.64   |
| 14  | aA    | 3113 | CL7  | OBD-CAD-C3D | -2.19 | 123.25      | 128.52   |
| 14  | cA    | 3117 | CL7  | OBD-CAD-C3D | -2.19 | 123.25      | 128.52   |
| 14  | bA    | 3103 | CL7  | C3D-C4D-ND  | 2.19  | 113.31      | 110.17   |
| 14  | aA    | 3127 | CL7  | CED-O2D-CGD | 2.19  | 120.89      | 115.94   |
| 14  | aA    | 3103 | CL7  | C5-C3-C2    | -2.19 | 116.68      | 121.12   |
| 14  | cB    | 803  | CL7  | C16-C15-C13 | -2.19 | 108.84      | 115.92   |
| 19  | bB    | 830  | LMG  | C12-C11-C10 | -2.19 | 105.66      | 113.62   |
| 14  | aA    | 3115 | CL7  | C2A-C1A-CHA | -2.19 | 121.98      | 126.36   |
| 14  | bA    | 3140 | CL7  | OBD-CAD-C3D | -2.19 | 123.25      | 128.52   |
| 14  | cB    | 803  | CL7  | C6-C7-C8    | -2.19 | 108.84      | 115.92   |
| 14  | bB    | 804  | CL7  | CAA-C2A-C3A | -2.19 | 106.78      | 112.78   |
| 14  | aB    | 3016 | CL7  | CBD-CHA-C4D | -2.19 | 103.91      | 109.14   |
| 14  | cB    | 804  | CL7  | CHB-C1B-NB  | -2.19 | 121.94      | 124.26   |
| 14  | cA    | 3133 | CL7  | CMB-C2B-C1B | 2.19  | 128.70      | 125.37   |
| 14  | bA    | 3125 | CL7  | CAA-C2A-C3A | -2.19 | 106.79      | 112.78   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | bB    | 815  | CL7  | C3D-C4D-ND  | 2.19  | 113.30      | 110.17   |
| 14  | bB    | 823  | CL7  | CHA-C1A-NA  | -2.19 | 120.81      | 125.98   |
| 14  | cA    | 3127 | CL7  | CHA-C1A-NA  | -2.19 | 120.81      | 125.98   |
| 14  | cA    | 3140 | CL7  | CBA-CAA-C2A | 2.19  | 120.31      | 113.86   |
| 14  | bL    | 205  | CL7  | CBD-CHA-C4D | -2.18 | 103.92      | 109.14   |
| 14  | cA    | 3116 | CL7  | C2D-C1D-ND  | 2.18  | 111.70      | 110.23   |
| 14  | bL    | 205  | CL7  | CHC-C1C-NC  | -2.18 | 122.45      | 124.45   |
| 14  | aB    | 3016 | CL7  | CAD-C3D-C2D | 2.18  | 149.15      | 144.44   |
| 14  | bB    | 803  | CL7  | CBD-CHA-C4D | -2.18 | 103.92      | 109.14   |
| 14  | bB    | 823  | CL7  | C2A-C1A-CHA | -2.18 | 120.98      | 124.42   |
| 14  | bA    | 3110 | CL7  | CMB-C2B-C1B | 2.18  | 128.69      | 125.37   |
| 14  | bA    | 3142 | CL7  | C4-C3-C2    | -2.18 | 118.09      | 123.68   |
| 14  | cB    | 803  | CL7  | C1-O2A-CGA  | -2.18 | 110.72      | 116.44   |
| 14  | aA    | 3115 | CL7  | CAA-C2A-C1A | -2.18 | 105.02      | 112.19   |
| 14  | bL    | 204  | CL7  | C11-C12-C13 | -2.18 | 108.88      | 115.92   |
| 14  | bA    | 3114 | CL7  | CBD-CHA-C4D | -2.18 | 103.93      | 109.14   |
| 14  | aB    | 3017 | CL7  | CHA-C1A-NA  | -2.18 | 120.83      | 125.98   |
| 14  | aB    | 3008 | CL7  | C4C-C3C-C2C | 2.18  | 109.96      | 107.13   |
| 14  | bA    | 3130 | CL7  | C3A-C4A-CHB | -2.18 | 120.47      | 123.70   |
| 14  | aB    | 3007 | CL7  | CBC-CAC-C3C | -2.18 | 106.43      | 112.43   |
| 14  | aA    | 3115 | CL7  | C5-C3-C2    | -2.18 | 116.71      | 121.12   |
| 14  | aB    | 3032 | CL7  | C6-C5-C3    | -2.18 | 107.75      | 113.45   |
| 14  | aA    | 3116 | CL7  | CMC-C2C-C3C | 2.18  | 132.02      | 126.12   |
| 14  | bA    | 3108 | CL7  | CAC-C3C-C2C | -2.18 | 123.81      | 127.53   |
| 14  | aA    | 3121 | CL7  | CAD-C3D-C2D | 2.18  | 149.14      | 144.44   |
| 14  | cB    | 809  | CL7  | O1D-CGD-CBD | -2.18 | 120.03      | 124.48   |
| 14  | bA    | 3109 | CL7  | C3A-C2A-C1A | -2.17 | 99.05       | 101.64   |
| 19  | aB    | 3029 | LMG  | O3-C3-C4    | -2.17 | 105.32      | 110.35   |
| 14  | bA    | 3124 | CL7  | C4C-C3C-C2C | 2.17  | 109.96      | 107.13   |
| 14  | bA    | 3124 | CL7  | O2A-CGA-CBA | 2.17  | 118.73      | 111.91   |
| 14  | aB    | 3006 | CL7  | CAA-C2A-C3A | -2.17 | 106.82      | 112.78   |
| 14  | bB    | 819  | CL7  | CMC-C2C-C1C | -2.17 | 120.88      | 124.71   |
| 14  | aA    | 3106 | CL7  | CHB-C1B-NB  | -2.17 | 121.96      | 124.26   |
| 14  | cA    | 3127 | CL7  | O2A-C1-C2   | -2.17 | 102.92      | 108.64   |
| 14  | aB    | 3010 | CL7  | CBD-CHA-C4D | -2.17 | 103.94      | 109.14   |
| 14  | cA    | 3103 | CL7  | C4C-C3C-C2C | 2.17  | 109.96      | 107.13   |
| 14  | aB    | 3024 | CL7  | CMA-C3A-C2A | -2.17 | 111.03      | 116.10   |
| 14  | bA    | 3132 | CL7  | C2D-C1D-ND  | -2.17 | 108.78      | 110.23   |
| 14  | bA    | 3108 | CL7  | CMC-C2C-C3C | 2.17  | 132.01      | 126.12   |
| 14  | bB    | 827  | CL7  | C1A-NA-C4A  | 2.17  | 107.62      | 106.30   |
| 14  | aB    | 3003 | CL7  | C4-C3-C5    | -2.17 | 111.62      | 115.27   |
| 14  | cA    | 3113 | CL7  | O1D-CGD-CBD | -2.17 | 120.04      | 124.48   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | cB    | 816  | CL7  | CGD-CBD-CAD | -2.17 | 103.70      | 110.73   |
| 14  | aB    | 3030 | CL7  | CHA-C1A-NA  | -2.17 | 120.85      | 125.98   |
| 14  | bB    | 812  | CL7  | CAD-C3D-C2D | 2.17  | 149.12      | 144.44   |
| 14  | aA    | 3117 | CL7  | CED-O2D-CGD | 2.17  | 120.84      | 115.94   |
| 14  | aA    | 3128 | CL7  | CAA-C2A-C3A | -2.17 | 106.84      | 112.78   |
| 14  | bA    | 3117 | CL7  | CGD-CBD-CAD | -2.17 | 105.41      | 114.30   |
| 14  | aB    | 3019 | CL7  | C6-C5-C3    | -2.17 | 107.77      | 113.45   |
| 14  | cA    | 3108 | CL7  | C3B-C4B-NB  | -2.17 | 108.50      | 110.52   |
| 14  | aA    | 3132 | CL7  | C3D-C4D-ND  | 2.17  | 113.28      | 110.17   |
| 14  | bB    | 831  | CL7  | C6-C5-C3    | -2.17 | 107.77      | 113.45   |
| 14  | bA    | 3128 | CL7  | O2D-CGD-O1D | -2.17 | 119.60      | 123.84   |
| 14  | cB    | 826  | CL7  | C1-C2-C3    | -2.17 | 122.30      | 126.04   |
| 14  | cA    | 3105 | CL7  | OBD-CAD-C3D | -2.17 | 123.31      | 128.52   |
| 14  | aA    | 3116 | CL7  | CBC-CAC-C3C | 2.17  | 118.40      | 112.43   |
| 14  | cB    | 822  | CL7  | CAD-C3D-C2D | 2.17  | 149.12      | 144.44   |
| 14  | aA    | 3112 | CL7  | C3B-C4B-NB  | -2.17 | 108.51      | 110.52   |
| 14  | cA    | 3140 | CL7  | CMB-C2B-C1B | 2.17  | 128.67      | 125.37   |
| 14  | bA    | 3131 | CL7  | C3D-C4D-ND  | 2.16  | 113.27      | 110.17   |
| 14  | bA    | 3120 | CL7  | CAC-C3C-C2C | -2.16 | 123.83      | 127.53   |
| 14  | bB    | 816  | CL7  | CAD-C3D-C2D | 2.16  | 149.11      | 144.44   |
| 14  | cB    | 826  | CL7  | O2A-CGA-O1A | -2.16 | 118.13      | 123.59   |
| 14  | cB    | 812  | CL7  | CAD-C3D-C2D | 2.16  | 149.11      | 144.44   |
| 14  | cA    | 3102 | CL7  | C7-C6-C5    | -2.16 | 107.48      | 113.36   |
| 14  | bA    | 3140 | CL7  | C1-O2A-CGA  | -2.16 | 110.77      | 116.44   |
| 14  | aA    | 3122 | CL7  | C4D-C3D-C2D | -2.16 | 104.48      | 107.30   |
| 14  | aA    | 3113 | CL7  | CMB-C2B-C1B | 2.16  | 128.66      | 125.37   |
| 14  | aA    | 3114 | CL7  | C3D-C4D-ND  | 2.16  | 113.27      | 110.17   |
| 14  | bA    | 3128 | CL7  | C2A-C1A-CHA | -2.16 | 122.04      | 126.36   |
| 13  | cB    | 801  | PHO  | CBA-CAA-C2A | -2.16 | 107.49      | 113.81   |
| 14  | aA    | 3125 | CL7  | C4C-C3C-C2C | 2.16  | 109.94      | 107.13   |
| 14  | bB    | 815  | CL7  | O1D-CGD-CBD | -2.16 | 120.06      | 124.48   |
| 14  | cB    | 820  | CL7  | C4C-C3C-C2C | 2.16  | 109.94      | 107.13   |
| 14  | bB    | 819  | CL7  | O2D-CGD-O1D | -2.16 | 119.61      | 123.84   |
| 19  | bB    | 830  | LMG  | O3-C3-C4    | -2.16 | 105.36      | 110.35   |
| 14  | aA    | 3132 | CL7  | CHC-C1C-NC  | -2.16 | 122.47      | 124.45   |
| 14  | aB    | 3006 | CL7  | CHD-C4C-NC  | -2.16 | 122.47      | 124.45   |
| 14  | cA    | 3125 | CL7  | CBD-CHA-C4D | -2.16 | 103.98      | 109.14   |
| 14  | aA    | 3142 | CL7  | C6-C5-C3    | -2.16 | 107.79      | 113.45   |
| 14  | bL    | 203  | CL7  | C6-C7-C8    | -2.16 | 108.94      | 115.92   |
| 14  | aA    | 3106 | CL7  | CHD-C1D-ND  | 2.16  | 126.54      | 124.26   |
| 14  | aB    | 3031 | CL7  | C16-C17-C18 | -2.16 | 105.81      | 115.98   |
| 12  | cA    | 3101 | G9R  | CMB-C2B-C3B | -2.16 | 121.36      | 126.59   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | cA    | 3114 | CL7  | C3A-C4A-CHB | -2.16 | 120.50      | 123.70   |
| 14  | cA    | 3132 | CL7  | CBD-CHA-C4D | -2.16 | 103.98      | 109.14   |
| 14  | bA    | 3131 | CL7  | O2D-CGD-O1D | -2.16 | 119.62      | 123.84   |
| 14  | bA    | 3106 | CL7  | C4C-C3C-C2C | 2.16  | 109.94      | 107.13   |
| 14  | aA    | 3124 | CL7  | C2A-C1A-CHA | -2.16 | 122.05      | 126.36   |
| 14  | bB    | 814  | CL7  | O2D-CGD-O1D | -2.16 | 119.62      | 123.84   |
| 14  | aB    | 3017 | CL7  | C3D-C4D-ND  | 2.16  | 113.26      | 110.17   |
| 14  | cA    | 3108 | CL7  | OBD-CAD-C3D | -2.15 | 123.34      | 128.52   |
| 14  | cB    | 816  | CL7  | CHB-C1B-NB  | -2.15 | 121.98      | 124.26   |
| 14  | cB    | 804  | CL7  | CGD-CBD-CAD | -2.15 | 103.76      | 110.73   |
| 14  | aB    | 3026 | CL7  | C4C-C3C-C2C | 2.15  | 109.93      | 107.13   |
| 14  | aA    | 3124 | CL7  | C1-O2A-CGA  | 2.15  | 122.09      | 116.44   |
| 14  | bB    | 810  | CL7  | C3A-C2A-C1A | 2.15  | 104.56      | 101.34   |
| 14  | cB    | 806  | CL7  | C3A-C2A-C1A | 2.15  | 104.56      | 101.34   |
| 14  | bB    | 815  | CL7  | CHA-C1A-NA  | -2.15 | 120.89      | 125.98   |
| 14  | bA    | 3117 | CL7  | OBD-CAD-C3D | -2.15 | 123.34      | 128.52   |
| 14  | cA    | 3116 | CL7  | CAA-C2A-C3A | -2.15 | 106.89      | 112.78   |
| 14  | bA    | 3128 | CL7  | CHC-C1C-NC  | 2.15  | 126.43      | 124.45   |
| 14  | aL    | 202  | CL7  | O2A-CGA-O1A | -2.15 | 118.17      | 123.59   |
| 14  | bB    | 824  | CL7  | C4C-C3C-C2C | 2.15  | 109.93      | 107.13   |
| 16  | aA    | 3139 | LHG  | C5-O7-C7    | 2.15  | 120.64      | 117.88   |
| 14  | bB    | 810  | CL7  | CHB-C1B-NB  | -2.15 | 121.98      | 124.26   |
| 14  | cA    | 3108 | CL7  | CMC-C2C-C3C | 2.15  | 131.95      | 126.12   |
| 14  | bA    | 3114 | CL7  | CHA-C1A-NA  | -2.15 | 120.89      | 125.98   |
| 14  | bA    | 3104 | CL7  | CBD-CHA-C4D | -2.15 | 104.00      | 109.14   |
| 14  | bA    | 3116 | CL7  | C3A-C2A-C1A | 2.15  | 104.56      | 101.34   |
| 14  | aA    | 3105 | CL7  | CHC-C1C-NC  | -2.15 | 122.48      | 124.45   |
| 14  | bA    | 3102 | CL7  | CHC-C4B-NB  | 2.15  | 126.53      | 124.26   |
| 14  | bA    | 3145 | CL7  | CHC-C4B-NB  | 2.15  | 126.53      | 124.26   |
| 14  | bB    | 816  | CL7  | CHA-C1A-NA  | -2.15 | 120.89      | 125.98   |
| 14  | cA    | 3128 | CL7  | C2B-C1B-NB  | 2.15  | 111.67      | 110.23   |
| 14  | cA    | 3142 | CL7  | C6-C7-C8    | -2.15 | 108.98      | 115.92   |
| 14  | bA    | 3123 | CL7  | C3D-C4D-ND  | 2.15  | 113.25      | 110.17   |
| 14  | cA    | 3103 | CL7  | C3D-C4D-ND  | 2.15  | 113.25      | 110.17   |
| 14  | cA    | 3116 | CL7  | CED-O2D-CGD | 2.15  | 120.79      | 115.94   |
| 14  | aA    | 3125 | CL7  | O2A-CGA-CBA | 2.15  | 118.64      | 111.91   |
| 14  | cB    | 807  | CL7  | C3D-C4D-ND  | 2.15  | 113.25      | 110.17   |
| 14  | bB    | 811  | CL7  | C3A-C2A-C1A | 2.15  | 104.21      | 101.64   |
| 13  | aB    | 3004 | PHO  | C11-C12-C13 | -2.15 | 108.98      | 115.92   |
| 14  | aB    | 3030 | CL7  | CAA-C2A-C3A | -2.15 | 106.90      | 112.78   |
| 14  | aB    | 3014 | CL7  | C3A-C4A-CHB | -2.15 | 120.52      | 123.70   |
| 14  | cB    | 815  | CL7  | C3A-C4A-CHB | -2.15 | 120.52      | 123.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | bA    | 3112 | CL7  | CAC-C3C-C2C | -2.15 | 123.86      | 127.53   |
| 14  | aA    | 3124 | CL7  | CMC-C2C-C1C | -2.14 | 120.93      | 124.71   |
| 14  | bB    | 809  | CL7  | C4C-C3C-C2C | 2.14  | 109.92      | 107.13   |
| 14  | cB    | 808  | CL7  | C4C-C3C-C2C | 2.14  | 109.92      | 107.13   |
| 14  | cA    | 3140 | CL7  | C11-C12-C13 | -2.14 | 108.99      | 115.92   |
| 14  | bA    | 3132 | CL7  | CBD-CHA-C4D | -2.14 | 104.01      | 109.14   |
| 14  | aA    | 3142 | CL7  | C3B-C4B-NB  | -2.14 | 108.53      | 110.52   |
| 14  | bA    | 3102 | CL7  | OBD-CAD-C3D | -2.14 | 123.36      | 128.52   |
| 14  | aB    | 3009 | CL7  | C9-C8-C7    | -2.14 | 103.53      | 111.29   |
| 14  | bB    | 820  | CL7  | O2D-CGD-O1D | -2.14 | 119.65      | 123.84   |
| 13  | aA    | 3102 | PHO  | CBA-CAA-C2A | -2.14 | 107.55      | 113.81   |
| 14  | bA    | 3130 | CL7  | CHC-C1C-NC  | -2.14 | 122.48      | 124.45   |
| 14  | bA    | 3106 | CL7  | CMB-C2B-C1B | 2.14  | 128.63      | 125.37   |
| 14  | aA    | 3130 | CL7  | C3D-C4D-ND  | 2.14  | 113.24      | 110.17   |
| 14  | bB    | 826  | CL7  | C11-C10-C8  | -2.14 | 109.00      | 115.92   |
| 14  | aA    | 3107 | CL7  | C6-C5-C3    | -2.14 | 107.84      | 113.45   |
| 14  | cA    | 3121 | CL7  | C3C-C4C-NC  | 2.14  | 111.73      | 110.18   |
| 14  | cA    | 3127 | CL7  | CGD-CBD-CAD | -2.14 | 103.80      | 110.73   |
| 14  | cB    | 810  | CL7  | O2D-CGD-O1D | -2.14 | 119.65      | 123.84   |
| 14  | bB    | 827  | CL7  | C3A-C2A-C1A | 2.14  | 104.54      | 101.34   |
| 14  | cA    | 3102 | CL7  | CHD-C4C-C3C | 2.14  | 128.40      | 124.94   |
| 14  | cA    | 3124 | CL7  | C16-C15-C13 | -2.14 | 109.01      | 115.92   |
| 14  | bA    | 3141 | CL7  | CAD-C3D-C2D | 2.14  | 149.06      | 144.44   |
| 14  | bB    | 804  | CL7  | C16-C15-C13 | -2.14 | 109.01      | 115.92   |
| 14  | bA    | 3115 | CL7  | CBC-CAC-C3C | 2.14  | 118.33      | 112.43   |
| 14  | bL    | 204  | CL7  | C3A-C4A-CHB | -2.14 | 120.53      | 123.70   |
| 14  | aA    | 3141 | CL7  | C3D-C4D-ND  | 2.14  | 113.23      | 110.17   |
| 14  | cA    | 3103 | CL7  | CHC-C1C-NC  | -2.14 | 122.49      | 124.45   |
| 14  | bB    | 833  | CL7  | C2A-C1A-CHA | -2.14 | 122.09      | 126.36   |
| 14  | bB    | 825  | CL7  | CHB-C1B-NB  | -2.14 | 122.00      | 124.26   |
| 14  | cA    | 3132 | CL7  | O2A-CGA-CBA | 2.14  | 118.61      | 111.91   |
| 14  | bA    | 3130 | CL7  | O1D-CGD-CBD | -2.14 | 120.11      | 124.48   |
| 14  | aA    | 3141 | CL7  | CMB-C2B-C1B | 2.13  | 128.62      | 125.37   |
| 14  | aB    | 3009 | CL7  | CAC-C3C-C2C | -2.13 | 123.88      | 127.53   |
| 14  | cA    | 3102 | CL7  | CAD-C3D-C2D | 2.13  | 149.05      | 144.44   |
| 14  | cB    | 823  | CL7  | OBD-CAD-C3D | -2.13 | 123.38      | 128.52   |
| 14  | aA    | 3128 | CL7  | CHC-C4B-NB  | 2.13  | 126.52      | 124.26   |
| 14  | aA    | 3142 | CL7  | CAD-C3D-C2D | 2.13  | 149.05      | 144.44   |
| 14  | aB    | 3014 | CL7  | C3D-C4D-ND  | 2.13  | 113.23      | 110.17   |
| 14  | aA    | 3125 | CL7  | C16-C15-C13 | -2.13 | 109.03      | 115.92   |
| 14  | cB    | 833  | CL7  | C6-C5-C3    | -2.13 | 107.87      | 113.45   |
| 14  | aA    | 3128 | CL7  | C2A-C1A-CHA | -2.13 | 122.10      | 126.36   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | bB    | 818  | CL7  | C3D-C4D-ND  | 2.13  | 113.22      | 110.17   |
| 14  | bA    | 3141 | CL7  | CAC-C3C-C2C | -2.13 | 123.89      | 127.53   |
| 14  | cB    | 833  | CL7  | C2A-C1A-CHA | -2.13 | 122.10      | 126.36   |
| 14  | cB    | 807  | CL7  | CHD-C4C-NC  | -2.13 | 122.50      | 124.45   |
| 12  | cA    | 3101 | G9R  | CHB-C4A-NA  | 2.13  | 127.45      | 124.51   |
| 14  | bB    | 810  | CL7  | CAD-C3D-C2D | 2.13  | 149.04      | 144.44   |
| 14  | cA    | 3123 | CL7  | C1D-ND-C4D  | -2.13 | 104.82      | 106.33   |
| 14  | aA    | 3104 | CL7  | C4C-C3C-C2C | 2.13  | 109.90      | 107.13   |
| 14  | cB    | 824  | CL7  | CHC-C4B-NB  | 2.13  | 126.51      | 124.26   |
| 14  | cA    | 3103 | CL7  | CAD-C3D-C2D | 2.13  | 149.03      | 144.44   |
| 14  | aB    | 3025 | CL7  | C3A-C4A-CHB | -2.13 | 120.55      | 123.70   |
| 14  | aB    | 3007 | CL7  | C4-C3-C2    | -2.12 | 118.23      | 123.68   |
| 17  | aB    | 3027 | PQN  | C19-C18-C20 | -2.12 | 103.60      | 111.29   |
| 14  | aJ    | 101  | CL7  | CAD-C3D-C2D | 2.12  | 149.03      | 144.44   |
| 14  | aA    | 3128 | CL7  | CHA-C1A-NA  | -2.12 | 120.96      | 125.98   |
| 14  | cA    | 3106 | CL7  | CAD-C3D-C2D | 2.12  | 149.02      | 144.44   |
| 14  | aB    | 3009 | CL7  | CHB-C1B-NB  | -2.12 | 122.01      | 124.26   |
| 14  | bB    | 820  | CL7  | O1A-CGA-CBA | -2.12 | 115.45      | 123.73   |
| 14  | aB    | 3007 | CL7  | C11-C12-C13 | -2.12 | 109.06      | 115.92   |
| 14  | cA    | 3125 | CL7  | C2A-C1A-CHA | -2.12 | 122.12      | 126.36   |
| 14  | cA    | 3126 | CL7  | OBD-CAD-C3D | -2.12 | 123.41      | 128.52   |
| 14  | bA    | 3102 | CL7  | C1D-ND-C4D  | -2.12 | 104.83      | 106.33   |
| 14  | bB    | 832  | CL7  | CAD-C3D-C2D | 2.12  | 149.02      | 144.44   |
| 14  | aB    | 3021 | CL7  | CMC-C2C-C1C | -2.12 | 120.98      | 124.71   |
| 14  | bB    | 833  | CL7  | CED-O2D-CGD | -2.12 | 111.14      | 115.94   |
| 14  | aA    | 3123 | CL7  | CAA-C2A-C3A | -2.12 | 106.97      | 112.78   |
| 14  | cB    | 803  | CL7  | CHB-C1B-NB  | -2.12 | 122.01      | 124.26   |
| 14  | bA    | 3106 | CL7  | CHA-C1A-NA  | -2.12 | 120.97      | 125.98   |
| 14  | bA    | 3103 | CL7  | C4C-C3C-C2C | 2.12  | 109.89      | 107.13   |
| 14  | aB    | 3008 | CL7  | O2A-CGA-O1A | -2.12 | 118.25      | 123.59   |
| 14  | aA    | 3132 | CL7  | CHC-C4B-NB  | 2.12  | 126.50      | 124.26   |
| 14  | bB    | 804  | CL7  | CAD-C3D-C2D | 2.12  | 149.01      | 144.44   |
| 14  | cA    | 3139 | CL7  | CHC-C4B-NB  | 2.12  | 126.50      | 124.26   |
| 14  | bA    | 3103 | CL7  | CAD-C3D-C2D | 2.12  | 149.01      | 144.44   |
| 14  | aA    | 3104 | CL7  | CAD-C3D-C2D | 2.12  | 149.01      | 144.44   |
| 14  | cA    | 3120 | CL7  | CBD-CHA-C4D | -2.12 | 104.08      | 109.14   |
| 14  | bL    | 204  | CL7  | CAD-C3D-C2D | 2.11  | 149.01      | 144.44   |
| 14  | bB    | 823  | CL7  | OBD-CAD-C3D | -2.11 | 123.43      | 128.52   |
| 14  | aA    | 3142 | CL7  | C1-C2-C3    | -2.11 | 122.39      | 126.04   |
| 14  | aB    | 3032 | CL7  | CBA-CAA-C2A | 2.11  | 120.10      | 113.86   |
| 14  | bB    | 803  | CL7  | CHB-C1B-NB  | -2.11 | 122.02      | 124.26   |
| 14  | aA    | 3117 | CL7  | C3A-C2A-C1A | 2.11  | 104.50      | 101.34   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | aB    | 3026 | CL7  | CMD-C2D-C1D | -2.11 | 122.15      | 125.37   |
| 14  | bB    | 824  | CL7  | CHC-C4B-NB  | 2.11  | 126.49      | 124.26   |
| 14  | aB    | 3013 | CL7  | O2D-CGD-O1D | -2.11 | 119.71      | 123.84   |
| 14  | aA    | 3113 | CL7  | C4D-C3D-CAD | 2.11  | 108.84      | 107.42   |
| 14  | bB    | 827  | CL7  | C4C-C3C-C2C | 2.11  | 109.88      | 107.13   |
| 14  | cB    | 823  | CL7  | C2A-C1A-CHA | -2.11 | 121.09      | 124.42   |
| 14  | aB    | 3013 | CL7  | CED-O2D-CGD | 2.11  | 120.71      | 115.94   |
| 14  | aA    | 3141 | CL7  | C11-C10-C8  | -2.11 | 109.10      | 115.92   |
| 14  | cA    | 3102 | CL7  | CHC-C1C-C2C | 2.11  | 129.91      | 125.48   |
| 14  | cL    | 204  | CL7  | C1D-CHD-C4C | -2.11 | 118.22      | 124.74   |
| 14  | aA    | 3109 | CL7  | CMC-C2C-C3C | 2.11  | 131.84      | 126.12   |
| 14  | cA    | 3132 | CL7  | CMA-C3A-C2A | -2.11 | 105.32      | 113.83   |
| 14  | cA    | 3104 | CL7  | CAD-C3D-C2D | 2.11  | 149.00      | 144.44   |
| 14  | cA    | 3116 | CL7  | C3A-C2A-C1A | 2.11  | 104.50      | 101.34   |
| 14  | bB    | 820  | CL7  | CMB-C2B-C1B | 2.11  | 128.58      | 125.37   |
| 14  | cA    | 3131 | CL7  | C3D-C4D-ND  | 2.11  | 113.19      | 110.17   |
| 14  | aB    | 3019 | CL7  | C6-C7-C8    | -2.11 | 109.11      | 115.92   |
| 14  | bB    | 816  | CL7  | CHD-C1D-ND  | 2.11  | 126.49      | 124.26   |
| 14  | bA    | 3104 | CL7  | CMB-C2B-C1B | 2.11  | 128.58      | 125.37   |
| 14  | bA    | 3104 | CL7  | CHC-C1C-NC  | -2.11 | 122.52      | 124.45   |
| 14  | bL    | 203  | CL7  | C3A-C2A-C1A | 2.11  | 104.49      | 101.34   |
| 14  | bF    | 201  | CL7  | CMC-C2C-C1C | -2.11 | 121.00      | 124.71   |
| 12  | bA    | 3101 | G9R  | C4-C3-C5    | 2.11  | 118.81      | 115.27   |
| 14  | cB    | 810  | CL7  | C2B-C1B-NB  | -2.10 | 108.82      | 110.23   |
| 14  | aB    | 3023 | CL7  | CMB-C2B-C3B | -2.10 | 121.49      | 126.59   |
| 14  | cA    | 3104 | CL7  | CBD-CHA-C4D | -2.10 | 104.11      | 109.14   |
| 14  | bA    | 3119 | CL7  | OBB-CAB-C3B | -2.10 | 120.93      | 125.69   |
| 14  | aA    | 3130 | CL7  | C2C-C1C-NC  | -2.10 | 108.55      | 110.10   |
| 19  | aB    | 3029 | LMG  | C12-C11-C10 | -2.10 | 105.97      | 113.62   |
| 14  | aA    | 3115 | CL7  | C11-C10-C8  | -2.10 | 109.12      | 115.92   |
| 16  | cA    | 3137 | LHG  | P-O3-C3     | -2.10 | 109.36      | 121.68   |
| 14  | bA    | 3109 | CL7  | CMA-C3A-C2A | -2.10 | 111.19      | 116.10   |
| 14  | bA    | 3108 | CL7  | C4D-C3D-C2D | -2.10 | 104.56      | 107.30   |
| 14  | aB    | 3017 | CL7  | CAD-C3D-C2D | 2.10  | 148.98      | 144.44   |
| 14  | bA    | 3123 | CL7  | C2C-C1C-NC  | -2.10 | 108.56      | 110.10   |
| 14  | cA    | 3141 | CL7  | C7-C6-C5    | -2.10 | 107.65      | 113.36   |
| 14  | aB    | 3016 | CL7  | OBD-CAD-C3D | -2.10 | 123.47      | 128.52   |
| 14  | cB    | 814  | CL7  | O2D-CGD-O1D | -2.10 | 119.73      | 123.84   |
| 14  | aB    | 3022 | CL7  | OBD-CAD-C3D | -2.10 | 123.47      | 128.52   |
| 14  | aA    | 3106 | CL7  | C4D-C3D-CAD | 2.10  | 108.84      | 107.42   |
| 14  | cA    | 3125 | CL7  | C4D-C3D-C2D | -2.10 | 104.56      | 107.30   |
| 14  | cB    | 803  | CL7  | C4C-C3C-C2C | 2.10  | 109.86      | 107.13   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | cB    | 831  | CL7  | C4-C3-C2    | -2.10 | 118.30      | 123.68   |
| 14  | cB    | 819  | CL7  | C3B-C2B-C1B | -2.10 | 104.63      | 107.16   |
| 14  | aA    | 3129 | CL7  | C4-C3-C5    | -2.10 | 111.74      | 115.27   |
| 14  | bA    | 3113 | CL7  | C3D-C4D-ND  | 2.10  | 113.17      | 110.17   |
| 14  | aA    | 3126 | CL7  | CBD-CHA-C4D | -2.10 | 104.13      | 109.14   |
| 14  | bL    | 204  | CL7  | CHB-C1B-NB  | -2.10 | 122.04      | 124.26   |
| 14  | bA    | 3131 | CL7  | CHC-C4B-NB  | 2.10  | 126.48      | 124.26   |
| 14  | cA    | 3111 | CL7  | CHC-C4B-NB  | 2.10  | 126.48      | 124.26   |
| 14  | aA    | 3109 | CL7  | CMC-C2C-C1C | -2.10 | 121.02      | 124.71   |
| 14  | cA    | 3103 | CL7  | CBD-CHA-C4D | -2.10 | 104.13      | 109.14   |
| 14  | cA    | 3140 | CL7  | C3A-C2A-C1A | 2.10  | 104.48      | 101.34   |
| 14  | aA    | 3107 | CL7  | CHA-C1A-NA  | -2.09 | 121.02      | 125.98   |
| 14  | aB    | 3026 | CL7  | C5-C3-C2    | -2.09 | 116.88      | 121.12   |
| 14  | cA    | 3123 | CL7  | O2A-CGA-CBA | 2.09  | 118.48      | 111.91   |
| 14  | cB    | 818  | CL7  | CHC-C1C-NC  | -2.09 | 122.53      | 124.45   |
| 14  | aA    | 3125 | CL7  | CAD-C3D-C2D | 2.09  | 148.96      | 144.44   |
| 14  | aB    | 3023 | CL7  | O1D-CGD-CBD | -2.09 | 120.20      | 124.48   |
| 14  | cA    | 3114 | CL7  | CBD-CHA-C4D | -2.09 | 104.14      | 109.14   |
| 14  | cB    | 807  | CL7  | CHC-C1C-NC  | -2.09 | 122.53      | 124.45   |
| 14  | aA    | 3123 | CL7  | CHB-C1B-NB  | -2.09 | 122.04      | 124.26   |
| 14  | cA    | 3133 | CL7  | C4D-C3D-CAD | 2.09  | 108.83      | 107.42   |
| 14  | aB    | 3008 | CL7  | C2C-C1C-NC  | -2.09 | 108.56      | 110.10   |
| 14  | bB    | 832  | CL7  | CBD-CHA-C4D | -2.09 | 104.14      | 109.14   |
| 14  | aA    | 3129 | CL7  | OBD-CAD-C3D | -2.09 | 123.49      | 128.52   |
| 14  | aA    | 3109 | CL7  | C4C-C3C-C2C | 2.09  | 109.85      | 107.13   |
| 14  | bA    | 3121 | CL7  | CHC-C4B-NB  | 2.09  | 126.47      | 124.26   |
| 14  | bA    | 3123 | CL7  | CHA-C1A-NA  | -2.09 | 121.04      | 125.98   |
| 14  | cB    | 832  | CL7  | C16-C15-C13 | -2.09 | 109.17      | 115.92   |
| 14  | bA    | 3119 | CL7  | C1D-ND-C4D  | -2.09 | 104.85      | 106.33   |
| 14  | cB    | 804  | CL7  | C9-C8-C7    | -2.09 | 103.73      | 111.29   |
| 14  | cL    | 204  | CL7  | CAD-C3D-C2D | 2.09  | 148.95      | 144.44   |
| 14  | cA    | 3115 | CL7  | CMC-C2C-C3C | 2.09  | 131.78      | 126.12   |
| 14  | aB    | 3020 | CL7  | C3A-C4A-CHB | -2.09 | 120.61      | 123.70   |
| 14  | aA    | 3143 | CL7  | C3D-C4D-ND  | 2.09  | 113.16      | 110.17   |
| 14  | aB    | 3014 | CL7  | O1D-CGD-CBD | -2.09 | 120.22      | 124.48   |
| 14  | cB    | 806  | CL7  | CHC-C4B-NB  | 2.09  | 126.47      | 124.26   |
| 14  | bA    | 3105 | CL7  | CBD-CHA-C4D | -2.09 | 104.15      | 109.14   |
| 14  | cA    | 3133 | CL7  | CBC-CAC-C3C | 2.09  | 118.18      | 112.43   |
| 14  | bB    | 816  | CL7  | C3D-C4D-ND  | 2.09  | 113.16      | 110.17   |
| 13  | cB    | 805  | PHO  | CMC-C2C-C1C | -2.09 | 120.79      | 124.73   |
| 14  | aB    | 3012 | CL7  | CHA-C1A-NA  | -2.08 | 121.05      | 125.98   |
| 14  | cA    | 3129 | CL7  | CMB-C2B-C3B | -2.08 | 121.54      | 126.59   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | bL    | 205  | CL7  | C4D-C3D-C2D | -2.08 | 104.58      | 107.30   |
| 14  | cB    | 808  | CL7  | C16-C17-C18 | -2.08 | 106.16      | 115.98   |
| 14  | bB    | 809  | CL7  | C3D-C4D-ND  | 2.08  | 113.16      | 110.17   |
| 14  | bL    | 203  | CL7  | C1A-NA-C4A  | 2.08  | 107.56      | 106.30   |
| 14  | bB    | 816  | CL7  | CBD-CHA-C4D | -2.08 | 104.16      | 109.14   |
| 14  | bB    | 832  | CL7  | C16-C15-C13 | -2.08 | 109.19      | 115.92   |
| 14  | bA    | 3118 | CL7  | OBD-CAD-C3D | -2.08 | 123.51      | 128.52   |
| 14  | cL    | 205  | CL7  | CAD-C3D-C2D | 2.08  | 148.94      | 144.44   |
| 14  | bA    | 3115 | CL7  | CMC-C2C-C3C | 2.08  | 131.77      | 126.12   |
| 14  | cB    | 821  | CL7  | C3A-C4A-CHB | -2.08 | 120.61      | 123.70   |
| 14  | cA    | 3130 | CL7  | C1D-ND-C4D  | -2.08 | 104.86      | 106.33   |
| 14  | aB    | 3005 | CL7  | CHC-C4B-NB  | 2.08  | 126.46      | 124.26   |
| 14  | cA    | 3125 | CL7  | C3D-C4D-ND  | 2.08  | 113.15      | 110.17   |
| 14  | aA    | 3106 | CL7  | C2D-C1D-ND  | -2.08 | 108.84      | 110.23   |
| 14  | aB    | 3015 | CL7  | CMC-C2C-C1C | -2.08 | 121.05      | 124.71   |
| 14  | bA    | 3141 | CL7  | C4C-C3C-C2C | 2.08  | 109.84      | 107.13   |
| 14  | bL    | 203  | CL7  | C4C-C3C-C2C | 2.08  | 109.84      | 107.13   |
| 17  | cA    | 3143 | PQN  | C17-C16-C15 | -2.08 | 107.71      | 113.36   |
| 19  | aB    | 3029 | LMG  | C3-C4-C5    | -2.08 | 106.53      | 110.24   |
| 14  | bA    | 3122 | CL7  | OBB-CAB-C3B | -2.08 | 120.99      | 125.69   |
| 14  | bL    | 204  | CL7  | C1-O2A-CGA  | -2.08 | 111.00      | 116.44   |
| 14  | bA    | 3111 | CL7  | C3A-C4A-CHB | -2.08 | 120.62      | 123.70   |
| 14  | aB    | 3021 | CL7  | CMB-C2B-C3B | -2.08 | 121.56      | 126.59   |
| 16  | bA    | 3137 | LHG  | P-O3-C3     | -2.08 | 109.51      | 121.68   |
| 14  | bB    | 827  | CL7  | CBD-CHA-C4D | -2.08 | 104.18      | 109.14   |
| 14  | aA    | 3118 | CL7  | CGD-CBD-CAD | -2.07 | 105.79      | 114.30   |
| 14  | aA    | 3146 | CL7  | C3A-C4A-CHB | -2.07 | 120.62      | 123.70   |
| 14  | bA    | 3116 | CL7  | C1D-CHD-C4C | -2.07 | 118.33      | 124.74   |
| 14  | bB    | 808  | CL7  | CAD-C3D-C2D | 2.07  | 148.91      | 144.44   |
| 14  | bB    | 814  | CL7  | CED-O2D-CGD | 2.07  | 120.62      | 115.94   |
| 14  | bL    | 203  | CL7  | C2C-C1C-NC  | 2.07  | 111.63      | 110.10   |
| 14  | aL    | 204  | CL7  | OBD-CAD-C3D | -2.07 | 123.54      | 128.52   |
| 14  | aA    | 3131 | CL7  | C1D-ND-C4D  | -2.07 | 104.87      | 106.33   |
| 14  | bA    | 3102 | CL7  | CBC-CAC-C3C | -2.07 | 106.73      | 112.43   |
| 14  | bB    | 827  | CL7  | C6-C7-C8    | -2.07 | 109.24      | 115.92   |
| 14  | aA    | 3104 | CL7  | CBD-CHA-C4D | -2.07 | 104.20      | 109.14   |
| 14  | cB    | 826  | CL7  | C16-C17-C18 | -2.07 | 106.25      | 115.98   |
| 14  | cA    | 3127 | CL7  | CHC-C4B-NB  | 2.07  | 126.44      | 124.26   |
| 14  | cA    | 3102 | CL7  | C2C-C1C-NC  | 2.07  | 111.63      | 110.10   |
| 14  | bA    | 3121 | CL7  | CAC-C3C-C2C | -2.06 | 124.00      | 127.53   |
| 14  | bA    | 3125 | CL7  | CAC-C3C-C2C | -2.06 | 124.00      | 127.53   |
| 14  | cA    | 3128 | CL7  | CAA-CBA-CGA | 2.06  | 119.28      | 113.25   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | bA    | 3142 | CL7  | CAD-C3D-C2D | 2.06  | 148.90      | 144.44   |
| 14  | cA    | 3108 | CL7  | C4D-C3D-CAD | 2.06  | 108.81      | 107.42   |
| 14  | bA    | 3106 | CL7  | CAD-C3D-C2D | 2.06  | 148.90      | 144.44   |
| 14  | bB    | 826  | CL7  | CHC-C4B-NB  | 2.06  | 126.44      | 124.26   |
| 14  | cB    | 804  | CL7  | CAD-C3D-C2D | 2.06  | 148.89      | 144.44   |
| 14  | bA    | 3115 | CL7  | OBD-CAD-C3D | -2.06 | 123.56      | 128.52   |
| 14  | cA    | 3139 | CL7  | CHB-C1B-NB  | -2.06 | 122.07      | 124.26   |
| 14  | bL    | 205  | CL7  | CAD-C3D-C2D | 2.06  | 148.89      | 144.44   |
| 14  | cA    | 3130 | CL7  | C1A-NA-C4A  | -2.06 | 105.05      | 106.30   |
| 14  | aA    | 3126 | CL7  | CAA-CBA-CGA | -2.06 | 107.23      | 113.25   |
| 14  | bA    | 3113 | CL7  | O1D-CGD-CBD | -2.06 | 120.27      | 124.48   |
| 14  | bA    | 3103 | CL7  | CBD-CHA-C4D | -2.06 | 104.21      | 109.14   |
| 14  | cA    | 3102 | CL7  | C3C-C4C-NC  | -2.06 | 108.68      | 110.18   |
| 14  | bB    | 808  | CL7  | C3C-C4C-NC  | 2.06  | 111.67      | 110.18   |
| 14  | bA    | 3124 | CL7  | CAC-C3C-C4C | 2.06  | 127.92      | 124.68   |
| 14  | aL    | 202  | CL7  | C4C-C3C-C2C | 2.06  | 109.81      | 107.13   |
| 14  | bB    | 827  | CL7  | O1A-CGA-CBA | -2.06 | 115.70      | 123.73   |
| 14  | bB    | 824  | CL7  | O1D-CGD-CBD | -2.06 | 120.27      | 124.48   |
| 14  | bB    | 826  | CL7  | CAC-C3C-C2C | -2.06 | 124.01      | 127.53   |
| 14  | aA    | 3109 | CL7  | O1D-CGD-CBD | -2.06 | 120.27      | 124.48   |
| 14  | aL    | 202  | CL7  | OBD-CAD-C3D | -2.06 | 123.57      | 128.52   |
| 14  | aL    | 204  | CL7  | CAA-C2A-C3A | -2.06 | 109.12      | 114.26   |
| 14  | cA    | 3132 | CL7  | C9-C8-C7    | -2.06 | 103.84      | 111.29   |
| 14  | cA    | 3141 | CL7  | CAD-C3D-C2D | 2.06  | 148.88      | 144.44   |
| 14  | bB    | 824  | CL7  | CBD-CHA-C4D | -2.06 | 104.22      | 109.14   |
| 14  | bA    | 3104 | CL7  | CAD-C3D-C2D | 2.06  | 148.88      | 144.44   |
| 14  | bA    | 3121 | CL7  | CMA-C3A-C2A | -2.06 | 111.30      | 116.10   |
| 14  | aB    | 3003 | CL7  | O2D-CGD-O1D | -2.05 | 119.82      | 123.84   |
| 14  | cB    | 826  | CL7  | C3A-C4A-CHB | -2.05 | 120.65      | 123.70   |
| 14  | aA    | 3108 | CL7  | CHC-C1C-NC  | -2.05 | 122.57      | 124.45   |
| 14  | aA    | 3127 | CL7  | C6-C5-C3    | -2.05 | 108.07      | 113.45   |
| 14  | aA    | 3103 | CL7  | C3D-C4D-ND  | 2.05  | 113.11      | 110.17   |
| 14  | cA    | 3142 | CL7  | CMC-C2C-C1C | -2.05 | 121.10      | 124.71   |
| 14  | bA    | 3123 | CL7  | CAD-C3D-C2D | 2.05  | 148.87      | 144.44   |
| 14  | cB    | 804  | CL7  | C3D-C4D-ND  | 2.05  | 113.11      | 110.17   |
| 14  | cA    | 3125 | CL7  | CAA-C2A-C3A | -2.05 | 107.16      | 112.78   |
| 14  | aA    | 3108 | CL7  | C16-C15-C13 | -2.05 | 109.29      | 115.92   |
| 14  | aA    | 3104 | CL7  | CHC-C1C-NC  | -2.05 | 122.57      | 124.45   |
| 14  | cA    | 3128 | CL7  | C2C-C1C-NC  | -2.05 | 108.59      | 110.10   |
| 14  | aA    | 3143 | CL7  | CBD-CHA-C4D | -2.05 | 104.24      | 109.14   |
| 14  | aB    | 3022 | CL7  | C2A-C1A-CHA | -2.05 | 121.19      | 124.42   |
| 14  | aA    | 3112 | CL7  | CGD-CBD-CAD | -2.05 | 105.90      | 114.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | aA    | 3141 | CL7  | C1-C2-C3    | -2.05 | 122.50      | 126.04   |
| 14  | aL    | 203  | CL7  | C11-C10-C8  | -2.05 | 109.30      | 115.92   |
| 14  | bB    | 815  | CL7  | C3A-C4A-CHB | -2.05 | 120.66      | 123.70   |
| 14  | aA    | 3120 | CL7  | O2D-CGD-O1D | -2.05 | 119.84      | 123.84   |
| 14  | bA    | 3132 | CL7  | CMA-C3A-C2A | -2.05 | 105.57      | 113.83   |
| 14  | bA    | 3121 | CL7  | CAD-C3D-C2D | 2.05  | 148.86      | 144.44   |
| 14  | aA    | 3134 | CL7  | CMB-C2B-C1B | 2.05  | 128.49      | 125.37   |
| 14  | aL    | 203  | CL7  | C6-C7-C8    | -2.05 | 109.31      | 115.92   |
| 14  | aA    | 3115 | CL7  | CAC-C3C-C2C | -2.05 | 124.03      | 127.53   |
| 14  | aA    | 3106 | CL7  | C3D-C4D-ND  | 2.04  | 113.10      | 110.17   |
| 14  | bA    | 3122 | CL7  | CAD-C3D-C2D | 2.04  | 148.85      | 144.44   |
| 14  | aA    | 3107 | CL7  | C1A-NA-C4A  | 2.04  | 107.54      | 106.30   |
| 14  | cA    | 3124 | CL7  | CAA-C2A-C3A | -2.04 | 107.18      | 112.78   |
| 17  | bA    | 3143 | PQN  | O4-C4-C5    | -2.04 | 118.26      | 121.56   |
| 14  | cB    | 810  | CL7  | OBD-CAD-C3D | -2.04 | 123.61      | 128.52   |
| 14  | bB    | 819  | CL7  | C1-O2A-CGA  | -2.04 | 111.09      | 116.44   |
| 14  | cA    | 3141 | CL7  | CMC-C2C-C1C | -2.04 | 121.12      | 124.71   |
| 14  | cB    | 822  | CL7  | CMC-C2C-C1C | -2.04 | 121.12      | 124.71   |
| 14  | aA    | 3126 | CL7  | C3A-C4A-CHB | -2.04 | 120.67      | 123.70   |
| 14  | aA    | 3114 | CL7  | CMB-C2B-C3B | -2.04 | 121.64      | 126.59   |
| 14  | cA    | 3115 | CL7  | OBD-CAD-C3D | -2.04 | 123.61      | 128.52   |
| 14  | cB    | 826  | CL7  | O2A-CGA-CBA | 2.04  | 118.31      | 111.91   |
| 14  | cB    | 826  | CL7  | O2D-CGD-CBD | 2.04  | 114.89      | 111.27   |
| 17  | aA    | 3144 | PQN  | O4-C4-C5    | -2.04 | 118.26      | 121.56   |
| 14  | cA    | 3105 | CL7  | CAD-C3D-C2D | 2.04  | 148.84      | 144.44   |
| 14  | aA    | 3133 | CL7  | C3A-C4A-CHB | -2.04 | 120.68      | 123.70   |
| 14  | aB    | 3007 | CL7  | C3C-C4C-NC  | 2.04  | 111.65      | 110.18   |
| 14  | aB    | 3026 | CL7  | CBD-CHA-C4D | -2.04 | 104.27      | 109.14   |
| 14  | aL    | 202  | CL7  | C1A-NA-C4A  | 2.04  | 107.53      | 106.30   |
| 12  | cA    | 3101 | G9R  | CBA-CAA-C2A | -2.04 | 107.85      | 113.86   |
| 14  | bA    | 3127 | CL7  | CHA-C1A-NA  | -2.04 | 121.16      | 125.98   |
| 14  | cA    | 3119 | CL7  | OBB-CAB-C3B | -2.04 | 121.08      | 125.69   |
| 14  | aL    | 203  | CL7  | C1D-CHD-C4C | -2.04 | 118.45      | 124.74   |
| 14  | bA    | 3102 | CL7  | C3B-C2B-C1B | -2.04 | 104.70      | 107.16   |
| 14  | bA    | 3132 | CL7  | C2A-C1A-CHA | -2.04 | 122.29      | 126.36   |
| 14  | aA    | 3132 | CL7  | CAD-C3D-C2D | 2.03  | 148.83      | 144.44   |
| 14  | bA    | 3105 | CL7  | CAD-C3D-C2D | 2.03  | 148.83      | 144.44   |
| 14  | bA    | 3119 | CL7  | CHA-C1A-NA  | -2.03 | 121.17      | 125.98   |
| 14  | bA    | 3102 | CL7  | CHD-C4C-C3C | 2.03  | 128.23      | 124.94   |
| 14  | cL    | 203  | CL7  | OBB-CAB-C3B | -2.03 | 121.09      | 125.69   |
| 14  | bA    | 3102 | CL7  | C3D-C4D-ND  | 2.03  | 113.08      | 110.17   |
| 13  | cB    | 805  | PHO  | CAA-CBA-CGA | -2.03 | 107.31      | 113.25   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | aB    | 3011 | CL7  | CAD-C3D-C2D | 2.03  | 148.83      | 144.44   |
| 14  | bB    | 818  | CL7  | CAD-C3D-C2D | 2.03  | 148.83      | 144.44   |
| 14  | cB    | 833  | CL7  | C1D-ND-C4D  | -2.03 | 104.89      | 106.33   |
| 14  | cL    | 203  | CL7  | C1D-ND-C4D  | -2.03 | 104.89      | 106.33   |
| 14  | aB    | 3003 | CL7  | CAD-C3D-C2D | 2.03  | 148.82      | 144.44   |
| 14  | cB    | 820  | CL7  | CMB-C2B-C1B | 2.03  | 128.46      | 125.37   |
| 14  | aB    | 3025 | CL7  | O2A-CGA-CBA | 2.03  | 118.28      | 111.91   |
| 14  | aA    | 3104 | CL7  | CHC-C4B-NB  | 2.03  | 126.41      | 124.26   |
| 14  | aA    | 3123 | CL7  | C1-O2A-CGA  | -2.03 | 111.12      | 116.44   |
| 14  | cA    | 3120 | CL7  | CAC-C3C-C2C | -2.03 | 124.06      | 127.53   |
| 14  | cB    | 810  | CL7  | CMD-C2D-C1D | -2.03 | 122.28      | 125.37   |
| 14  | aL    | 204  | CL7  | C1D-CHD-C4C | -2.03 | 118.47      | 124.74   |
| 14  | aA    | 3124 | CL7  | C1-C2-C3    | -2.03 | 122.54      | 126.04   |
| 14  | bB    | 831  | CL7  | C4-C3-C2    | -2.03 | 118.48      | 123.68   |
| 14  | aB    | 3019 | CL7  | O1A-CGA-CBA | -2.03 | 115.83      | 123.73   |
| 14  | cB    | 803  | CL7  | C3D-C4D-ND  | 2.03  | 113.07      | 110.17   |
| 14  | aB    | 3021 | CL7  | C2B-C1B-NB  | -2.03 | 108.87      | 110.23   |
| 14  | bB    | 824  | CL7  | C3D-C4D-ND  | 2.03  | 113.07      | 110.17   |
| 14  | aB    | 3023 | CL7  | CHC-C1C-NC  | -2.03 | 122.59      | 124.45   |
| 14  | aB    | 3017 | CL7  | CHC-C1C-NC  | -2.02 | 122.59      | 124.45   |
| 14  | aB    | 3030 | CL7  | C3A-C4A-CHB | -2.02 | 120.70      | 123.70   |
| 14  | aA    | 3142 | CL7  | C4C-C3C-C2C | 2.02  | 109.76      | 107.13   |
| 14  | cA    | 3103 | CL7  | CHC-C4B-NB  | 2.02  | 126.40      | 124.26   |
| 14  | cB    | 831  | CL7  | C6-C5-C3    | -2.02 | 108.15      | 113.45   |
| 14  | aA    | 3132 | CL7  | C3A-C4A-CHB | -2.02 | 120.70      | 123.70   |
| 14  | aA    | 3132 | CL7  | O1D-CGD-CBD | -2.02 | 120.35      | 124.48   |
| 14  | bA    | 3142 | CL7  | CMC-C2C-C1C | -2.02 | 121.15      | 124.71   |
| 14  | cB    | 803  | CL7  | C3A-C2A-C1A | 2.02  | 104.37      | 101.34   |
| 14  | cB    | 825  | CL7  | CHC-C1C-NC  | -2.02 | 122.60      | 124.45   |
| 14  | aA    | 3124 | CL7  | CHB-C1B-NB  | -2.02 | 122.12      | 124.26   |
| 14  | cB    | 816  | CL7  | CAD-C3D-C2D | 2.02  | 148.80      | 144.44   |
| 14  | cA    | 3105 | CL7  | CBD-CHA-C4D | -2.02 | 104.31      | 109.14   |
| 14  | cA    | 3106 | CL7  | C16-C17-C18 | -2.02 | 106.47      | 115.98   |
| 14  | bB    | 827  | CL7  | CGD-CBD-CAD | -2.02 | 104.19      | 110.73   |
| 14  | bB    | 804  | CL7  | CGD-CBD-CAD | -2.02 | 104.19      | 110.73   |
| 14  | aF    | 201  | CL7  | CMB-C2B-C1B | 2.02  | 128.44      | 125.37   |
| 14  | aB    | 3019 | CL7  | CHB-C1B-NB  | -2.02 | 122.12      | 124.26   |
| 14  | cA    | 3142 | CL7  | O2A-CGA-O1A | -2.02 | 118.50      | 123.59   |
| 14  | aA    | 3114 | CL7  | O1D-CGD-CBD | -2.02 | 120.36      | 124.48   |
| 14  | aB    | 3009 | CL7  | C2B-C1B-NB  | -2.02 | 108.88      | 110.23   |
| 14  | bA    | 3125 | CL7  | C3A-C4A-CHB | -2.02 | 120.71      | 123.70   |
| 14  | bA    | 3112 | CL7  | O2D-CGD-O1D | -2.02 | 119.90      | 123.84   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | cA    | 3112 | CL7  | O2D-CGD-O1D | -2.02 | 119.90      | 123.84   |
| 14  | aA    | 3107 | CL7  | C4C-C3C-C2C | 2.01  | 109.75      | 107.13   |
| 14  | cB    | 814  | CL7  | CED-O2D-CGD | 2.01  | 120.49      | 115.94   |
| 19  | cB    | 830  | LMG  | C30-C29-C28 | -2.01 | 106.30      | 113.62   |
| 14  | cB    | 810  | CL7  | C9-C8-C7    | -2.01 | 104.00      | 111.29   |
| 14  | cA    | 3140 | CL7  | C3D-C4D-ND  | 2.01  | 113.06      | 110.17   |
| 14  | aB    | 3018 | CL7  | CHA-C1A-NA  | -2.01 | 121.22      | 125.98   |
| 14  | cB    | 815  | CL7  | CHA-C1A-NA  | -2.01 | 121.22      | 125.98   |
| 14  | bB    | 813  | CL7  | CHA-C1A-NA  | -2.01 | 121.22      | 125.98   |
| 14  | bA    | 3110 | CL7  | C3D-C4D-ND  | 2.01  | 113.05      | 110.17   |
| 14  | cB    | 819  | CL7  | CBC-CAC-C3C | 2.01  | 117.97      | 112.43   |
| 14  | aB    | 3012 | CL7  | CHC-C1C-NC  | -2.01 | 122.61      | 124.45   |
| 14  | aA    | 3146 | CL7  | CHA-C1A-NA  | -2.01 | 121.23      | 125.98   |
| 14  | aB    | 3025 | CL7  | CHC-C4B-NB  | 2.01  | 126.38      | 124.26   |
| 14  | aA    | 3103 | CL7  | CHC-C1C-C2C | 2.01  | 129.69      | 125.48   |
| 14  | bA    | 3132 | CL7  | CAA-C2A-C3A | -2.01 | 107.28      | 112.78   |
| 14  | aB    | 3025 | CL7  | CAD-C3D-C2D | 2.01  | 148.78      | 144.44   |
| 14  | bA    | 3142 | CL7  | C3D-C4D-ND  | 2.01  | 113.05      | 110.17   |
| 14  | cB    | 804  | CL7  | C3B-C2B-C1B | -2.01 | 104.74      | 107.16   |
| 14  | aB    | 3025 | CL7  | C16-C17-C18 | -2.01 | 106.52      | 115.98   |
| 14  | cA    | 3123 | CL7  | C2A-C1A-CHA | -2.01 | 122.35      | 126.36   |
| 14  | aB    | 3030 | CL7  | C4-C3-C2    | -2.01 | 118.53      | 123.68   |
| 14  | cA    | 3120 | CL7  | CAD-C3D-C2D | 2.01  | 148.77      | 144.44   |
| 14  | cA    | 3125 | CL7  | C1D-ND-C4D  | -2.01 | 104.91      | 106.33   |
| 14  | bA    | 3106 | CL7  | C16-C17-C18 | -2.01 | 106.53      | 115.98   |
| 14  | aB    | 3024 | CL7  | CHA-C1A-NA  | -2.00 | 121.24      | 125.98   |
| 14  | aA    | 3103 | CL7  | C1D-ND-C4D  | -2.00 | 104.91      | 106.33   |
| 14  | bB    | 827  | CL7  | C2A-C1A-CHA | -2.00 | 122.35      | 126.36   |
| 14  | bB    | 804  | CL7  | O1D-CGD-CBD | -2.00 | 120.38      | 124.48   |
| 14  | bL    | 205  | CL7  | OBD-CAD-C3D | -2.00 | 123.70      | 128.52   |
| 14  | cB    | 816  | CL7  | C3D-C4D-ND  | 2.00  | 113.04      | 110.17   |
| 14  | bA    | 3121 | CL7  | OBD-CAD-C3D | -2.00 | 123.70      | 128.52   |
| 14  | cA    | 3142 | CL7  | OBD-CAD-C3D | -2.00 | 123.70      | 128.52   |
| 14  | aB    | 3025 | CL7  | CHD-C1D-ND  | 2.00  | 126.38      | 124.26   |
| 14  | aA    | 3110 | CL7  | CAD-C3D-C2D | 2.00  | 148.76      | 144.44   |
| 14  | cL    | 204  | CL7  | C4C-C3C-C2C | 2.00  | 109.73      | 107.13   |
| 14  | aB    | 3015 | CL7  | OBD-CAD-C3D | -2.00 | 123.70      | 128.52   |
| 14  | cB    | 832  | CL7  | CHD-C1D-ND  | 2.00  | 126.38      | 124.26   |
| 14  | cA    | 3142 | CL7  | O1A-CGA-CBA | -2.00 | 115.93      | 123.73   |
| 14  | aB    | 3024 | CL7  | C3A-C2A-C1A | 2.00  | 104.03      | 101.64   |
| 14  | bB    | 809  | CL7  | CHC-C1C-NC  | -2.00 | 122.62      | 124.45   |

All (376) chirality outliers are listed below:



| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 12  | aA    | 3101 | G9R  | ND   |
| 12  | cA    | 3101 | G9R  | ND   |
| 14  | aA    | 3103 | CL7  | NC   |
| 14  | aA    | 3104 | CL7  | NA   |
| 14  | aA    | 3104 | CL7  | NC   |
| 14  | aA    | 3105 | CL7  | NA   |
| 14  | aA    | 3105 | CL7  | NC   |
| 14  | aA    | 3106 | CL7  | NA   |
| 14  | aA    | 3106 | CL7  | NC   |
| 14  | aA    | 3107 | CL7  | NA   |
| 14  | aA    | 3107 | CL7  | NC   |
| 14  | aA    | 3108 | CL7  | NC   |
| 14  | aA    | 3109 | CL7  | NC   |
| 14  | aA    | 3110 | CL7  | NA   |
| 14  | aA    | 3110 | CL7  | NC   |
| 14  | aA    | 3111 | CL7  | NC   |
| 14  | aA    | 3112 | CL7  | NA   |
| 14  | aA    | 3112 | CL7  | NC   |
| 14  | aA    | 3113 | CL7  | NA   |
| 14  | aA    | 3113 | CL7  | NC   |
| 14  | aA    | 3114 | CL7  | NA   |
| 14  | aA    | 3114 | CL7  | NC   |
| 14  | aA    | 3115 | CL7  | NA   |
| 14  | aA    | 3115 | CL7  | NC   |
| 14  | aA    | 3116 | CL7  | NC   |
| 14  | aA    | 3117 | CL7  | NA   |
| 14  | aA    | 3117 | CL7  | NC   |
| 14  | aA    | 3118 | CL7  | NA   |
| 14  | aA    | 3118 | CL7  | NC   |
| 14  | aA    | 3119 | CL7  | NC   |
| 14  | aA    | 3120 | CL7  | NA   |
| 14  | aA    | 3120 | CL7  | NC   |
| 14  | aA    | 3121 | CL7  | NA   |
| 14  | aA    | 3121 | CL7  | NC   |
| 14  | aA    | 3122 | CL7  | NC   |
| 14  | aA    | 3123 | CL7  | NA   |
| 14  | aA    | 3123 | CL7  | NC   |
| 14  | aA    | 3124 | CL7  | NA   |
| 14  | aA    | 3124 | CL7  | NC   |
| 14  | aA    | 3125 | CL7  | NA   |
| 14  | aA    | 3125 | CL7  | NC   |
| 14  | aA    | 3126 | CL7  | NA   |
| 14  | aA    | 3126 | CL7  | NC   |

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| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 14  | aA    | 3127 | CL7  | NC   |
| 14  | aA    | 3128 | CL7  | NA   |
| 14  | aA    | 3128 | CL7  | NC   |
| 14  | aA    | 3129 | CL7  | NA   |
| 14  | aA    | 3129 | CL7  | NC   |
| 14  | aA    | 3130 | CL7  | NC   |
| 14  | aA    | 3131 | CL7  | NC   |
| 14  | aA    | 3132 | CL7  | NA   |
| 14  | aA    | 3132 | CL7  | NC   |
| 14  | aA    | 3133 | CL7  | NA   |
| 14  | aA    | 3133 | CL7  | NC   |
| 14  | aA    | 3134 | CL7  | NA   |
| 14  | aA    | 3134 | CL7  | NC   |
| 14  | aA    | 3140 | CL7  | NA   |
| 14  | aA    | 3140 | CL7  | NC   |
| 14  | aA    | 3141 | CL7  | NA   |
| 14  | aA    | 3141 | CL7  | NC   |
| 14  | aA    | 3142 | CL7  | NA   |
| 14  | aA    | 3142 | CL7  | NC   |
| 14  | aA    | 3143 | CL7  | NC   |
| 14  | aA    | 3146 | CL7  | NA   |
| 14  | aA    | 3146 | CL7  | NC   |
| 14  | aB    | 3002 | CL7  | NA   |
| 14  | aB    | 3002 | CL7  | NC   |
| 14  | aB    | 3003 | CL7  | NA   |
| 14  | aB    | 3003 | CL7  | NC   |
| 14  | aB    | 3005 | CL7  | NA   |
| 14  | aB    | 3005 | CL7  | NC   |
| 14  | aB    | 3006 | CL7  | NC   |
| 14  | aB    | 3007 | CL7  | NA   |
| 14  | aB    | 3007 | CL7  | NC   |
| 14  | aB    | 3008 | CL7  | NA   |
| 14  | aB    | 3008 | CL7  | NC   |
| 14  | aB    | 3009 | CL7  | NA   |
| 14  | aB    | 3009 | CL7  | NC   |
| 14  | aB    | 3010 | CL7  | NA   |
| 14  | aB    | 3010 | CL7  | NC   |
| 14  | aB    | 3011 | CL7  | NA   |
| 14  | aB    | 3011 | CL7  | NC   |
| 14  | aB    | 3012 | CL7  | NA   |
| 14  | aB    | 3012 | CL7  | NC   |
| 14  | aB    | 3013 | CL7  | NC   |

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| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 14  | aB    | 3014 | CL7  | NC   |
| 14  | aB    | 3015 | CL7  | NA   |
| 14  | aB    | 3015 | CL7  | NC   |
| 14  | aB    | 3016 | CL7  | NA   |
| 14  | aB    | 3016 | CL7  | NC   |
| 14  | aB    | 3017 | CL7  | NA   |
| 14  | aB    | 3017 | CL7  | NC   |
| 14  | aB    | 3018 | CL7  | NA   |
| 14  | aB    | 3018 | CL7  | NC   |
| 14  | aB    | 3019 | CL7  | NA   |
| 14  | aB    | 3019 | CL7  | NC   |
| 14  | aB    | 3020 | CL7  | NC   |
| 14  | aB    | 3021 | CL7  | NC   |
| 14  | aB    | 3022 | CL7  | NA   |
| 14  | aB    | 3022 | CL7  | NC   |
| 14  | aB    | 3023 | CL7  | NA   |
| 14  | aB    | 3023 | CL7  | NC   |
| 14  | aB    | 3024 | CL7  | NA   |
| 14  | aB    | 3024 | CL7  | NC   |
| 14  | aB    | 3025 | CL7  | NA   |
| 14  | aB    | 3025 | CL7  | NC   |
| 14  | aB    | 3026 | CL7  | NA   |
| 14  | aB    | 3026 | CL7  | NC   |
| 14  | aB    | 3030 | CL7  | NA   |
| 14  | aB    | 3030 | CL7  | NC   |
| 14  | aB    | 3031 | CL7  | NA   |
| 14  | aB    | 3031 | CL7  | NC   |
| 14  | aB    | 3032 | CL7  | NA   |
| 14  | aB    | 3032 | CL7  | NC   |
| 14  | aF    | 201  | CL7  | NA   |
| 14  | aF    | 201  | CL7  | NC   |
| 14  | aJ    | 101  | CL7  | NC   |
| 14  | aK    | 101  | CL7  | NA   |
| 14  | aK    | 101  | CL7  | NC   |
| 14  | aL    | 202  | CL7  | NA   |
| 14  | aL    | 202  | CL7  | NC   |
| 14  | aL    | 203  | CL7  | NA   |
| 14  | aL    | 203  | CL7  | NC   |
| 14  | aL    | 204  | CL7  | NA   |
| 14  | aL    | 204  | CL7  | NC   |
| 14  | bA    | 3102 | CL7  | NC   |
| 14  | bA    | 3103 | CL7  | NA   |

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| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 14  | bA    | 3103 | CL7  | NC   |
| 14  | bA    | 3104 | CL7  | NA   |
| 14  | bA    | 3104 | CL7  | NC   |
| 14  | bA    | 3105 | CL7  | NA   |
| 14  | bA    | 3105 | CL7  | NC   |
| 14  | bA    | 3106 | CL7  | NA   |
| 14  | bA    | 3106 | CL7  | NC   |
| 14  | bA    | 3107 | CL7  | NC   |
| 14  | bA    | 3108 | CL7  | NC   |
| 14  | bA    | 3109 | CL7  | NA   |
| 14  | bA    | 3109 | CL7  | NC   |
| 14  | bA    | 3110 | CL7  | NA   |
| 14  | bA    | 3110 | CL7  | NC   |
| 14  | bA    | 3111 | CL7  | NA   |
| 14  | bA    | 3111 | CL7  | NC   |
| 14  | bA    | 3112 | CL7  | NA   |
| 14  | bA    | 3112 | CL7  | NC   |
| 14  | bA    | 3113 | CL7  | NC   |
| 14  | bA    | 3114 | CL7  | NA   |
| 14  | bA    | 3114 | CL7  | NC   |
| 14  | bA    | 3115 | CL7  | NC   |
| 14  | bA    | 3116 | CL7  | NA   |
| 14  | bA    | 3116 | CL7  | NC   |
| 14  | bA    | 3117 | CL7  | NA   |
| 14  | bA    | 3117 | CL7  | NC   |
| 14  | bA    | 3118 | CL7  | NA   |
| 14  | bA    | 3118 | CL7  | NC   |
| 14  | bA    | 3119 | CL7  | NA   |
| 14  | bA    | 3119 | CL7  | NC   |
| 14  | bA    | 3120 | CL7  | NA   |
| 14  | bA    | 3120 | CL7  | NC   |
| 14  | bA    | 3121 | CL7  | NA   |
| 14  | bA    | 3121 | CL7  | NC   |
| 14  | bA    | 3122 | CL7  | NA   |
| 14  | bA    | 3122 | CL7  | NC   |
| 14  | bA    | 3123 | CL7  | NA   |
| 14  | bA    | 3123 | CL7  | NC   |
| 14  | bA    | 3124 | CL7  | NA   |
| 14  | bA    | 3124 | CL7  | NC   |
| 14  | bA    | 3125 | CL7  | NA   |
| 14  | bA    | 3125 | CL7  | NC   |
| 14  | bA    | 3126 | CL7  | NC   |

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| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 14  | bA    | 3127 | CL7  | NA   |
| 14  | bA    | 3127 | CL7  | NC   |
| 14  | bA    | 3128 | CL7  | NA   |
| 14  | bA    | 3128 | CL7  | NC   |
| 14  | bA    | 3129 | CL7  | NC   |
| 14  | bA    | 3130 | CL7  | NA   |
| 14  | bA    | 3130 | CL7  | NC   |
| 14  | bA    | 3131 | CL7  | NA   |
| 14  | bA    | 3131 | CL7  | NC   |
| 14  | bA    | 3132 | CL7  | NA   |
| 14  | bA    | 3132 | CL7  | NC   |
| 14  | bA    | 3133 | CL7  | NA   |
| 14  | bA    | 3133 | CL7  | NC   |
| 14  | bA    | 3139 | CL7  | NA   |
| 14  | bA    | 3139 | CL7  | NC   |
| 14  | bA    | 3140 | CL7  | NA   |
| 14  | bA    | 3140 | CL7  | NC   |
| 14  | bA    | 3141 | CL7  | NA   |
| 14  | bA    | 3141 | CL7  | NC   |
| 14  | bA    | 3142 | CL7  | NA   |
| 14  | bA    | 3142 | CL7  | NC   |
| 14  | bA    | 3145 | CL7  | NA   |
| 14  | bA    | 3145 | CL7  | NC   |
| 14  | bB    | 803  | CL7  | NA   |
| 14  | bB    | 803  | CL7  | NC   |
| 14  | bB    | 804  | CL7  | NA   |
| 14  | bB    | 804  | CL7  | NC   |
| 14  | bB    | 806  | CL7  | NA   |
| 14  | bB    | 806  | CL7  | NC   |
| 14  | bB    | 807  | CL7  | NC   |
| 14  | bB    | 808  | CL7  | NA   |
| 14  | bB    | 808  | CL7  | NC   |
| 14  | bB    | 809  | CL7  | NA   |
| 14  | bB    | 809  | CL7  | NC   |
| 14  | bB    | 810  | CL7  | NA   |
| 14  | bB    | 810  | CL7  | NC   |
| 14  | bB    | 811  | CL7  | NA   |
| 14  | bB    | 811  | CL7  | NC   |
| 14  | bB    | 812  | CL7  | NA   |
| 14  | bB    | 812  | CL7  | NC   |
| 14  | bB    | 813  | CL7  | NA   |
| 14  | bB    | 813  | CL7  | NC   |

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| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 14  | bB    | 814  | CL7  | NC   |
| 14  | bB    | 815  | CL7  | NA   |
| 14  | bB    | 815  | CL7  | NC   |
| 14  | bB    | 816  | CL7  | NC   |
| 14  | bB    | 817  | CL7  | NA   |
| 14  | bB    | 817  | CL7  | NC   |
| 14  | bB    | 818  | CL7  | NA   |
| 14  | bB    | 818  | CL7  | NC   |
| 14  | bB    | 819  | CL7  | NA   |
| 14  | bB    | 819  | CL7  | NC   |
| 14  | bB    | 820  | CL7  | NA   |
| 14  | bB    | 820  | CL7  | NC   |
| 14  | bB    | 821  | CL7  | NC   |
| 14  | bB    | 822  | CL7  | NC   |
| 14  | bB    | 823  | CL7  | NA   |
| 14  | bB    | 823  | CL7  | NC   |
| 14  | bB    | 824  | CL7  | NA   |
| 14  | bB    | 824  | CL7  | NC   |
| 14  | bB    | 825  | CL7  | NA   |
| 14  | bB    | 825  | CL7  | NC   |
| 14  | bB    | 826  | CL7  | NA   |
| 14  | bB    | 826  | CL7  | NC   |
| 14  | bB    | 827  | CL7  | NA   |
| 14  | bB    | 827  | CL7  | NC   |
| 14  | bB    | 831  | CL7  | NA   |
| 14  | bB    | 831  | CL7  | NC   |
| 14  | bB    | 832  | CL7  | NA   |
| 14  | bB    | 832  | CL7  | NC   |
| 14  | bB    | 833  | CL7  | NA   |
| 14  | bB    | 833  | CL7  | NC   |
| 14  | bF    | 201  | CL7  | NA   |
| 14  | bF    | 201  | CL7  | NC   |
| 14  | bJ    | 101  | CL7  | NC   |
| 14  | bK    | 101  | CL7  | NA   |
| 14  | bK    | 101  | CL7  | NC   |
| 14  | bL    | 203  | CL7  | NA   |
| 14  | bL    | 203  | CL7  | NC   |
| 14  | bL    | 204  | CL7  | NA   |
| 14  | bL    | 204  | CL7  | NC   |
| 14  | bL    | 205  | CL7  | NA   |
| 14  | bL    | 205  | CL7  | NC   |
| 14  | cA    | 3102 | CL7  | NC   |

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| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 14  | cA    | 3103 | CL7  | NA   |
| 14  | cA    | 3103 | CL7  | NC   |
| 14  | cA    | 3104 | CL7  | NA   |
| 14  | cA    | 3104 | CL7  | NC   |
| 14  | cA    | 3105 | CL7  | NA   |
| 14  | cA    | 3105 | CL7  | NC   |
| 14  | cA    | 3106 | CL7  | NA   |
| 14  | cA    | 3106 | CL7  | NC   |
| 14  | cA    | 3107 | CL7  | NC   |
| 14  | cA    | 3108 | CL7  | NC   |
| 14  | cA    | 3109 | CL7  | NA   |
| 14  | cA    | 3109 | CL7  | NC   |
| 14  | cA    | 3110 | CL7  | NC   |
| 14  | cA    | 3111 | CL7  | NA   |
| 14  | cA    | 3111 | CL7  | NC   |
| 14  | cA    | 3112 | CL7  | NA   |
| 14  | cA    | 3112 | CL7  | NC   |
| 14  | cA    | 3113 | CL7  | NC   |
| 14  | cA    | 3114 | CL7  | NC   |
| 14  | cA    | 3115 | CL7  | NC   |
| 14  | cA    | 3116 | CL7  | NA   |
| 14  | cA    | 3116 | CL7  | NC   |
| 14  | cA    | 3117 | CL7  | NA   |
| 14  | cA    | 3117 | CL7  | NC   |
| 14  | cA    | 3118 | CL7  | NC   |
| 14  | cA    | 3119 | CL7  | NA   |
| 14  | cA    | 3119 | CL7  | NC   |
| 14  | cA    | 3120 | CL7  | NA   |
| 14  | cA    | 3120 | CL7  | NC   |
| 14  | cA    | 3121 | CL7  | NA   |
| 14  | cA    | 3121 | CL7  | NC   |
| 14  | cA    | 3122 | CL7  | NA   |
| 14  | cA    | 3122 | CL7  | NC   |
| 14  | cA    | 3123 | CL7  | NA   |
| 14  | cA    | 3123 | CL7  | NC   |
| 14  | cA    | 3124 | CL7  | NA   |
| 14  | cA    | 3124 | CL7  | NC   |
| 14  | cA    | 3125 | CL7  | NA   |
| 14  | cA    | 3125 | CL7  | NC   |
| 14  | cA    | 3126 | CL7  | NA   |
| 14  | cA    | 3126 | CL7  | NC   |
| 14  | cA    | 3127 | CL7  | NA   |

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| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 14  | cA    | 3127 | CL7  | NC   |
| 14  | cA    | 3128 | CL7  | NA   |
| 14  | cA    | 3128 | CL7  | NC   |
| 14  | cA    | 3129 | CL7  | NC   |
| 14  | cA    | 3130 | CL7  | NA   |
| 14  | cA    | 3130 | CL7  | NC   |
| 14  | cA    | 3131 | CL7  | NA   |
| 14  | cA    | 3131 | CL7  | NC   |
| 14  | cA    | 3132 | CL7  | NA   |
| 14  | cA    | 3132 | CL7  | NC   |
| 14  | cA    | 3133 | CL7  | NA   |
| 14  | cA    | 3133 | CL7  | NC   |
| 14  | cA    | 3139 | CL7  | NA   |
| 14  | cA    | 3139 | CL7  | NC   |
| 14  | cA    | 3140 | CL7  | NA   |
| 14  | cA    | 3140 | CL7  | NC   |
| 14  | cA    | 3141 | CL7  | NA   |
| 14  | cA    | 3141 | CL7  | NC   |
| 14  | cA    | 3142 | CL7  | NA   |
| 14  | cA    | 3142 | CL7  | NC   |
| 14  | cA    | 3144 | CL7  | NA   |
| 14  | cA    | 3144 | CL7  | NC   |
| 14  | cB    | 803  | CL7  | NA   |
| 14  | cB    | 803  | CL7  | NC   |
| 14  | cB    | 804  | CL7  | NC   |
| 14  | cB    | 806  | CL7  | NA   |
| 14  | cB    | 806  | CL7  | NC   |
| 14  | cB    | 807  | CL7  | NC   |
| 14  | cB    | 808  | CL7  | NA   |
| 14  | cB    | 808  | CL7  | NC   |
| 14  | cB    | 809  | CL7  | NA   |
| 14  | cB    | 809  | CL7  | NC   |
| 14  | cB    | 810  | CL7  | NA   |
| 14  | cB    | 810  | CL7  | NC   |
| 14  | cB    | 811  | CL7  | NA   |
| 14  | cB    | 811  | CL7  | NC   |
| 14  | cB    | 812  | CL7  | NA   |
| 14  | cB    | 812  | CL7  | NC   |
| 14  | cB    | 813  | CL7  | NA   |
| 14  | cB    | 813  | CL7  | NC   |
| 14  | cB    | 814  | CL7  | NC   |
| 14  | cB    | 815  | CL7  | NA   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 14  | cB    | 815 | CL7  | NC   |
| 14  | cB    | 816 | CL7  | NA   |
| 14  | cB    | 816 | CL7  | NC   |
| 14  | cB    | 817 | CL7  | NA   |
| 14  | cB    | 817 | CL7  | NC   |
| 14  | cB    | 818 | CL7  | NA   |
| 14  | cB    | 818 | CL7  | NC   |
| 14  | cB    | 819 | CL7  | NA   |
| 14  | cB    | 819 | CL7  | NC   |
| 14  | cB    | 820 | CL7  | NA   |
| 14  | cB    | 820 | CL7  | NC   |
| 14  | cB    | 821 | CL7  | NC   |
| 14  | cB    | 822 | CL7  | NC   |
| 14  | cB    | 823 | CL7  | NA   |
| 14  | cB    | 823 | CL7  | NC   |
| 14  | cB    | 824 | CL7  | NA   |
| 14  | cB    | 824 | CL7  | NC   |
| 14  | cB    | 825 | CL7  | NA   |
| 14  | cB    | 825 | CL7  | NC   |
| 14  | cB    | 826 | CL7  | NA   |
| 14  | cB    | 826 | CL7  | NC   |
| 14  | cB    | 827 | CL7  | NC   |
| 14  | cB    | 831 | CL7  | NA   |
| 14  | cB    | 831 | CL7  | NC   |
| 14  | cB    | 832 | CL7  | NA   |
| 14  | cB    | 832 | CL7  | NC   |
| 14  | cB    | 833 | CL7  | NA   |
| 14  | cB    | 833 | CL7  | NC   |
| 14  | cF    | 201 | CL7  | NA   |
| 14  | cF    | 201 | CL7  | NC   |
| 14  | cJ    | 101 | CL7  | NC   |
| 14  | cK    | 101 | CL7  | NA   |
| 14  | cK    | 101 | CL7  | NC   |
| 14  | cL    | 203 | CL7  | NA   |
| 14  | cL    | 203 | CL7  | NC   |
| 14  | cL    | 204 | CL7  | NA   |
| 14  | cL    | 204 | CL7  | NC   |
| 14  | cL    | 205 | CL7  | NA   |
| 14  | cL    | 205 | CL7  | NC   |

All (2107) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 13  | aA    | 3102 | PHO  | CBA-CGA-O2A-C1  |
| 13  | aA    | 3102 | PHO  | O1A-CGA-O2A-C1  |
| 13  | bB    | 801  | PHO  | CBA-CGA-O2A-C1  |
| 13  | bB    | 801  | PHO  | O1A-CGA-O2A-C1  |
| 13  | bB    | 805  | PHO  | CHA-CBD-CGD-O1D |
| 13  | cB    | 801  | PHO  | CBA-CGA-O2A-C1  |
| 13  | cB    | 801  | PHO  | O1A-CGA-O2A-C1  |
| 13  | cB    | 805  | PHO  | C11-C10-C8-C9   |
| 14  | aA    | 3103 | CL7  | C1-C2-C3-C4     |
| 14  | aA    | 3103 | CL7  | C2B-C3B-CAB-OBB |
| 14  | aA    | 3103 | CL7  | C4B-C3B-CAB-OBB |
| 14  | aA    | 3105 | CL7  | CAD-CBD-CGD-O1D |
| 14  | aA    | 3105 | CL7  | CBD-CGD-O2D-CED |
| 14  | aA    | 3105 | CL7  | C2B-C3B-CAB-OBB |
| 14  | aA    | 3105 | CL7  | C4B-C3B-CAB-OBB |
| 14  | aA    | 3106 | CL7  | CHA-CBD-CGD-O2D |
| 14  | aA    | 3106 | CL7  | C2B-C3B-CAB-OBB |
| 14  | aA    | 3106 | CL7  | C4B-C3B-CAB-OBB |
| 14  | aA    | 3107 | CL7  | C1-C2-C3-C4     |
| 14  | aA    | 3107 | CL7  | C1A-C2A-CAA-CBA |
| 14  | aA    | 3108 | CL7  | C1A-C2A-CAA-CBA |
| 14  | aA    | 3109 | CL7  | C1A-C2A-CAA-CBA |
| 14  | aA    | 3109 | CL7  | C4B-C3B-CAB-OBB |
| 14  | aA    | 3110 | CL7  | C2B-C3B-CAB-OBB |
| 14  | aA    | 3110 | CL7  | C4B-C3B-CAB-OBB |
| 14  | aA    | 3111 | CL7  | CBD-CGD-O2D-CED |
| 14  | aA    | 3112 | CL7  | C2B-C3B-CAB-OBB |
| 14  | aA    | 3112 | CL7  | C4B-C3B-CAB-OBB |
| 14  | aA    | 3113 | CL7  | C2B-C3B-CAB-OBB |
| 14  | aA    | 3113 | CL7  | C4B-C3B-CAB-OBB |
| 14  | aA    | 3115 | CL7  | CBD-CGD-O2D-CED |
| 14  | aA    | 3116 | CL7  | C2B-C3B-CAB-OBB |
| 14  | aA    | 3116 | CL7  | C4B-C3B-CAB-OBB |
| 14  | aA    | 3117 | CL7  | C1-C2-C3-C5     |
| 14  | aA    | 3117 | CL7  | C1-C2-C3-C4     |
| 14  | aA    | 3123 | CL7  | C1-C2-C3-C5     |
| 14  | aA    | 3123 | CL7  | C1A-C2A-CAA-CBA |
| 14  | aA    | 3123 | CL7  | CHA-CBD-CGD-O1D |
| 14  | aA    | 3123 | CL7  | CAD-CBD-CGD-O1D |
| 14  | aA    | 3123 | CL7  | C2B-C3B-CAB-OBB |
| 14  | aA    | 3123 | CL7  | C4B-C3B-CAB-OBB |
| 14  | aA    | 3124 | CL7  | C1-C2-C3-C5     |
| 14  | aA    | 3124 | CL7  | C2B-C3B-CAB-OBB |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | aA    | 3124 | CL7  | C4B-C3B-CAB-OBB |
| 14  | aA    | 3125 | CL7  | C1-C2-C3-C4     |
| 14  | aA    | 3125 | CL7  | C4B-C3B-CAB-OBB |
| 14  | aA    | 3126 | CL7  | C1A-C2A-CAA-CBA |
| 14  | aA    | 3126 | CL7  | C4B-C3B-CAB-OBB |
| 14  | aA    | 3127 | CL7  | CHA-CBD-CGD-O1D |
| 14  | aA    | 3127 | CL7  | C2B-C3B-CAB-OBB |
| 14  | aA    | 3127 | CL7  | C4B-C3B-CAB-OBB |
| 14  | aA    | 3128 | CL7  | C1-C2-C3-C5     |
| 14  | aA    | 3129 | CL7  | C1-C2-C3-C5     |
| 14  | aA    | 3129 | CL7  | C1-C2-C3-C4     |
| 14  | aA    | 3129 | CL7  | CHA-CBD-CGD-O2D |
| 14  | aA    | 3130 | CL7  | CHA-CBD-CGD-O2D |
| 14  | aA    | 3131 | CL7  | CHA-CBD-CGD-O2D |
| 14  | aA    | 3132 | CL7  | CBD-CGD-O2D-CED |
| 14  | aA    | 3132 | CL7  | C2B-C3B-CAB-OBB |
| 14  | aA    | 3132 | CL7  | C4B-C3B-CAB-OBB |
| 14  | aA    | 3133 | CL7  | C1-C2-C3-C5     |
| 14  | aA    | 3133 | CL7  | C1-C2-C3-C4     |
| 14  | aA    | 3133 | CL7  | C1A-C2A-CAA-CBA |
| 14  | aA    | 3134 | CL7  | CHA-CBD-CGD-O1D |
| 14  | aA    | 3134 | CL7  | CAD-CBD-CGD-O1D |
| 14  | aA    | 3134 | CL7  | CBD-CGD-O2D-CED |
| 14  | aA    | 3140 | CL7  | C1-C2-C3-C4     |
| 14  | aA    | 3140 | CL7  | C11-C10-C8-C9   |
| 14  | aA    | 3140 | CL7  | CHA-CBD-CGD-O1D |
| 14  | aA    | 3140 | CL7  | CAD-CBD-CGD-O2D |
| 14  | aA    | 3140 | CL7  | CBD-CGD-O2D-CED |
| 14  | aA    | 3140 | CL7  | O1D-CGD-O2D-CED |
| 14  | aA    | 3140 | CL7  | C2B-C3B-CAB-OBB |
| 14  | aA    | 3140 | CL7  | C4B-C3B-CAB-OBB |
| 14  | aA    | 3141 | CL7  | O2A-C1-C2-C3    |
| 14  | aA    | 3141 | CL7  | C1-C2-C3-C4     |
| 14  | aA    | 3141 | CL7  | CHA-CBD-CGD-O2D |
| 14  | aA    | 3141 | CL7  | C2B-C3B-CAB-OBB |
| 14  | aA    | 3141 | CL7  | C4B-C3B-CAB-OBB |
| 14  | aA    | 3142 | CL7  | C11-C12-C13-C14 |
| 14  | aA    | 3142 | CL7  | CBD-CGD-O2D-CED |
| 14  | aA    | 3143 | CL7  | C1-C2-C3-C5     |
| 14  | aA    | 3143 | CL7  | C1-C2-C3-C4     |
| 14  | aA    | 3143 | CL7  | C1A-C2A-CAA-CBA |
| 14  | aA    | 3146 | CL7  | C2B-C3B-CAB-OBB |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | aA    | 3146 | CL7  | C4B-C3B-CAB-OBB |
| 14  | aB    | 3002 | CL7  | C1-C2-C3-C4     |
| 14  | aB    | 3002 | CL7  | CHA-CBD-CGD-O2D |
| 14  | aB    | 3002 | CL7  | CAD-CBD-CGD-O2D |
| 14  | aB    | 3002 | CL7  | C2B-C3B-CAB-OBB |
| 14  | aB    | 3002 | CL7  | C4B-C3B-CAB-OBB |
| 14  | aB    | 3003 | CL7  | C1-C2-C3-C5     |
| 14  | aB    | 3003 | CL7  | C1-C2-C3-C4     |
| 14  | aB    | 3005 | CL7  | C1-C2-C3-C4     |
| 14  | aB    | 3005 | CL7  | C6-C7-C8-C9     |
| 14  | aB    | 3006 | CL7  | C1-C2-C3-C4     |
| 14  | aB    | 3006 | CL7  | CHA-CBD-CGD-O2D |
| 14  | aB    | 3006 | CL7  | C2B-C3B-CAB-OBB |
| 14  | aB    | 3006 | CL7  | C4B-C3B-CAB-OBB |
| 14  | aB    | 3007 | CL7  | C1-C2-C3-C4     |
| 14  | aB    | 3007 | CL7  | C14-C13-C15-C16 |
| 14  | aB    | 3008 | CL7  | C1-C2-C3-C5     |
| 14  | aB    | 3008 | CL7  | C1-C2-C3-C4     |
| 14  | aB    | 3008 | CL7  | C4B-C3B-CAB-OBB |
| 14  | aB    | 3009 | CL7  | C1-C2-C3-C4     |
| 14  | aB    | 3009 | CL7  | C14-C13-C15-C16 |
| 14  | aB    | 3009 | CL7  | C4B-C3B-CAB-OBB |
| 14  | aB    | 3011 | CL7  | C2B-C3B-CAB-OBB |
| 14  | aB    | 3011 | CL7  | C4B-C3B-CAB-OBB |
| 14  | aB    | 3013 | CL7  | CAD-CBD-CGD-O1D |
| 14  | aB    | 3015 | CL7  | C1-C2-C3-C5     |
| 14  | aB    | 3015 | CL7  | C1-C2-C3-C4     |
| 14  | aB    | 3015 | CL7  | CAD-CBD-CGD-O1D |
| 14  | aB    | 3016 | CL7  | CHA-CBD-CGD-O1D |
| 14  | aB    | 3016 | CL7  | C4B-C3B-CAB-OBB |
| 14  | aB    | 3017 | CL7  | CHA-CBD-CGD-O2D |
| 14  | aB    | 3017 | CL7  | C2B-C3B-CAB-OBB |
| 14  | aB    | 3017 | CL7  | C4B-C3B-CAB-OBB |
| 14  | aB    | 3018 | CL7  | C11-C10-C8-C7   |
| 14  | aB    | 3018 | CL7  | C3A-C2A-CAA-CBA |
| 14  | aB    | 3018 | CL7  | C2B-C3B-CAB-OBB |
| 14  | aB    | 3018 | CL7  | C4B-C3B-CAB-OBB |
| 14  | aB    | 3019 | CL7  | C1A-C2A-CAA-CBA |
| 14  | aB    | 3020 | CL7  | C4B-C3B-CAB-OBB |
| 14  | aB    | 3021 | CL7  | CBD-CGD-O2D-CED |
| 14  | aB    | 3021 | CL7  | C2B-C3B-CAB-OBB |
| 14  | aB    | 3021 | CL7  | C4B-C3B-CAB-OBB |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | aB    | 3022 | CL7  | C2B-C3B-CAB-OBB |
| 14  | aB    | 3022 | CL7  | C4B-C3B-CAB-OBB |
| 14  | aB    | 3023 | CL7  | C1-C2-C3-C4     |
| 14  | aB    | 3023 | CL7  | C1A-C2A-CAA-CBA |
| 14  | aB    | 3023 | CL7  | C2B-C3B-CAB-OBB |
| 14  | aB    | 3023 | CL7  | C4B-C3B-CAB-OBB |
| 14  | aB    | 3025 | CL7  | O2A-C1-C2-C3    |
| 14  | aB    | 3025 | CL7  | C1-C2-C3-C5     |
| 14  | aB    | 3025 | CL7  | C1-C2-C3-C4     |
| 14  | aB    | 3025 | CL7  | C2B-C3B-CAB-OBB |
| 14  | aB    | 3025 | CL7  | C4B-C3B-CAB-OBB |
| 14  | aB    | 3026 | CL7  | C1-C2-C3-C5     |
| 14  | aB    | 3030 | CL7  | C1A-C2A-CAA-CBA |
| 14  | aB    | 3030 | CL7  | C2B-C3B-CAB-OBB |
| 14  | aB    | 3030 | CL7  | C4B-C3B-CAB-OBB |
| 14  | aB    | 3031 | CL7  | C1-C2-C3-C4     |
| 14  | aB    | 3031 | CL7  | C2B-C3B-CAB-OBB |
| 14  | aB    | 3031 | CL7  | C4B-C3B-CAB-OBB |
| 14  | aB    | 3032 | CL7  | C1-C2-C3-C5     |
| 14  | aB    | 3032 | CL7  | C1-C2-C3-C4     |
| 14  | aB    | 3032 | CL7  | C1A-C2A-CAA-CBA |
| 14  | aB    | 3032 | CL7  | C3A-C2A-CAA-CBA |
| 14  | aK    | 101  | CL7  | C2B-C3B-CAB-OBB |
| 14  | aK    | 101  | CL7  | C4B-C3B-CAB-OBB |
| 14  | aL    | 202  | CL7  | O1A-CGA-O2A-C1  |
| 14  | aL    | 202  | CL7  | C1A-C2A-CAA-CBA |
| 14  | aL    | 202  | CL7  | C3A-C2A-CAA-CBA |
| 14  | aL    | 203  | CL7  | CHA-CBD-CGD-O2D |
| 14  | aL    | 203  | CL7  | C2B-C3B-CAB-OBB |
| 14  | aL    | 203  | CL7  | C4B-C3B-CAB-OBB |
| 14  | aL    | 204  | CL7  | C4B-C3B-CAB-OBB |
| 14  | bA    | 3102 | CL7  | C1-C2-C3-C4     |
| 14  | bA    | 3102 | CL7  | C2B-C3B-CAB-OBB |
| 14  | bA    | 3102 | CL7  | C4B-C3B-CAB-OBB |
| 14  | bA    | 3103 | CL7  | CHA-CBD-CGD-O2D |
| 14  | bA    | 3104 | CL7  | CBD-CGD-O2D-CED |
| 14  | bA    | 3104 | CL7  | C2B-C3B-CAB-OBB |
| 14  | bA    | 3104 | CL7  | C4B-C3B-CAB-OBB |
| 14  | bA    | 3105 | CL7  | CHA-CBD-CGD-O2D |
| 14  | bA    | 3105 | CL7  | C4B-C3B-CAB-OBB |
| 14  | bA    | 3106 | CL7  | C1-C2-C3-C4     |
| 14  | bA    | 3106 | CL7  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | bA    | 3106 | CL7  | C4B-C3B-CAB-OBB |
| 14  | bA    | 3108 | CL7  | C1A-C2A-CAA-CBA |
| 14  | bA    | 3108 | CL7  | C4B-C3B-CAB-OBB |
| 14  | bA    | 3109 | CL7  | C2B-C3B-CAB-OBB |
| 14  | bA    | 3109 | CL7  | C4B-C3B-CAB-OBB |
| 14  | bA    | 3110 | CL7  | CBD-CGD-O2D-CED |
| 14  | bA    | 3112 | CL7  | C2B-C3B-CAB-OBB |
| 14  | bA    | 3112 | CL7  | C4B-C3B-CAB-OBB |
| 14  | bA    | 3113 | CL7  | C2B-C3B-CAB-OBB |
| 14  | bA    | 3113 | CL7  | C4B-C3B-CAB-OBB |
| 14  | bA    | 3114 | CL7  | CBD-CGD-O2D-CED |
| 14  | bA    | 3115 | CL7  | C2B-C3B-CAB-OBB |
| 14  | bA    | 3115 | CL7  | C4B-C3B-CAB-OBB |
| 14  | bA    | 3116 | CL7  | C1-C2-C3-C5     |
| 14  | bA    | 3116 | CL7  | C2-C3-C5-C6     |
| 14  | bA    | 3120 | CL7  | C1A-C2A-CAA-CBA |
| 14  | bA    | 3120 | CL7  | C3A-C2A-CAA-CBA |
| 14  | bA    | 3122 | CL7  | C1-C2-C3-C5     |
| 14  | bA    | 3122 | CL7  | C1-C2-C3-C4     |
| 14  | bA    | 3122 | CL7  | C1A-C2A-CAA-CBA |
| 14  | bA    | 3122 | CL7  | CHA-CBD-CGD-O1D |
| 14  | bA    | 3122 | CL7  | CAD-CBD-CGD-O1D |
| 14  | bA    | 3122 | CL7  | C2B-C3B-CAB-OBB |
| 14  | bA    | 3122 | CL7  | C4B-C3B-CAB-OBB |
| 14  | bA    | 3124 | CL7  | C2B-C3B-CAB-OBB |
| 14  | bA    | 3124 | CL7  | C4B-C3B-CAB-OBB |
| 14  | bA    | 3125 | CL7  | C1A-C2A-CAA-CBA |
| 14  | bA    | 3125 | CL7  | CBD-CGD-O2D-CED |
| 14  | bA    | 3126 | CL7  | CHA-CBD-CGD-O1D |
| 14  | bA    | 3126 | CL7  | C2B-C3B-CAB-OBB |
| 14  | bA    | 3126 | CL7  | C4B-C3B-CAB-OBB |
| 14  | bA    | 3127 | CL7  | C1-C2-C3-C5     |
| 14  | bA    | 3127 | CL7  | C4-C3-C5-C6     |
| 14  | bA    | 3128 | CL7  | C1-C2-C3-C5     |
| 14  | bA    | 3128 | CL7  | C1-C2-C3-C4     |
| 14  | bA    | 3128 | CL7  | C12-C13-C15-C16 |
| 14  | bA    | 3128 | CL7  | CHA-CBD-CGD-O2D |
| 14  | bA    | 3129 | CL7  | CHA-CBD-CGD-O2D |
| 14  | bA    | 3129 | CL7  | CBD-CGD-O2D-CED |
| 14  | bA    | 3130 | CL7  | CHA-CBD-CGD-O2D |
| 14  | bA    | 3131 | CL7  | CBD-CGD-O2D-CED |
| 14  | bA    | 3131 | CL7  | C2B-C3B-CAB-OBB |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | bA    | 3131 | CL7  | C4B-C3B-CAB-OBB |
| 14  | bA    | 3132 | CL7  | C1-C2-C3-C5     |
| 14  | bA    | 3132 | CL7  | C1-C2-C3-C4     |
| 14  | bA    | 3132 | CL7  | C1A-C2A-CAA-CBA |
| 14  | bA    | 3132 | CL7  | C3A-C2A-CAA-CBA |
| 14  | bA    | 3133 | CL7  | C2B-C3B-CAB-OBB |
| 14  | bA    | 3133 | CL7  | C4B-C3B-CAB-OBB |
| 14  | bA    | 3139 | CL7  | CAD-CBD-CGD-O2D |
| 14  | bA    | 3139 | CL7  | CBD-CGD-O2D-CED |
| 14  | bA    | 3139 | CL7  | C2B-C3B-CAB-OBB |
| 14  | bA    | 3139 | CL7  | C4B-C3B-CAB-OBB |
| 14  | bA    | 3140 | CL7  | CHA-CBD-CGD-O2D |
| 14  | bA    | 3140 | CL7  | C4B-C3B-CAB-OBB |
| 14  | bA    | 3142 | CL7  | C1-C2-C3-C5     |
| 14  | bA    | 3142 | CL7  | C1-C2-C3-C4     |
| 14  | bA    | 3142 | CL7  | C2-C3-C5-C6     |
| 14  | bA    | 3142 | CL7  | C4-C3-C5-C6     |
| 14  | bA    | 3142 | CL7  | C11-C10-C8-C9   |
| 14  | bA    | 3145 | CL7  | CHA-CBD-CGD-O2D |
| 14  | bA    | 3145 | CL7  | C2B-C3B-CAB-OBB |
| 14  | bA    | 3145 | CL7  | C4B-C3B-CAB-OBB |
| 14  | bB    | 803  | CL7  | C1-C2-C3-C4     |
| 14  | bB    | 803  | CL7  | CHA-CBD-CGD-O2D |
| 14  | bB    | 803  | CL7  | C2B-C3B-CAB-OBB |
| 14  | bB    | 803  | CL7  | C4B-C3B-CAB-OBB |
| 14  | bB    | 804  | CL7  | C1-C2-C3-C4     |
| 14  | bB    | 806  | CL7  | C1-C2-C3-C4     |
| 14  | bB    | 807  | CL7  | C1-C2-C3-C4     |
| 14  | bB    | 807  | CL7  | C2B-C3B-CAB-OBB |
| 14  | bB    | 807  | CL7  | C4B-C3B-CAB-OBB |
| 14  | bB    | 808  | CL7  | C1-C2-C3-C4     |
| 14  | bB    | 808  | CL7  | C14-C13-C15-C16 |
| 14  | bB    | 809  | CL7  | C1-C2-C3-C5     |
| 14  | bB    | 809  | CL7  | C1-C2-C3-C4     |
| 14  | bB    | 809  | CL7  | C2B-C3B-CAB-OBB |
| 14  | bB    | 809  | CL7  | C4B-C3B-CAB-OBB |
| 14  | bB    | 810  | CL7  | C1-C2-C3-C4     |
| 14  | bB    | 810  | CL7  | C4B-C3B-CAB-OBB |
| 14  | bB    | 814  | CL7  | CAD-CBD-CGD-O1D |
| 14  | bB    | 817  | CL7  | CHA-CBD-CGD-O1D |
| 14  | bB    | 817  | CL7  | C4B-C3B-CAB-OBB |
| 14  | bB    | 818  | CL7  | CHA-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | bB    | 818 | CL7  | C2B-C3B-CAB-OBB |
| 14  | bB    | 818 | CL7  | C4B-C3B-CAB-OBB |
| 14  | bB    | 819 | CL7  | C1-C2-C3-C5     |
| 14  | bB    | 819 | CL7  | C3A-C2A-CAA-CBA |
| 14  | bB    | 819 | CL7  | C4B-C3B-CAB-OBB |
| 14  | bB    | 820 | CL7  | C1A-C2A-CAA-CBA |
| 14  | bB    | 820 | CL7  | C3A-C2A-CAA-CBA |
| 14  | bB    | 822 | CL7  | CBD-CGD-O2D-CED |
| 14  | bB    | 822 | CL7  | C2B-C3B-CAB-OBB |
| 14  | bB    | 822 | CL7  | C4B-C3B-CAB-OBB |
| 14  | bB    | 823 | CL7  | C2B-C3B-CAB-OBB |
| 14  | bB    | 823 | CL7  | C4B-C3B-CAB-OBB |
| 14  | bB    | 824 | CL7  | C1-C2-C3-C4     |
| 14  | bB    | 824 | CL7  | C1A-C2A-CAA-CBA |
| 14  | bB    | 824 | CL7  | CHA-CBD-CGD-O1D |
| 14  | bB    | 824 | CL7  | C2B-C3B-CAB-OBB |
| 14  | bB    | 824 | CL7  | C4B-C3B-CAB-OBB |
| 14  | bB    | 826 | CL7  | C1-C2-C3-C5     |
| 14  | bB    | 826 | CL7  | C1-C2-C3-C4     |
| 14  | bB    | 826 | CL7  | C4-C3-C5-C6     |
| 14  | bB    | 826 | CL7  | C11-C12-C13-C14 |
| 14  | bB    | 826 | CL7  | C2B-C3B-CAB-OBB |
| 14  | bB    | 826 | CL7  | C4B-C3B-CAB-OBB |
| 14  | bB    | 827 | CL7  | C1-C2-C3-C5     |
| 14  | bB    | 831 | CL7  | C1-C2-C3-C4     |
| 14  | bB    | 831 | CL7  | CHA-CBD-CGD-O2D |
| 14  | bB    | 831 | CL7  | C2B-C3B-CAB-OBB |
| 14  | bB    | 831 | CL7  | C4B-C3B-CAB-OBB |
| 14  | bB    | 832 | CL7  | C1-C2-C3-C4     |
| 14  | bB    | 832 | CL7  | C2B-C3B-CAB-OBB |
| 14  | bB    | 832 | CL7  | C4B-C3B-CAB-OBB |
| 14  | bB    | 833 | CL7  | C2-C3-C5-C6     |
| 14  | bB    | 833 | CL7  | C1A-C2A-CAA-CBA |
| 14  | bK    | 101 | CL7  | C2B-C3B-CAB-OBB |
| 14  | bK    | 101 | CL7  | C4B-C3B-CAB-OBB |
| 14  | bL    | 203 | CL7  | O1A-CGA-O2A-C1  |
| 14  | bL    | 203 | CL7  | C1A-C2A-CAA-CBA |
| 14  | bL    | 203 | CL7  | CBD-CGD-O2D-CED |
| 14  | bL    | 203 | CL7  | C2B-C3B-CAB-OBB |
| 14  | bL    | 203 | CL7  | C4B-C3B-CAB-OBB |
| 14  | bL    | 204 | CL7  | CHA-CBD-CGD-O2D |
| 14  | bL    | 205 | CL7  | C2B-C3B-CAB-OBB |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | bL    | 205  | CL7  | C4B-C3B-CAB-OBB |
| 14  | cA    | 3102 | CL7  | C1-C2-C3-C4     |
| 14  | cA    | 3102 | CL7  | CHA-CBD-CGD-O1D |
| 14  | cA    | 3103 | CL7  | CHA-CBD-CGD-O2D |
| 14  | cA    | 3104 | CL7  | CBD-CGD-O2D-CED |
| 14  | cA    | 3104 | CL7  | C2B-C3B-CAB-OBB |
| 14  | cA    | 3104 | CL7  | C4B-C3B-CAB-OBB |
| 14  | cA    | 3105 | CL7  | CHA-CBD-CGD-O2D |
| 14  | cA    | 3106 | CL7  | C1A-C2A-CAA-CBA |
| 14  | cA    | 3107 | CL7  | C1A-C2A-CAA-CBA |
| 14  | cA    | 3108 | CL7  | C2B-C3B-CAB-OBB |
| 14  | cA    | 3108 | CL7  | C4B-C3B-CAB-OBB |
| 14  | cA    | 3109 | CL7  | C2B-C3B-CAB-OBB |
| 14  | cA    | 3109 | CL7  | C4B-C3B-CAB-OBB |
| 14  | cA    | 3110 | CL7  | CBD-CGD-O2D-CED |
| 14  | cA    | 3112 | CL7  | C2B-C3B-CAB-OBB |
| 14  | cA    | 3112 | CL7  | C4B-C3B-CAB-OBB |
| 14  | cA    | 3114 | CL7  | CBD-CGD-O2D-CED |
| 14  | cA    | 3115 | CL7  | C2B-C3B-CAB-OBB |
| 14  | cA    | 3115 | CL7  | C4B-C3B-CAB-OBB |
| 14  | cA    | 3116 | CL7  | C1-C2-C3-C5     |
| 14  | cA    | 3116 | CL7  | C1-C2-C3-C4     |
| 14  | cA    | 3116 | CL7  | CBD-CGD-O2D-CED |
| 14  | cA    | 3116 | CL7  | C4B-C3B-CAB-OBB |
| 14  | cA    | 3120 | CL7  | C1A-C2A-CAA-CBA |
| 14  | cA    | 3120 | CL7  | C3A-C2A-CAA-CBA |
| 14  | cA    | 3120 | CL7  | C2B-C3B-CAB-OBB |
| 14  | cA    | 3120 | CL7  | C4B-C3B-CAB-OBB |
| 14  | cA    | 3122 | CL7  | C1-C2-C3-C5     |
| 14  | cA    | 3122 | CL7  | C1-C2-C3-C4     |
| 14  | cA    | 3122 | CL7  | C1A-C2A-CAA-CBA |
| 14  | cA    | 3122 | CL7  | CHA-CBD-CGD-O1D |
| 14  | cA    | 3122 | CL7  | CAD-CBD-CGD-O1D |
| 14  | cA    | 3122 | CL7  | C2B-C3B-CAB-OBB |
| 14  | cA    | 3122 | CL7  | C4B-C3B-CAB-OBB |
| 14  | cA    | 3125 | CL7  | C1A-C2A-CAA-CBA |
| 14  | cA    | 3125 | CL7  | C3A-C2A-CAA-CBA |
| 14  | cA    | 3125 | CL7  | CBD-CGD-O2D-CED |
| 14  | cA    | 3125 | CL7  | C4B-C3B-CAB-OBB |
| 14  | cA    | 3126 | CL7  | C1-C2-C3-C4     |
| 14  | cA    | 3126 | CL7  | C1A-C2A-CAA-CBA |
| 14  | cA    | 3126 | CL7  | C2B-C3B-CAB-OBB |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | cA    | 3126 | CL7  | C4B-C3B-CAB-OBB |
| 14  | cA    | 3127 | CL7  | C1-C2-C3-C5     |
| 14  | cA    | 3128 | CL7  | C1-C2-C3-C5     |
| 14  | cA    | 3128 | CL7  | C1-C2-C3-C4     |
| 14  | cA    | 3128 | CL7  | CHA-CBD-CGD-O2D |
| 14  | cA    | 3128 | CL7  | CHA-CBD-CGD-O1D |
| 14  | cA    | 3129 | CL7  | CHA-CBD-CGD-O2D |
| 14  | cA    | 3130 | CL7  | CHA-CBD-CGD-O2D |
| 14  | cA    | 3131 | CL7  | CBD-CGD-O2D-CED |
| 14  | cA    | 3131 | CL7  | C2B-C3B-CAB-OBB |
| 14  | cA    | 3131 | CL7  | C4B-C3B-CAB-OBB |
| 14  | cA    | 3132 | CL7  | C1-C2-C3-C5     |
| 14  | cA    | 3132 | CL7  | C1-C2-C3-C4     |
| 14  | cA    | 3132 | CL7  | C1A-C2A-CAA-CBA |
| 14  | cA    | 3132 | CL7  | C3A-C2A-CAA-CBA |
| 14  | cA    | 3133 | CL7  | C2B-C3B-CAB-OBB |
| 14  | cA    | 3133 | CL7  | C4B-C3B-CAB-OBB |
| 14  | cA    | 3139 | CL7  | C1-C2-C3-C4     |
| 14  | cA    | 3139 | CL7  | CHA-CBD-CGD-O1D |
| 14  | cA    | 3139 | CL7  | CAD-CBD-CGD-O2D |
| 14  | cA    | 3139 | CL7  | CBD-CGD-O2D-CED |
| 14  | cA    | 3139 | CL7  | O1D-CGD-O2D-CED |
| 14  | cA    | 3139 | CL7  | C4B-C3B-CAB-OBB |
| 14  | cA    | 3140 | CL7  | O2A-C1-C2-C3    |
| 14  | cA    | 3140 | CL7  | C1-C2-C3-C5     |
| 14  | cA    | 3140 | CL7  | C1-C2-C3-C4     |
| 14  | cA    | 3140 | CL7  | C4-C3-C5-C6     |
| 14  | cA    | 3140 | CL7  | CHA-CBD-CGD-O2D |
| 14  | cA    | 3140 | CL7  | C2B-C3B-CAB-OBB |
| 14  | cA    | 3140 | CL7  | C4B-C3B-CAB-OBB |
| 14  | cA    | 3142 | CL7  | C1-C2-C3-C4     |
| 14  | cA    | 3142 | CL7  | C2-C3-C5-C6     |
| 14  | cA    | 3144 | CL7  | CHA-CBD-CGD-O2D |
| 14  | cA    | 3144 | CL7  | C2B-C3B-CAB-OBB |
| 14  | cA    | 3144 | CL7  | C4B-C3B-CAB-OBB |
| 14  | cB    | 803  | CL7  | C1-C2-C3-C5     |
| 14  | cB    | 803  | CL7  | C2B-C3B-CAB-OBB |
| 14  | cB    | 803  | CL7  | C4B-C3B-CAB-OBB |
| 14  | cB    | 804  | CL7  | C1-C2-C3-C5     |
| 14  | cB    | 804  | CL7  | C1-C2-C3-C4     |
| 14  | cB    | 806  | CL7  | C1-C2-C3-C4     |
| 14  | cB    | 806  | CL7  | C2-C3-C5-C6     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | cB    | 807 | CL7  | C1-C2-C3-C4     |
| 14  | cB    | 807 | CL7  | CHA-CBD-CGD-O2D |
| 14  | cB    | 807 | CL7  | C2B-C3B-CAB-OBB |
| 14  | cB    | 807 | CL7  | C4B-C3B-CAB-OBB |
| 14  | cB    | 808 | CL7  | C1-C2-C3-C4     |
| 14  | cB    | 808 | CL7  | C6-C7-C8-C9     |
| 14  | cB    | 808 | CL7  | CBD-CGD-O2D-CED |
| 14  | cB    | 809 | CL7  | C1-C2-C3-C5     |
| 14  | cB    | 809 | CL7  | C1-C2-C3-C4     |
| 14  | cB    | 809 | CL7  | C4B-C3B-CAB-OBB |
| 14  | cB    | 810 | CL7  | C1-C2-C3-C4     |
| 14  | cB    | 810 | CL7  | C4B-C3B-CAB-OBB |
| 14  | cB    | 811 | CL7  | CHA-CBD-CGD-O1D |
| 14  | cB    | 811 | CL7  | CAD-CBD-CGD-O2D |
| 14  | cB    | 811 | CL7  | CAD-CBD-CGD-O1D |
| 14  | cB    | 812 | CL7  | C2B-C3B-CAB-OBB |
| 14  | cB    | 812 | CL7  | C4B-C3B-CAB-OBB |
| 14  | cB    | 814 | CL7  | CAD-CBD-CGD-O1D |
| 14  | cB    | 817 | CL7  | CHA-CBD-CGD-O1D |
| 14  | cB    | 817 | CL7  | C4B-C3B-CAB-OBB |
| 14  | cB    | 818 | CL7  | C2B-C3B-CAB-OBB |
| 14  | cB    | 818 | CL7  | C4B-C3B-CAB-OBB |
| 14  | cB    | 819 | CL7  | C1A-C2A-CAA-CBA |
| 14  | cB    | 819 | CL7  | C3A-C2A-CAA-CBA |
| 14  | cB    | 819 | CL7  | C4B-C3B-CAB-OBB |
| 14  | cB    | 820 | CL7  | CHA-CBD-CGD-O2D |
| 14  | cB    | 820 | CL7  | CHA-CBD-CGD-O1D |
| 14  | cB    | 820 | CL7  | CAD-CBD-CGD-O2D |
| 14  | cB    | 820 | CL7  | CAD-CBD-CGD-O1D |
| 14  | cB    | 821 | CL7  | C2B-C3B-CAB-OBB |
| 14  | cB    | 821 | CL7  | C4B-C3B-CAB-OBB |
| 14  | cB    | 822 | CL7  | CAD-CBD-CGD-O2D |
| 14  | cB    | 822 | CL7  | C4B-C3B-CAB-OBB |
| 14  | cB    | 823 | CL7  | C2B-C3B-CAB-OBB |
| 14  | cB    | 823 | CL7  | C4B-C3B-CAB-OBB |
| 14  | cB    | 824 | CL7  | C1-C2-C3-C4     |
| 14  | cB    | 824 | CL7  | C1A-C2A-CAA-CBA |
| 14  | cB    | 824 | CL7  | CHA-CBD-CGD-O1D |
| 14  | cB    | 824 | CL7  | C2B-C3B-CAB-OBB |
| 14  | cB    | 824 | CL7  | C4B-C3B-CAB-OBB |
| 14  | cB    | 826 | CL7  | O2A-C1-C2-C3    |
| 14  | cB    | 826 | CL7  | C1-C2-C3-C5     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | cB    | 826  | CL7  | C1-C2-C3-C4     |
| 14  | cB    | 826  | CL7  | C4-C3-C5-C6     |
| 14  | cB    | 826  | CL7  | C2B-C3B-CAB-OBB |
| 14  | cB    | 826  | CL7  | C4B-C3B-CAB-OBB |
| 14  | cB    | 827  | CL7  | O2A-C1-C2-C3    |
| 14  | cB    | 827  | CL7  | C1-C2-C3-C4     |
| 14  | cB    | 827  | CL7  | C11-C10-C8-C9   |
| 14  | cB    | 827  | CL7  | C1A-C2A-CAA-CBA |
| 14  | cB    | 831  | CL7  | C1-C2-C3-C4     |
| 14  | cB    | 831  | CL7  | CHA-CBD-CGD-O2D |
| 14  | cB    | 831  | CL7  | C2B-C3B-CAB-OBB |
| 14  | cB    | 831  | CL7  | C4B-C3B-CAB-OBB |
| 14  | cB    | 832  | CL7  | C1-C2-C3-C4     |
| 14  | cB    | 832  | CL7  | C2B-C3B-CAB-OBB |
| 14  | cB    | 832  | CL7  | C4B-C3B-CAB-OBB |
| 14  | cB    | 833  | CL7  | C1-C2-C3-C5     |
| 14  | cB    | 833  | CL7  | C1-C2-C3-C4     |
| 14  | cB    | 833  | CL7  | C1A-C2A-CAA-CBA |
| 14  | cK    | 101  | CL7  | C2B-C3B-CAB-OBB |
| 14  | cK    | 101  | CL7  | C4B-C3B-CAB-OBB |
| 14  | cL    | 203  | CL7  | O1A-CGA-O2A-C1  |
| 14  | cL    | 204  | CL7  | C1A-C2A-CAA-CBA |
| 14  | cL    | 204  | CL7  | C3A-C2A-CAA-CBA |
| 14  | cL    | 204  | CL7  | CHA-CBD-CGD-O2D |
| 14  | cL    | 204  | CL7  | C4B-C3B-CAB-OBB |
| 16  | aA    | 3138 | LHG  | C4-O6-P-O4      |
| 16  | aA    | 3138 | LHG  | C4-O6-P-O5      |
| 16  | aA    | 3139 | LHG  | O1-C1-C2-O2     |
| 16  | aA    | 3139 | LHG  | O1-C1-C2-C3     |
| 16  | aA    | 3139 | LHG  | C1-C2-C3-O3     |
| 16  | aA    | 3139 | LHG  | O2-C2-C3-O3     |
| 16  | aA    | 3139 | LHG  | C3-O3-P-O5      |
| 16  | aA    | 3139 | LHG  | O6-C4-C5-C6     |
| 16  | aA    | 3139 | LHG  | O6-C4-C5-O7     |
| 16  | bA    | 3137 | LHG  | O1-C1-C2-C3     |
| 16  | bA    | 3137 | LHG  | C3-O3-P-O4      |
| 16  | bA    | 3137 | LHG  | C4-O6-P-O4      |
| 16  | bA    | 3137 | LHG  | C4-O6-P-O5      |
| 16  | bA    | 3138 | LHG  | O1-C1-C2-C3     |
| 16  | bA    | 3138 | LHG  | C1-C2-C3-O3     |
| 16  | bA    | 3138 | LHG  | O2-C2-C3-O3     |
| 16  | bA    | 3138 | LHG  | C3-O3-P-O5      |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 16  | bA    | 3138 | LHG  | O6-C4-C5-C6     |
| 16  | bA    | 3138 | LHG  | O6-C4-C5-O7     |
| 16  | cA    | 3137 | LHG  | O1-C1-C2-O2     |
| 16  | cA    | 3137 | LHG  | O1-C1-C2-C3     |
| 16  | cA    | 3137 | LHG  | C3-O3-P-O4      |
| 16  | cA    | 3137 | LHG  | C4-O6-P-O4      |
| 16  | cA    | 3137 | LHG  | C4-O6-P-O5      |
| 16  | cA    | 3138 | LHG  | O1-C1-C2-C3     |
| 16  | cA    | 3138 | LHG  | C1-C2-C3-O3     |
| 16  | cA    | 3138 | LHG  | O2-C2-C3-O3     |
| 16  | cA    | 3138 | LHG  | C3-O3-P-O5      |
| 16  | cA    | 3138 | LHG  | O6-C4-C5-C6     |
| 16  | cA    | 3138 | LHG  | O6-C4-C5-O7     |
| 17  | aA    | 3144 | PQN  | C24-C23-C25-C26 |
| 19  | aB    | 3029 | LMG  | C2-C1-O1-C7     |
| 19  | aB    | 3029 | LMG  | O6-C1-O1-C7     |
| 14  | aA    | 3105 | CL7  | O1D-CGD-O2D-CED |
| 14  | aA    | 3134 | CL7  | O1D-CGD-O2D-CED |
| 14  | aA    | 3142 | CL7  | O1D-CGD-O2D-CED |
| 14  | aB    | 3031 | CL7  | O1D-CGD-O2D-CED |
| 14  | aL    | 202  | CL7  | O1D-CGD-O2D-CED |
| 14  | bA    | 3104 | CL7  | O1D-CGD-O2D-CED |
| 14  | bA    | 3139 | CL7  | O1D-CGD-O2D-CED |
| 14  | cA    | 3104 | CL7  | O1D-CGD-O2D-CED |
| 14  | cA    | 3110 | CL7  | O1D-CGD-O2D-CED |
| 14  | cA    | 3126 | CL7  | O1D-CGD-O2D-CED |
| 14  | cA    | 3141 | CL7  | O1D-CGD-O2D-CED |
| 14  | cL    | 203  | CL7  | O1D-CGD-O2D-CED |
| 14  | aA    | 3116 | CL7  | C2C-C3C-CAC-CBC |
| 14  | aA    | 3116 | CL7  | C4C-C3C-CAC-CBC |
| 14  | bA    | 3115 | CL7  | C2C-C3C-CAC-CBC |
| 14  | bA    | 3115 | CL7  | C4C-C3C-CAC-CBC |
| 14  | cA    | 3115 | CL7  | C2C-C3C-CAC-CBC |
| 14  | cA    | 3115 | CL7  | C4C-C3C-CAC-CBC |
| 14  | aA    | 3111 | CL7  | O1D-CGD-O2D-CED |
| 14  | aA    | 3125 | CL7  | O1D-CGD-O2D-CED |
| 14  | aA    | 3129 | CL7  | O1D-CGD-O2D-CED |
| 14  | aA    | 3132 | CL7  | O1D-CGD-O2D-CED |
| 14  | aA    | 3146 | CL7  | O1D-CGD-O2D-CED |
| 14  | aB    | 3016 | CL7  | O1D-CGD-O2D-CED |
| 14  | aB    | 3017 | CL7  | O1D-CGD-O2D-CED |
| 14  | aB    | 3026 | CL7  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | bA    | 3124 | CL7  | O1D-CGD-O2D-CED |
| 14  | bA    | 3131 | CL7  | O1D-CGD-O2D-CED |
| 14  | bA    | 3140 | CL7  | O1D-CGD-O2D-CED |
| 14  | bA    | 3141 | CL7  | O1D-CGD-O2D-CED |
| 14  | bB    | 817  | CL7  | O1D-CGD-O2D-CED |
| 14  | bB    | 827  | CL7  | O1D-CGD-O2D-CED |
| 14  | bL    | 203  | CL7  | O1D-CGD-O2D-CED |
| 14  | cA    | 3124 | CL7  | O1D-CGD-O2D-CED |
| 14  | cA    | 3131 | CL7  | O1D-CGD-O2D-CED |
| 14  | cB    | 817  | CL7  | O1D-CGD-O2D-CED |
| 14  | cB    | 827  | CL7  | O1D-CGD-O2D-CED |
| 14  | cB    | 832  | CL7  | O1D-CGD-O2D-CED |
| 14  | aA    | 3107 | CL7  | CBD-CGD-O2D-CED |
| 14  | aA    | 3117 | CL7  | CBD-CGD-O2D-CED |
| 14  | aA    | 3126 | CL7  | CBD-CGD-O2D-CED |
| 14  | aA    | 3127 | CL7  | CBD-CGD-O2D-CED |
| 14  | aA    | 3129 | CL7  | CBD-CGD-O2D-CED |
| 14  | aA    | 3130 | CL7  | CBD-CGD-O2D-CED |
| 14  | aA    | 3131 | CL7  | CBD-CGD-O2D-CED |
| 14  | aA    | 3141 | CL7  | CBD-CGD-O2D-CED |
| 14  | aA    | 3146 | CL7  | CBD-CGD-O2D-CED |
| 14  | aB    | 3007 | CL7  | CBD-CGD-O2D-CED |
| 14  | aB    | 3013 | CL7  | CBD-CGD-O2D-CED |
| 14  | aB    | 3016 | CL7  | CBD-CGD-O2D-CED |
| 14  | aB    | 3017 | CL7  | CBD-CGD-O2D-CED |
| 14  | aB    | 3031 | CL7  | CBD-CGD-O2D-CED |
| 14  | aL    | 202  | CL7  | CBD-CGD-O2D-CED |
| 14  | bA    | 3116 | CL7  | CBD-CGD-O2D-CED |
| 14  | bA    | 3126 | CL7  | CBD-CGD-O2D-CED |
| 14  | bA    | 3130 | CL7  | CBD-CGD-O2D-CED |
| 14  | bA    | 3140 | CL7  | CBD-CGD-O2D-CED |
| 14  | bA    | 3141 | CL7  | CBD-CGD-O2D-CED |
| 14  | bB    | 808  | CL7  | CBD-CGD-O2D-CED |
| 14  | bB    | 814  | CL7  | CBD-CGD-O2D-CED |
| 14  | bB    | 817  | CL7  | CBD-CGD-O2D-CED |
| 14  | bB    | 818  | CL7  | CBD-CGD-O2D-CED |
| 14  | cA    | 3112 | CL7  | CBD-CGD-O2D-CED |
| 14  | cA    | 3126 | CL7  | CBD-CGD-O2D-CED |
| 14  | cA    | 3129 | CL7  | CBD-CGD-O2D-CED |
| 14  | cA    | 3130 | CL7  | CBD-CGD-O2D-CED |
| 14  | cA    | 3140 | CL7  | CBD-CGD-O2D-CED |
| 14  | cA    | 3141 | CL7  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | cB    | 810  | CL7  | CBD-CGD-O2D-CED |
| 14  | cB    | 816  | CL7  | CBD-CGD-O2D-CED |
| 14  | cB    | 817  | CL7  | CBD-CGD-O2D-CED |
| 14  | cB    | 822  | CL7  | CBD-CGD-O2D-CED |
| 14  | cB    | 832  | CL7  | CBD-CGD-O2D-CED |
| 14  | cL    | 203  | CL7  | CBD-CGD-O2D-CED |
| 14  | aA    | 3141 | CL7  | O1D-CGD-O2D-CED |
| 14  | bB    | 818  | CL7  | O1D-CGD-O2D-CED |
| 14  | cA    | 3140 | CL7  | O1D-CGD-O2D-CED |
| 14  | cB    | 810  | CL7  | O1D-CGD-O2D-CED |
| 14  | aA    | 3127 | CL7  | O1D-CGD-O2D-CED |
| 14  | bA    | 3128 | CL7  | O1D-CGD-O2D-CED |
| 14  | aA    | 3133 | CL7  | CBA-CGA-O2A-C1  |
| 14  | bB    | 810  | CL7  | CBA-CGA-O2A-C1  |
| 14  | aA    | 3113 | CL7  | CBD-CGD-O2D-CED |
| 14  | aA    | 3122 | CL7  | CBD-CGD-O2D-CED |
| 14  | aB    | 3008 | CL7  | CBD-CGD-O2D-CED |
| 14  | aB    | 3010 | CL7  | CBD-CGD-O2D-CED |
| 14  | aB    | 3026 | CL7  | CBD-CGD-O2D-CED |
| 14  | bA    | 3103 | CL7  | CBD-CGD-O2D-CED |
| 14  | bA    | 3106 | CL7  | CBD-CGD-O2D-CED |
| 14  | bA    | 3112 | CL7  | CBD-CGD-O2D-CED |
| 14  | bA    | 3127 | CL7  | CBD-CGD-O2D-CED |
| 14  | bA    | 3128 | CL7  | CBD-CGD-O2D-CED |
| 14  | bB    | 809  | CL7  | CBD-CGD-O2D-CED |
| 14  | bB    | 811  | CL7  | CBD-CGD-O2D-CED |
| 14  | bB    | 827  | CL7  | CBD-CGD-O2D-CED |
| 14  | cA    | 3102 | CL7  | CBD-CGD-O2D-CED |
| 14  | cA    | 3106 | CL7  | CBD-CGD-O2D-CED |
| 14  | cA    | 3127 | CL7  | CBD-CGD-O2D-CED |
| 14  | cB    | 809  | CL7  | CBD-CGD-O2D-CED |
| 14  | cB    | 814  | CL7  | CBD-CGD-O2D-CED |
| 14  | bL    | 204  | CL7  | O1A-CGA-O2A-C1  |
| 14  | cL    | 204  | CL7  | O1A-CGA-O2A-C1  |
| 14  | bA    | 3126 | CL7  | O1D-CGD-O2D-CED |
| 14  | bA    | 3124 | CL7  | CBD-CGD-O2D-CED |
| 14  | cB    | 827  | CL7  | CBD-CGD-O2D-CED |
| 14  | cA    | 3107 | CL7  | O1A-CGA-O2A-C1  |
| 14  | aA    | 3140 | CL7  | C3-C5-C6-C7     |
| 14  | aB    | 3025 | CL7  | C3-C5-C6-C7     |
| 14  | bA    | 3140 | CL7  | C3-C5-C6-C7     |
| 14  | cA    | 3114 | CL7  | C3-C5-C6-C7     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | cA    | 3142 | CL7  | C3-C5-C6-C7     |
| 14  | aB    | 3009 | CL7  | CBA-CGA-O2A-C1  |
| 14  | aB    | 3031 | CL7  | CBA-CGA-O2A-C1  |
| 14  | aL    | 202  | CL7  | CBA-CGA-O2A-C1  |
| 14  | bA    | 3132 | CL7  | CBA-CGA-O2A-C1  |
| 14  | bB    | 832  | CL7  | CBA-CGA-O2A-C1  |
| 14  | cA    | 3132 | CL7  | CBA-CGA-O2A-C1  |
| 14  | cB    | 810  | CL7  | CBA-CGA-O2A-C1  |
| 14  | cB    | 832  | CL7  | CBA-CGA-O2A-C1  |
| 14  | bB    | 826  | CL7  | C5-C6-C7-C8     |
| 14  | aA    | 3125 | CL7  | CBD-CGD-O2D-CED |
| 14  | bA    | 3119 | CL7  | O1A-CGA-O2A-C1  |
| 14  | cA    | 3119 | CL7  | O1A-CGA-O2A-C1  |
| 14  | cB    | 807  | CL7  | C2C-C3C-CAC-CBC |
| 14  | aA    | 3133 | CL7  | C4-C3-C5-C6     |
| 14  | aB    | 3023 | CL7  | C2-C3-C5-C6     |
| 14  | bA    | 3132 | CL7  | C2-C3-C5-C6     |
| 14  | aA    | 3128 | CL7  | CBD-CGD-O2D-CED |
| 14  | aB    | 3015 | CL7  | CBD-CGD-O2D-CED |
| 14  | bA    | 3108 | CL7  | CBD-CGD-O2D-CED |
| 14  | bA    | 3121 | CL7  | CBD-CGD-O2D-CED |
| 14  | bB    | 807  | CL7  | CBD-CGD-O2D-CED |
| 14  | cB    | 803  | CL7  | CBD-CGD-O2D-CED |
| 14  | cB    | 818  | CL7  | CBD-CGD-O2D-CED |
| 14  | aA    | 3108 | CL7  | C2A-CAA-CBA-CGA |
| 14  | aB    | 3002 | CL7  | C2A-CAA-CBA-CGA |
| 14  | aB    | 3025 | CL7  | C2A-CAA-CBA-CGA |
| 14  | bA    | 3107 | CL7  | C2A-CAA-CBA-CGA |
| 14  | bB    | 803  | CL7  | C2A-CAA-CBA-CGA |
| 14  | bB    | 816  | CL7  | C2A-CAA-CBA-CGA |
| 14  | bB    | 826  | CL7  | C2A-CAA-CBA-CGA |
| 14  | cA    | 3107 | CL7  | C2A-CAA-CBA-CGA |
| 14  | cB    | 816  | CL7  | C2A-CAA-CBA-CGA |
| 14  | aB    | 3006 | CL7  | C2C-C3C-CAC-CBC |
| 14  | bB    | 807  | CL7  | C2C-C3C-CAC-CBC |
| 14  | aA    | 3120 | CL7  | O1A-CGA-O2A-C1  |
| 14  | aB    | 3026 | CL7  | C3-C5-C6-C7     |
| 14  | cB    | 803  | CL7  | C3-C5-C6-C7     |
| 14  | aB    | 3023 | CL7  | CBA-CGA-O2A-C1  |
| 14  | bB    | 824  | CL7  | CBA-CGA-O2A-C1  |
| 14  | bL    | 203  | CL7  | CBA-CGA-O2A-C1  |
| 14  | cB    | 824  | CL7  | CBA-CGA-O2A-C1  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | cL    | 203  | CL7  | CBA-CGA-O2A-C1  |
| 14  | aA    | 3141 | CL7  | C1-C2-C3-C5     |
| 14  | aB    | 3009 | CL7  | C1-C2-C3-C5     |
| 14  | aB    | 3030 | CL7  | C1-C2-C3-C5     |
| 14  | bA    | 3139 | CL7  | C1-C2-C3-C5     |
| 14  | bB    | 810  | CL7  | C1-C2-C3-C5     |
| 14  | bB    | 831  | CL7  | C1-C2-C3-C5     |
| 14  | cA    | 3139 | CL7  | C1-C2-C3-C5     |
| 14  | cB    | 810  | CL7  | C1-C2-C3-C5     |
| 14  | cB    | 827  | CL7  | C1-C2-C3-C5     |
| 14  | cB    | 831  | CL7  | C1-C2-C3-C5     |
| 14  | aA    | 3104 | CL7  | CBD-CGD-O2D-CED |
| 14  | bB    | 816  | CL7  | CBD-CGD-O2D-CED |
| 14  | cB    | 815  | CL7  | CBD-CGD-O2D-CED |
| 14  | bA    | 3110 | CL7  | O1D-CGD-O2D-CED |
| 14  | aA    | 3108 | CL7  | O1A-CGA-O2A-C1  |
| 14  | aA    | 3133 | CL7  | O1A-CGA-O2A-C1  |
| 14  | aB    | 3009 | CL7  | O1A-CGA-O2A-C1  |
| 14  | aB    | 3031 | CL7  | O1A-CGA-O2A-C1  |
| 14  | aL    | 203  | CL7  | O1A-CGA-O2A-C1  |
| 14  | bA    | 3107 | CL7  | O1A-CGA-O2A-C1  |
| 14  | bA    | 3132 | CL7  | O1A-CGA-O2A-C1  |
| 14  | bB    | 810  | CL7  | O1A-CGA-O2A-C1  |
| 14  | bB    | 832  | CL7  | O1A-CGA-O2A-C1  |
| 14  | cA    | 3132 | CL7  | O1A-CGA-O2A-C1  |
| 14  | cA    | 3141 | CL7  | O1A-CGA-O2A-C1  |
| 14  | cB    | 832  | CL7  | O1A-CGA-O2A-C1  |
| 14  | bA    | 3109 | CL7  | CBD-CGD-O2D-CED |
| 14  | bB    | 815  | CL7  | CBD-CGD-O2D-CED |
| 14  | cA    | 3103 | CL7  | CBD-CGD-O2D-CED |
| 14  | cA    | 3108 | CL7  | CBD-CGD-O2D-CED |
| 14  | cA    | 3124 | CL7  | CBD-CGD-O2D-CED |
| 14  | cA    | 3128 | CL7  | CBD-CGD-O2D-CED |
| 16  | aA    | 3138 | LHG  | O2-C2-C3-O3     |
| 14  | aA    | 3143 | CL7  | C3-C5-C6-C7     |
| 14  | bB    | 827  | CL7  | C3-C5-C6-C7     |
| 14  | bA    | 3123 | CL7  | CBA-CGA-O2A-C1  |
| 14  | aA    | 3142 | CL7  | O1A-CGA-O2A-C1  |
| 14  | cB    | 810  | CL7  | O1A-CGA-O2A-C1  |
| 14  | aB    | 3014 | CL7  | CBD-CGD-O2D-CED |
| 14  | bB    | 832  | CL7  | CBD-CGD-O2D-CED |
| 14  | cB    | 826  | CL7  | C5-C6-C7-C8     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | bA    | 3139 | CL7  | O1A-CGA-O2A-C1  |
| 14  | bA    | 3141 | CL7  | O1A-CGA-O2A-C1  |
| 14  | bL    | 203  | CL7  | C3-C5-C6-C7     |
| 14  | cA    | 3123 | CL7  | CBA-CGA-O2A-C1  |
| 14  | aA    | 3143 | CL7  | C4-C3-C5-C6     |
| 14  | aB    | 3025 | CL7  | C4-C3-C5-C6     |
| 14  | bA    | 3116 | CL7  | C4-C3-C5-C6     |
| 14  | bB    | 833  | CL7  | C4-C3-C5-C6     |
| 14  | cA    | 3116 | CL7  | C4-C3-C5-C6     |
| 14  | cA    | 3142 | CL7  | C4-C3-C5-C6     |
| 17  | aA    | 3144 | PQN  | C14-C13-C15-C16 |
| 17  | bA    | 3143 | PQN  | C14-C13-C15-C16 |
| 17  | cA    | 3143 | PQN  | C14-C13-C15-C16 |
| 14  | aA    | 3117 | CL7  | C2-C3-C5-C6     |
| 14  | cA    | 3116 | CL7  | C2-C3-C5-C6     |
| 17  | aA    | 3144 | PQN  | C12-C13-C15-C16 |
| 17  | bA    | 3143 | PQN  | C12-C13-C15-C16 |
| 17  | cA    | 3143 | PQN  | C12-C13-C15-C16 |
| 14  | cB    | 826  | CL7  | C2A-CAA-CBA-CGA |
| 14  | cA    | 3139 | CL7  | O1A-CGA-O2A-C1  |
| 19  | bB    | 830  | LMG  | O6-C1-O1-C7     |
| 14  | cL    | 204  | CL7  | CBA-CGA-O2A-C1  |
| 14  | aB    | 3002 | CL7  | CBD-CGD-O2D-CED |
| 14  | bA    | 3140 | CL7  | C10-C11-C12-C13 |
| 14  | bA    | 3127 | CL7  | O1A-CGA-O2A-C1  |
| 14  | cA    | 3128 | CL7  | O1A-CGA-O2A-C1  |
| 14  | cA    | 3140 | CL7  | O1A-CGA-O2A-C1  |
| 14  | aA    | 3141 | CL7  | C3-C5-C6-C7     |
| 14  | bB    | 803  | CL7  | C3-C5-C6-C7     |
| 14  | cB    | 827  | CL7  | C3-C5-C6-C7     |
| 14  | bA    | 3123 | CL7  | O1D-CGD-O2D-CED |
| 12  | bA    | 3101 | G9R  | CBA-CGA-O2A-C1  |
| 12  | cA    | 3101 | G9R  | CBA-CGA-O2A-C1  |
| 14  | bA    | 3107 | CL7  | CBA-CGA-O2A-C1  |
| 14  | cA    | 3107 | CL7  | CBA-CGA-O2A-C1  |
| 14  | cA    | 3105 | CL7  | CBD-CGD-O2D-CED |
| 14  | cA    | 3132 | CL7  | C5-C6-C7-C8     |
| 14  | aA    | 3142 | CL7  | C15-C16-C17-C18 |
| 14  | bA    | 3124 | CL7  | C15-C16-C17-C18 |
| 14  | cA    | 3128 | CL7  | C13-C15-C16-C17 |
| 12  | bA    | 3101 | G9R  | O1A-CGA-O2A-C1  |
| 14  | cA    | 3132 | CL7  | C2-C3-C5-C6     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | cB    | 803  | CL7  | C2-C3-C5-C6     |
| 13  | aB    | 3004 | PHO  | C11-C10-C8-C9   |
| 13  | aB    | 3004 | PHO  | C14-C13-C15-C16 |
| 13  | bB    | 805  | PHO  | C11-C10-C8-C9   |
| 14  | aA    | 3108 | CL7  | C11-C12-C13-C14 |
| 14  | aA    | 3129 | CL7  | C11-C12-C13-C14 |
| 14  | aA    | 3133 | CL7  | C11-C12-C13-C14 |
| 14  | aA    | 3143 | CL7  | C11-C10-C8-C9   |
| 14  | aA    | 3143 | CL7  | C14-C13-C15-C16 |
| 14  | aB    | 3007 | CL7  | C6-C7-C8-C9     |
| 14  | aB    | 3009 | CL7  | C6-C7-C8-C9     |
| 14  | aB    | 3025 | CL7  | C11-C12-C13-C14 |
| 14  | aL    | 203  | CL7  | C6-C7-C8-C9     |
| 14  | bA    | 3107 | CL7  | C11-C12-C13-C14 |
| 14  | bA    | 3114 | CL7  | C6-C7-C8-C9     |
| 14  | bA    | 3124 | CL7  | C11-C10-C8-C9   |
| 14  | bA    | 3132 | CL7  | C11-C12-C13-C14 |
| 14  | bA    | 3142 | CL7  | C14-C13-C15-C16 |
| 14  | bB    | 808  | CL7  | C6-C7-C8-C9     |
| 14  | bB    | 810  | CL7  | C6-C7-C8-C9     |
| 14  | bB    | 810  | CL7  | C14-C13-C15-C16 |
| 14  | bB    | 820  | CL7  | C14-C13-C15-C16 |
| 14  | bB    | 832  | CL7  | C11-C12-C13-C14 |
| 14  | cA    | 3107 | CL7  | C11-C12-C13-C14 |
| 14  | cA    | 3114 | CL7  | C6-C7-C8-C9     |
| 14  | cA    | 3132 | CL7  | C11-C12-C13-C14 |
| 14  | cA    | 3141 | CL7  | C11-C12-C13-C14 |
| 14  | cA    | 3142 | CL7  | C11-C10-C8-C9   |
| 14  | cB    | 808  | CL7  | C11-C12-C13-C14 |
| 14  | cB    | 808  | CL7  | C14-C13-C15-C16 |
| 14  | cB    | 810  | CL7  | C6-C7-C8-C9     |
| 14  | cB    | 810  | CL7  | C14-C13-C15-C16 |
| 14  | cB    | 820  | CL7  | C14-C13-C15-C16 |
| 14  | cB    | 826  | CL7  | C11-C12-C13-C14 |
| 14  | cB    | 832  | CL7  | C11-C12-C13-C14 |
| 14  | cL    | 204  | CL7  | C11-C10-C8-C9   |
| 17  | aA    | 3144 | PQN  | C19-C18-C20-C21 |
| 17  | aA    | 3144 | PQN  | C21-C22-C23-C24 |
| 17  | bA    | 3143 | PQN  | C19-C18-C20-C21 |
| 17  | bA    | 3143 | PQN  | C21-C22-C23-C24 |
| 17  | bA    | 3143 | PQN  | C24-C23-C25-C26 |
| 17  | cA    | 3143 | PQN  | C19-C18-C20-C21 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | bA    | 3133 | CL7  | O1D-CGD-O2D-CED |
| 14  | cA    | 3144 | CL7  | O1D-CGD-O2D-CED |
| 14  | aA    | 3103 | CL7  | C2A-CAA-CBA-CGA |
| 14  | aA    | 3128 | CL7  | O1A-CGA-O2A-C1  |
| 14  | aA    | 3129 | CL7  | O1A-CGA-O2A-C1  |
| 14  | aA    | 3141 | CL7  | O1A-CGA-O2A-C1  |
| 14  | cA    | 3127 | CL7  | O1A-CGA-O2A-C1  |
| 14  | cB    | 820  | CL7  | O1A-CGA-O2A-C1  |
| 14  | bA    | 3132 | CL7  | C5-C6-C7-C8     |
| 14  | bA    | 3145 | CL7  | O1D-CGD-O2D-CED |
| 14  | bA    | 3114 | CL7  | C3-C5-C6-C7     |
| 14  | bA    | 3114 | CL7  | C8-C10-C11-C12  |
| 14  | bA    | 3128 | CL7  | C13-C15-C16-C17 |
| 14  | bA    | 3128 | CL7  | C15-C16-C17-C18 |
| 14  | bB    | 827  | CL7  | C8-C10-C11-C12  |
| 14  | cA    | 3114 | CL7  | C8-C10-C11-C12  |
| 14  | cL    | 203  | CL7  | C5-C6-C7-C8     |
| 14  | bA    | 3109 | CL7  | O1D-CGD-O2D-CED |
| 14  | aB    | 3032 | CL7  | CBD-CGD-O2D-CED |
| 14  | aA    | 3125 | CL7  | C15-C16-C17-C18 |
| 14  | bA    | 3139 | CL7  | C13-C15-C16-C17 |
| 14  | bL    | 203  | CL7  | C5-C6-C7-C8     |
| 14  | bL    | 204  | CL7  | C8-C10-C11-C12  |
| 14  | bL    | 204  | CL7  | C10-C11-C12-C13 |
| 14  | cB    | 820  | CL7  | C5-C6-C7-C8     |
| 17  | aB    | 3027 | PQN  | C18-C20-C21-C22 |
| 19  | cB    | 830  | LMG  | C28-C29-C30-C31 |
| 14  | cB    | 807  | CL7  | C4C-C3C-CAC-CBC |
| 14  | bB    | 820  | CL7  | C5-C6-C7-C8     |
| 14  | cA    | 3141 | CL7  | C5-C6-C7-C8     |
| 14  | cA    | 3141 | CL7  | C15-C16-C17-C18 |
| 14  | cL    | 203  | CL7  | C3-C5-C6-C7     |
| 14  | aA    | 3108 | CL7  | CBA-CGA-O2A-C1  |
| 14  | bL    | 204  | CL7  | CBA-CGA-O2A-C1  |
| 14  | aA    | 3140 | CL7  | C5-C6-C7-C8     |
| 14  | bA    | 3133 | CL7  | CBD-CGD-O2D-CED |
| 14  | cB    | 823  | CL7  | CBD-CGD-O2D-CED |
| 14  | aA    | 3133 | CL7  | C5-C6-C7-C8     |
| 14  | aA    | 3117 | CL7  | O1D-CGD-O2D-CED |
| 14  | bA    | 3116 | CL7  | O1D-CGD-O2D-CED |
| 14  | aA    | 3115 | CL7  | C12-C13-C15-C16 |
| 14  | aA    | 3143 | CL7  | C11-C10-C8-C7   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | aB    | 3007 | CL7  | C6-C7-C8-C10    |
| 14  | aL    | 202  | CL7  | C6-C7-C8-C10    |
| 14  | bA    | 3107 | CL7  | C12-C13-C15-C16 |
| 14  | bA    | 3114 | CL7  | C12-C13-C15-C16 |
| 14  | bL    | 203  | CL7  | C11-C12-C13-C15 |
| 14  | cA    | 3107 | CL7  | C12-C13-C15-C16 |
| 14  | cA    | 3114 | CL7  | C12-C13-C15-C16 |
| 14  | cA    | 3128 | CL7  | C12-C13-C15-C16 |
| 14  | cA    | 3141 | CL7  | C12-C13-C15-C16 |
| 14  | cB    | 820  | CL7  | C12-C13-C15-C16 |
| 17  | aB    | 3027 | PQN  | C17-C18-C20-C21 |
| 17  | bB    | 828  | PQN  | C17-C18-C20-C21 |
| 17  | cB    | 828  | PQN  | C17-C18-C20-C21 |
| 12  | aA    | 3101 | G9R  | C3-C5-C6-C7     |
| 14  | aL    | 202  | CL7  | C3-C5-C6-C7     |
| 14  | bB    | 833  | CL7  | O1A-CGA-O2A-C1  |
| 14  | aA    | 3121 | CL7  | O1D-CGD-O2D-CED |
| 14  | cA    | 3133 | CL7  | O1D-CGD-O2D-CED |
| 14  | aB    | 3026 | CL7  | C8-C10-C11-C12  |
| 14  | bB    | 807  | CL7  | C4C-C3C-CAC-CBC |
| 14  | bB    | 820  | CL7  | O1A-CGA-O2A-C1  |
| 14  | cB    | 824  | CL7  | O1A-CGA-O2A-C1  |
| 14  | aB    | 3022 | CL7  | CBD-CGD-O2D-CED |
| 14  | aA    | 3129 | CL7  | C5-C6-C7-C8     |
| 14  | aA    | 3129 | CL7  | C15-C16-C17-C18 |
| 14  | aA    | 3133 | CL7  | C10-C11-C12-C13 |
| 14  | cA    | 3132 | CL7  | C10-C11-C12-C13 |
| 14  | aL    | 203  | CL7  | O1D-CGD-O2D-CED |
| 14  | aB    | 3006 | CL7  | C4C-C3C-CAC-CBC |
| 14  | aL    | 202  | CL7  | C5-C6-C7-C8     |
| 14  | bB    | 803  | CL7  | C15-C16-C17-C18 |
| 14  | bB    | 807  | CL7  | C5-C6-C7-C8     |
| 14  | bB    | 832  | CL7  | C10-C11-C12-C13 |
| 14  | bB    | 824  | CL7  | O1A-CGA-O2A-C1  |
| 14  | aB    | 3031 | CL7  | C8-C10-C11-C12  |
| 14  | bA    | 3114 | CL7  | C15-C16-C17-C18 |
| 14  | bA    | 3132 | CL7  | C10-C11-C12-C13 |
| 14  | cA    | 3106 | CL7  | C5-C6-C7-C8     |
| 14  | cA    | 3114 | CL7  | C15-C16-C17-C18 |
| 14  | cB    | 803  | CL7  | C5-C6-C7-C8     |
| 14  | cB    | 807  | CL7  | C5-C6-C7-C8     |
| 14  | cB    | 827  | CL7  | C13-C15-C16-C17 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | cB    | 827  | CL7  | C15-C16-C17-C18 |
| 14  | bA    | 3108 | CL7  | O1D-CGD-O2D-CED |
| 14  | bB    | 823  | CL7  | CBD-CGD-O2D-CED |
| 14  | aB    | 3019 | CL7  | O1A-CGA-O2A-C1  |
| 16  | bA    | 3137 | LHG  | C9-C10-C11-C12  |
| 14  | aB    | 3026 | CL7  | C13-C15-C16-C17 |
| 14  | aB    | 3026 | CL7  | C15-C16-C17-C18 |
| 14  | cA    | 3128 | CL7  | C5-C6-C7-C8     |
| 14  | cB    | 806  | CL7  | C10-C11-C12-C13 |
| 14  | cB    | 832  | CL7  | C10-C11-C12-C13 |
| 17  | bA    | 3143 | PQN  | C18-C20-C21-C22 |
| 17  | cA    | 3143 | PQN  | C23-C25-C26-C27 |
| 16  | aA    | 3138 | LHG  | C4-O6-P-O3      |
| 16  | bA    | 3137 | LHG  | C3-O3-P-O6      |
| 16  | bA    | 3137 | LHG  | C4-O6-P-O3      |
| 16  | cA    | 3137 | LHG  | C3-O3-P-O6      |
| 16  | cA    | 3137 | LHG  | C4-O6-P-O3      |
| 16  | cA    | 3138 | LHG  | C4-O6-P-O3      |
| 14  | bB    | 827  | CL7  | C13-C15-C16-C17 |
| 17  | aA    | 3144 | PQN  | C23-C25-C26-C27 |
| 14  | aA    | 3107 | CL7  | O1A-CGA-O2A-C1  |
| 16  | aA    | 3138 | LHG  | C9-C10-C11-C12  |
| 14  | aB    | 3015 | CL7  | C2A-CAA-CBA-CGA |
| 14  | aB    | 3018 | CL7  | C2A-CAA-CBA-CGA |
| 14  | aB    | 3023 | CL7  | C2A-CAA-CBA-CGA |
| 14  | bA    | 3102 | CL7  | C2A-CAA-CBA-CGA |
| 14  | bB    | 819  | CL7  | C2A-CAA-CBA-CGA |
| 14  | cB    | 803  | CL7  | C2A-CAA-CBA-CGA |
| 14  | cB    | 819  | CL7  | C2A-CAA-CBA-CGA |
| 14  | aA    | 3115 | CL7  | C3-C5-C6-C7     |
| 14  | cB    | 826  | CL7  | C3-C5-C6-C7     |
| 12  | aA    | 3101 | G9R  | CBA-CGA-O2A-C1  |
| 14  | aB    | 3026 | CL7  | CBA-CGA-O2A-C1  |
| 14  | aL    | 203  | CL7  | CBA-CGA-O2A-C1  |
| 14  | bB    | 827  | CL7  | CBA-CGA-O2A-C1  |
| 14  | aA    | 3142 | CL7  | C10-C11-C12-C13 |
| 14  | bB    | 827  | CL7  | C10-C11-C12-C13 |
| 14  | aB    | 3002 | CL7  | C3-C5-C6-C7     |
| 14  | aL    | 203  | CL7  | C3-C5-C6-C7     |
| 14  | cA    | 3132 | CL7  | C16-C17-C18-C19 |
| 17  | aA    | 3144 | PQN  | C26-C27-C28-C29 |
| 17  | bB    | 828  | PQN  | C26-C27-C28-C30 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | cA    | 3143 | PQN  | C26-C27-C28-C30 |
| 14  | aA    | 3142 | CL7  | C13-C15-C16-C17 |
| 17  | cB    | 828  | PQN  | C18-C20-C21-C22 |
| 19  | aB    | 3029 | LMG  | C38-C39-C40-C41 |
| 14  | cA    | 3128 | CL7  | C15-C16-C17-C18 |
| 14  | bA    | 3132 | CL7  | C3-C5-C6-C7     |
| 14  | cB    | 818  | CL7  | O1D-CGD-O2D-CED |
| 19  | bB    | 830  | LMG  | C2-C1-O1-C7     |
| 14  | bA    | 3123 | CL7  | C1-C2-C3-C5     |
| 14  | aB    | 3006 | CL7  | C5-C6-C7-C8     |
| 14  | bB    | 810  | CL7  | C15-C16-C17-C18 |
| 14  | aB    | 3006 | CL7  | O1A-CGA-O2A-C1  |
| 14  | bA    | 3122 | CL7  | O1A-CGA-O2A-C1  |
| 17  | aA    | 3144 | PQN  | C26-C27-C28-C30 |
| 17  | aB    | 3027 | PQN  | C26-C27-C28-C30 |
| 16  | cA    | 3137 | LHG  | C27-C28-C29-C30 |
| 19  | aB    | 3029 | LMG  | C14-C15-C16-C17 |
| 13  | aA    | 3102 | PHO  | C6-C7-C8-C9     |
| 14  | aB    | 3019 | CL7  | C11-C10-C8-C9   |
| 14  | aL    | 202  | CL7  | C11-C12-C13-C14 |
| 14  | bA    | 3128 | CL7  | C14-C13-C15-C16 |
| 14  | bA    | 3141 | CL7  | C6-C7-C8-C9     |
| 14  | bL    | 203  | CL7  | C6-C7-C8-C9     |
| 14  | bL    | 203  | CL7  | C11-C12-C13-C14 |
| 14  | cA    | 3128 | CL7  | C14-C13-C15-C16 |
| 14  | cL    | 203  | CL7  | C6-C7-C8-C9     |
| 14  | cL    | 203  | CL7  | C11-C12-C13-C14 |
| 17  | bB    | 828  | PQN  | C19-C18-C20-C21 |
| 14  | aA    | 3122 | CL7  | O1D-CGD-O2D-CED |
| 19  | aB    | 3029 | LMG  | C16-C17-C18-C19 |
| 14  | bB    | 827  | CL7  | C15-C16-C17-C18 |
| 17  | bA    | 3143 | PQN  | C23-C25-C26-C27 |
| 14  | bB    | 824  | CL7  | C2A-CAA-CBA-CGA |
| 14  | bA    | 3106 | CL7  | O1A-CGA-O2A-C1  |
| 14  | cA    | 3122 | CL7  | O1A-CGA-O2A-C1  |
| 14  | cA    | 3126 | CL7  | O1A-CGA-O2A-C1  |
| 16  | aA    | 3138 | LHG  | O1-C1-C2-C3     |
| 17  | aA    | 3144 | PQN  | C13-C15-C16-C17 |
| 14  | aA    | 3129 | CL7  | C8-C10-C11-C12  |
| 19  | cB    | 830  | LMG  | C38-C39-C40-C41 |
| 14  | cA    | 3141 | CL7  | CBA-CGA-O2A-C1  |
| 19  | aB    | 3029 | LMG  | C28-C29-C30-C31 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | aA    | 3115 | CL7  | O1D-CGD-O2D-CED |
| 14  | bA    | 3132 | CL7  | C16-C17-C18-C19 |
| 17  | aB    | 3027 | PQN  | C26-C27-C28-C29 |
| 17  | bA    | 3143 | PQN  | C26-C27-C28-C29 |
| 17  | bA    | 3143 | PQN  | C26-C27-C28-C30 |
| 17  | bB    | 828  | PQN  | C26-C27-C28-C29 |
| 17  | cB    | 828  | PQN  | C26-C27-C28-C29 |
| 17  | cB    | 828  | PQN  | C26-C27-C28-C30 |
| 14  | cA    | 3140 | CL7  | C15-C16-C17-C18 |
| 14  | aB    | 3006 | CL7  | CBD-CGD-O2D-CED |
| 14  | cB    | 816  | CL7  | C2C-C3C-CAC-CBC |
| 19  | bB    | 830  | LMG  | C28-C29-C30-C31 |
| 14  | aA    | 3142 | CL7  | C8-C10-C11-C12  |
| 14  | aB    | 3009 | CL7  | C15-C16-C17-C18 |
| 14  | aB    | 3019 | CL7  | C15-C16-C17-C18 |
| 14  | aL    | 203  | CL7  | C8-C10-C11-C12  |
| 14  | bB    | 806  | CL7  | C15-C16-C17-C18 |
| 14  | aA    | 3140 | CL7  | O1A-CGA-O2A-C1  |
| 14  | bB    | 807  | CL7  | O1A-CGA-O2A-C1  |
| 14  | bA    | 3114 | CL7  | O1D-CGD-O2D-CED |
| 14  | cB    | 819  | CL7  | C2C-C3C-CAC-CBC |
| 12  | bA    | 3101 | G9R  | C3A-C2A-CAA-CBA |
| 12  | cA    | 3101 | G9R  | C3A-C2A-CAA-CBA |
| 13  | aB    | 3004 | PHO  | C3A-C2A-CAA-CBA |
| 13  | bB    | 805  | PHO  | C3A-C2A-CAA-CBA |
| 13  | cB    | 805  | PHO  | C3A-C2A-CAA-CBA |
| 14  | aA    | 3107 | CL7  | C3A-C2A-CAA-CBA |
| 14  | aA    | 3121 | CL7  | C3A-C2A-CAA-CBA |
| 14  | aA    | 3126 | CL7  | C3A-C2A-CAA-CBA |
| 14  | aA    | 3133 | CL7  | C3A-C2A-CAA-CBA |
| 14  | aB    | 3019 | CL7  | C3A-C2A-CAA-CBA |
| 14  | aB    | 3023 | CL7  | C3A-C2A-CAA-CBA |
| 14  | aB    | 3030 | CL7  | C3A-C2A-CAA-CBA |
| 14  | bA    | 3102 | CL7  | C3A-C2A-CAA-CBA |
| 14  | bA    | 3106 | CL7  | C3A-C2A-CAA-CBA |
| 14  | bA    | 3122 | CL7  | C3A-C2A-CAA-CBA |
| 14  | bA    | 3125 | CL7  | C3A-C2A-CAA-CBA |
| 14  | bB    | 824  | CL7  | C3A-C2A-CAA-CBA |
| 14  | bB    | 833  | CL7  | C3A-C2A-CAA-CBA |
| 14  | cA    | 3102 | CL7  | C3A-C2A-CAA-CBA |
| 14  | cA    | 3106 | CL7  | C3A-C2A-CAA-CBA |
| 14  | cA    | 3122 | CL7  | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | cB    | 824  | CL7  | C3A-C2A-CAA-CBA |
| 14  | cB    | 827  | CL7  | C3A-C2A-CAA-CBA |
| 14  | aB    | 3032 | CL7  | C5-C6-C7-C8     |
| 14  | cB    | 827  | CL7  | C5-C6-C7-C8     |
| 14  | cB    | 827  | CL7  | C8-C10-C11-C12  |
| 14  | bB    | 832  | CL7  | O1D-CGD-O2D-CED |
| 14  | cA    | 3106 | CL7  | O1A-CGA-O2A-C1  |
| 14  | cB    | 807  | CL7  | O1A-CGA-O2A-C1  |
| 14  | aB    | 3025 | CL7  | C16-C17-C18-C19 |
| 14  | bA    | 3132 | CL7  | C16-C17-C18-C20 |
| 14  | cA    | 3132 | CL7  | C16-C17-C18-C20 |
| 17  | cA    | 3143 | PQN  | C26-C27-C28-C29 |
| 14  | bA    | 3121 | CL7  | O1D-CGD-O2D-CED |
| 14  | bB    | 824  | CL7  | O2A-C1-C2-C3    |
| 14  | cB    | 824  | CL7  | O2A-C1-C2-C3    |
| 17  | cA    | 3143 | PQN  | C13-C15-C16-C17 |
| 13  | bB    | 805  | PHO  | C10-C11-C12-C13 |
| 14  | aB    | 3032 | CL7  | C2-C3-C5-C6     |
| 14  | cB    | 833  | CL7  | C2-C3-C5-C6     |
| 16  | aA    | 3138 | LHG  | O1-C1-C2-O2     |
| 16  | bA    | 3137 | LHG  | O1-C1-C2-O2     |
| 16  | bA    | 3138 | LHG  | O1-C1-C2-O2     |
| 16  | cA    | 3138 | LHG  | O1-C1-C2-O2     |
| 14  | cB    | 833  | CL7  | C5-C6-C7-C8     |
| 16  | aA    | 3138 | LHG  | C24-C25-C26-C27 |
| 19  | bB    | 830  | LMG  | C14-C15-C16-C17 |
| 14  | aA    | 3127 | CL7  | O1A-CGA-O2A-C1  |
| 14  | aB    | 3032 | CL7  | O1A-CGA-O2A-C1  |
| 14  | bA    | 3126 | CL7  | O1A-CGA-O2A-C1  |
| 14  | bB    | 820  | CL7  | C16-C17-C18-C19 |
| 17  | aB    | 3027 | PQN  | C13-C15-C16-C17 |
| 17  | bA    | 3143 | PQN  | C13-C15-C16-C17 |
| 13  | cB    | 805  | PHO  | C10-C11-C12-C13 |
| 19  | cB    | 830  | LMG  | O6-C5-C6-O5     |
| 14  | cA    | 3141 | CL7  | C8-C10-C11-C12  |
| 14  | cB    | 810  | CL7  | C15-C16-C17-C18 |
| 19  | bB    | 830  | LMG  | C18-C19-C20-C21 |
| 14  | aA    | 3108 | CL7  | C3-C5-C6-C7     |
| 14  | aB    | 3031 | CL7  | C15-C16-C17-C18 |
| 14  | bB    | 806  | CL7  | C10-C11-C12-C13 |
| 14  | cB    | 803  | CL7  | C15-C16-C17-C18 |
| 16  | cA    | 3137 | LHG  | C8-C7-O7-C5     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | bB    | 803  | CL7  | CBD-CGD-O2D-CED |
| 14  | cB    | 824  | CL7  | C11-C10-C8-C9   |
| 14  | bA    | 3140 | CL7  | C5-C6-C7-C8     |
| 14  | cA    | 3140 | CL7  | C8-C10-C11-C12  |
| 14  | bB    | 822  | CL7  | O1D-CGD-O2D-CED |
| 12  | bA    | 3101 | G9R  | C12-C13-C15-C16 |
| 13  | aB    | 3004 | PHO  | C6-C7-C8-C10    |
| 13  | aB    | 3004 | PHO  | C12-C13-C15-C16 |
| 13  | bB    | 801  | PHO  | C2-C3-C5-C6     |
| 13  | bB    | 805  | PHO  | C11-C10-C8-C7   |
| 13  | cB    | 805  | PHO  | C11-C10-C8-C7   |
| 14  | aA    | 3140 | CL7  | C6-C7-C8-C10    |
| 14  | aA    | 3142 | CL7  | C12-C13-C15-C16 |
| 14  | aB    | 3002 | CL7  | C11-C10-C8-C7   |
| 14  | aB    | 3019 | CL7  | C11-C10-C8-C7   |
| 14  | aB    | 3026 | CL7  | C6-C7-C8-C10    |
| 14  | aB    | 3026 | CL7  | C11-C12-C13-C15 |
| 14  | aL    | 202  | CL7  | C11-C12-C13-C15 |
| 14  | bA    | 3114 | CL7  | C11-C12-C13-C15 |
| 14  | bA    | 3139 | CL7  | C6-C7-C8-C10    |
| 14  | bB    | 804  | CL7  | C6-C7-C8-C10    |
| 14  | bB    | 808  | CL7  | C6-C7-C8-C10    |
| 14  | bB    | 827  | CL7  | C11-C12-C13-C15 |
| 14  | bL    | 203  | CL7  | C6-C7-C8-C10    |
| 14  | cA    | 3106 | CL7  | C12-C13-C15-C16 |
| 14  | cA    | 3140 | CL7  | C11-C12-C13-C15 |
| 14  | cA    | 3142 | CL7  | C11-C10-C8-C7   |
| 14  | cB    | 808  | CL7  | C6-C7-C8-C10    |
| 14  | cB    | 827  | CL7  | C11-C10-C8-C7   |
| 14  | cL    | 203  | CL7  | C6-C7-C8-C10    |
| 14  | cL    | 203  | CL7  | C11-C12-C13-C15 |
| 14  | cL    | 203  | CL7  | C12-C13-C15-C16 |
| 17  | aA    | 3144 | PQN  | C17-C18-C20-C21 |
| 17  | aA    | 3144 | PQN  | C21-C22-C23-C25 |
| 17  | bA    | 3143 | PQN  | C21-C22-C23-C25 |
| 14  | aB    | 3018 | CL7  | C2C-C3C-CAC-CBC |
| 14  | cA    | 3106 | CL7  | C16-C17-C18-C20 |
| 14  | aB    | 3021 | CL7  | O1D-CGD-O2D-CED |
| 14  | aA    | 3142 | CL7  | CBA-CGA-O2A-C1  |
| 14  | bB    | 833  | CL7  | C2A-CAA-CBA-CGA |
| 14  | cA    | 3102 | CL7  | C2A-CAA-CBA-CGA |
| 14  | cL    | 204  | CL7  | C15-C16-C17-C18 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | aA    | 3127 | CL7  | C5-C6-C7-C8     |
| 14  | cB    | 819  | CL7  | C11-C10-C8-C7   |
| 14  | cA    | 3119 | CL7  | CBA-CGA-O2A-C1  |
| 13  | aB    | 3004 | PHO  | C3-C5-C6-C7     |
| 14  | cA    | 3132 | CL7  | C3-C5-C6-C7     |
| 14  | aA    | 3107 | CL7  | C16-C17-C18-C20 |
| 19  | cB    | 830  | LMG  | O6-C1-O1-C7     |
| 13  | aB    | 3004 | PHO  | C10-C11-C12-C13 |
| 14  | cB    | 820  | CL7  | C15-C16-C17-C18 |
| 17  | aA    | 3144 | PQN  | C18-C20-C21-C22 |
| 14  | cB    | 816  | CL7  | O1D-CGD-O2D-CED |
| 16  | aA    | 3138 | LHG  | C28-C29-C30-C31 |
| 19  | cB    | 830  | LMG  | C12-C13-C14-C15 |
| 16  | aA    | 3138 | LHG  | C8-C7-O7-C5     |
| 14  | bB    | 803  | CL7  | C8-C10-C11-C12  |
| 14  | bB    | 804  | CL7  | C5-C6-C7-C8     |
| 16  | cA    | 3137 | LHG  | O9-C7-O7-C5     |
| 19  | cB    | 830  | LMG  | C2-C1-O1-C7     |
| 17  | cA    | 3143 | PQN  | C18-C20-C21-C22 |
| 14  | aB    | 3019 | CL7  | C16-C17-C18-C19 |
| 14  | bA    | 3106 | CL7  | C13-C15-C16-C17 |
| 14  | bA    | 3139 | CL7  | C15-C16-C17-C18 |
| 13  | bB    | 801  | PHO  | C4-C3-C5-C6     |
| 14  | aA    | 3143 | CL7  | C2-C3-C5-C6     |
| 19  | aB    | 3029 | LMG  | C31-C32-C33-C34 |
| 13  | aB    | 3004 | PHO  | C6-C7-C8-C9     |
| 13  | bB    | 805  | PHO  | C11-C12-C13-C14 |
| 13  | bB    | 805  | PHO  | C14-C13-C15-C16 |
| 13  | cB    | 805  | PHO  | C11-C12-C13-C14 |
| 14  | aA    | 3107 | CL7  | C14-C13-C15-C16 |
| 14  | aA    | 3115 | CL7  | C14-C13-C15-C16 |
| 14  | aA    | 3140 | CL7  | C6-C7-C8-C9     |
| 14  | aA    | 3142 | CL7  | C11-C10-C8-C9   |
| 14  | aB    | 3002 | CL7  | C11-C10-C8-C9   |
| 14  | aB    | 3026 | CL7  | C11-C12-C13-C14 |
| 14  | aL    | 202  | CL7  | C6-C7-C8-C9     |
| 14  | bA    | 3106 | CL7  | C14-C13-C15-C16 |
| 14  | bA    | 3114 | CL7  | C11-C12-C13-C14 |
| 14  | bB    | 806  | CL7  | C6-C7-C8-C9     |
| 14  | bB    | 827  | CL7  | C11-C12-C13-C14 |
| 14  | cA    | 3107 | CL7  | C14-C13-C15-C16 |
| 14  | cA    | 3125 | CL7  | C11-C12-C13-C14 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | cA    | 3140 | CL7  | C11-C12-C13-C14 |
| 14  | cA    | 3141 | CL7  | C6-C7-C8-C9     |
| 17  | cB    | 828  | PQN  | C19-C18-C20-C21 |
| 12  | cA    | 3101 | G9R  | O1A-CGA-O2A-C1  |
| 14  | cA    | 3123 | CL7  | C2A-CAA-CBA-CGA |
| 14  | cB    | 824  | CL7  | C2A-CAA-CBA-CGA |
| 19  | aB    | 3029 | LMG  | C20-C21-C22-C23 |
| 14  | cA    | 3108 | CL7  | O1D-CGD-O2D-CED |
| 14  | bA    | 3128 | CL7  | C8-C10-C11-C12  |
| 17  | bB    | 828  | PQN  | C18-C20-C21-C22 |
| 14  | cB    | 824  | CL7  | CBD-CGD-O2D-CED |
| 14  | aA    | 3120 | CL7  | CBA-CGA-O2A-C1  |
| 14  | aB    | 3018 | CL7  | C1A-C2A-CAA-CBA |
| 14  | aL    | 203  | CL7  | C1A-C2A-CAA-CBA |
| 14  | bA    | 3107 | CL7  | C1A-C2A-CAA-CBA |
| 14  | bB    | 819  | CL7  | C1A-C2A-CAA-CBA |
| 14  | bJ    | 101  | CL7  | C1A-C2A-CAA-CBA |
| 14  | bL    | 204  | CL7  | C1A-C2A-CAA-CBA |
| 14  | cL    | 203  | CL7  | C1A-C2A-CAA-CBA |
| 19  | bB    | 830  | LMG  | C22-C23-C24-C25 |
| 14  | bA    | 3140 | CL7  | C15-C16-C17-C18 |
| 14  | bB    | 820  | CL7  | C15-C16-C17-C18 |
| 14  | cB    | 808  | CL7  | C8-C10-C11-C12  |
| 17  | cB    | 828  | PQN  | C13-C15-C16-C17 |
| 14  | bA    | 3126 | CL7  | C5-C6-C7-C8     |
| 14  | bA    | 3128 | CL7  | C5-C6-C7-C8     |
| 19  | cB    | 830  | LMG  | C29-C30-C31-C32 |
| 12  | cA    | 3101 | G9R  | C5-C6-C7-C8     |
| 13  | cB    | 805  | PHO  | C13-C15-C16-C17 |
| 14  | cA    | 3124 | CL7  | C5-C6-C7-C8     |
| 14  | cB    | 820  | CL7  | C16-C17-C18-C19 |
| 14  | aA    | 3115 | CL7  | C8-C10-C11-C12  |
| 14  | cL    | 204  | CL7  | C5-C6-C7-C8     |
| 19  | cB    | 830  | LMG  | C15-C16-C17-C18 |
| 16  | aA    | 3138 | LHG  | C1-C2-C3-O3     |
| 14  | bA    | 3139 | CL7  | C4-C3-C5-C6     |
| 14  | aA    | 3109 | CL7  | C3A-C2A-CAA-CBA |
| 14  | cL    | 205  | CL7  | C3A-C2A-CAA-CBA |
| 14  | aB    | 3026 | CL7  | C10-C11-C12-C13 |
| 14  | bA    | 3124 | CL7  | C5-C6-C7-C8     |
| 14  | bA    | 3116 | CL7  | O1A-CGA-O2A-C1  |
| 14  | bA    | 3124 | CL7  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | aB    | 3005 | CL7  | C13-C15-C16-C17 |
| 17  | bB    | 828  | PQN  | C25-C26-C27-C28 |
| 14  | bB    | 833  | CL7  | C6-C7-C8-C9     |
| 14  | cA    | 3141 | CL7  | C16-C17-C18-C20 |
| 19  | aB    | 3029 | LMG  | O1-C7-C8-C9     |
| 19  | aB    | 3029 | LMG  | C37-C38-C39-C40 |
| 19  | bB    | 830  | LMG  | O1-C7-C8-C9     |
| 19  | cB    | 830  | LMG  | O1-C7-C8-C9     |
| 14  | cA    | 3124 | CL7  | O1A-CGA-O2A-C1  |
| 19  | cB    | 830  | LMG  | C14-C15-C16-C17 |
| 14  | cA    | 3124 | CL7  | C15-C16-C17-C18 |
| 19  | aB    | 3029 | LMG  | C29-C30-C31-C32 |
| 14  | aA    | 3104 | CL7  | C2B-C3B-CAB-OBB |
| 14  | aA    | 3109 | CL7  | C2B-C3B-CAB-OBB |
| 14  | aA    | 3114 | CL7  | C2B-C3B-CAB-OBB |
| 14  | aA    | 3117 | CL7  | C2B-C3B-CAB-OBB |
| 14  | aA    | 3118 | CL7  | C2B-C3B-CAB-OBB |
| 14  | aA    | 3125 | CL7  | C2B-C3B-CAB-OBB |
| 14  | aA    | 3126 | CL7  | C2B-C3B-CAB-OBB |
| 14  | aB    | 3008 | CL7  | C2B-C3B-CAB-OBB |
| 14  | aB    | 3019 | CL7  | C2B-C3B-CAB-OBB |
| 14  | aB    | 3020 | CL7  | C2B-C3B-CAB-OBB |
| 14  | bA    | 3103 | CL7  | C2B-C3B-CAB-OBB |
| 14  | bA    | 3105 | CL7  | C2B-C3B-CAB-OBB |
| 14  | bA    | 3108 | CL7  | C2B-C3B-CAB-OBB |
| 14  | bA    | 3116 | CL7  | C2B-C3B-CAB-OBB |
| 14  | bA    | 3125 | CL7  | C2B-C3B-CAB-OBB |
| 14  | bB    | 812  | CL7  | C2B-C3B-CAB-OBB |
| 14  | cA    | 3105 | CL7  | C2B-C3B-CAB-OBB |
| 14  | cA    | 3111 | CL7  | C2B-C3B-CAB-OBB |
| 14  | cA    | 3116 | CL7  | C2B-C3B-CAB-OBB |
| 14  | cA    | 3117 | CL7  | C2B-C3B-CAB-OBB |
| 14  | cA    | 3124 | CL7  | C2B-C3B-CAB-OBB |
| 14  | cA    | 3125 | CL7  | C2B-C3B-CAB-OBB |
| 14  | cA    | 3139 | CL7  | C2B-C3B-CAB-OBB |
| 14  | cB    | 809  | CL7  | C2B-C3B-CAB-OBB |
| 14  | aB    | 3032 | CL7  | C4-C3-C5-C6     |
| 14  | cB    | 833  | CL7  | C4-C3-C5-C6     |
| 19  | aB    | 3029 | LMG  | C36-C37-C38-C39 |
| 14  | bA    | 3141 | CL7  | CBA-CGA-O2A-C1  |
| 14  | cB    | 811  | CL7  | CBD-CGD-O2D-CED |
| 14  | aA    | 3104 | CL7  | C4B-C3B-CAB-OBB |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | aA    | 3114 | CL7  | C4B-C3B-CAB-OBB |
| 14  | bA    | 3116 | CL7  | C4B-C3B-CAB-OBB |
| 14  | bB    | 812  | CL7  | C4B-C3B-CAB-OBB |
| 14  | bL    | 204  | CL7  | C4B-C3B-CAB-OBB |
| 14  | cA    | 3105 | CL7  | C4B-C3B-CAB-OBB |
| 14  | cA    | 3117 | CL7  | C4B-C3B-CAB-OBB |
| 14  | cA    | 3124 | CL7  | C4B-C3B-CAB-OBB |
| 14  | bB    | 819  | CL7  | CAA-CBA-CGA-O2A |
| 14  | aA    | 3124 | CL7  | C2A-CAA-CBA-CGA |
| 14  | cA    | 3123 | CL7  | C2-C1-O2A-CGA   |
| 14  | bA    | 3107 | CL7  | C3-C5-C6-C7     |
| 14  | cA    | 3107 | CL7  | C3-C5-C6-C7     |
| 14  | aL    | 203  | CL7  | C10-C11-C12-C13 |
| 14  | aB    | 3018 | CL7  | CAA-CBA-CGA-O2A |
| 14  | bB    | 826  | CL7  | C16-C17-C18-C19 |
| 14  | bB    | 803  | CL7  | C5-C6-C7-C8     |
| 16  | cA    | 3137 | LHG  | C13-C14-C15-C16 |
| 13  | bB    | 805  | PHO  | C13-C15-C16-C17 |
| 14  | cB    | 819  | CL7  | CAA-CBA-CGA-O2A |
| 14  | aA    | 3127 | CL7  | C6-C7-C8-C9     |
| 14  | bA    | 3126 | CL7  | C6-C7-C8-C9     |
| 13  | aA    | 3102 | PHO  | CHA-CBD-CGD-O1D |
| 13  | aA    | 3102 | PHO  | CHA-CBD-CGD-O2D |
| 13  | aB    | 3004 | PHO  | CHA-CBD-CGD-O2D |
| 13  | bB    | 805  | PHO  | CHA-CBD-CGD-O2D |
| 13  | cB    | 801  | PHO  | CHA-CBD-CGD-O1D |
| 13  | cB    | 801  | PHO  | CHA-CBD-CGD-O2D |
| 13  | cB    | 805  | PHO  | CHA-CBD-CGD-O1D |
| 13  | cB    | 805  | PHO  | CHA-CBD-CGD-O2D |
| 13  | cB    | 801  | PHO  | C4-C3-C5-C6     |
| 13  | aB    | 3004 | PHO  | C11-C12-C13-C15 |
| 13  | bB    | 805  | PHO  | C6-C7-C8-C10    |
| 13  | bB    | 805  | PHO  | C11-C12-C13-C15 |
| 13  | cB    | 801  | PHO  | C2-C3-C5-C6     |
| 13  | cB    | 805  | PHO  | C6-C7-C8-C10    |
| 13  | cB    | 805  | PHO  | C11-C12-C13-C15 |
| 14  | aA    | 3107 | CL7  | C12-C13-C15-C16 |
| 14  | aA    | 3115 | CL7  | C11-C12-C13-C15 |
| 14  | aA    | 3133 | CL7  | C11-C12-C13-C15 |
| 14  | aA    | 3140 | CL7  | C11-C12-C13-C15 |
| 14  | aA    | 3142 | CL7  | C11-C10-C8-C7   |
| 14  | aB    | 3007 | CL7  | C12-C13-C15-C16 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | aB    | 3009 | CL7  | C6-C7-C8-C10    |
| 14  | bA    | 3124 | CL7  | C11-C10-C8-C7   |
| 14  | bA    | 3128 | CL7  | C2-C3-C5-C6     |
| 14  | bA    | 3128 | CL7  | C6-C7-C8-C10    |
| 14  | bA    | 3142 | CL7  | C11-C12-C13-C15 |
| 14  | bB    | 806  | CL7  | C2-C3-C5-C6     |
| 14  | bB    | 806  | CL7  | C11-C10-C8-C7   |
| 14  | bB    | 806  | CL7  | C11-C12-C13-C15 |
| 14  | bB    | 808  | CL7  | C12-C13-C15-C16 |
| 14  | bB    | 810  | CL7  | C12-C13-C15-C16 |
| 14  | bB    | 820  | CL7  | C12-C13-C15-C16 |
| 14  | bB    | 827  | CL7  | C6-C7-C8-C10    |
| 14  | bB    | 832  | CL7  | C11-C12-C13-C15 |
| 14  | cA    | 3125 | CL7  | C11-C12-C13-C15 |
| 14  | cA    | 3139 | CL7  | C6-C7-C8-C10    |
| 14  | cA    | 3139 | CL7  | C12-C13-C15-C16 |
| 14  | cA    | 3141 | CL7  | C6-C7-C8-C10    |
| 14  | cB    | 803  | CL7  | C6-C7-C8-C10    |
| 14  | cB    | 808  | CL7  | C11-C12-C13-C15 |
| 14  | cB    | 810  | CL7  | C6-C7-C8-C10    |
| 17  | bA    | 3143 | PQN  | C17-C18-C20-C21 |
| 17  | cA    | 3143 | PQN  | C17-C18-C20-C21 |
| 14  | cA    | 3126 | CL7  | C3-C5-C6-C7     |
| 14  | aB    | 3003 | CL7  | O1A-CGA-O2A-C1  |
| 13  | aB    | 3004 | PHO  | C11-C12-C13-C14 |
| 13  | bB    | 805  | PHO  | C6-C7-C8-C9     |
| 13  | cB    | 805  | PHO  | C6-C7-C8-C9     |
| 13  | cB    | 805  | PHO  | C14-C13-C15-C16 |
| 14  | aA    | 3115 | CL7  | C6-C7-C8-C9     |
| 14  | aA    | 3115 | CL7  | C11-C12-C13-C14 |
| 14  | aA    | 3126 | CL7  | C11-C12-C13-C14 |
| 14  | aA    | 3140 | CL7  | C11-C12-C13-C14 |
| 14  | aB    | 3002 | CL7  | C6-C7-C8-C9     |
| 14  | aB    | 3009 | CL7  | C11-C10-C8-C9   |
| 14  | aB    | 3019 | CL7  | C14-C13-C15-C16 |
| 14  | aB    | 3026 | CL7  | C6-C7-C8-C9     |
| 14  | aB    | 3031 | CL7  | C11-C10-C8-C9   |
| 14  | bA    | 3107 | CL7  | C14-C13-C15-C16 |
| 14  | bA    | 3139 | CL7  | C14-C13-C15-C16 |
| 14  | bB    | 806  | CL7  | C11-C12-C13-C14 |
| 14  | bB    | 827  | CL7  | C6-C7-C8-C9     |
| 14  | bB    | 832  | CL7  | C11-C10-C8-C9   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | cA    | 3114 | CL7  | C14-C13-C15-C16 |
| 14  | cA    | 3124 | CL7  | C11-C10-C8-C9   |
| 14  | cA    | 3139 | CL7  | C14-C13-C15-C16 |
| 14  | cA    | 3141 | CL7  | C14-C13-C15-C16 |
| 14  | cB    | 810  | CL7  | C11-C10-C8-C9   |
| 14  | aA    | 3141 | CL7  | CBA-CGA-O2A-C1  |
| 14  | bA    | 3107 | CL7  | C5-C6-C7-C8     |
| 14  | bA    | 3142 | CL7  | C5-C6-C7-C8     |
| 14  | cA    | 3128 | CL7  | O1D-CGD-O2D-CED |
| 14  | bA    | 3142 | CL7  | C3-C5-C6-C7     |
| 19  | cB    | 830  | LMG  | C22-C23-C24-C25 |
| 14  | cA    | 3128 | CL7  | CBA-CGA-O2A-C1  |
| 14  | bA    | 3128 | CL7  | C10-C11-C12-C13 |
| 14  | cA    | 3128 | CL7  | C8-C10-C11-C12  |
| 14  | aB    | 3002 | CL7  | C10-C11-C12-C13 |
| 14  | cB    | 803  | CL7  | C8-C10-C11-C12  |
| 14  | cB    | 806  | CL7  | C15-C16-C17-C18 |
| 17  | cB    | 828  | PQN  | C25-C26-C27-C28 |
| 14  | aB    | 3002 | CL7  | C5-C6-C7-C8     |
| 14  | aB    | 3018 | CL7  | C11-C10-C8-C9   |
| 19  | aB    | 3029 | LMG  | C13-C14-C15-C16 |
| 14  | cL    | 204  | CL7  | O1D-CGD-O2D-CED |
| 14  | cB    | 819  | CL7  | C3-C5-C6-C7     |
| 14  | bL    | 203  | CL7  | C16-C17-C18-C19 |
| 14  | cB    | 816  | CL7  | C4C-C3C-CAC-CBC |
| 14  | cA    | 3141 | CL7  | C13-C15-C16-C17 |
| 14  | aA    | 3117 | CL7  | CBA-CGA-O2A-C1  |
| 14  | bA    | 3139 | CL7  | CBA-CGA-O2A-C1  |
| 14  | aA    | 3108 | CL7  | C3A-C2A-CAA-CBA |
| 14  | aA    | 3143 | CL7  | C3A-C2A-CAA-CBA |
| 14  | bA    | 3107 | CL7  | C3A-C2A-CAA-CBA |
| 14  | bJ    | 101  | CL7  | C3A-C2A-CAA-CBA |
| 14  | bL    | 203  | CL7  | C3A-C2A-CAA-CBA |
| 14  | cA    | 3107 | CL7  | C3A-C2A-CAA-CBA |
| 14  | cB    | 833  | CL7  | C3A-C2A-CAA-CBA |
| 14  | aA    | 3133 | CL7  | C16-C17-C18-C20 |
| 14  | cB    | 833  | CL7  | CBA-CGA-O2A-C1  |
| 14  | cA    | 3139 | CL7  | O2A-C1-C2-C3    |
| 14  | aB    | 3031 | CL7  | C10-C11-C12-C13 |
| 14  | aA    | 3107 | CL7  | C16-C17-C18-C19 |
| 14  | bB    | 820  | CL7  | C16-C17-C18-C20 |
| 16  | bA    | 3137 | LHG  | C8-C7-O7-C5     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 19  | aB    | 3029 | LMG  | C12-C13-C14-C15 |
| 14  | bB    | 804  | CL7  | O1A-CGA-O2A-C1  |
| 14  | aB    | 3019 | CL7  | C16-C17-C18-C20 |
| 14  | aB    | 3025 | CL7  | C16-C17-C18-C20 |
| 14  | bB    | 833  | CL7  | C6-C7-C8-C10    |
| 14  | cA    | 3141 | CL7  | C16-C17-C18-C19 |
| 13  | bB    | 801  | PHO  | C5-C6-C7-C8     |
| 14  | aA    | 3115 | CL7  | C5-C6-C7-C8     |
| 14  | cA    | 3107 | CL7  | C5-C6-C7-C8     |
| 13  | aB    | 3004 | PHO  | C2C-C3C-CAC-CBC |
| 14  | aA    | 3115 | CL7  | C15-C16-C17-C18 |
| 14  | aA    | 3125 | CL7  | O1A-CGA-O2A-C1  |
| 14  | cB    | 809  | CL7  | O1D-CGD-O2D-CED |
| 14  | aB    | 3002 | CL7  | C15-C16-C17-C18 |
| 16  | bA    | 3137 | LHG  | C27-C28-C29-C30 |
| 16  | aA    | 3138 | LHG  | O9-C7-O7-C5     |
| 16  | bA    | 3137 | LHG  | O9-C7-O7-C5     |
| 14  | aA    | 3107 | CL7  | C2-C1-O2A-CGA   |
| 14  | aA    | 3128 | CL7  | C2-C1-O2A-CGA   |
| 14  | aB    | 3023 | CL7  | C2-C1-O2A-CGA   |
| 14  | cA    | 3126 | CL7  | C2-C1-O2A-CGA   |
| 14  | cA    | 3128 | CL7  | C2-C1-O2A-CGA   |
| 14  | cB    | 810  | CL7  | C2-C1-O2A-CGA   |
| 14  | aA    | 3131 | CL7  | O1D-CGD-O2D-CED |
| 14  | cA    | 3121 | CL7  | O1D-CGD-O2D-CED |
| 13  | aA    | 3102 | PHO  | C2-C3-C5-C6     |
| 14  | aB    | 3007 | CL7  | C10-C11-C12-C13 |
| 13  | cB    | 801  | PHO  | C6-C7-C8-C9     |
| 14  | aA    | 3141 | CL7  | C11-C10-C8-C9   |
| 14  | aA    | 3141 | CL7  | C11-C12-C13-C14 |
| 14  | aB    | 3026 | CL7  | C14-C13-C15-C16 |
| 14  | bA    | 3114 | CL7  | C11-C10-C8-C9   |
| 14  | bA    | 3140 | CL7  | C11-C12-C13-C14 |
| 14  | bA    | 3141 | CL7  | C11-C10-C8-C9   |
| 14  | bB    | 827  | CL7  | C14-C13-C15-C16 |
| 14  | cA    | 3114 | CL7  | C11-C10-C8-C9   |
| 14  | cA    | 3114 | CL7  | C11-C12-C13-C14 |
| 14  | cB    | 803  | CL7  | C6-C7-C8-C9     |
| 14  | cB    | 806  | CL7  | C11-C12-C13-C14 |
| 14  | cB    | 827  | CL7  | C14-C13-C15-C16 |
| 17  | cA    | 3143 | PQN  | C21-C22-C23-C24 |
| 17  | cA    | 3143 | PQN  | C24-C23-C25-C26 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | cA    | 3139 | CL7  | CBA-CGA-O2A-C1  |
| 13  | aB    | 3004 | PHO  | C13-C15-C16-C17 |
| 14  | aA    | 3141 | CL7  | C8-C10-C11-C12  |
| 17  | aA    | 3144 | PQN  | C15-C16-C17-C18 |
| 13  | aB    | 3004 | PHO  | C1A-C2A-CAA-CBA |
| 13  | bB    | 805  | PHO  | C1A-C2A-CAA-CBA |
| 13  | cB    | 805  | PHO  | C1A-C2A-CAA-CBA |
| 14  | aB    | 3005 | CL7  | O1A-CGA-O2A-C1  |
| 19  | cB    | 830  | LMG  | C18-C19-C20-C21 |
| 14  | cB    | 820  | CL7  | C16-C17-C18-C20 |
| 14  | bA    | 3107 | CL7  | C1-C2-C3-C5     |
| 14  | bA    | 3141 | CL7  | C1-C2-C3-C5     |
| 14  | cA    | 3128 | CL7  | C10-C11-C12-C13 |
| 14  | bB    | 816  | CL7  | CAA-CBA-CGA-O2A |
| 19  | aB    | 3029 | LMG  | C35-C36-C37-C38 |
| 19  | bB    | 830  | LMG  | C29-C30-C31-C32 |
| 14  | cA    | 3108 | CL7  | C1A-C2A-CAA-CBA |
| 14  | cL    | 205  | CL7  | C1A-C2A-CAA-CBA |
| 14  | bA    | 3125 | CL7  | C5-C6-C7-C8     |
| 17  | bA    | 3143 | PQN  | C20-C21-C22-C23 |
| 12  | bA    | 3101 | G9R  | C5-C6-C7-C8     |
| 14  | aL    | 202  | CL7  | C16-C17-C18-C19 |
| 14  | cA    | 3106 | CL7  | C16-C17-C18-C19 |
| 14  | aB    | 3023 | CL7  | C11-C10-C8-C9   |
| 14  | cB    | 819  | CL7  | C11-C10-C8-C9   |
| 14  | aB    | 3023 | CL7  | O1A-CGA-O2A-C1  |
| 14  | aB    | 3030 | CL7  | O1D-CGD-O2D-CED |
| 14  | aB    | 3002 | CL7  | C8-C10-C11-C12  |
| 16  | aA    | 3138 | LHG  | O6-C4-C5-C6     |
| 13  | aA    | 3102 | PHO  | C4-C3-C5-C6     |
| 14  | aA    | 3125 | CL7  | C11-C12-C13-C15 |
| 14  | aA    | 3126 | CL7  | C11-C12-C13-C15 |
| 14  | aA    | 3129 | CL7  | C11-C12-C13-C15 |
| 14  | aA    | 3140 | CL7  | C11-C10-C8-C7   |
| 14  | aA    | 3141 | CL7  | C11-C12-C13-C15 |
| 14  | aA    | 3142 | CL7  | C11-C12-C13-C15 |
| 14  | aA    | 3143 | CL7  | C11-C12-C13-C15 |
| 14  | aA    | 3143 | CL7  | C12-C13-C15-C16 |
| 14  | aB    | 3002 | CL7  | C6-C7-C8-C10    |
| 14  | aB    | 3005 | CL7  | C6-C7-C8-C10    |
| 14  | aB    | 3009 | CL7  | C11-C10-C8-C7   |
| 14  | aB    | 3009 | CL7  | C12-C13-C15-C16 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | aB    | 3019 | CL7  | C12-C13-C15-C16 |
| 14  | aB    | 3025 | CL7  | C12-C13-C15-C16 |
| 14  | bA    | 3106 | CL7  | C12-C13-C15-C16 |
| 14  | bA    | 3107 | CL7  | C11-C12-C13-C15 |
| 14  | bA    | 3114 | CL7  | C6-C7-C8-C10    |
| 14  | bA    | 3114 | CL7  | C11-C10-C8-C7   |
| 14  | bA    | 3132 | CL7  | C11-C12-C13-C15 |
| 14  | bA    | 3139 | CL7  | C12-C13-C15-C16 |
| 14  | bA    | 3140 | CL7  | C11-C12-C13-C15 |
| 14  | bA    | 3142 | CL7  | C11-C10-C8-C7   |
| 14  | bB    | 807  | CL7  | C12-C13-C15-C16 |
| 14  | bB    | 810  | CL7  | C6-C7-C8-C10    |
| 14  | bB    | 826  | CL7  | C6-C7-C8-C10    |
| 14  | bB    | 826  | CL7  | C11-C12-C13-C15 |
| 14  | bB    | 826  | CL7  | C12-C13-C15-C16 |
| 14  | bB    | 832  | CL7  | C11-C10-C8-C7   |
| 14  | cA    | 3107 | CL7  | C11-C12-C13-C15 |
| 14  | cA    | 3114 | CL7  | C6-C7-C8-C10    |
| 14  | cA    | 3114 | CL7  | C11-C12-C13-C15 |
| 14  | cA    | 3128 | CL7  | C6-C7-C8-C10    |
| 14  | cA    | 3132 | CL7  | C11-C12-C13-C15 |
| 14  | cB    | 806  | CL7  | C11-C10-C8-C7   |
| 14  | cB    | 806  | CL7  | C11-C12-C13-C15 |
| 14  | cB    | 807  | CL7  | C12-C13-C15-C16 |
| 14  | cB    | 810  | CL7  | C11-C10-C8-C7   |
| 14  | cB    | 810  | CL7  | C12-C13-C15-C16 |
| 14  | cB    | 826  | CL7  | C11-C12-C13-C15 |
| 14  | cB    | 826  | CL7  | C12-C13-C15-C16 |
| 14  | cB    | 832  | CL7  | C11-C12-C13-C15 |
| 14  | cL    | 203  | CL7  | C11-C10-C8-C7   |
| 14  | bA    | 3106 | CL7  | C3-C5-C6-C7     |
| 14  | aA    | 3121 | CL7  | O1A-CGA-O2A-C1  |
| 14  | aA    | 3143 | CL7  | O1A-CGA-O2A-C1  |
| 14  | aB    | 3009 | CL7  | C13-C15-C16-C17 |
| 14  | aB    | 3003 | CL7  | C8-C10-C11-C12  |
| 14  | cA    | 3139 | CL7  | C13-C15-C16-C17 |
| 14  | aA    | 3124 | CL7  | O1A-CGA-O2A-C1  |
| 19  | bB    | 830  | LMG  | C16-C17-C18-C19 |
| 17  | bB    | 828  | PQN  | C13-C15-C16-C17 |
| 14  | aA    | 3108 | CL7  | C5-C6-C7-C8     |
| 14  | aA    | 3141 | CL7  | C15-C16-C17-C18 |
| 14  | cA    | 3114 | CL7  | C5-C6-C7-C8     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | aA    | 3120 | CL7  | CAD-CBD-CGD-O2D |
| 14  | bA    | 3106 | CL7  | CAD-CBD-CGD-O2D |
| 14  | bA    | 3110 | CL7  | CAD-CBD-CGD-O2D |
| 14  | bA    | 3131 | CL7  | CAD-CBD-CGD-O2D |
| 14  | bB    | 810  | CL7  | CAD-CBD-CGD-O2D |
| 14  | bB    | 818  | CL7  | CAD-CBD-CGD-O2D |
| 14  | cA    | 3108 | CL7  | CAD-CBD-CGD-O2D |
| 14  | cA    | 3112 | CL7  | CAD-CBD-CGD-O2D |
| 14  | cA    | 3119 | CL7  | CAD-CBD-CGD-O2D |
| 14  | cA    | 3131 | CL7  | CAD-CBD-CGD-O2D |
| 14  | aL    | 202  | CL7  | C8-C10-C11-C12  |
| 14  | bA    | 3139 | CL7  | C5-C6-C7-C8     |
| 14  | cA    | 3140 | CL7  | CBA-CGA-O2A-C1  |
| 14  | bA    | 3106 | CL7  | C16-C17-C18-C19 |
| 14  | aA    | 3106 | CL7  | CBD-CGD-O2D-CED |
| 14  | aB    | 3009 | CL7  | CBD-CGD-O2D-CED |
| 16  | aA    | 3138 | LHG  | O6-C4-C5-O7     |
| 16  | cA    | 3137 | LHG  | O6-C4-C5-O7     |
| 14  | bB    | 810  | CL7  | C8-C10-C11-C12  |
| 14  | cL    | 203  | CL7  | C8-C10-C11-C12  |
| 14  | cA    | 3126 | CL7  | C5-C6-C7-C8     |
| 14  | aB    | 3006 | CL7  | C2A-CAA-CBA-CGA |
| 17  | bA    | 3143 | PQN  | C15-C16-C17-C18 |
| 14  | bB    | 826  | CL7  | C16-C17-C18-C20 |
| 14  | aA    | 3104 | CL7  | CHA-CBD-CGD-O2D |
| 14  | aA    | 3108 | CL7  | CHA-CBD-CGD-O2D |
| 14  | aA    | 3126 | CL7  | CHA-CBD-CGD-O2D |
| 14  | aA    | 3126 | CL7  | CHA-CBD-CGD-O1D |
| 14  | aA    | 3127 | CL7  | CHA-CBD-CGD-O2D |
| 14  | aA    | 3132 | CL7  | CHA-CBD-CGD-O1D |
| 14  | aA    | 3146 | CL7  | CHA-CBD-CGD-O1D |
| 14  | aB    | 3002 | CL7  | CHA-CBD-CGD-O1D |
| 14  | aB    | 3016 | CL7  | CHA-CBD-CGD-O2D |
| 14  | aB    | 3019 | CL7  | CHA-CBD-CGD-O2D |
| 14  | aB    | 3019 | CL7  | CHA-CBD-CGD-O1D |
| 14  | aB    | 3022 | CL7  | CHA-CBD-CGD-O1D |
| 14  | aB    | 3023 | CL7  | CHA-CBD-CGD-O1D |
| 14  | aB    | 3031 | CL7  | CHA-CBD-CGD-O2D |
| 14  | bA    | 3107 | CL7  | CHA-CBD-CGD-O2D |
| 14  | bA    | 3125 | CL7  | CHA-CBD-CGD-O2D |
| 14  | bA    | 3126 | CL7  | CHA-CBD-CGD-O2D |
| 14  | bA    | 3131 | CL7  | CHA-CBD-CGD-O1D |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | bA    | 3139 | CL7  | CHA-CBD-CGD-O1D |
| 14  | bA    | 3145 | CL7  | CHA-CBD-CGD-O1D |
| 14  | bB    | 807  | CL7  | CHA-CBD-CGD-O2D |
| 14  | bB    | 817  | CL7  | CHA-CBD-CGD-O2D |
| 14  | bB    | 818  | CL7  | CHA-CBD-CGD-O1D |
| 14  | cA    | 3107 | CL7  | CHA-CBD-CGD-O2D |
| 14  | cA    | 3120 | CL7  | CHA-CBD-CGD-O1D |
| 14  | cA    | 3125 | CL7  | CHA-CBD-CGD-O2D |
| 14  | cA    | 3131 | CL7  | CHA-CBD-CGD-O1D |
| 14  | cB    | 803  | CL7  | CHA-CBD-CGD-O2D |
| 14  | cB    | 822  | CL7  | CHA-CBD-CGD-O1D |
| 14  | cB    | 823  | CL7  | CHA-CBD-CGD-O1D |
| 14  | cB    | 831  | CL7  | CHA-CBD-CGD-O1D |
| 14  | bB    | 819  | CL7  | C2C-C3C-CAC-CBC |
| 14  | aB    | 3005 | CL7  | C3-C5-C6-C7     |
| 14  | bA    | 3142 | CL7  | O1A-CGA-O2A-C1  |
| 17  | aB    | 3027 | PQN  | C15-C16-C17-C18 |
| 14  | cA    | 3126 | CL7  | C6-C7-C8-C9     |
| 16  | aA    | 3138 | LHG  | C34-C35-C36-C37 |
| 19  | aB    | 3029 | LMG  | O1-C7-C8-O7     |
| 19  | bB    | 830  | LMG  | O1-C7-C8-O7     |
| 19  | cB    | 830  | LMG  | O1-C7-C8-O7     |
| 14  | aA    | 3126 | CL7  | C1-C2-C3-C5     |
| 19  | bB    | 830  | LMG  | C15-C16-C17-C18 |
| 14  | bB    | 808  | CL7  | C10-C11-C12-C13 |
| 12  | aA    | 3101 | G9R  | O1A-CGA-O2A-C1  |
| 14  | cA    | 3102 | CL7  | C4-C3-C5-C6     |
| 16  | bA    | 3137 | LHG  | C29-C30-C31-C32 |
| 14  | aB    | 3002 | CL7  | C11-C12-C13-C14 |
| 14  | bA    | 3114 | CL7  | C14-C13-C15-C16 |
| 14  | bB    | 826  | CL7  | C14-C13-C15-C16 |
| 14  | cB    | 806  | CL7  | C11-C10-C8-C9   |
| 14  | cB    | 807  | CL7  | C14-C13-C15-C16 |
| 14  | cB    | 826  | CL7  | C14-C13-C15-C16 |
| 17  | aB    | 3027 | PQN  | C19-C18-C20-C21 |
| 14  | cA    | 3109 | CL7  | O1D-CGD-O2D-CED |
| 14  | cA    | 3142 | CL7  | O1A-CGA-O2A-C1  |
| 14  | cB    | 808  | CL7  | O1A-CGA-O2A-C1  |
| 13  | cB    | 805  | PHO  | C2C-C3C-CAC-CBC |
| 14  | cB    | 833  | CL7  | C2A-CAA-CBA-CGA |
| 14  | bB    | 819  | CL7  | C11-C10-C8-C9   |
| 14  | bB    | 810  | CL7  | C13-C15-C16-C17 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 19  | bB    | 830  | LMG  | C20-C21-C22-C23 |
| 14  | aB    | 3018 | CL7  | C3-C5-C6-C7     |
| 14  | aA    | 3103 | CL7  | C1A-C2A-CAA-CBA |
| 14  | aA    | 3121 | CL7  | C1A-C2A-CAA-CBA |
| 14  | aA    | 3128 | CL7  | C1A-C2A-CAA-CBA |
| 14  | aB    | 3026 | CL7  | C1A-C2A-CAA-CBA |
| 14  | bA    | 3102 | CL7  | C1A-C2A-CAA-CBA |
| 14  | cA    | 3102 | CL7  | C1A-C2A-CAA-CBA |
| 14  | cB    | 826  | CL7  | C16-C17-C18-C19 |
| 14  | cB    | 832  | CL7  | C16-C17-C18-C20 |
| 14  | aB    | 3008 | CL7  | O1D-CGD-O2D-CED |
| 14  | bL    | 203  | CL7  | C8-C10-C11-C12  |
| 14  | aA    | 3117 | CL7  | C4-C3-C5-C6     |
| 14  | bA    | 3106 | CL7  | C4-C3-C5-C6     |
| 14  | aB    | 3007 | CL7  | C3-C5-C6-C7     |
| 14  | bB    | 806  | CL7  | O1A-CGA-O2A-C1  |
| 16  | cA    | 3138 | LHG  | C4-O6-P-O5      |
| 14  | cL    | 203  | CL7  | C16-C17-C18-C19 |
| 14  | cA    | 3125 | CL7  | C5-C6-C7-C8     |
| 16  | cA    | 3137 | LHG  | O6-C4-C5-C6     |
| 14  | cA    | 3130 | CL7  | O1D-CGD-O2D-CED |
| 14  | cA    | 3114 | CL7  | C2A-CAA-CBA-CGA |
| 14  | aA    | 3121 | CL7  | CAD-CBD-CGD-O1D |
| 14  | aA    | 3128 | CL7  | CAD-CBD-CGD-O1D |
| 14  | aB    | 3002 | CL7  | CAD-CBD-CGD-O1D |
| 14  | aB    | 3017 | CL7  | CAD-CBD-CGD-O1D |
| 14  | aB    | 3019 | CL7  | CAD-CBD-CGD-O1D |
| 14  | aB    | 3022 | CL7  | CAD-CBD-CGD-O1D |
| 14  | bA    | 3104 | CL7  | CAD-CBD-CGD-O1D |
| 14  | bA    | 3120 | CL7  | CAD-CBD-CGD-O1D |
| 14  | bA    | 3127 | CL7  | CAD-CBD-CGD-O1D |
| 14  | bB    | 818  | CL7  | CAD-CBD-CGD-O1D |
| 14  | bB    | 823  | CL7  | CAD-CBD-CGD-O1D |
| 14  | bL    | 203  | CL7  | CAD-CBD-CGD-O1D |
| 14  | cA    | 3104 | CL7  | CAD-CBD-CGD-O1D |
| 14  | cA    | 3112 | CL7  | CAD-CBD-CGD-O1D |
| 14  | cA    | 3120 | CL7  | CAD-CBD-CGD-O1D |
| 14  | cA    | 3127 | CL7  | CAD-CBD-CGD-O1D |
| 14  | cB    | 823  | CL7  | CAD-CBD-CGD-O1D |
| 14  | bB    | 808  | CL7  | C3-C5-C6-C7     |
| 14  | bB    | 814  | CL7  | O1D-CGD-O2D-CED |
| 19  | bB    | 830  | LMG  | O6-C5-C6-O5     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | aA    | 3107 | CL7  | C11-C12-C13-C15 |
| 14  | aA    | 3115 | CL7  | C11-C10-C8-C7   |
| 14  | aA    | 3127 | CL7  | C1A-C2A-CAA-CBA |
| 14  | aB    | 3006 | CL7  | C12-C13-C15-C16 |
| 14  | aB    | 3019 | CL7  | C11-C12-C13-C15 |
| 14  | aB    | 3025 | CL7  | C11-C12-C13-C15 |
| 14  | aB    | 3031 | CL7  | C11-C10-C8-C7   |
| 14  | aL    | 203  | CL7  | C11-C10-C8-C7   |
| 14  | aL    | 203  | CL7  | C12-C13-C15-C16 |
| 14  | bA    | 3126 | CL7  | C1A-C2A-CAA-CBA |
| 14  | bA    | 3141 | CL7  | C11-C10-C8-C7   |
| 14  | bA    | 3142 | CL7  | C12-C13-C15-C16 |
| 14  | bB    | 810  | CL7  | C11-C10-C8-C7   |
| 14  | bB    | 820  | CL7  | C11-C12-C13-C15 |
| 14  | bB    | 832  | CL7  | C12-C13-C15-C16 |
| 14  | bL    | 203  | CL7  | C11-C10-C8-C7   |
| 14  | bL    | 205  | CL7  | C3A-C2A-CAA-CBA |
| 14  | cA    | 3106 | CL7  | C11-C12-C13-C15 |
| 14  | cA    | 3114 | CL7  | C11-C10-C8-C7   |
| 14  | cA    | 3124 | CL7  | C11-C12-C13-C15 |
| 14  | cA    | 3132 | CL7  | C12-C13-C15-C16 |
| 14  | cA    | 3141 | CL7  | C11-C12-C13-C15 |
| 14  | cA    | 3142 | CL7  | C11-C12-C13-C15 |
| 14  | cB    | 826  | CL7  | C6-C7-C8-C10    |
| 14  | cB    | 832  | CL7  | C11-C10-C8-C7   |
| 14  | cL    | 204  | CL7  | C6-C7-C8-C10    |
| 19  | bB    | 830  | LMG  | C35-C36-C37-C38 |
| 13  | bB    | 805  | PHO  | C2C-C3C-CAC-CBC |
| 14  | aA    | 3142 | CL7  | C16-C17-C18-C19 |
| 14  | bB    | 832  | CL7  | C16-C17-C18-C20 |
| 14  | bB    | 826  | CL7  | C3-C5-C6-C7     |
| 19  | bB    | 830  | LMG  | C13-C14-C15-C16 |
| 14  | bA    | 3106 | CL7  | C16-C17-C18-C20 |
| 14  | bB    | 806  | CL7  | C16-C17-C18-C19 |
| 14  | cA    | 3114 | CL7  | C2C-C3C-CAC-CBC |
| 14  | aB    | 3019 | CL7  | C4-C3-C5-C6     |
| 14  | cB    | 816  | CL7  | CAA-CBA-CGA-O2A |
| 14  | bB    | 807  | CL7  | C15-C16-C17-C18 |
| 14  | cA    | 3139 | CL7  | C5-C6-C7-C8     |
| 14  | aA    | 3115 | CL7  | C11-C10-C8-C9   |
| 14  | aA    | 3125 | CL7  | C11-C12-C13-C14 |
| 14  | aA    | 3140 | CL7  | C14-C13-C15-C16 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | aA    | 3143 | CL7  | C11-C12-C13-C14 |
| 14  | aB    | 3006 | CL7  | C14-C13-C15-C16 |
| 14  | bB    | 806  | CL7  | C11-C10-C8-C9   |
| 14  | bB    | 810  | CL7  | C11-C10-C8-C9   |
| 14  | bB    | 826  | CL7  | C6-C7-C8-C9     |
| 14  | cA    | 3106 | CL7  | C14-C13-C15-C16 |
| 14  | cA    | 3128 | CL7  | C6-C7-C8-C9     |
| 14  | cL    | 203  | CL7  | C14-C13-C15-C16 |
| 14  | cL    | 204  | CL7  | C6-C7-C8-C9     |
| 14  | bA    | 3141 | CL7  | C5-C6-C7-C8     |
| 14  | cB    | 804  | CL7  | O1A-CGA-O2A-C1  |
| 14  | aB    | 3026 | CL7  | C5-C6-C7-C8     |
| 14  | cB    | 832  | CL7  | C15-C16-C17-C18 |
| 16  | bA    | 3137 | LHG  | C11-C12-C13-C14 |
| 14  | aB    | 3016 | CL7  | C2B-C3B-CAB-OBB |
| 14  | aL    | 204  | CL7  | C2B-C3B-CAB-OBB |
| 14  | bA    | 3106 | CL7  | C2B-C3B-CAB-OBB |
| 14  | bA    | 3140 | CL7  | C2B-C3B-CAB-OBB |
| 14  | bB    | 810  | CL7  | C2B-C3B-CAB-OBB |
| 14  | bB    | 817  | CL7  | C2B-C3B-CAB-OBB |
| 14  | bB    | 819  | CL7  | C2B-C3B-CAB-OBB |
| 14  | cB    | 817  | CL7  | C2B-C3B-CAB-OBB |
| 14  | cB    | 819  | CL7  | C2B-C3B-CAB-OBB |
| 14  | cB    | 822  | CL7  | C2B-C3B-CAB-OBB |
| 14  | cL    | 204  | CL7  | C2B-C3B-CAB-OBB |
| 14  | bL    | 203  | CL7  | C16-C17-C18-C20 |
| 14  | cB    | 826  | CL7  | C16-C17-C18-C20 |
| 16  | cA    | 3137 | LHG  | C34-C35-C36-C37 |
| 13  | cB    | 801  | PHO  | C8-C10-C11-C12  |
| 14  | cA    | 3116 | CL7  | O1D-CGD-O2D-CED |
| 17  | aB    | 3027 | PQN  | C25-C26-C27-C28 |
| 17  | cA    | 3143 | PQN  | C15-C16-C17-C18 |
| 14  | aA    | 3133 | CL7  | C16-C17-C18-C19 |
| 14  | aA    | 3108 | CL7  | C4B-C3B-CAB-OBB |
| 14  | aA    | 3117 | CL7  | C4B-C3B-CAB-OBB |
| 14  | aA    | 3118 | CL7  | C4B-C3B-CAB-OBB |
| 14  | aA    | 3131 | CL7  | C4B-C3B-CAB-OBB |
| 14  | aA    | 3133 | CL7  | C4B-C3B-CAB-OBB |
| 14  | aA    | 3134 | CL7  | C4B-C3B-CAB-OBB |
| 14  | aA    | 3143 | CL7  | C4B-C3B-CAB-OBB |
| 14  | aB    | 3019 | CL7  | C4B-C3B-CAB-OBB |
| 14  | bA    | 3103 | CL7  | C4B-C3B-CAB-OBB |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | bA    | 3111 | CL7  | C4B-C3B-CAB-OBB |
| 14  | bA    | 3117 | CL7  | C4B-C3B-CAB-OBB |
| 14  | bA    | 3119 | CL7  | C4B-C3B-CAB-OBB |
| 14  | bA    | 3125 | CL7  | C4B-C3B-CAB-OBB |
| 14  | bA    | 3127 | CL7  | C4B-C3B-CAB-OBB |
| 14  | bA    | 3130 | CL7  | C4B-C3B-CAB-OBB |
| 14  | bA    | 3132 | CL7  | C4B-C3B-CAB-OBB |
| 14  | bA    | 3142 | CL7  | C4B-C3B-CAB-OBB |
| 14  | bB    | 821  | CL7  | C4B-C3B-CAB-OBB |
| 14  | bB    | 827  | CL7  | C4B-C3B-CAB-OBB |
| 14  | bJ    | 101  | CL7  | C4B-C3B-CAB-OBB |
| 14  | cA    | 3103 | CL7  | C4B-C3B-CAB-OBB |
| 14  | cA    | 3107 | CL7  | C4B-C3B-CAB-OBB |
| 14  | cA    | 3111 | CL7  | C4B-C3B-CAB-OBB |
| 14  | cB    | 813  | CL7  | C4B-C3B-CAB-OBB |
| 19  | cB    | 830  | LMG  | C4-C5-C6-O5     |
| 14  | aA    | 3115 | CL7  | C2A-CAA-CBA-CGA |
| 14  | aB    | 3032 | CL7  | C2A-CAA-CBA-CGA |
| 14  | bA    | 3114 | CL7  | C2A-CAA-CBA-CGA |
| 14  | bB    | 807  | CL7  | C2A-CAA-CBA-CGA |
| 14  | bB    | 810  | CL7  | C2A-CAA-CBA-CGA |
| 14  | cB    | 808  | CL7  | C1-C2-C3-C5     |
| 14  | bA    | 3114 | CL7  | C2C-C3C-CAC-CBC |
| 14  | aA    | 3107 | CL7  | C13-C15-C16-C17 |
| 14  | aA    | 3127 | CL7  | C2-C1-O2A-CGA   |
| 14  | aB    | 3009 | CL7  | C2-C1-O2A-CGA   |
| 14  | bA    | 3106 | CL7  | C2-C1-O2A-CGA   |
| 14  | bA    | 3126 | CL7  | C2-C1-O2A-CGA   |
| 14  | bB    | 810  | CL7  | C2-C1-O2A-CGA   |
| 14  | cA    | 3106 | CL7  | C2-C1-O2A-CGA   |
| 14  | bB    | 808  | CL7  | O1A-CGA-O2A-C1  |
| 14  | cB    | 808  | CL7  | C3-C5-C6-C7     |
| 12  | bA    | 3101 | G9R  | O1D-CGD-O2D-CED |
| 19  | aB    | 3029 | LMG  | C18-C19-C20-C21 |
| 14  | cB    | 824  | CL7  | C2-C3-C5-C6     |
| 14  | bA    | 3141 | CL7  | C10-C11-C12-C13 |
| 14  | bB    | 833  | CL7  | C1-C2-C3-C5     |
| 16  | aA    | 3138 | LHG  | C3-O3-P-O6      |
| 16  | aA    | 3139 | LHG  | C3-O3-P-O6      |
| 16  | bA    | 3138 | LHG  | C3-O3-P-O6      |
| 16  | bA    | 3138 | LHG  | C4-O6-P-O3      |
| 16  | cA    | 3138 | LHG  | C3-O3-P-O6      |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 13  | aB    | 3004 | PHO  | CHA-CBD-CGD-O1D |
| 13  | bB    | 801  | PHO  | CHA-CBD-CGD-O1D |
| 13  | bB    | 801  | PHO  | CHA-CBD-CGD-O2D |
| 14  | aA    | 3130 | CL7  | O1D-CGD-O2D-CED |
| 14  | aB    | 3005 | CL7  | C2-C3-C5-C6     |
| 14  | bA    | 3141 | CL7  | C6-C7-C8-C10    |
| 14  | bB    | 803  | CL7  | C6-C7-C8-C10    |
| 14  | bB    | 806  | CL7  | C6-C7-C8-C10    |
| 14  | cL    | 204  | CL7  | C11-C10-C8-C7   |
| 17  | aA    | 3144 | PQN  | C22-C23-C25-C26 |
| 17  | cA    | 3143 | PQN  | C21-C22-C23-C25 |
| 13  | bB    | 801  | PHO  | C6-C7-C8-C9     |
| 14  | aA    | 3107 | CL7  | C11-C12-C13-C14 |
| 14  | aA    | 3108 | CL7  | C14-C13-C15-C16 |
| 14  | aB    | 3019 | CL7  | C11-C12-C13-C14 |
| 14  | aB    | 3025 | CL7  | C14-C13-C15-C16 |
| 14  | aL    | 203  | CL7  | C11-C10-C8-C9   |
| 14  | aL    | 203  | CL7  | C14-C13-C15-C16 |
| 14  | bA    | 3128 | CL7  | C6-C7-C8-C9     |
| 14  | bA    | 3142 | CL7  | C11-C12-C13-C14 |
| 14  | bB    | 807  | CL7  | C14-C13-C15-C16 |
| 14  | bB    | 820  | CL7  | C11-C12-C13-C14 |
| 14  | bL    | 203  | CL7  | C11-C10-C8-C9   |
| 14  | cA    | 3106 | CL7  | C11-C12-C13-C14 |
| 14  | cA    | 3124 | CL7  | C11-C12-C13-C14 |
| 14  | cA    | 3142 | CL7  | C11-C12-C13-C14 |
| 14  | cB    | 832  | CL7  | C11-C10-C8-C9   |
| 14  | cL    | 203  | CL7  | C11-C10-C8-C9   |
| 19  | bB    | 830  | LMG  | C12-C13-C14-C15 |
| 14  | aB    | 3025 | CL7  | C13-C15-C16-C17 |
| 14  | cB    | 806  | CL7  | C16-C17-C18-C19 |
| 14  | aA    | 3126 | CL7  | C5-C6-C7-C8     |
| 14  | bB    | 808  | CL7  | C13-C15-C16-C17 |
| 14  | aB    | 3023 | CL7  | C11-C10-C8-C7   |
| 14  | bB    | 819  | CL7  | C11-C10-C8-C7   |
| 14  | cB    | 824  | CL7  | C11-C10-C8-C7   |
| 14  | bB    | 819  | CL7  | CBA-CGA-O2A-C1  |
| 14  | aA    | 3107 | CL7  | O1D-CGD-O2D-CED |
| 14  | cB    | 806  | CL7  | C13-C15-C16-C17 |
| 14  | aA    | 3134 | CL7  | C4C-C3C-CAC-CBC |
| 14  | cB    | 807  | CL7  | C2A-CAA-CBA-CGA |
| 14  | cA    | 3120 | CL7  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | cB    | 806  | CL7  | O1A-CGA-O2A-C1  |
| 14  | aA    | 3134 | CL7  | C2C-C3C-CAC-CBC |
| 16  | cA    | 3137 | LHG  | C24-C25-C26-C27 |
| 14  | aA    | 3123 | CL7  | O1A-CGA-O2A-C1  |
| 14  | aA    | 3129 | CL7  | C10-C11-C12-C13 |
| 14  | aA    | 3103 | CL7  | C4-C3-C5-C6     |
| 14  | aA    | 3107 | CL7  | C4-C3-C5-C6     |
| 14  | aJ    | 101  | CL7  | CAA-CBA-CGA-O1A |
| 14  | cJ    | 101  | CL7  | CAA-CBA-CGA-O1A |
| 14  | aA    | 3133 | CL7  | C2-C3-C5-C6     |
| 14  | bA    | 3123 | CL7  | O1A-CGA-O2A-C1  |
| 14  | cA    | 3116 | CL7  | O1A-CGA-O2A-C1  |
| 14  | aA    | 3129 | CL7  | C2-C1-O2A-CGA   |
| 14  | bA    | 3140 | CL7  | C2-C1-O2A-CGA   |
| 14  | cA    | 3127 | CL7  | C2-C1-O2A-CGA   |
| 14  | bL    | 203  | CL7  | C10-C11-C12-C13 |
| 14  | bA    | 3140 | CL7  | C2A-CAA-CBA-CGA |
| 14  | bA    | 3120 | CL7  | O1D-CGD-O2D-CED |
| 14  | aA    | 3128 | CL7  | C3A-C2A-CAA-CBA |
| 14  | bA    | 3127 | CL7  | C3A-C2A-CAA-CBA |
| 14  | bB    | 807  | CL7  | C3A-C2A-CAA-CBA |
| 14  | bB    | 831  | CL7  | C3A-C2A-CAA-CBA |
| 14  | cB    | 807  | CL7  | C3A-C2A-CAA-CBA |
| 14  | cB    | 831  | CL7  | C3A-C2A-CAA-CBA |
| 14  | cL    | 203  | CL7  | C3A-C2A-CAA-CBA |
| 14  | aL    | 202  | CL7  | C16-C17-C18-C20 |
| 14  | cL    | 204  | CL7  | C16-C17-C18-C19 |
| 13  | cB    | 801  | PHO  | C13-C15-C16-C17 |
| 14  | aB    | 3031 | CL7  | C6-C7-C8-C9     |
| 14  | bA    | 3140 | CL7  | C11-C10-C8-C9   |
| 14  | cA    | 3132 | CL7  | C14-C13-C15-C16 |
| 19  | cB    | 830  | LMG  | C20-C21-C22-C23 |
| 14  | aB    | 3015 | CL7  | O2A-C1-C2-C3    |
| 14  | aB    | 3023 | CL7  | O2A-C1-C2-C3    |
| 14  | bA    | 3139 | CL7  | O2A-C1-C2-C3    |
| 14  | bB    | 826  | CL7  | O2A-C1-C2-C3    |
| 14  | cA    | 3114 | CL7  | O1D-CGD-O2D-CED |
| 14  | aA    | 3107 | CL7  | C5-C6-C7-C8     |
| 12  | bA    | 3101 | G9R  | C1A-C2A-CAA-CBA |
| 12  | cA    | 3101 | G9R  | C1A-C2A-CAA-CBA |
| 14  | bA    | 3127 | CL7  | C1A-C2A-CAA-CBA |
| 14  | bA    | 3139 | CL7  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | cA    | 3142 | CL7  | C1A-C2A-CAA-CBA |
| 19  | aB    | 3029 | LMG  | C19-C20-C21-C22 |
| 13  | aB    | 3004 | PHO  | C11-C10-C8-C7   |
| 13  | bB    | 801  | PHO  | C11-C10-C8-C7   |
| 14  | aA    | 3129 | CL7  | C6-C7-C8-C10    |
| 14  | aB    | 3002 | CL7  | C12-C13-C15-C16 |
| 14  | aL    | 202  | CL7  | C11-C10-C8-C7   |
| 14  | bA    | 3124 | CL7  | C11-C12-C13-C15 |
| 14  | bA    | 3132 | CL7  | C12-C13-C15-C16 |
| 14  | bA    | 3140 | CL7  | C11-C10-C8-C7   |
| 14  | cB    | 808  | CL7  | C12-C13-C15-C16 |
| 14  | cB    | 820  | CL7  | C11-C12-C13-C15 |
| 14  | cL    | 204  | CL7  | C12-C13-C15-C16 |
| 17  | bA    | 3143 | PQN  | C22-C23-C25-C26 |
| 14  | aA    | 3129 | CL7  | C13-C15-C16-C17 |
| 14  | aB    | 3007 | CL7  | C13-C15-C16-C17 |
| 14  | cB    | 832  | CL7  | C8-C10-C11-C12  |
| 14  | bA    | 3120 | CL7  | O1A-CGA-O2A-C1  |
| 14  | aA    | 3143 | CL7  | CAA-CBA-CGA-O2A |
| 14  | aA    | 3103 | CL7  | O1A-CGA-O2A-C1  |
| 16  | bA    | 3137 | LHG  | C32-C33-C34-C35 |
| 14  | cA    | 3142 | CL7  | C10-C11-C12-C13 |
| 14  | cA    | 3142 | CL7  | CAA-CBA-CGA-O2A |
| 14  | bJ    | 101  | CL7  | CAA-CBA-CGA-O1A |
| 14  | bJ    | 101  | CL7  | CAA-CBA-CGA-O2A |
| 14  | bL    | 204  | CL7  | C15-C16-C17-C18 |
| 14  | cB    | 810  | CL7  | C13-C15-C16-C17 |
| 14  | aA    | 3140 | CL7  | C15-C16-C17-C18 |
| 14  | aB    | 3007 | CL7  | C4-C3-C5-C6     |
| 14  | aB    | 3009 | CL7  | C4-C3-C5-C6     |
| 14  | aB    | 3018 | CL7  | C4-C3-C5-C6     |
| 14  | cA    | 3114 | CL7  | C4-C3-C5-C6     |
| 14  | cA    | 3106 | CL7  | C8-C10-C11-C12  |
| 14  | bA    | 3106 | CL7  | C5-C6-C7-C8     |
| 14  | cA    | 3106 | CL7  | C10-C11-C12-C13 |
| 14  | aB    | 3007 | CL7  | O1A-CGA-O2A-C1  |
| 14  | cA    | 3112 | CL7  | O1D-CGD-O2D-CED |
| 14  | bB    | 809  | CL7  | O1D-CGD-O2D-CED |
| 12  | aA    | 3101 | G9R  | C5-C6-C7-C8     |
| 13  | cB    | 805  | PHO  | C8-C10-C11-C12  |
| 14  | bA    | 3114 | CL7  | C4-C3-C5-C6     |
| 14  | bA    | 3128 | CL7  | C4-C3-C5-C6     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | cA    | 3128 | CL7  | C4-C3-C5-C6     |
| 14  | aA    | 3133 | CL7  | C2-C1-O2A-CGA   |
| 14  | cB    | 804  | CL7  | C2-C1-O2A-CGA   |
| 14  | bB    | 806  | CL7  | C13-C15-C16-C17 |
| 14  | cB    | 804  | CL7  | C5-C6-C7-C8     |
| 16  | cA    | 3138 | LHG  | C9-C10-C11-C12  |
| 14  | bB    | 803  | CL7  | C6-C7-C8-C9     |
| 14  | aA    | 3128 | CL7  | C4-C3-C5-C6     |
| 14  | cA    | 3127 | CL7  | C4-C3-C5-C6     |
| 16  | cA    | 3138 | LHG  | C2-C3-O3-P      |
| 14  | bA    | 3140 | CL7  | CAA-CBA-CGA-O2A |
| 14  | aB    | 3009 | CL7  | C2A-CAA-CBA-CGA |
| 13  | cB    | 805  | PHO  | C16-C17-C18-C20 |
| 14  | bB    | 806  | CL7  | C16-C17-C18-C20 |
| 14  | bB    | 808  | CL7  | C1-C2-C3-C5     |
| 14  | cA    | 3142 | CL7  | C1-C2-C3-C5     |
| 13  | bB    | 801  | PHO  | C13-C15-C16-C17 |
| 12  | aA    | 3101 | G9R  | CAA-CBA-CGA-O2A |
| 14  | bA    | 3114 | CL7  | C5-C6-C7-C8     |
| 19  | bB    | 830  | LMG  | C31-C32-C33-C34 |
| 16  | bA    | 3137 | LHG  | C33-C34-C35-C36 |
| 14  | aA    | 3129 | CL7  | C4-C3-C5-C6     |
| 14  | bA    | 3102 | CL7  | C4-C3-C5-C6     |
| 14  | cB    | 810  | CL7  | C4-C3-C5-C6     |
| 14  | cB    | 819  | CL7  | C4-C3-C5-C6     |
| 14  | cL    | 203  | CL7  | C16-C17-C18-C20 |
| 14  | aB    | 3006 | CL7  | C15-C16-C17-C18 |
| 14  | aA    | 3143 | CL7  | C10-C11-C12-C13 |
| 13  | cB    | 805  | PHO  | C16-C17-C18-C19 |
| 14  | aA    | 3127 | CL7  | C3-C5-C6-C7     |
| 14  | aA    | 3107 | CL7  | C15-C16-C17-C18 |
| 16  | bA    | 3137 | LHG  | O6-C4-C5-O7     |
| 14  | cA    | 3123 | CL7  | C1-C2-C3-C5     |
| 14  | bA    | 3130 | CL7  | O1D-CGD-O2D-CED |
| 13  | bB    | 805  | PHO  | C12-C13-C15-C16 |
| 14  | aA    | 3103 | CL7  | C11-C10-C8-C7   |
| 14  | aA    | 3140 | CL7  | C12-C13-C15-C16 |
| 14  | aA    | 3143 | CL7  | C6-C7-C8-C10    |
| 14  | cA    | 3142 | CL7  | C6-C7-C8-C10    |
| 13  | bB    | 801  | PHO  | C8-C10-C11-C12  |
| 14  | aA    | 3115 | CL7  | C1-C2-C3-C4     |
| 14  | aA    | 3124 | CL7  | C1-C2-C3-C4     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | aA    | 3128 | CL7  | C1-C2-C3-C4     |
| 14  | aA    | 3142 | CL7  | C1-C2-C3-C4     |
| 14  | aB    | 3030 | CL7  | C1-C2-C3-C4     |
| 14  | bA    | 3114 | CL7  | C1-C2-C3-C4     |
| 14  | bA    | 3116 | CL7  | C1-C2-C3-C4     |
| 14  | bA    | 3123 | CL7  | C1-C2-C3-C4     |
| 14  | cA    | 3114 | CL7  | C1-C2-C3-C4     |
| 14  | cA    | 3124 | CL7  | C1-C2-C3-C4     |
| 14  | cA    | 3127 | CL7  | C1-C2-C3-C4     |
| 14  | aA    | 3108 | CL7  | C2B-C3B-CAB-OBB |
| 14  | aA    | 3131 | CL7  | C2B-C3B-CAB-OBB |
| 14  | aA    | 3134 | CL7  | C2B-C3B-CAB-OBB |
| 14  | aA    | 3143 | CL7  | C2B-C3B-CAB-OBB |
| 14  | bA    | 3117 | CL7  | C2B-C3B-CAB-OBB |
| 14  | bA    | 3130 | CL7  | C2B-C3B-CAB-OBB |
| 14  | bA    | 3142 | CL7  | C2B-C3B-CAB-OBB |
| 14  | bB    | 821  | CL7  | C2B-C3B-CAB-OBB |
| 14  | bJ    | 101  | CL7  | C2B-C3B-CAB-OBB |
| 14  | cA    | 3102 | CL7  | C2B-C3B-CAB-OBB |
| 14  | cA    | 3103 | CL7  | C2B-C3B-CAB-OBB |
| 14  | cA    | 3107 | CL7  | C2B-C3B-CAB-OBB |
| 14  | cB    | 813  | CL7  | C2B-C3B-CAB-OBB |
| 12  | bA    | 3101 | G9R  | CAA-CBA-CGA-O2A |
| 13  | aB    | 3004 | PHO  | C8-C10-C11-C12  |
| 14  | aA    | 3129 | CL7  | CBA-CGA-O2A-C1  |
| 14  | cA    | 3123 | CL7  | O1A-CGA-O2A-C1  |
| 14  | aA    | 3126 | CL7  | C4-C3-C5-C6     |
| 14  | bA    | 3125 | CL7  | C4-C3-C5-C6     |
| 14  | bB    | 808  | CL7  | C4-C3-C5-C6     |
| 14  | cA    | 3125 | CL7  | C4-C3-C5-C6     |
| 14  | cB    | 808  | CL7  | C4-C3-C5-C6     |
| 14  | cB    | 827  | CL7  | C4-C3-C5-C6     |
| 16  | aA    | 3139 | LHG  | C4-O6-P-O3      |
| 12  | bA    | 3101 | G9R  | C14-C13-C15-C16 |
| 14  | aA    | 3142 | CL7  | C14-C13-C15-C16 |
| 14  | aB    | 3002 | CL7  | C14-C13-C15-C16 |
| 14  | aL    | 202  | CL7  | C11-C10-C8-C9   |
| 14  | bA    | 3106 | CL7  | C11-C12-C13-C14 |
| 14  | bL    | 204  | CL7  | C14-C13-C15-C16 |
| 14  | cB    | 826  | CL7  | C6-C7-C8-C9     |
| 14  | cA    | 3132 | CL7  | C4B-C3B-CAB-OBB |
| 14  | cJ    | 101  | CL7  | C4B-C3B-CAB-OBB |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | aA    | 3103 | CL7  | C3A-C2A-CAA-CBA |
| 14  | aA    | 3123 | CL7  | C3A-C2A-CAA-CBA |
| 14  | aB    | 3006 | CL7  | C3A-C2A-CAA-CBA |
| 14  | cA    | 3142 | CL7  | C3A-C2A-CAA-CBA |
| 14  | aA    | 3107 | CL7  | CAD-CBD-CGD-O2D |
| 14  | aA    | 3109 | CL7  | CAD-CBD-CGD-O2D |
| 14  | aA    | 3113 | CL7  | CAD-CBD-CGD-O2D |
| 14  | aA    | 3128 | CL7  | CAD-CBD-CGD-O2D |
| 14  | aA    | 3132 | CL7  | CAD-CBD-CGD-O2D |
| 14  | aA    | 3143 | CL7  | CAD-CBD-CGD-O2D |
| 14  | aA    | 3146 | CL7  | CAD-CBD-CGD-O2D |
| 14  | aB    | 3009 | CL7  | CAD-CBD-CGD-O2D |
| 14  | aB    | 3010 | CL7  | CAD-CBD-CGD-O2D |
| 14  | aB    | 3017 | CL7  | CAD-CBD-CGD-O2D |
| 14  | aB    | 3022 | CL7  | CAD-CBD-CGD-O2D |
| 14  | bA    | 3104 | CL7  | CAD-CBD-CGD-O2D |
| 14  | bA    | 3108 | CL7  | CAD-CBD-CGD-O2D |
| 14  | bA    | 3112 | CL7  | CAD-CBD-CGD-O2D |
| 14  | bA    | 3120 | CL7  | CAD-CBD-CGD-O2D |
| 14  | bA    | 3127 | CL7  | CAD-CBD-CGD-O2D |
| 14  | bA    | 3133 | CL7  | CAD-CBD-CGD-O2D |
| 14  | bA    | 3141 | CL7  | CAD-CBD-CGD-O2D |
| 14  | bB    | 803  | CL7  | CAD-CBD-CGD-O2D |
| 14  | bB    | 823  | CL7  | CAD-CBD-CGD-O2D |
| 14  | bB    | 832  | CL7  | CAD-CBD-CGD-O2D |
| 14  | cA    | 3104 | CL7  | CAD-CBD-CGD-O2D |
| 14  | cA    | 3106 | CL7  | CAD-CBD-CGD-O2D |
| 14  | cA    | 3127 | CL7  | CAD-CBD-CGD-O2D |
| 14  | cA    | 3133 | CL7  | CAD-CBD-CGD-O2D |
| 14  | cA    | 3142 | CL7  | CAD-CBD-CGD-O2D |
| 14  | cB    | 823  | CL7  | CAD-CBD-CGD-O2D |
| 13  | bB    | 805  | PHO  | C16-C17-C18-C19 |
| 14  | bB    | 804  | CL7  | C8-C10-C11-C12  |
| 14  | bB    | 810  | CL7  | CAA-CBA-CGA-O2A |
| 14  | aB    | 3031 | CL7  | C13-C15-C16-C17 |
| 14  | bB    | 810  | CL7  | C5-C6-C7-C8     |
| 14  | cB    | 808  | CL7  | C5-C6-C7-C8     |
| 14  | aB    | 3005 | CL7  | CAA-CBA-CGA-O2A |
| 14  | cB    | 810  | CL7  | CAA-CBA-CGA-O2A |
| 19  | cB    | 830  | LMG  | C31-C32-C33-C34 |
| 14  | aA    | 3115 | CL7  | CAA-CBA-CGA-O2A |
| 14  | cB    | 806  | CL7  | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | cB    | 831  | CL7  | CAA-CBA-CGA-O2A |
| 13  | aB    | 3004 | PHO  | O2A-C1-C2-C3    |
| 13  | bB    | 805  | PHO  | O2A-C1-C2-C3    |
| 13  | cB    | 805  | PHO  | O2A-C1-C2-C3    |
| 14  | bB    | 804  | CL7  | O2A-C1-C2-C3    |
| 14  | cA    | 3126 | CL7  | O2A-C1-C2-C3    |
| 14  | cB    | 804  | CL7  | O2A-C1-C2-C3    |
| 14  | cB    | 806  | CL7  | O2A-C1-C2-C3    |
| 14  | bB    | 824  | CL7  | CAA-CBA-CGA-O2A |
| 14  | aA    | 3107 | CL7  | C3-C5-C6-C7     |
| 14  | aA    | 3126 | CL7  | O1D-CGD-O2D-CED |
| 14  | aB    | 3013 | CL7  | O1D-CGD-O2D-CED |
| 14  | cA    | 3122 | CL7  | O1D-CGD-O2D-CED |
| 14  | aA    | 3106 | CL7  | CHA-CBD-CGD-O1D |
| 14  | aA    | 3107 | CL7  | CHA-CBD-CGD-O1D |
| 14  | aA    | 3132 | CL7  | CHA-CBD-CGD-O2D |
| 14  | aA    | 3141 | CL7  | CHA-CBD-CGD-O1D |
| 14  | aA    | 3146 | CL7  | CHA-CBD-CGD-O2D |
| 14  | aB    | 3007 | CL7  | CHA-CBD-CGD-O2D |
| 14  | aB    | 3017 | CL7  | CHA-CBD-CGD-O1D |
| 14  | aB    | 3021 | CL7  | CHA-CBD-CGD-O2D |
| 14  | aB    | 3030 | CL7  | CHA-CBD-CGD-O2D |
| 14  | aL    | 202  | CL7  | CHA-CBD-CGD-O2D |
| 14  | bA    | 3102 | CL7  | CHA-CBD-CGD-O1D |
| 14  | bA    | 3105 | CL7  | CHA-CBD-CGD-O1D |
| 14  | bA    | 3106 | CL7  | CHA-CBD-CGD-O1D |
| 14  | bA    | 3120 | CL7  | CHA-CBD-CGD-O1D |
| 14  | bA    | 3130 | CL7  | CHA-CBD-CGD-O1D |
| 14  | bA    | 3141 | CL7  | CHA-CBD-CGD-O1D |
| 14  | bB    | 808  | CL7  | CHA-CBD-CGD-O2D |
| 14  | bB    | 810  | CL7  | CHA-CBD-CGD-O2D |
| 14  | bB    | 823  | CL7  | CHA-CBD-CGD-O1D |
| 14  | bB    | 831  | CL7  | CHA-CBD-CGD-O1D |
| 14  | bL    | 203  | CL7  | CHA-CBD-CGD-O2D |
| 14  | cA    | 3102 | CL7  | CHA-CBD-CGD-O2D |
| 14  | cA    | 3103 | CL7  | CHA-CBD-CGD-O1D |
| 14  | cA    | 3105 | CL7  | CHA-CBD-CGD-O1D |
| 14  | cA    | 3106 | CL7  | CHA-CBD-CGD-O1D |
| 14  | cA    | 3130 | CL7  | CHA-CBD-CGD-O1D |
| 14  | cA    | 3131 | CL7  | CHA-CBD-CGD-O2D |
| 14  | cA    | 3144 | CL7  | CHA-CBD-CGD-O1D |
| 14  | cB    | 817  | CL7  | CHA-CBD-CGD-O2D |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | cB    | 818  | CL7  | CHA-CBD-CGD-O2D |
| 14  | cB    | 832  | CL7  | CHA-CBD-CGD-O2D |
| 14  | cB    | 833  | CL7  | CHA-CBD-CGD-O2D |
| 14  | cL    | 203  | CL7  | CHA-CBD-CGD-O2D |
| 14  | bA    | 3121 | CL7  | C2C-C3C-CAC-CBC |
| 16  | bA    | 3137 | LHG  | O6-C4-C5-C6     |
| 14  | bA    | 3106 | CL7  | C15-C16-C17-C18 |
| 14  | bB    | 806  | CL7  | CAA-CBA-CGA-O2A |
| 14  | cA    | 3114 | CL7  | CAA-CBA-CGA-O2A |
| 14  | cB    | 824  | CL7  | CAA-CBA-CGA-O2A |
| 19  | bB    | 830  | LMG  | O7-C8-C9-O8     |
| 19  | cB    | 830  | LMG  | O7-C8-C9-O8     |
| 14  | cA    | 3125 | CL7  | CBA-CGA-O2A-C1  |
| 14  | cB    | 820  | CL7  | CBA-CGA-O2A-C1  |
| 14  | aA    | 3133 | CL7  | C3-C5-C6-C7     |
| 14  | aB    | 3009 | CL7  | CAA-CBA-CGA-O2A |
| 14  | cB    | 820  | CL7  | CAA-CBA-CGA-O2A |
| 14  | aA    | 3108 | CL7  | C4-C3-C5-C6     |
| 14  | cB    | 823  | CL7  | C4C-C3C-CAC-CBC |
| 14  | aA    | 3103 | CL7  | C11-C12-C13-C15 |
| 14  | aA    | 3108 | CL7  | C11-C12-C13-C15 |
| 14  | aB    | 3026 | CL7  | C12-C13-C15-C16 |
| 14  | bA    | 3142 | CL7  | C6-C7-C8-C10    |
| 13  | aB    | 3004 | PHO  | C16-C17-C18-C20 |
| 14  | cL    | 204  | CL7  | C16-C17-C18-C20 |
| 14  | cB    | 827  | CL7  | C10-C11-C12-C13 |
| 13  | bB    | 801  | PHO  | C11-C10-C8-C9   |
| 14  | bA    | 3124 | CL7  | C11-C12-C13-C14 |
| 14  | bB    | 832  | CL7  | C14-C13-C15-C16 |
| 14  | cB    | 803  | CL7  | C11-C10-C8-C9   |
| 14  | cB    | 820  | CL7  | C11-C12-C13-C14 |
| 14  | cL    | 204  | CL7  | C14-C13-C15-C16 |
| 17  | cB    | 828  | PQN  | C15-C16-C17-C18 |
| 14  | aA    | 3107 | CL7  | CAA-CBA-CGA-O2A |
| 14  | bB    | 831  | CL7  | CAA-CBA-CGA-O2A |
| 14  | cA    | 3106 | CL7  | CAA-CBA-CGA-O2A |
| 13  | aB    | 3004 | PHO  | C16-C17-C18-C19 |
| 14  | bB    | 804  | CL7  | C1-C2-C3-C5     |
| 14  | bB    | 823  | CL7  | C4C-C3C-CAC-CBC |
| 14  | bB    | 824  | CL7  | C11-C10-C8-C9   |
| 14  | bA    | 3106 | CL7  | CAA-CBA-CGA-O2A |
| 14  | bA    | 3126 | CL7  | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | bB    | 810  | CL7  | C4-C3-C5-C6     |
| 14  | cB    | 833  | CL7  | CAA-CBA-CGA-O1A |
| 14  | aA    | 3141 | CL7  | C2C-C3C-CAC-CBC |
| 14  | cB    | 831  | CL7  | CBA-CGA-O2A-C1  |
| 14  | bA    | 3140 | CL7  | C1A-C2A-CAA-CBA |
| 14  | cA    | 3127 | CL7  | C1A-C2A-CAA-CBA |
| 14  | cB    | 803  | CL7  | C1A-C2A-CAA-CBA |
| 14  | aB    | 3023 | CL7  | CAA-CBA-CGA-O2A |
| 19  | aB    | 3029 | LMG  | C21-C22-C23-C24 |
| 14  | bA    | 3116 | CL7  | C2-C1-O2A-CGA   |
| 14  | bL    | 204  | CL7  | C2-C1-O2A-CGA   |
| 14  | cB    | 826  | CL7  | C2-C1-O2A-CGA   |
| 14  | cB    | 832  | CL7  | CAA-CBA-CGA-O2A |
| 14  | bB    | 833  | CL7  | CBD-CGD-O2D-CED |
| 14  | aA    | 3117 | CL7  | CAA-CBA-CGA-O1A |
| 14  | aB    | 3031 | CL7  | C2-C3-C5-C6     |
| 14  | cA    | 3142 | CL7  | C13-C15-C16-C17 |
| 16  | bA    | 3138 | LHG  | C4-O6-P-O5      |
| 14  | cA    | 3132 | CL7  | C15-C16-C17-C18 |
| 14  | bB    | 809  | CL7  | O1A-CGA-O2A-C1  |
| 13  | bB    | 805  | PHO  | C8-C10-C11-C12  |
| 14  | bA    | 3119 | CL7  | C4C-C3C-CAC-CBC |
| 14  | cA    | 3132 | CL7  | CAA-CBA-CGA-O2A |
| 13  | bB    | 805  | PHO  | C16-C17-C18-C20 |
| 14  | cA    | 3140 | CL7  | C16-C17-C18-C19 |
| 14  | bL    | 204  | CL7  | O1D-CGD-O2D-CED |
| 14  | cJ    | 101  | CL7  | CAA-CBA-CGA-O2A |
| 14  | bB    | 807  | CL7  | CAA-CBA-CGA-O2A |
| 14  | aB    | 3007 | CL7  | C1-C2-C3-C5     |
| 14  | aB    | 3026 | CL7  | C4-C3-C5-C6     |
| 14  | bA    | 3107 | CL7  | C4-C3-C5-C6     |
| 14  | cA    | 3107 | CL7  | C4-C3-C5-C6     |
| 14  | cB    | 807  | CL7  | O1D-CGD-O2D-CED |
| 19  | cB    | 830  | LMG  | C21-C22-C23-C24 |
| 14  | aA    | 3113 | CL7  | CAD-CBD-CGD-O1D |
| 14  | aA    | 3129 | CL7  | CAD-CBD-CGD-O1D |
| 14  | aB    | 3010 | CL7  | CAD-CBD-CGD-O1D |
| 14  | bA    | 3112 | CL7  | CAD-CBD-CGD-O1D |
| 14  | bB    | 820  | CL7  | CAD-CBD-CGD-O1D |
| 14  | cB    | 807  | CL7  | CAD-CBD-CGD-O1D |
| 14  | cB    | 808  | CL7  | CAD-CBD-CGD-O1D |
| 14  | cL    | 203  | CL7  | CAD-CBD-CGD-O1D |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | aA    | 3127 | CL7  | CAA-CBA-CGA-O1A |
| 14  | cA    | 3116 | CL7  | CAA-CBA-CGA-O1A |
| 14  | cL    | 204  | CL7  | C10-C11-C12-C13 |
| 13  | cB    | 801  | PHO  | C11-C10-C8-C9   |
| 14  | bA    | 3132 | CL7  | C14-C13-C15-C16 |
| 14  | cB    | 832  | CL7  | C14-C13-C15-C16 |
| 14  | aB    | 3025 | CL7  | C5-C6-C7-C8     |
| 14  | bB    | 832  | CL7  | C8-C10-C11-C12  |
| 14  | aB    | 3030 | CL7  | O1A-CGA-O2A-C1  |
| 14  | bA    | 3128 | CL7  | CBA-CGA-O2A-C1  |
| 14  | aA    | 3121 | CL7  | CAA-CBA-CGA-O2A |
| 14  | bB    | 832  | CL7  | CAA-CBA-CGA-O2A |
| 14  | bA    | 3125 | CL7  | C8-C10-C11-C12  |
| 14  | cA    | 3106 | CL7  | O1D-CGD-O2D-CED |
| 14  | aB    | 3006 | CL7  | CAA-CBA-CGA-O2A |
| 14  | bA    | 3139 | CL7  | CAA-CBA-CGA-O2A |
| 14  | aJ    | 101  | CL7  | CAA-CBA-CGA-O2A |
| 14  | bB    | 833  | CL7  | CAA-CBA-CGA-O1A |
| 16  | bA    | 3138 | LHG  | C2-C3-O3-P      |
| 14  | aA    | 3115 | CL7  | C4-C3-C5-C6     |
| 14  | bA    | 3106 | CL7  | C8-C10-C11-C12  |
| 13  | aA    | 3102 | PHO  | C6-C7-C8-C10    |
| 13  | cB    | 805  | PHO  | C12-C13-C15-C16 |
| 14  | aA    | 3108 | CL7  | C6-C7-C8-C10    |
| 14  | aA    | 3108 | CL7  | C12-C13-C15-C16 |
| 14  | aA    | 3140 | CL7  | C3A-C2A-CAA-CBA |
| 14  | aB    | 3023 | CL7  | C6-C7-C8-C10    |
| 14  | aL    | 202  | CL7  | C12-C13-C15-C16 |
| 14  | aL    | 203  | CL7  | C6-C7-C8-C10    |
| 14  | bL    | 203  | CL7  | C12-C13-C15-C16 |
| 14  | bL    | 204  | CL7  | C12-C13-C15-C16 |
| 14  | cA    | 3139 | CL7  | C3A-C2A-CAA-CBA |
| 14  | cB    | 827  | CL7  | C12-C13-C15-C16 |
| 14  | cB    | 832  | CL7  | C2-C3-C5-C6     |
| 14  | cB    | 832  | CL7  | C12-C13-C15-C16 |
| 14  | bA    | 3123 | CL7  | CAA-CBA-CGA-O1A |
| 19  | aB    | 3029 | LMG  | C15-C16-C17-C18 |
| 14  | aB    | 3031 | CL7  | CAA-CBA-CGA-O2A |
| 14  | bA    | 3114 | CL7  | CAA-CBA-CGA-O2A |
| 14  | cA    | 3140 | CL7  | CAA-CBA-CGA-O2A |
| 14  | cB    | 807  | CL7  | CAA-CBA-CGA-O2A |
| 14  | bA    | 3116 | CL7  | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | bB    | 827  | CL7  | CAA-CBA-CGA-O1A |
| 14  | aA    | 3123 | CL7  | CAA-CBA-CGA-O2A |
| 14  | cB    | 808  | CL7  | C15-C16-C17-C18 |
| 14  | cA    | 3139 | CL7  | CAA-CBA-CGA-O2A |
| 13  | aA    | 3102 | PHO  | C13-C15-C16-C17 |
| 14  | cB    | 807  | CL7  | C15-C16-C17-C18 |

There are no ring outliers.

169 monomers are involved in 415 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 14  | aA    | 3142 | CL7  | 3       | 0            |
| 14  | cA    | 3113 | CL7  | 1       | 0            |
| 14  | cL    | 205  | CL7  | 1       | 0            |
| 14  | cB    | 808  | CL7  | 5       | 0            |
| 14  | bL    | 203  | CL7  | 5       | 0            |
| 14  | aA    | 3120 | CL7  | 1       | 0            |
| 13  | cB    | 805  | PHO  | 8       | 0            |
| 14  | aF    | 201  | CL7  | 1       | 0            |
| 14  | bB    | 827  | CL7  | 3       | 0            |
| 14  | bA    | 3103 | CL7  | 1       | 0            |
| 14  | bA    | 3129 | CL7  | 1       | 0            |
| 14  | cB    | 816  | CL7  | 1       | 0            |
| 14  | aA    | 3140 | CL7  | 3       | 0            |
| 14  | aB    | 3009 | CL7  | 2       | 0            |
| 14  | cA    | 3139 | CL7  | 2       | 0            |
| 14  | bA    | 3118 | CL7  | 1       | 0            |
| 14  | aA    | 3122 | CL7  | 3       | 0            |
| 14  | cB    | 823  | CL7  | 1       | 0            |
| 14  | bB    | 814  | CL7  | 1       | 0            |
| 14  | bB    | 817  | CL7  | 2       | 0            |
| 14  | aB    | 3006 | CL7  | 5       | 0            |
| 14  | bB    | 832  | CL7  | 8       | 0            |
| 14  | cA    | 3124 | CL7  | 2       | 0            |
| 14  | cA    | 3106 | CL7  | 3       | 0            |
| 14  | cB    | 810  | CL7  | 2       | 0            |
| 14  | aA    | 3114 | CL7  | 1       | 0            |
| 14  | aA    | 3108 | CL7  | 2       | 0            |
| 14  | bA    | 3139 | CL7  | 1       | 0            |
| 14  | cB    | 833  | CL7  | 3       | 0            |
| 14  | bA    | 3105 | CL7  | 1       | 0            |
| 16  | cA    | 3137 | LHG  | 2       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 17  | bB    | 828  | PQN  | 3       | 0            |
| 14  | bL    | 204  | CL7  | 7       | 0            |
| 14  | cA    | 3125 | CL7  | 4       | 0            |
| 14  | aA    | 3109 | CL7  | 1       | 0            |
| 14  | aA    | 3117 | CL7  | 2       | 0            |
| 14  | aB    | 3021 | CL7  | 4       | 0            |
| 14  | cB    | 826  | CL7  | 4       | 0            |
| 17  | cB    | 828  | PQN  | 1       | 0            |
| 14  | cA    | 3131 | CL7  | 1       | 0            |
| 14  | aA    | 3106 | CL7  | 1       | 0            |
| 13  | aA    | 3102 | PHO  | 7       | 0            |
| 14  | cB    | 815  | CL7  | 1       | 0            |
| 14  | cB    | 819  | CL7  | 5       | 0            |
| 19  | cB    | 830  | LMG  | 2       | 0            |
| 14  | cB    | 820  | CL7  | 4       | 0            |
| 14  | bA    | 3123 | CL7  | 2       | 0            |
| 14  | bA    | 3116 | CL7  | 2       | 0            |
| 13  | bB    | 805  | PHO  | 9       | 0            |
| 14  | aB    | 3013 | CL7  | 1       | 0            |
| 14  | bA    | 3131 | CL7  | 1       | 0            |
| 14  | cB    | 807  | CL7  | 5       | 0            |
| 16  | bA    | 3137 | LHG  | 3       | 0            |
| 14  | aA    | 3111 | CL7  | 1       | 0            |
| 14  | cA    | 3115 | CL7  | 3       | 0            |
| 14  | aB    | 3019 | CL7  | 9       | 0            |
| 17  | aA    | 3144 | PQN  | 1       | 0            |
| 13  | bB    | 801  | PHO  | 8       | 0            |
| 14  | cA    | 3114 | CL7  | 3       | 0            |
| 14  | cF    | 201  | CL7  | 1       | 0            |
| 14  | aA    | 3127 | CL7  | 1       | 0            |
| 14  | cA    | 3103 | CL7  | 1       | 0            |
| 14  | cA    | 3119 | CL7  | 2       | 0            |
| 14  | aB    | 3022 | CL7  | 1       | 0            |
| 14  | cB    | 804  | CL7  | 5       | 0            |
| 14  | aB    | 3031 | CL7  | 6       | 0            |
| 14  | bB    | 808  | CL7  | 4       | 0            |
| 14  | bJ    | 101  | CL7  | 1       | 0            |
| 16  | cA    | 3138 | LHG  | 1       | 0            |
| 16  | bA    | 3138 | LHG  | 1       | 0            |
| 14  | aA    | 3129 | CL7  | 3       | 0            |
| 14  | aA    | 3116 | CL7  | 3       | 0            |
| 14  | bB    | 809  | CL7  | 1       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 14  | bA    | 3119 | CL7  | 2       | 0            |
| 14  | cB    | 831  | CL7  | 1       | 0            |
| 14  | aL    | 202  | CL7  | 4       | 0            |
| 14  | bA    | 3113 | CL7  | 1       | 0            |
| 14  | aL    | 203  | CL7  | 7       | 0            |
| 14  | bB    | 826  | CL7  | 6       | 0            |
| 14  | cA    | 3121 | CL7  | 1       | 0            |
| 14  | bA    | 3125 | CL7  | 4       | 0            |
| 14  | cA    | 3116 | CL7  | 4       | 0            |
| 14  | cB    | 822  | CL7  | 3       | 0            |
| 14  | aA    | 3143 | CL7  | 1       | 0            |
| 14  | cA    | 3102 | CL7  | 2       | 0            |
| 14  | bB    | 815  | CL7  | 1       | 0            |
| 14  | cA    | 3142 | CL7  | 4       | 0            |
| 14  | cA    | 3105 | CL7  | 2       | 0            |
| 14  | bB    | 804  | CL7  | 2       | 0            |
| 14  | aB    | 3016 | CL7  | 2       | 0            |
| 13  | aB    | 3004 | PHO  | 9       | 0            |
| 14  | bB    | 803  | CL7  | 5       | 0            |
| 14  | cA    | 3112 | CL7  | 1       | 0            |
| 14  | bA    | 3124 | CL7  | 3       | 0            |
| 14  | bA    | 3121 | CL7  | 1       | 0            |
| 14  | bA    | 3106 | CL7  | 6       | 0            |
| 14  | cL    | 204  | CL7  | 8       | 0            |
| 14  | bB    | 819  | CL7  | 4       | 0            |
| 14  | cA    | 3140 | CL7  | 5       | 0            |
| 14  | bA    | 3141 | CL7  | 5       | 0            |
| 14  | cL    | 203  | CL7  | 6       | 0            |
| 14  | aB    | 3030 | CL7  | 2       | 0            |
| 14  | cB    | 809  | CL7  | 1       | 0            |
| 14  | aA    | 3107 | CL7  | 7       | 0            |
| 14  | cB    | 814  | CL7  | 1       | 0            |
| 14  | aA    | 3103 | CL7  | 2       | 0            |
| 14  | bL    | 205  | CL7  | 1       | 0            |
| 14  | cA    | 3123 | CL7  | 4       | 0            |
| 14  | bF    | 201  | CL7  | 1       | 0            |
| 17  | bA    | 3143 | PQN  | 3       | 0            |
| 14  | aA    | 3104 | CL7  | 1       | 0            |
| 14  | cB    | 827  | CL7  | 3       | 0            |
| 14  | cB    | 832  | CL7  | 8       | 0            |
| 16  | aA    | 3138 | LHG  | 2       | 0            |
| 14  | bA    | 3132 | CL7  | 2       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 14  | aB    | 3005 | CL7  | 3       | 0            |
| 14  | bB    | 820  | CL7  | 6       | 0            |
| 14  | bB    | 810  | CL7  | 1       | 0            |
| 14  | cA    | 3107 | CL7  | 1       | 0            |
| 14  | cA    | 3118 | CL7  | 1       | 0            |
| 17  | aB    | 3027 | PQN  | 1       | 0            |
| 14  | aA    | 3125 | CL7  | 2       | 0            |
| 14  | cB    | 817  | CL7  | 2       | 0            |
| 14  | bA    | 3128 | CL7  | 5       | 0            |
| 14  | bB    | 816  | CL7  | 2       | 0            |
| 19  | aB    | 3029 | LMG  | 1       | 0            |
| 19  | bB    | 830  | LMG  | 1       | 0            |
| 14  | aB    | 3018 | CL7  | 6       | 0            |
| 14  | cA    | 3126 | CL7  | 2       | 0            |
| 14  | aA    | 3123 | CL7  | 2       | 0            |
| 14  | bA    | 3115 | CL7  | 3       | 0            |
| 14  | bB    | 822  | CL7  | 4       | 0            |
| 14  | aA    | 3119 | CL7  | 1       | 0            |
| 14  | aA    | 3121 | CL7  | 1       | 0            |
| 14  | aB    | 3008 | CL7  | 2       | 0            |
| 14  | aB    | 3032 | CL7  | 2       | 0            |
| 14  | bB    | 831  | CL7  | 1       | 0            |
| 14  | aA    | 3141 | CL7  | 6       | 0            |
| 14  | bB    | 823  | CL7  | 1       | 0            |
| 14  | aA    | 3134 | CL7  | 1       | 0            |
| 16  | aA    | 3139 | LHG  | 1       | 0            |
| 14  | aB    | 3002 | CL7  | 4       | 0            |
| 14  | aB    | 3014 | CL7  | 1       | 0            |
| 14  | bA    | 3140 | CL7  | 2       | 0            |
| 14  | bB    | 833  | CL7  | 5       | 0            |
| 14  | cA    | 3128 | CL7  | 2       | 0            |
| 14  | bB    | 807  | CL7  | 5       | 0            |
| 14  | aA    | 3124 | CL7  | 2       | 0            |
| 14  | bA    | 3122 | CL7  | 2       | 0            |
| 14  | bA    | 3102 | CL7  | 2       | 0            |
| 14  | cB    | 803  | CL7  | 4       | 0            |
| 14  | aB    | 3003 | CL7  | 3       | 0            |
| 14  | aB    | 3025 | CL7  | 3       | 0            |
| 14  | cA    | 3141 | CL7  | 8       | 0            |
| 14  | aB    | 3007 | CL7  | 7       | 0            |
| 14  | bA    | 3142 | CL7  | 6       | 0            |
| 14  | bA    | 3114 | CL7  | 4       | 0            |

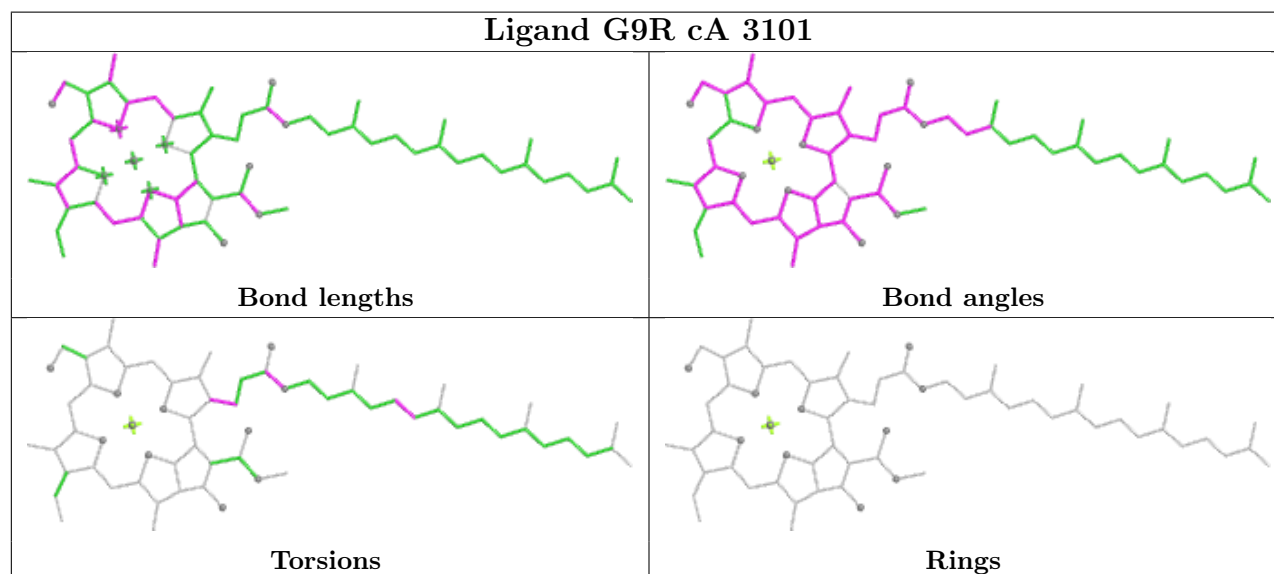
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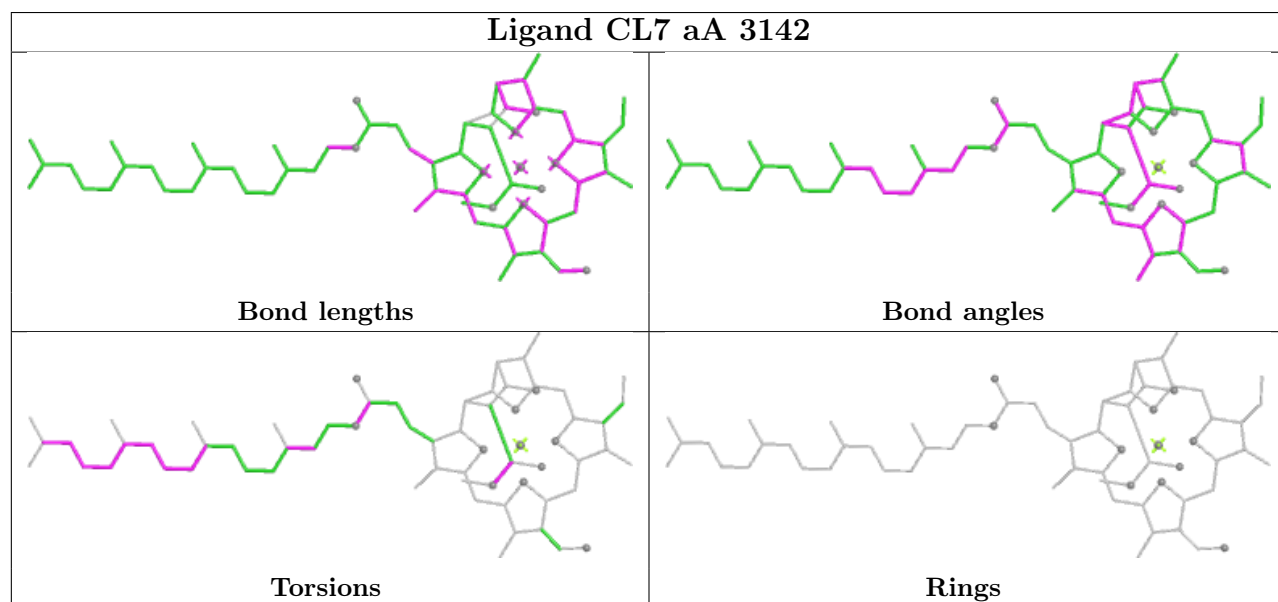
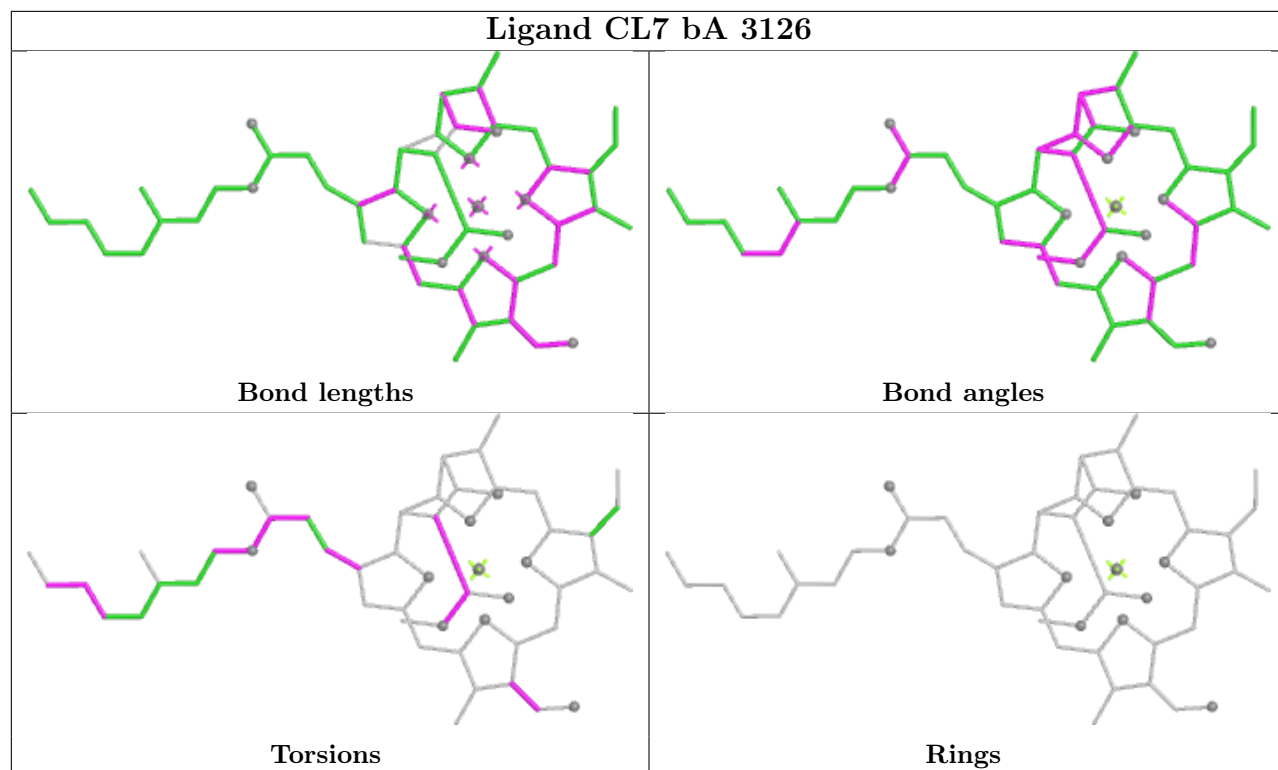


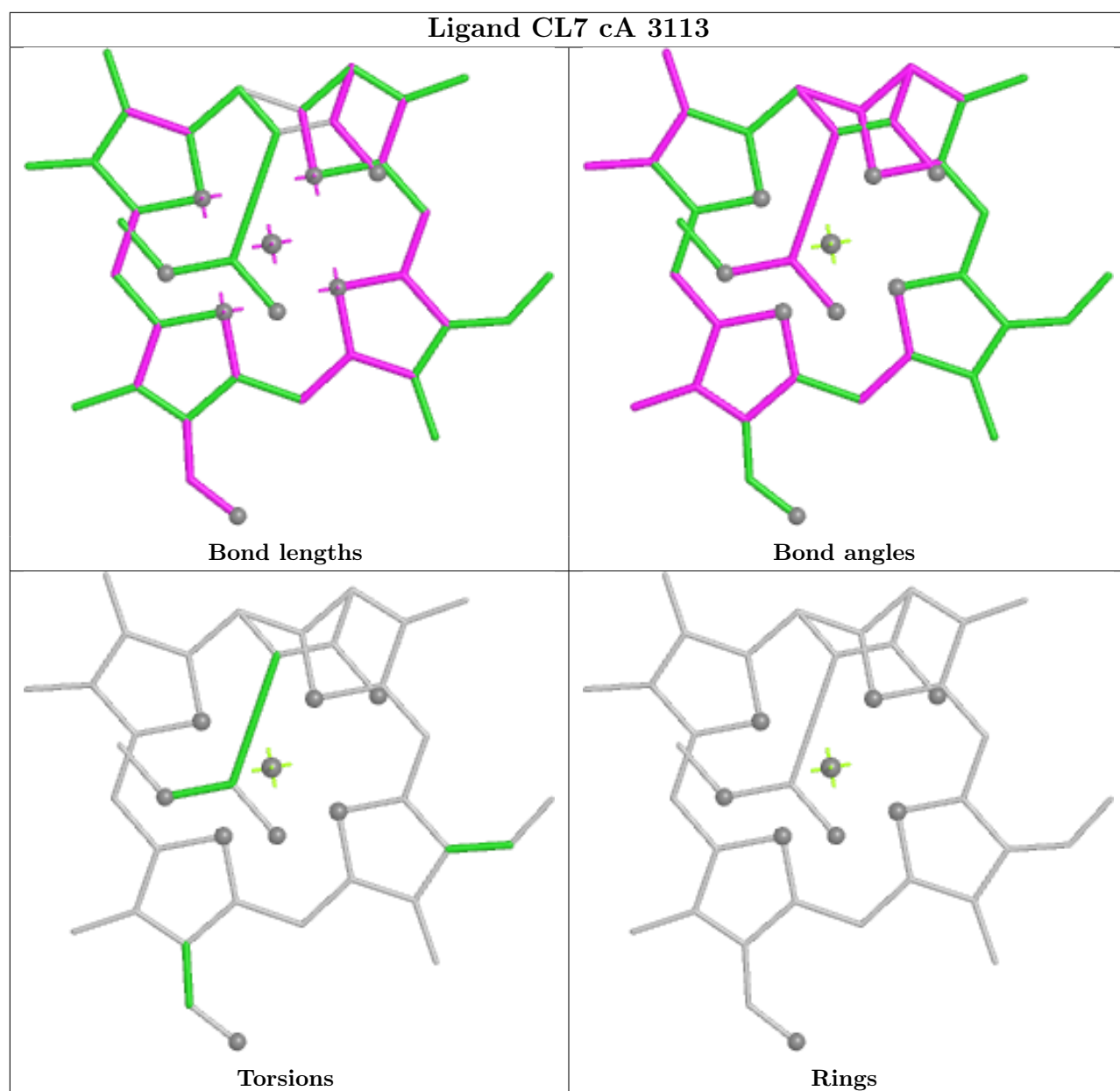
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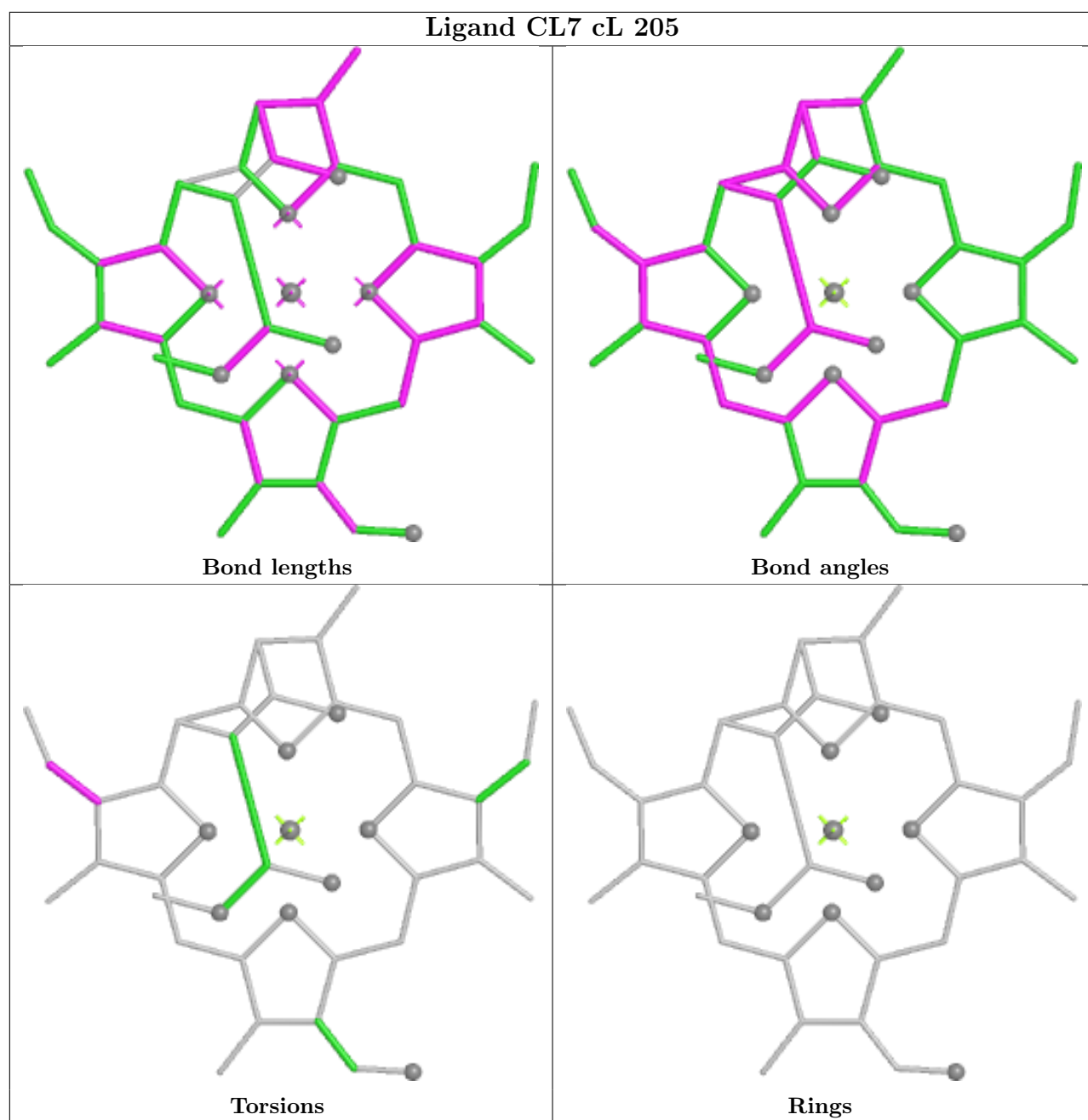
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 14  | cA    | 3120 | CL7  | 2       | 0            |
| 14  | aB    | 3026 | CL7  | 4       | 0            |
| 14  | bB    | 806  | CL7  | 4       | 0            |
| 14  | cB    | 806  | CL7  | 1       | 0            |
| 17  | cA    | 3143 | PQN  | 2       | 0            |
| 14  | aB    | 3023 | CL7  | 1       | 0            |
| 14  | bA    | 3112 | CL7  | 1       | 0            |
| 13  | cB    | 801  | PHO  | 11      | 0            |
| 14  | aA    | 3126 | CL7  | 4       | 0            |
| 14  | aA    | 3115 | CL7  | 2       | 0            |
| 14  | aA    | 3133 | CL7  | 2       | 0            |
| 14  | bA    | 3120 | CL7  | 2       | 0            |

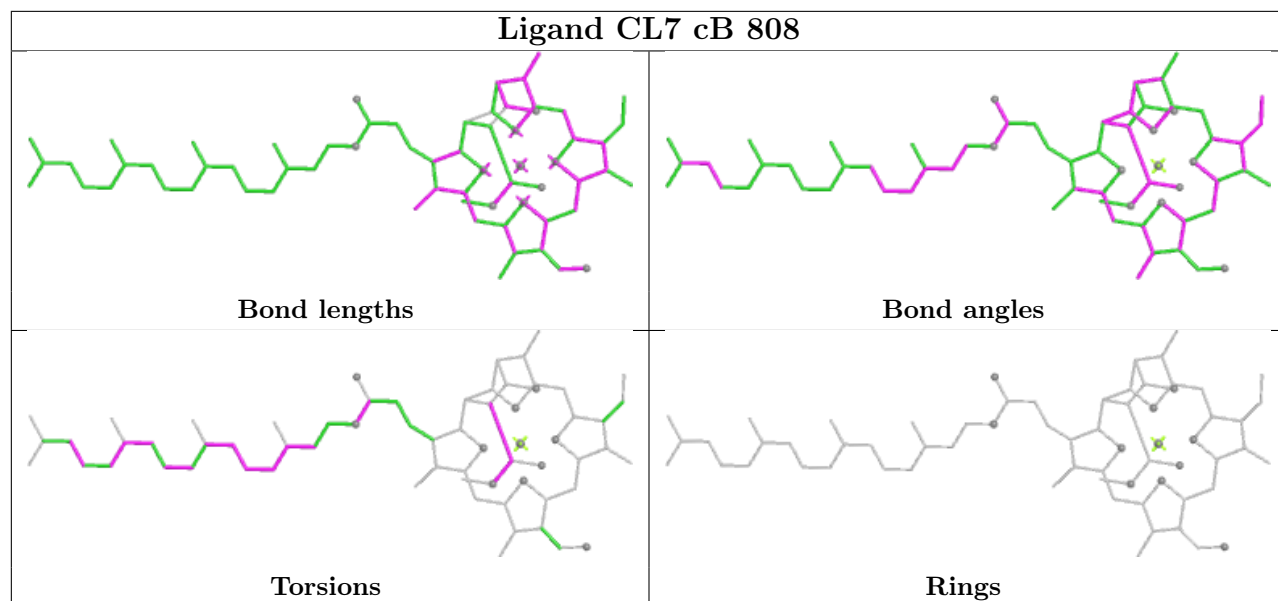
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

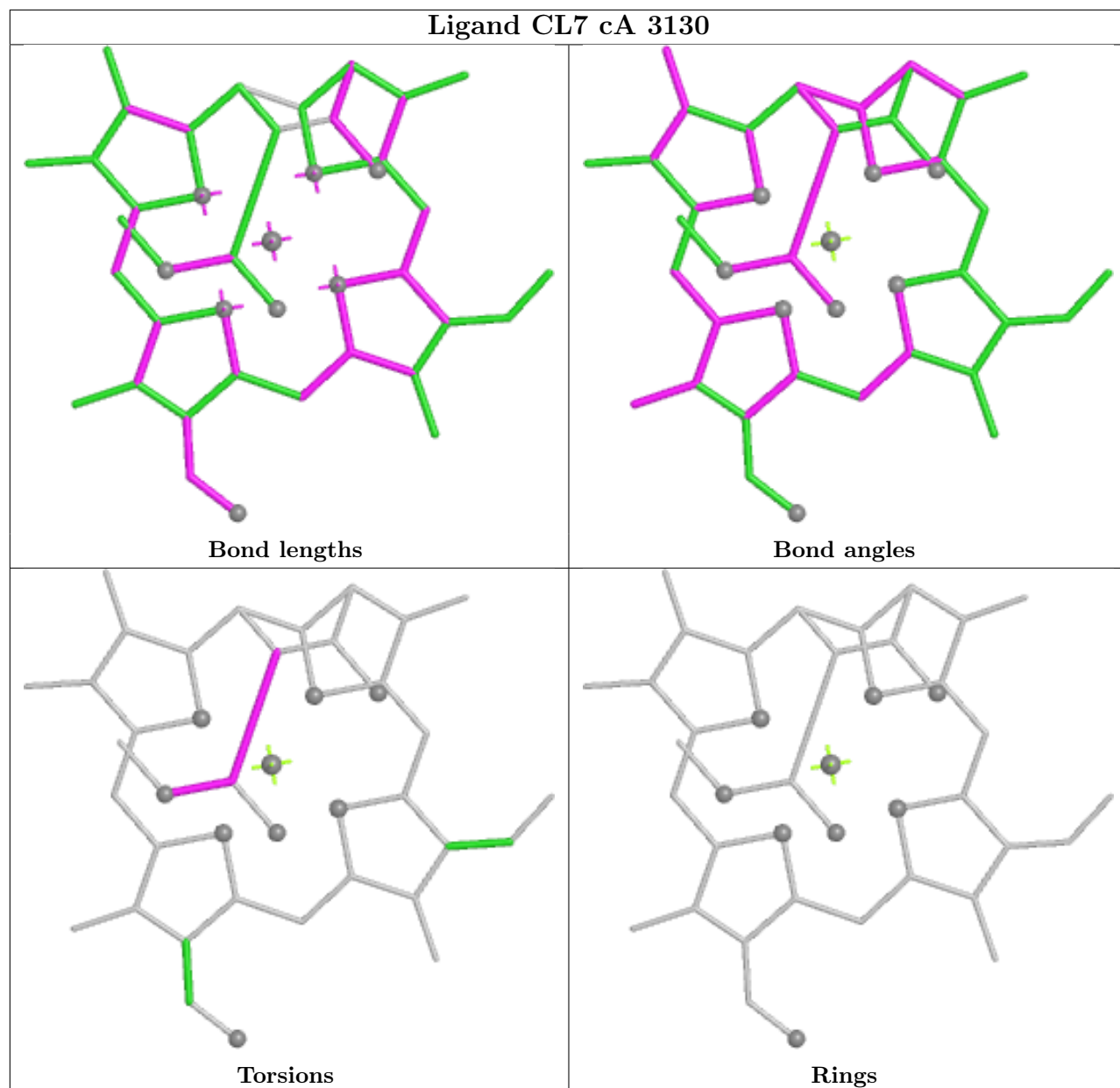


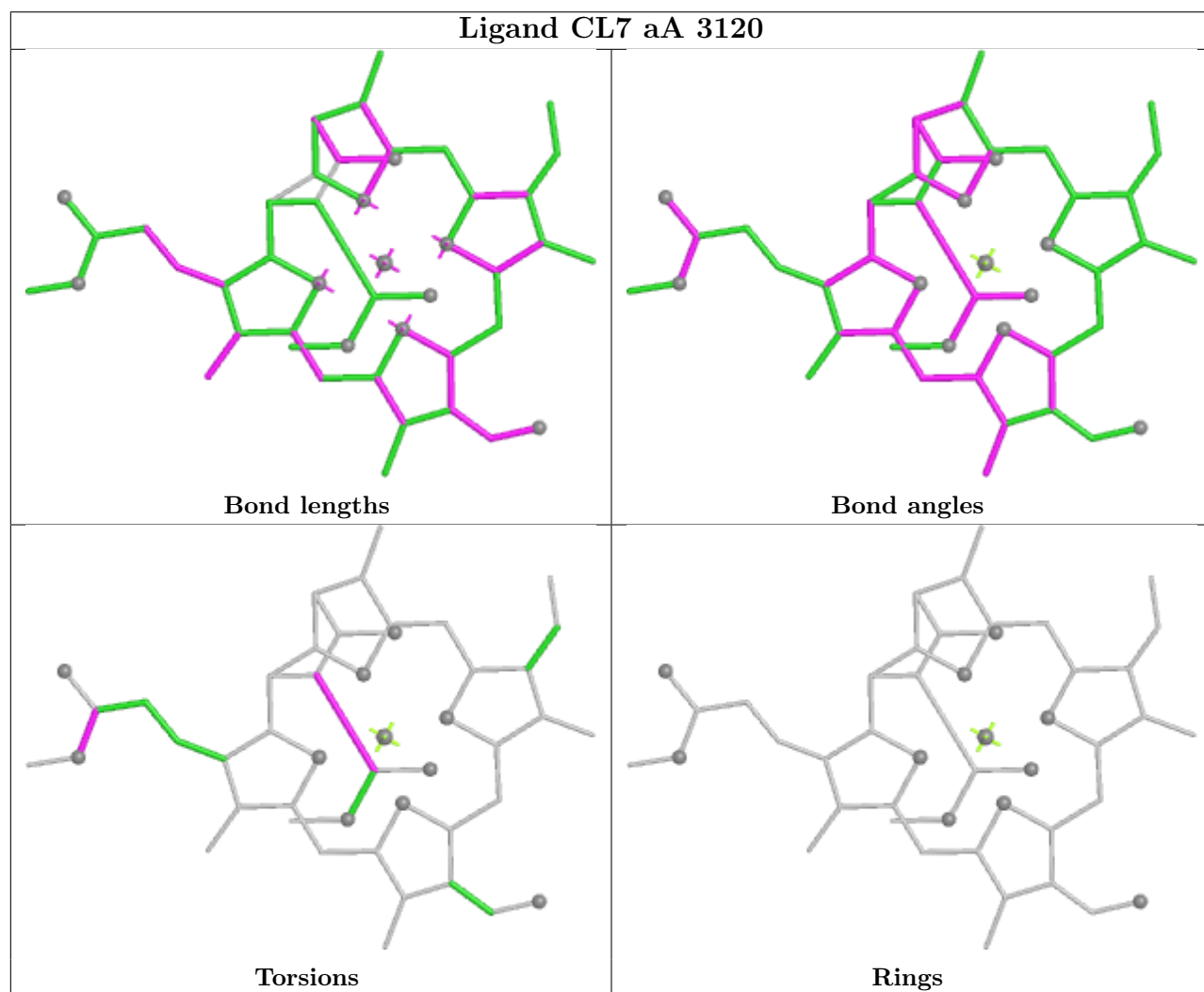
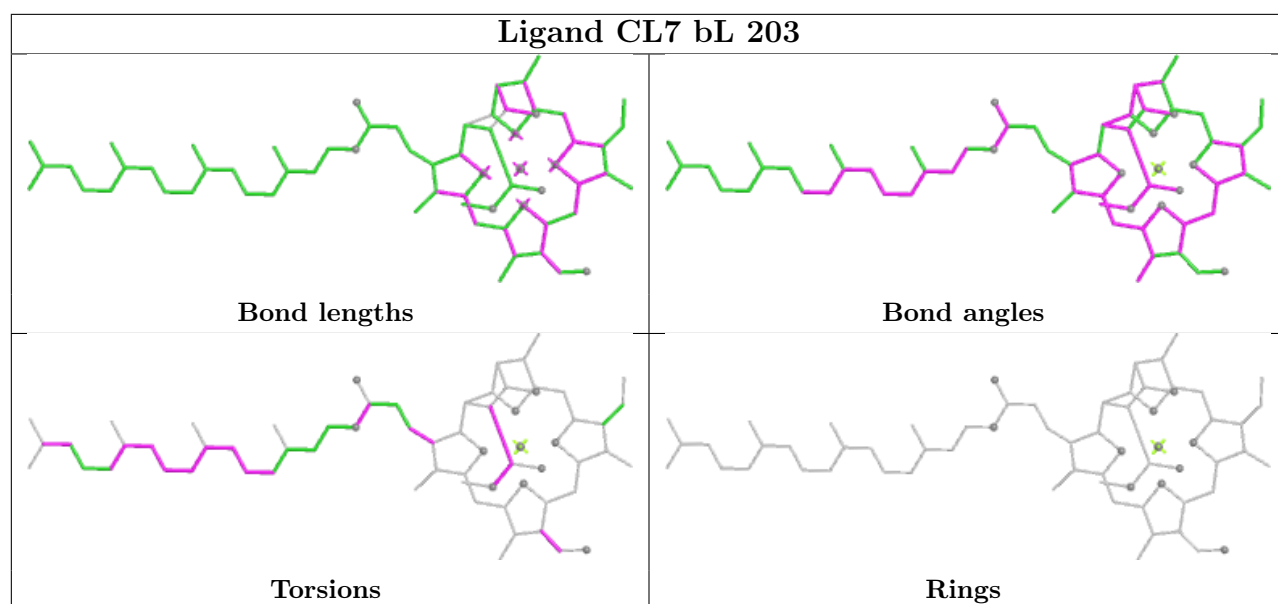






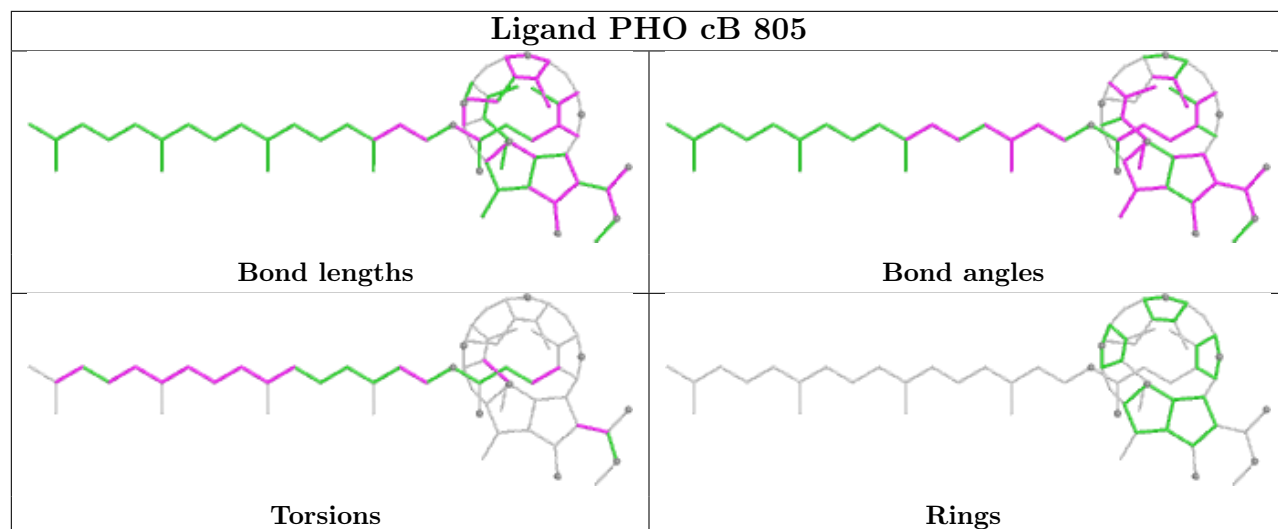




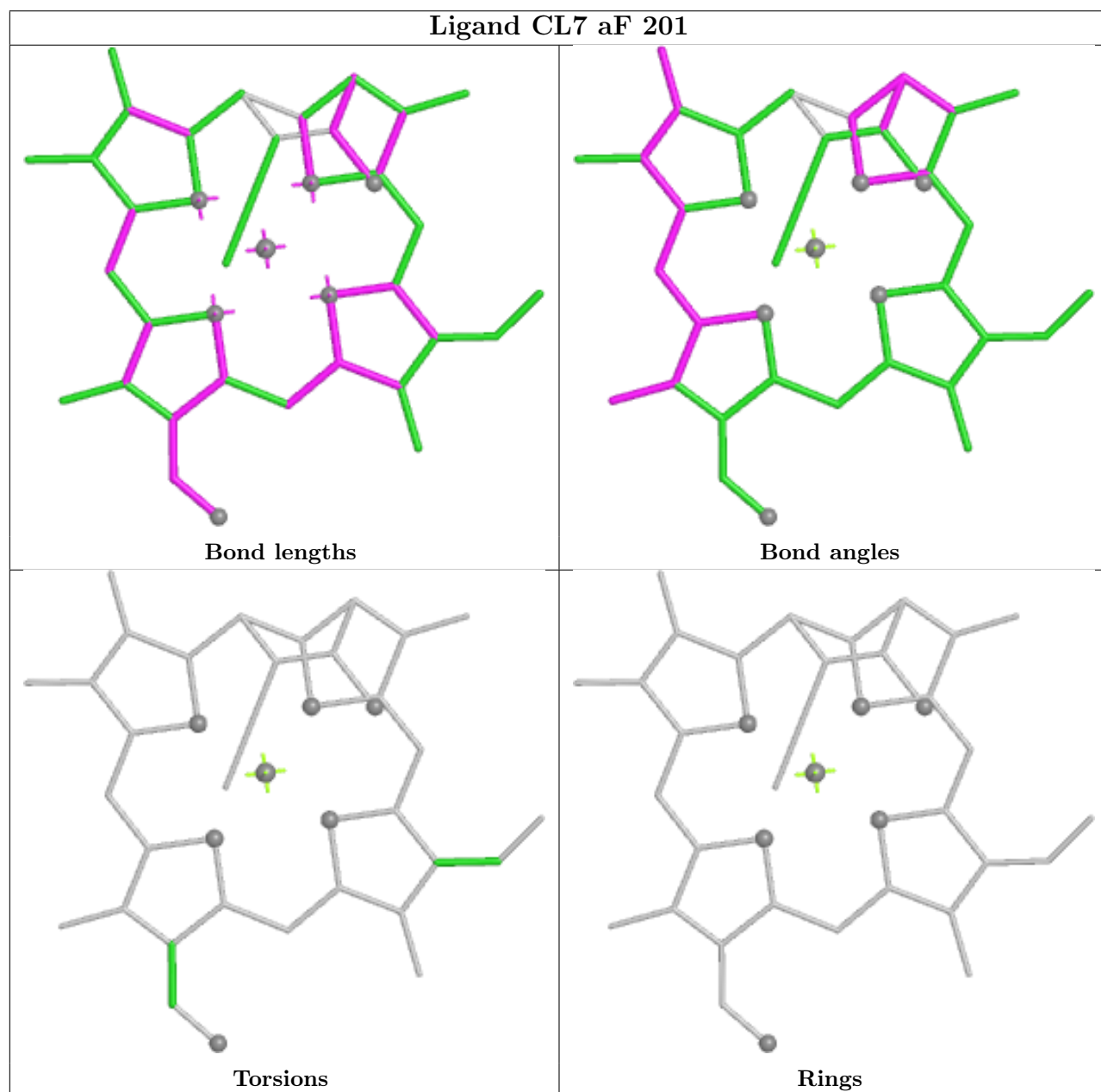




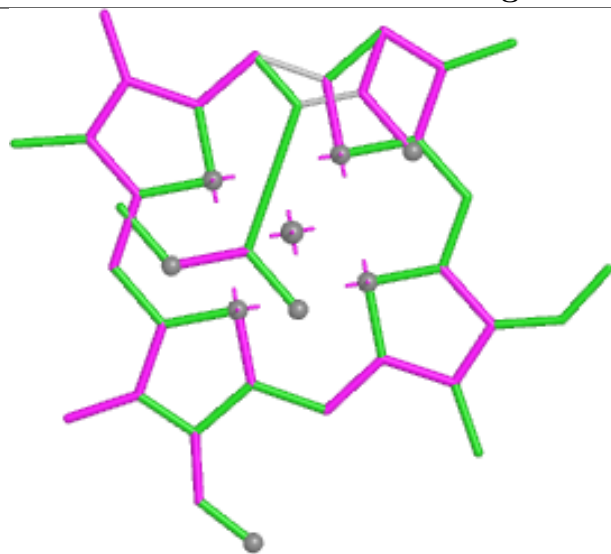
## Ligand PHO cB 805



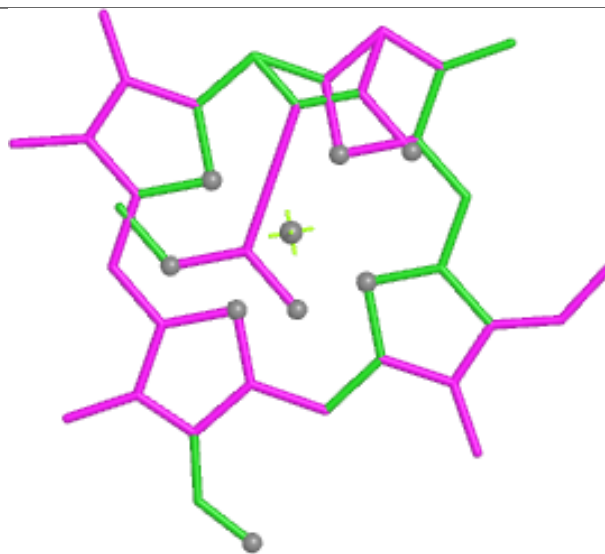
## Ligand CL7 aF 201



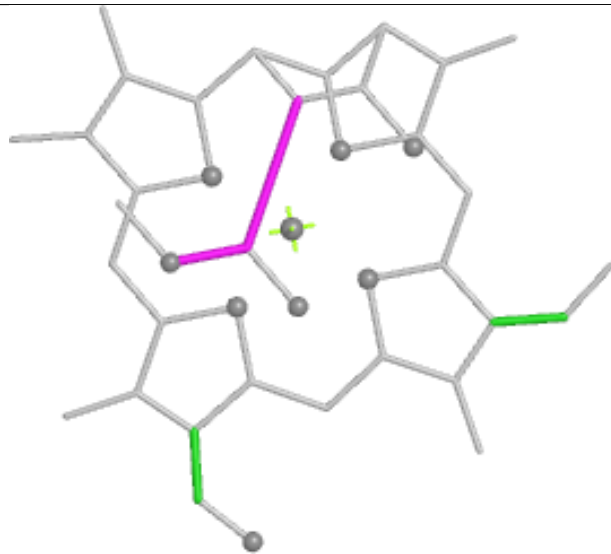
## Ligand CL7 cA 3129



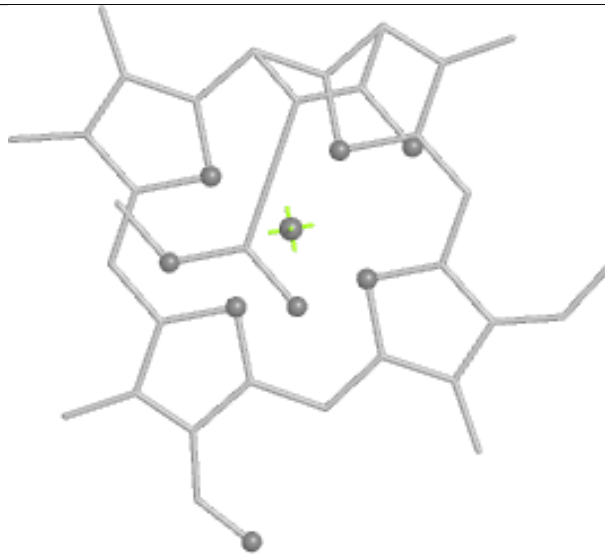
Bond lengths



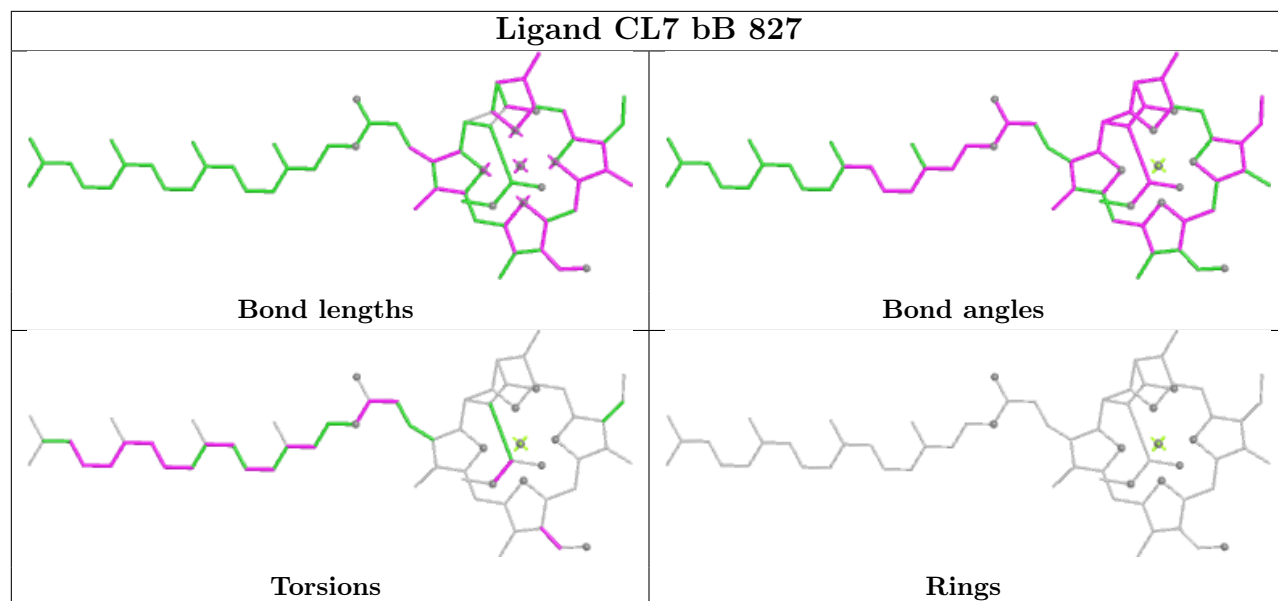
Bond angles

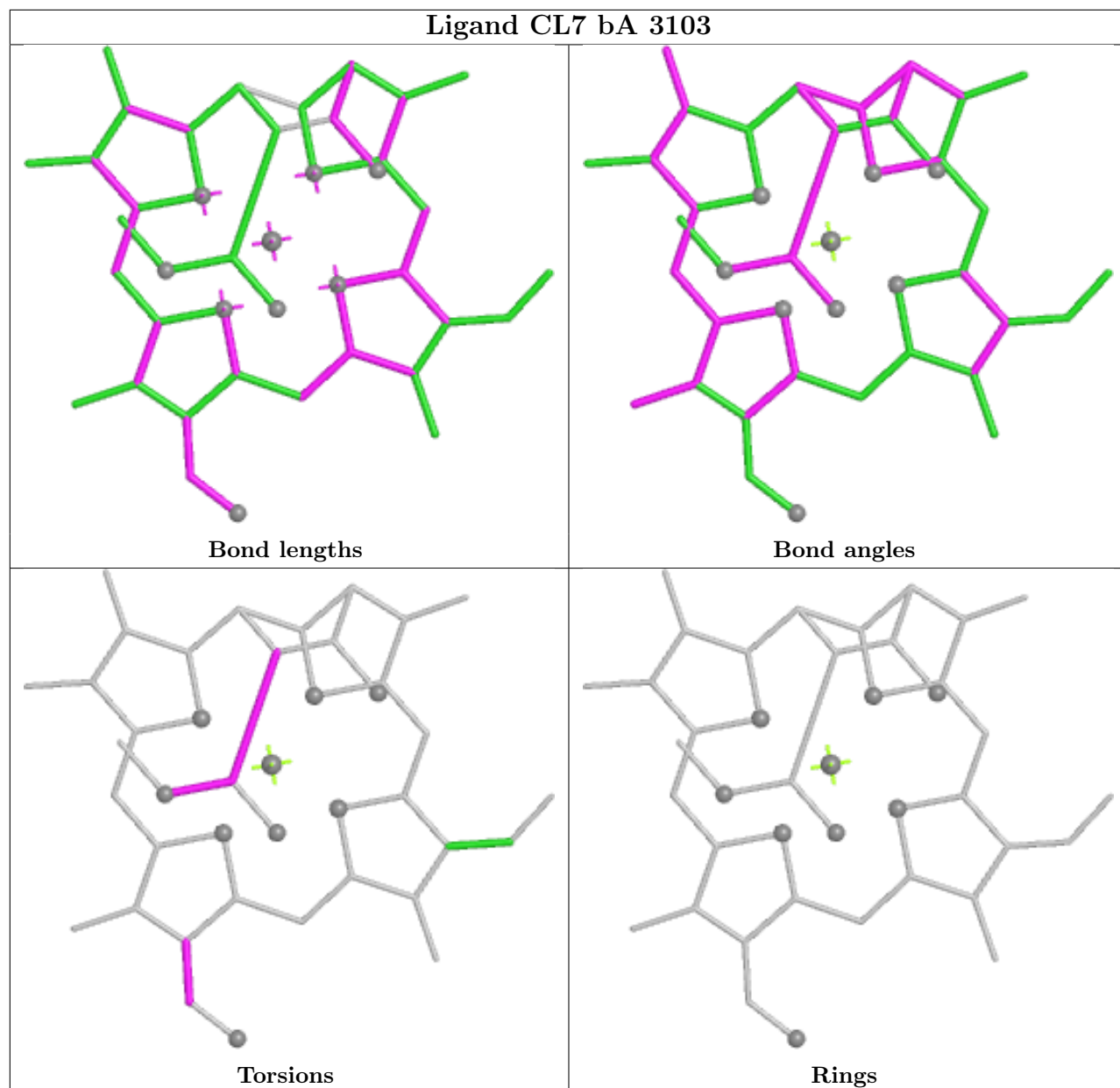


Torsions

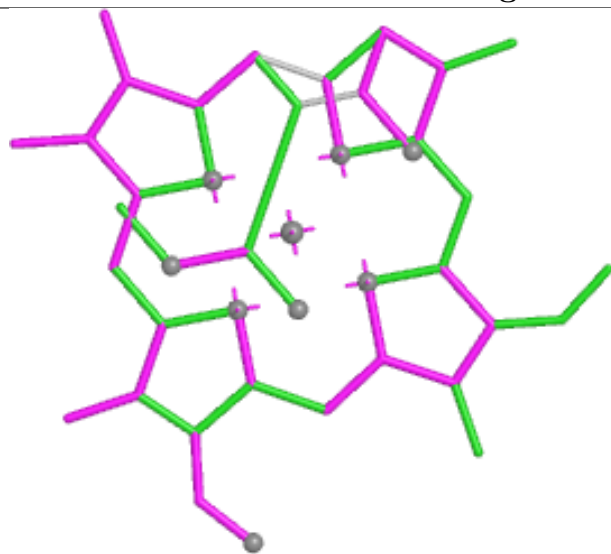


Rings

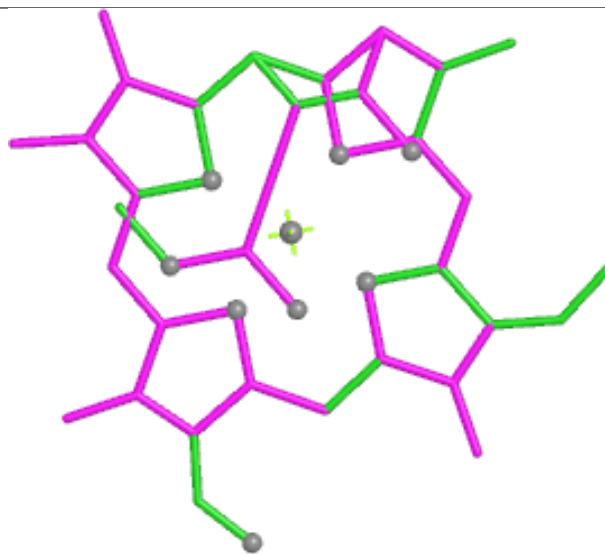




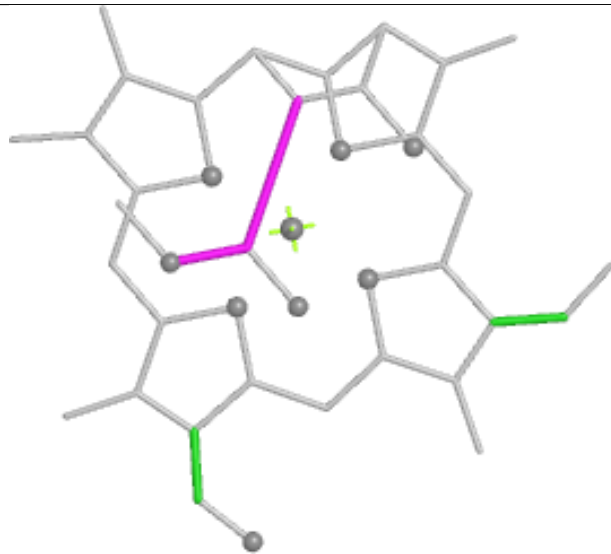
## Ligand CL7 bA 3129



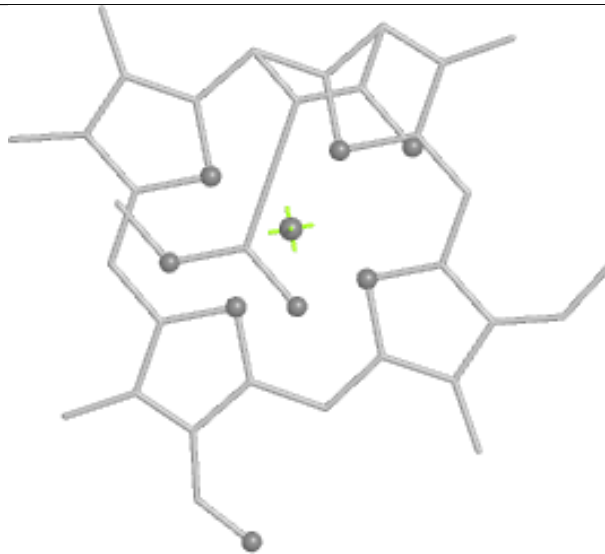
Bond lengths



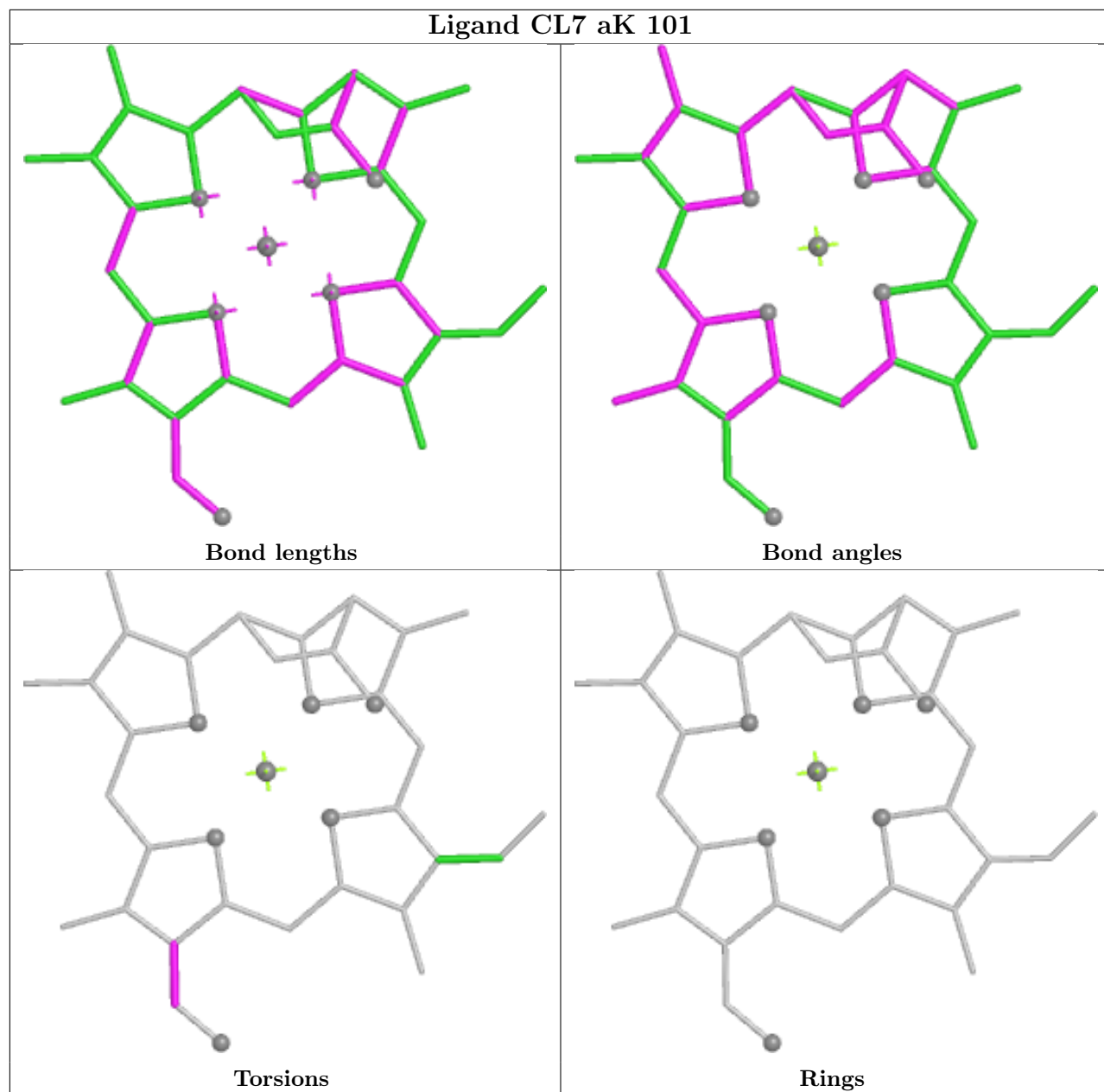
Bond angles

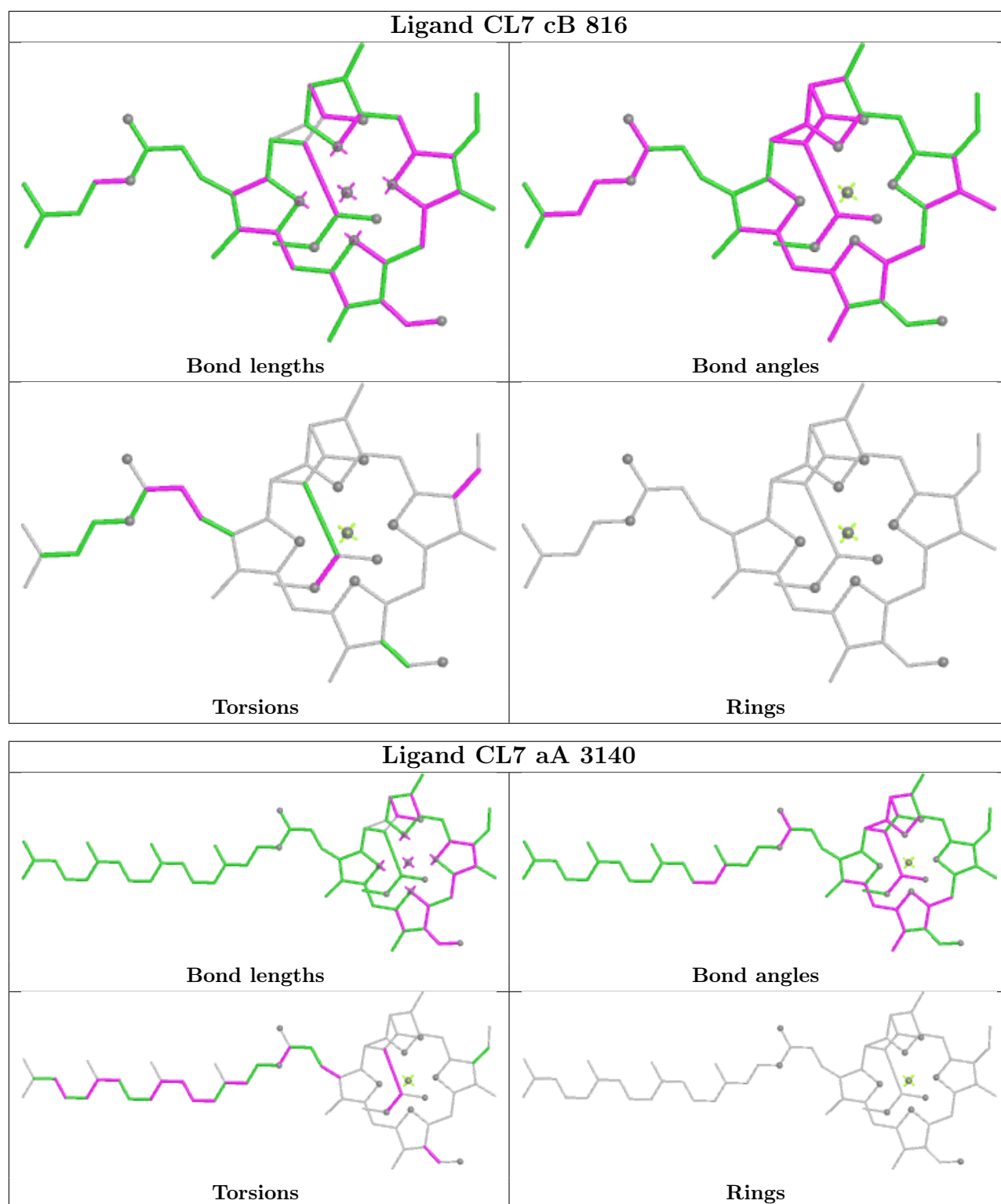


Torsions

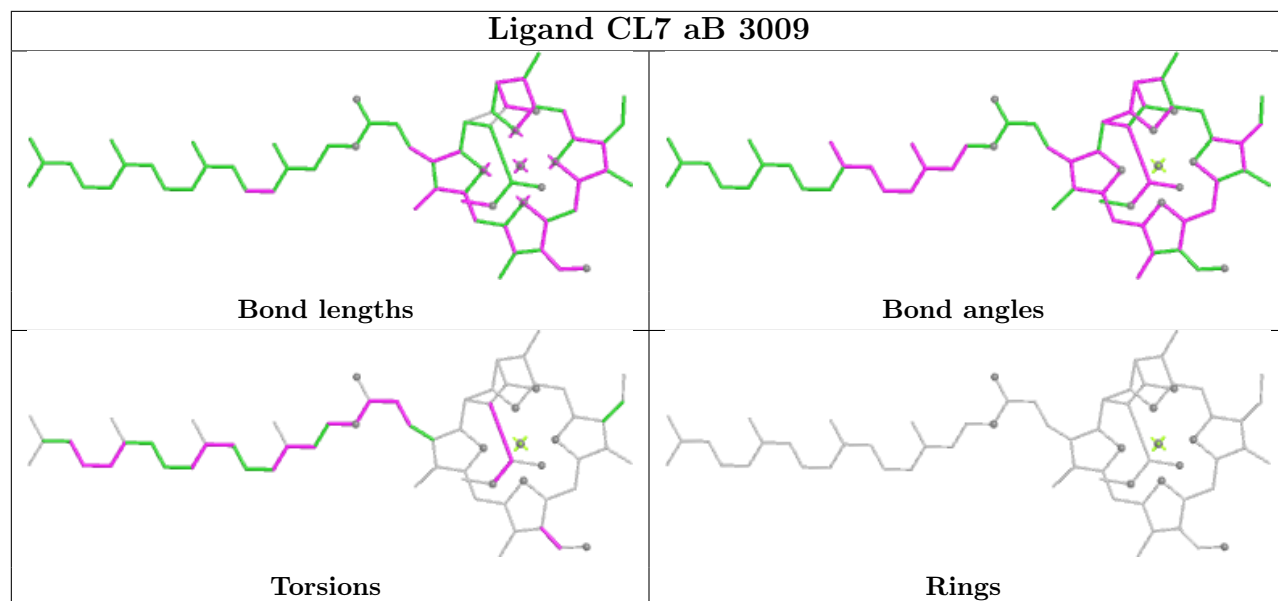


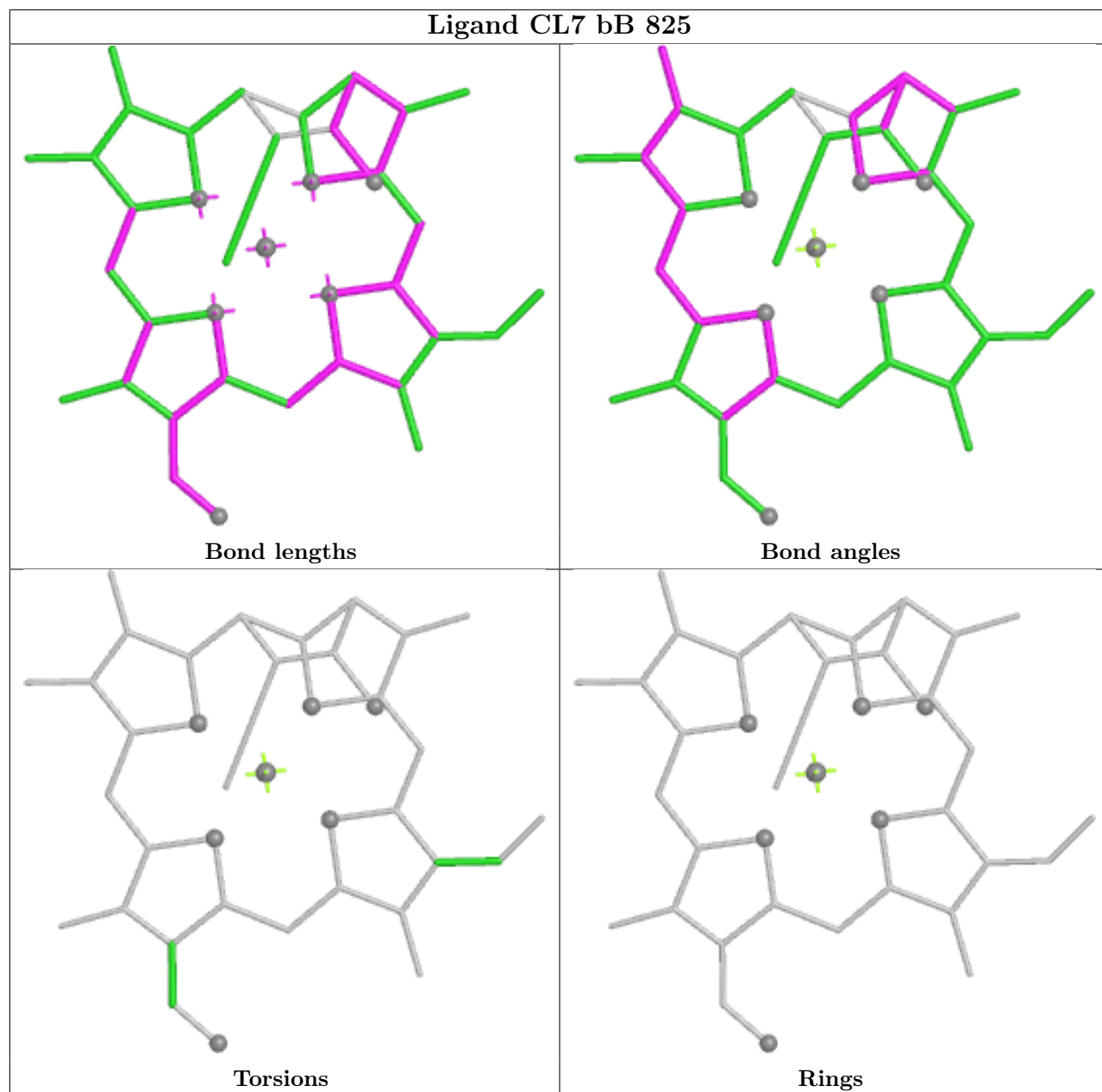
Rings

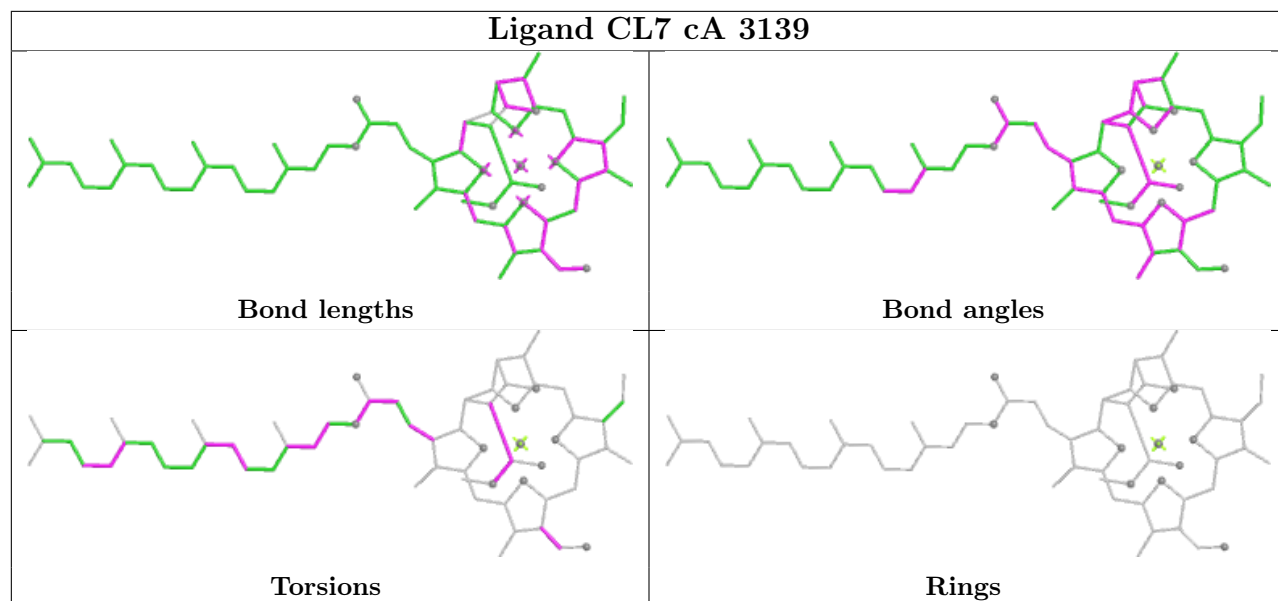




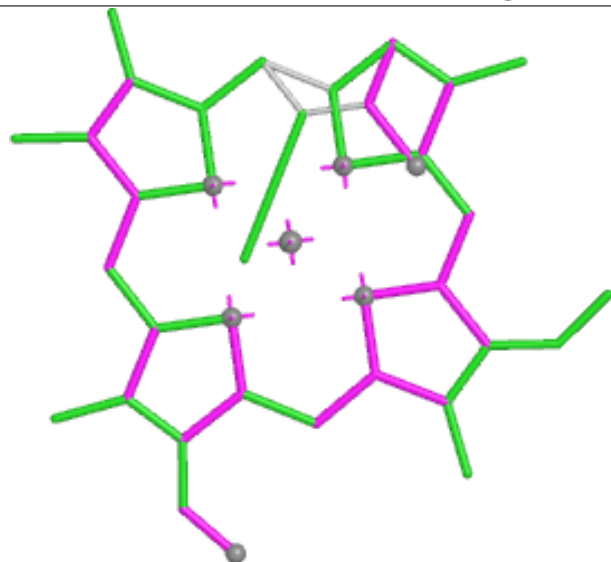




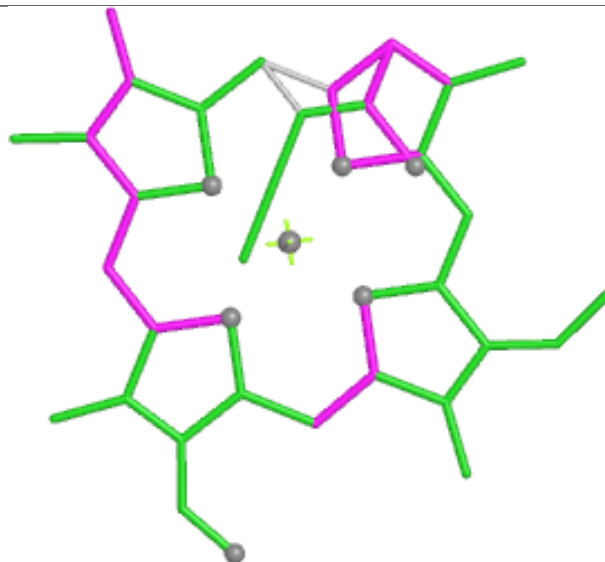




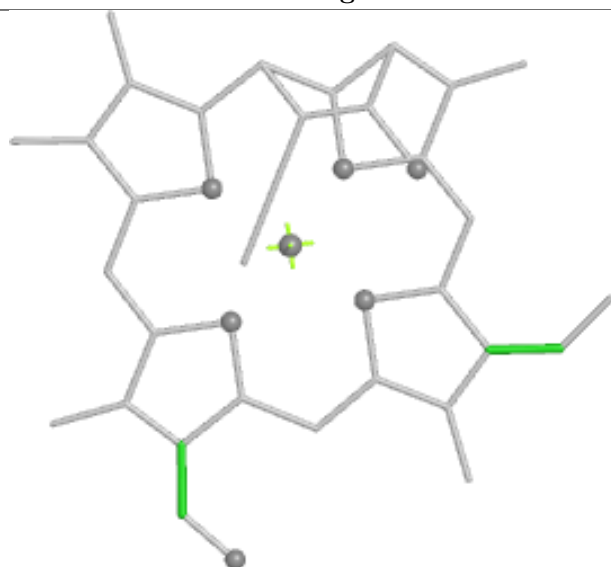
## Ligand CL7 bA 3118



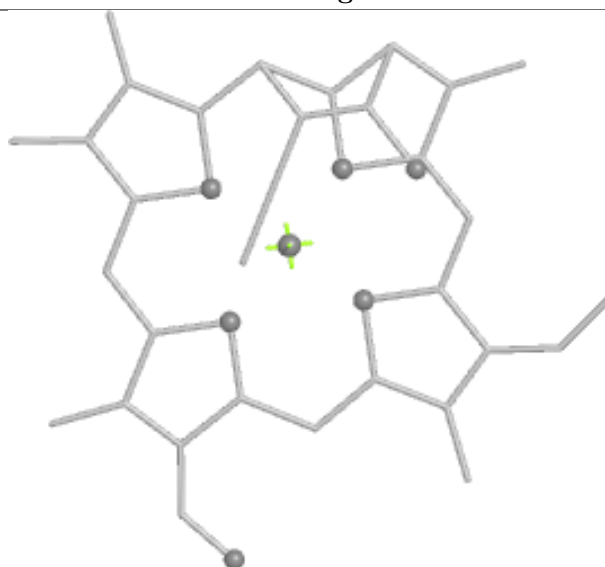
Bond lengths



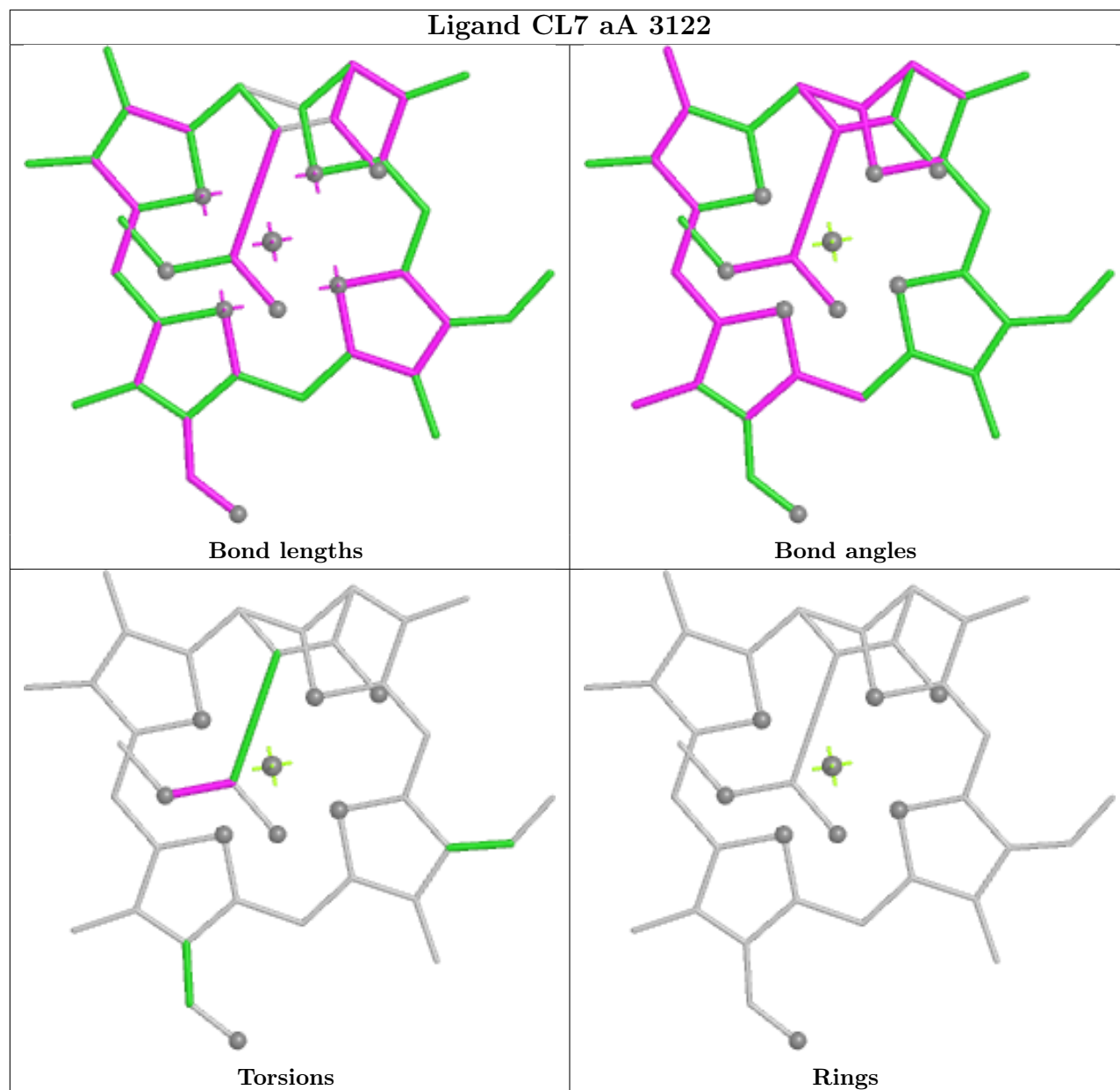
Bond angles

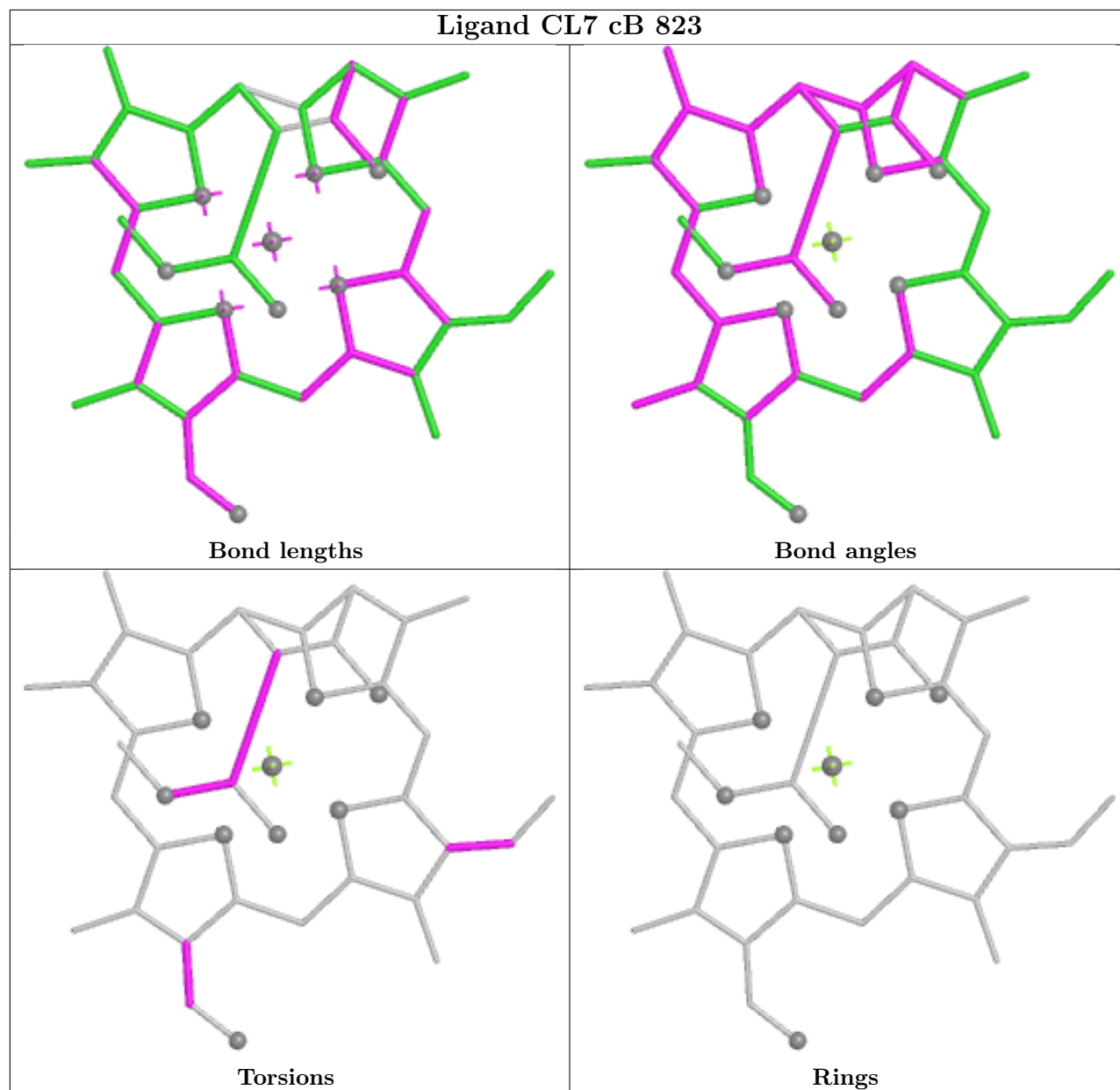


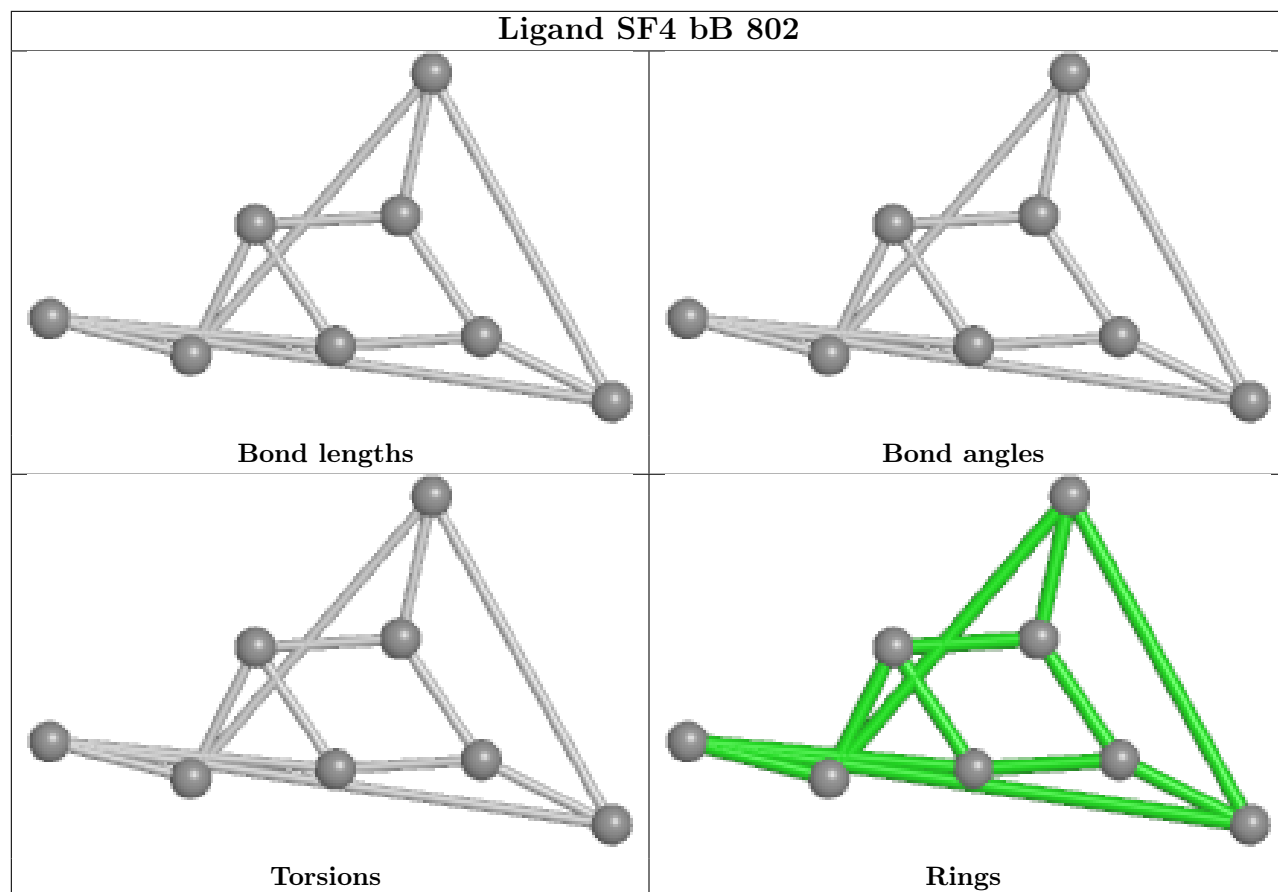
Torsions

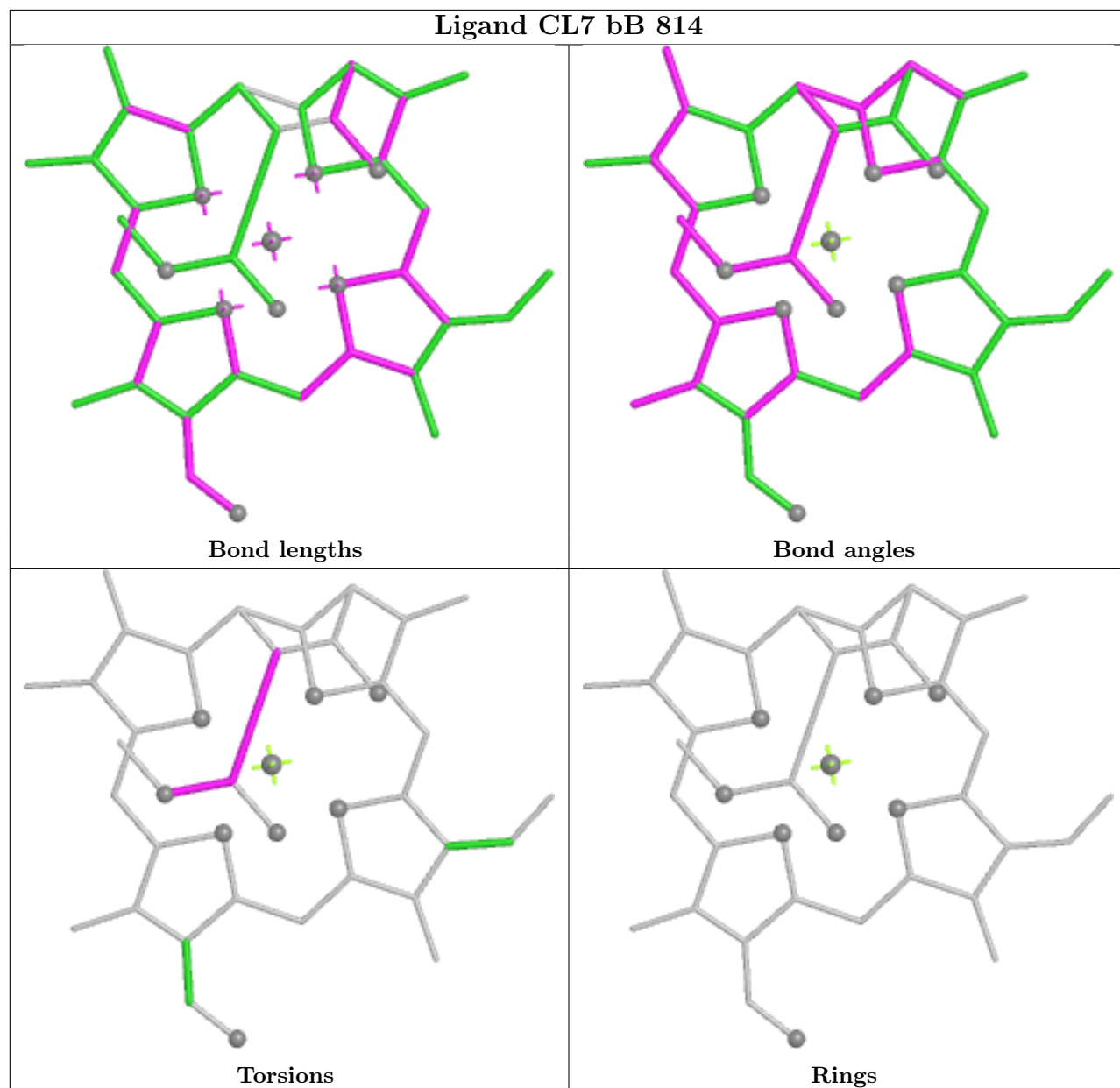


Rings



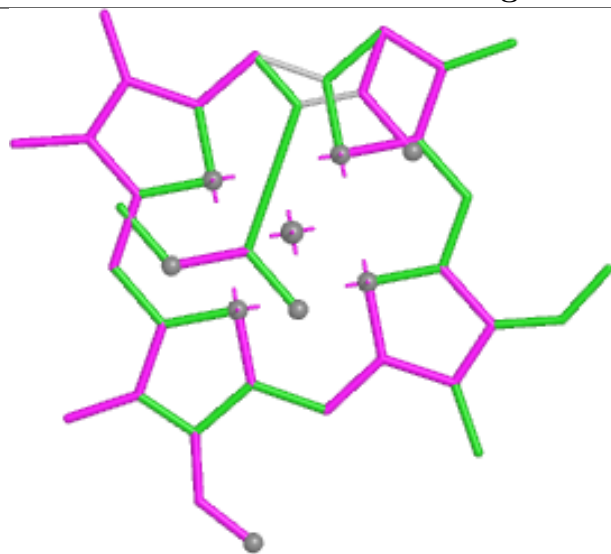




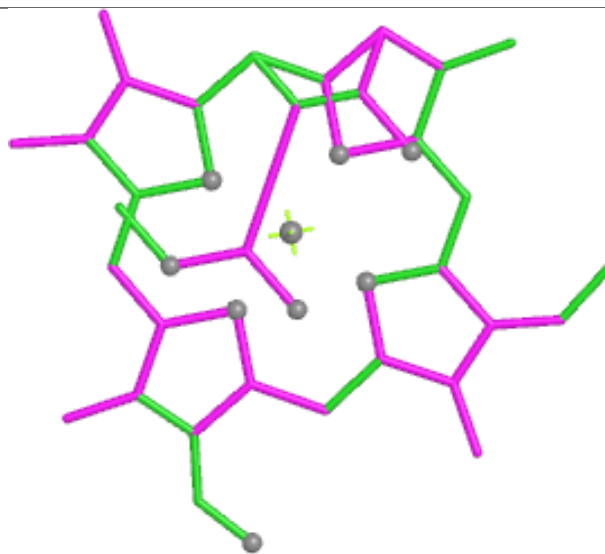




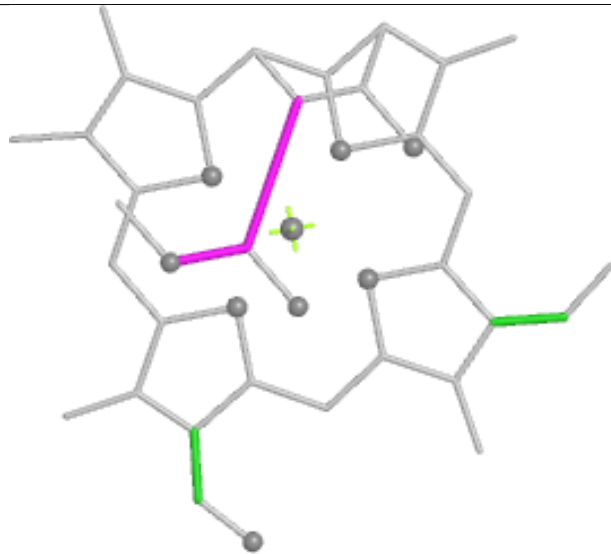
## Ligand CL7 aA 3130



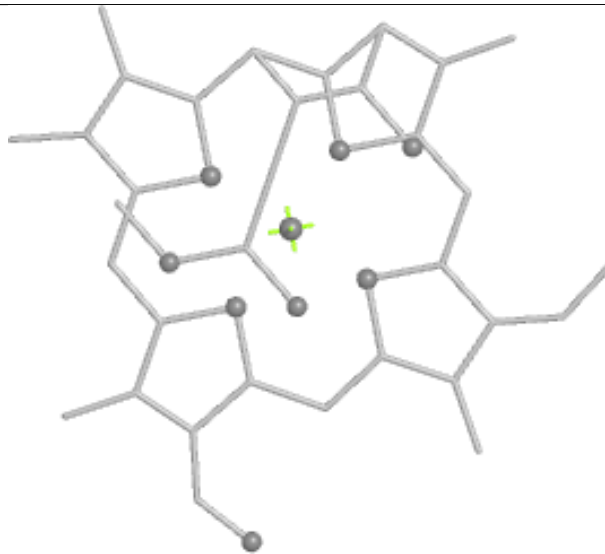
Bond lengths



Bond angles

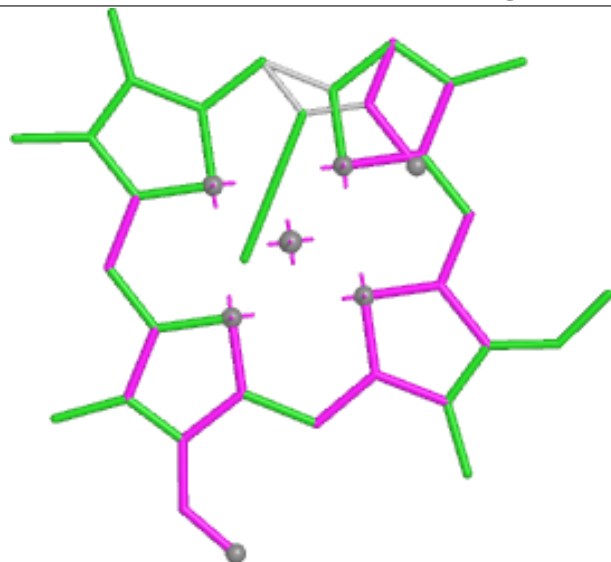


Torsions

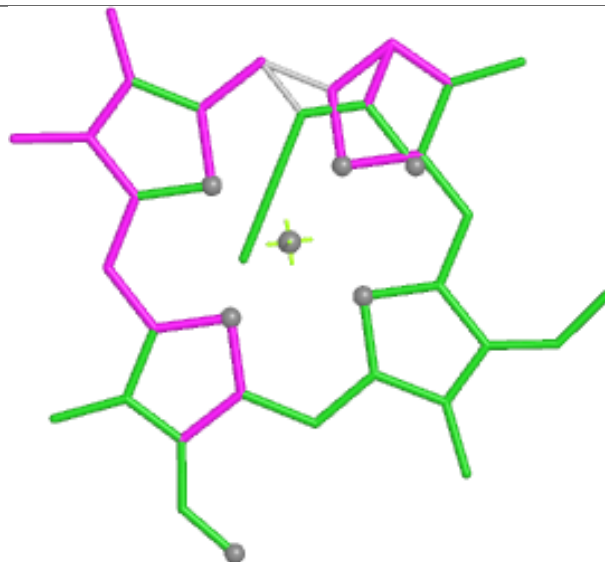


Rings

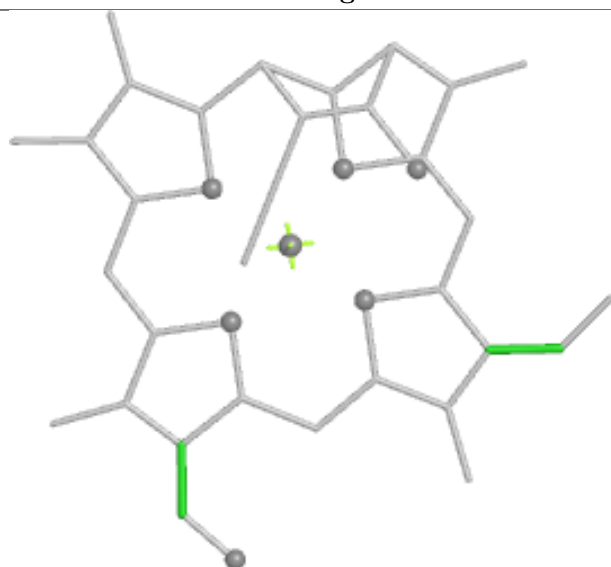
## Ligand CL7 aB 3024



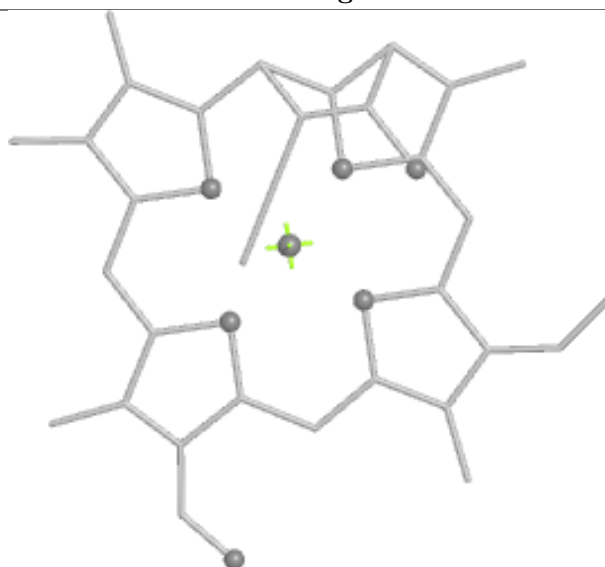
Bond lengths



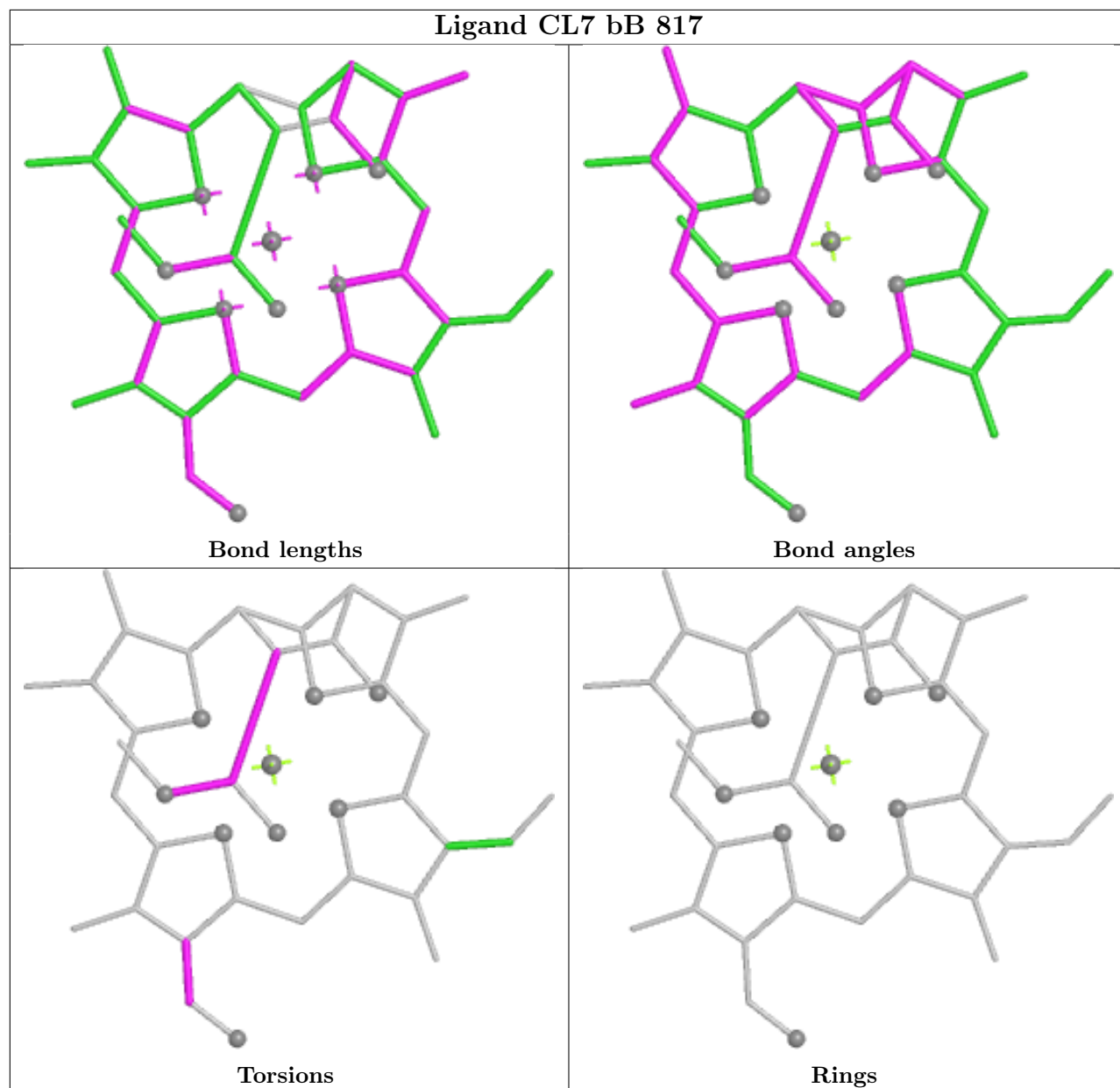
Bond angles

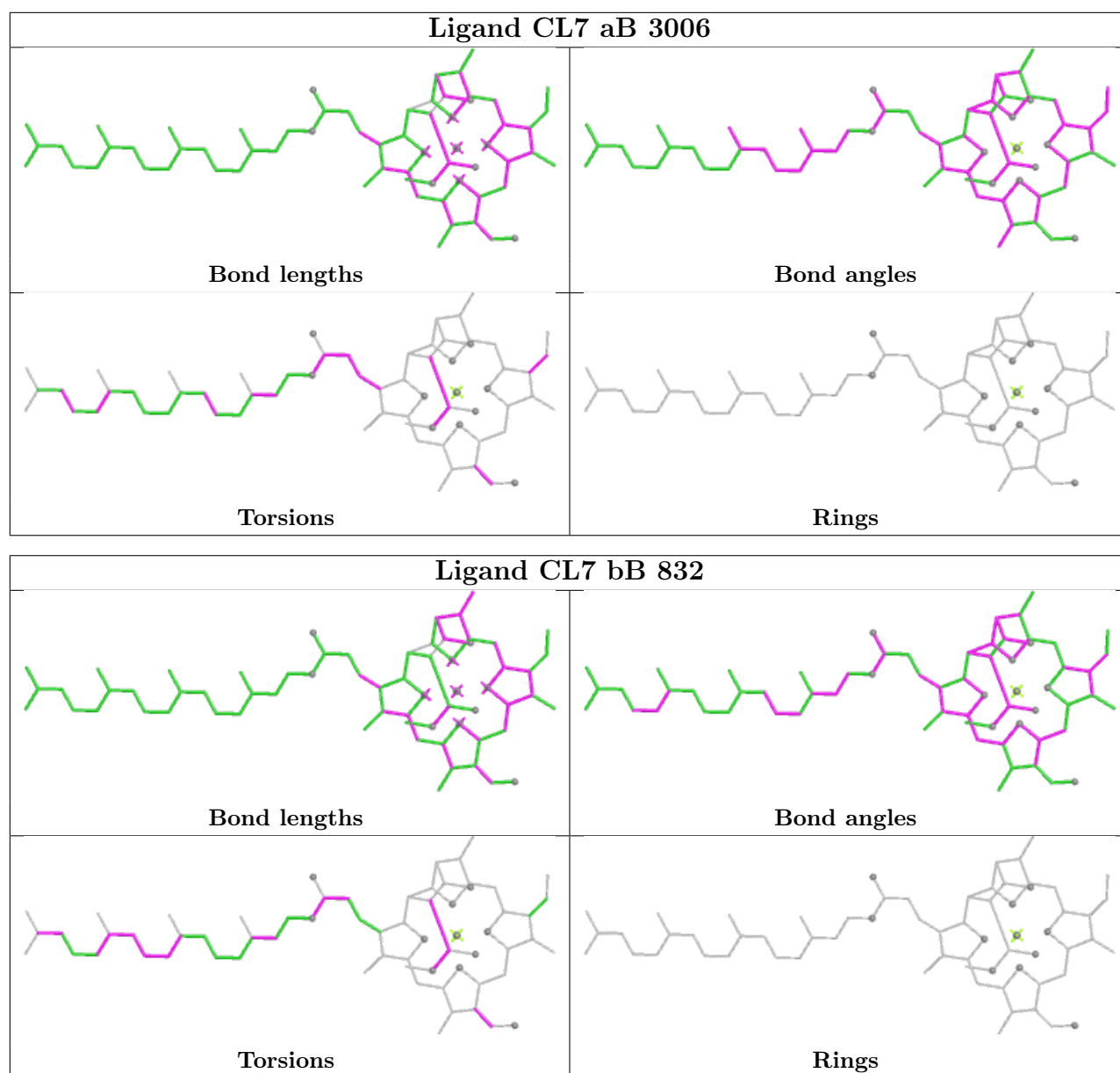


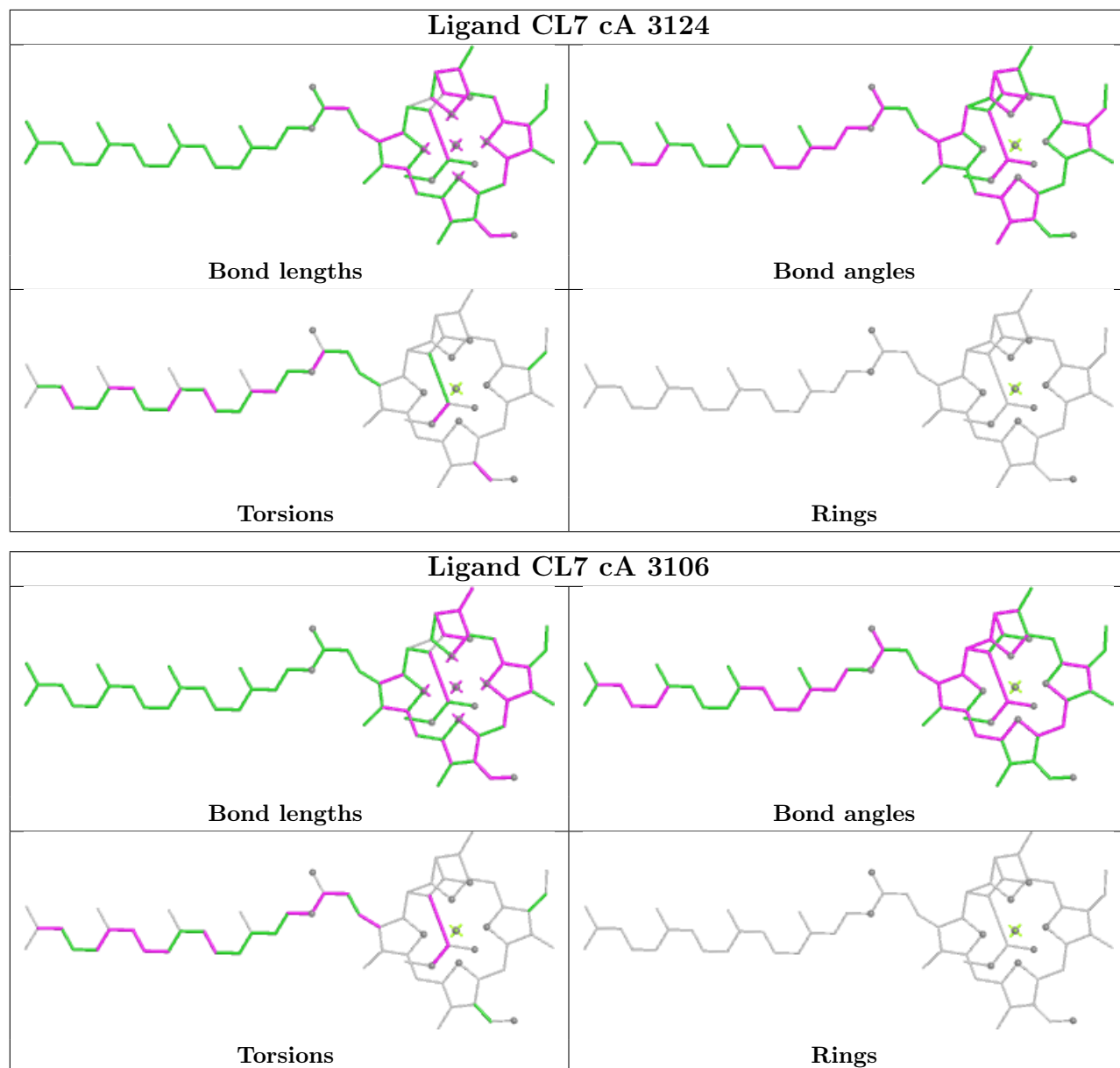
Torsions

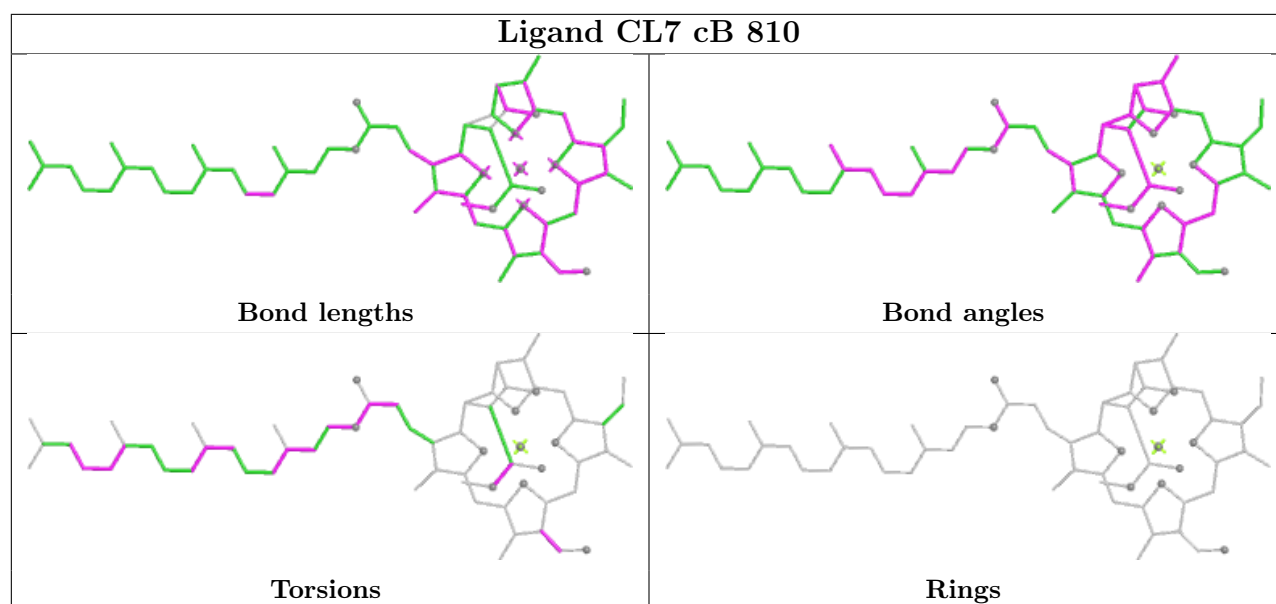


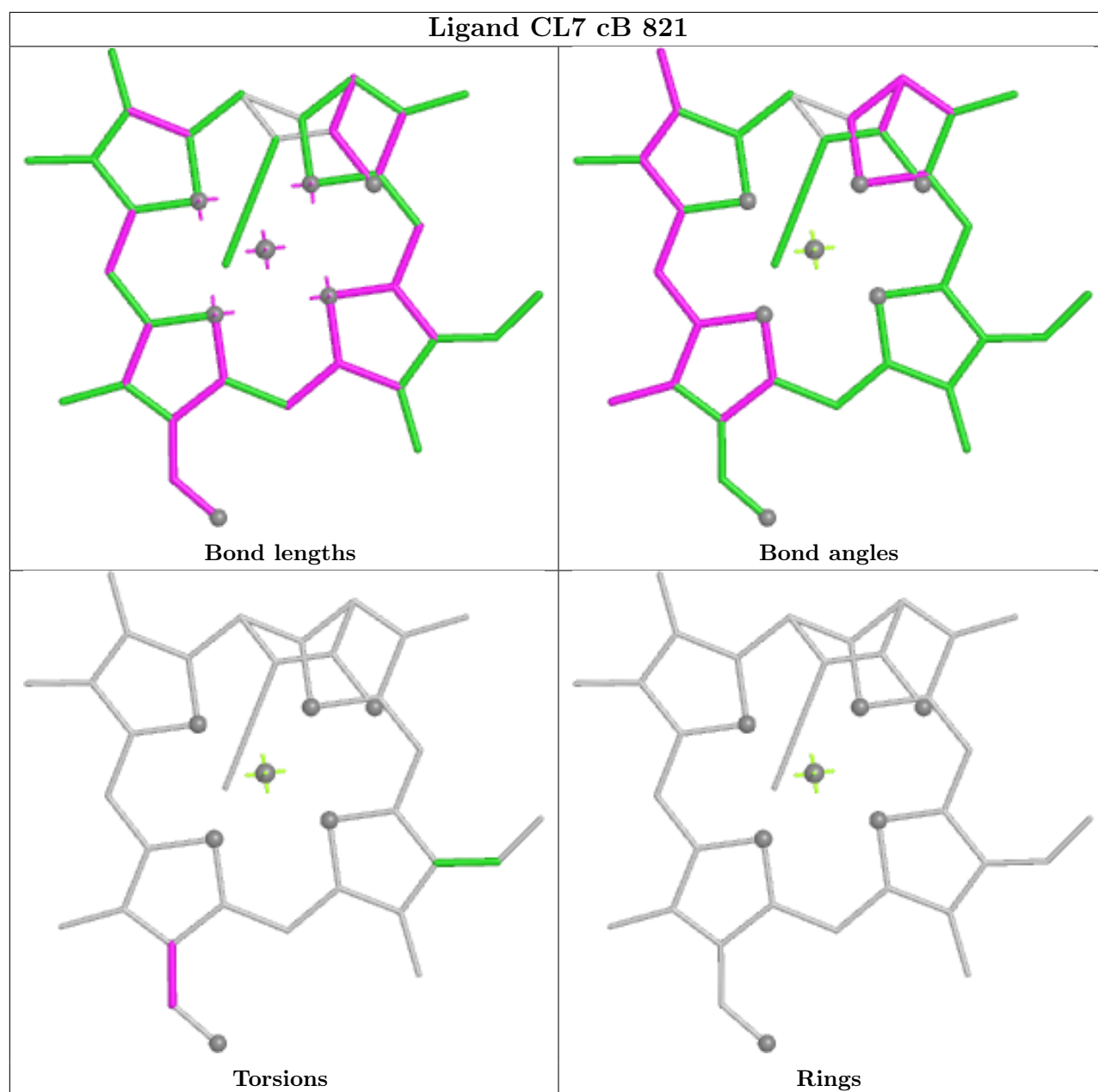
Rings

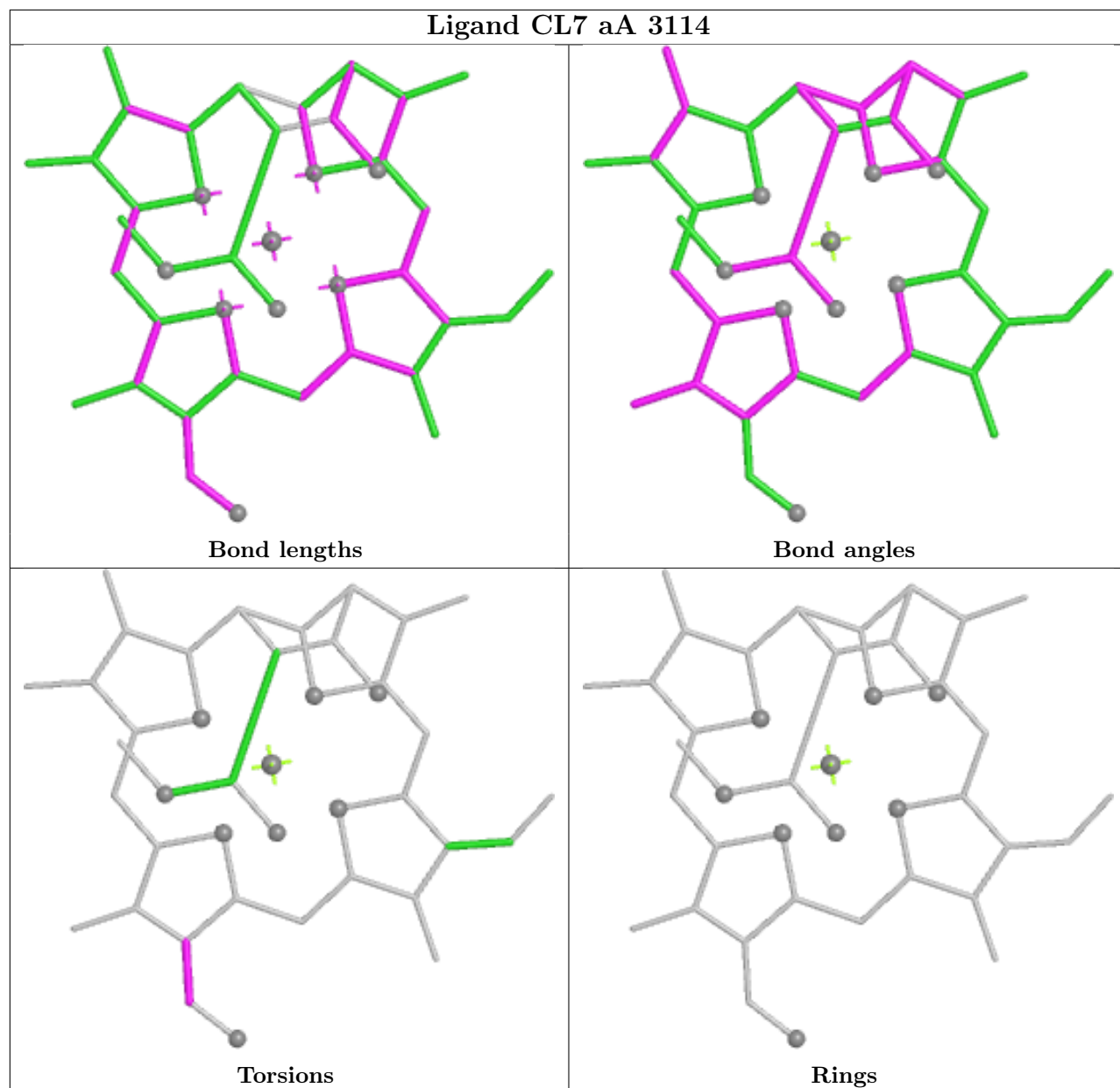




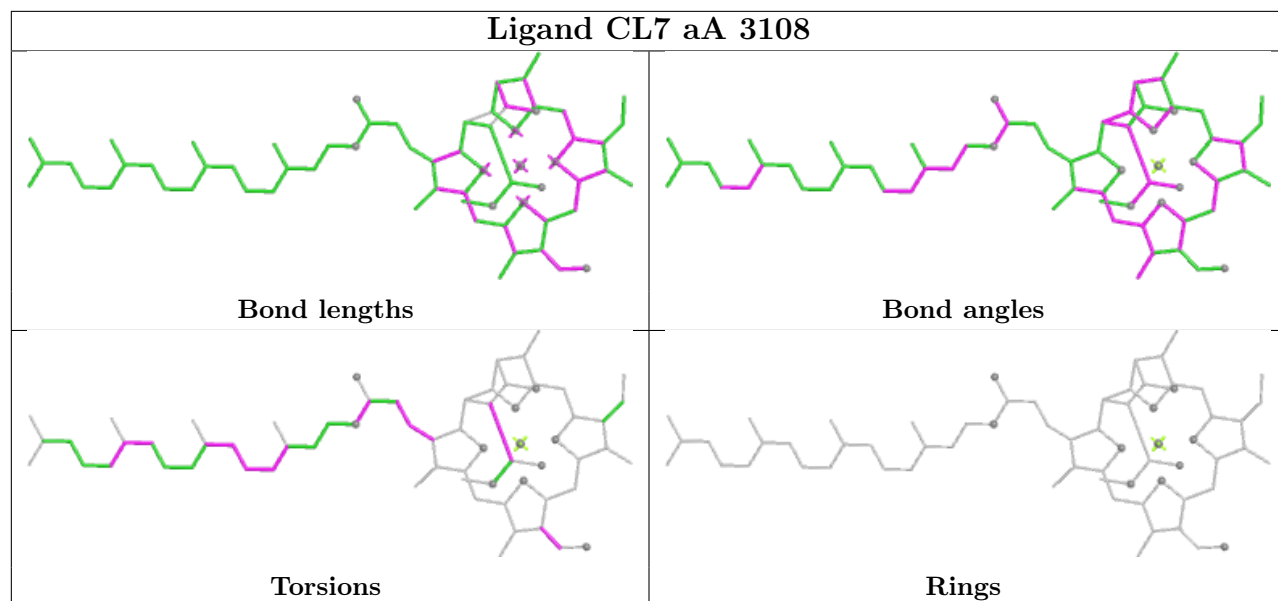


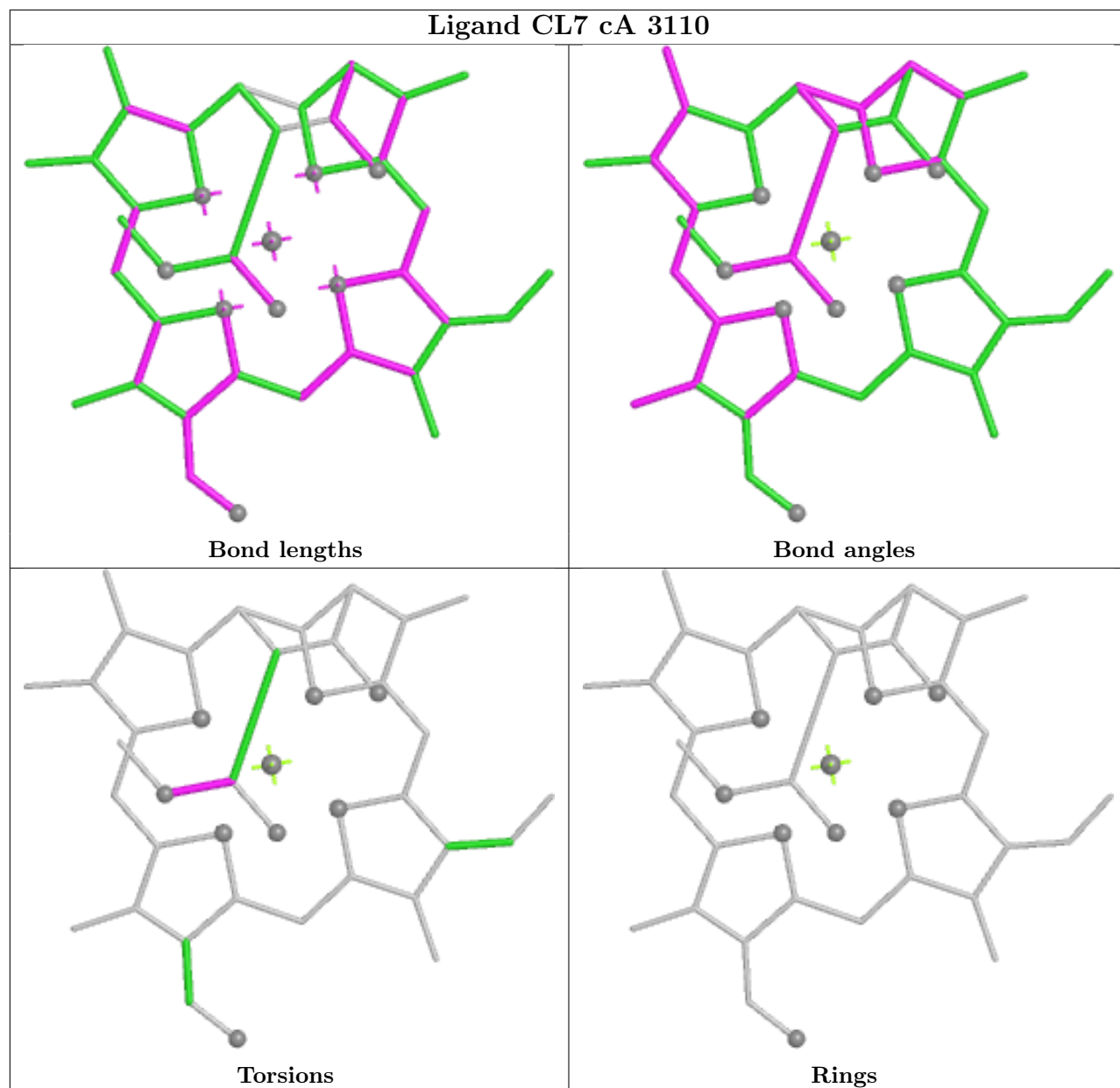


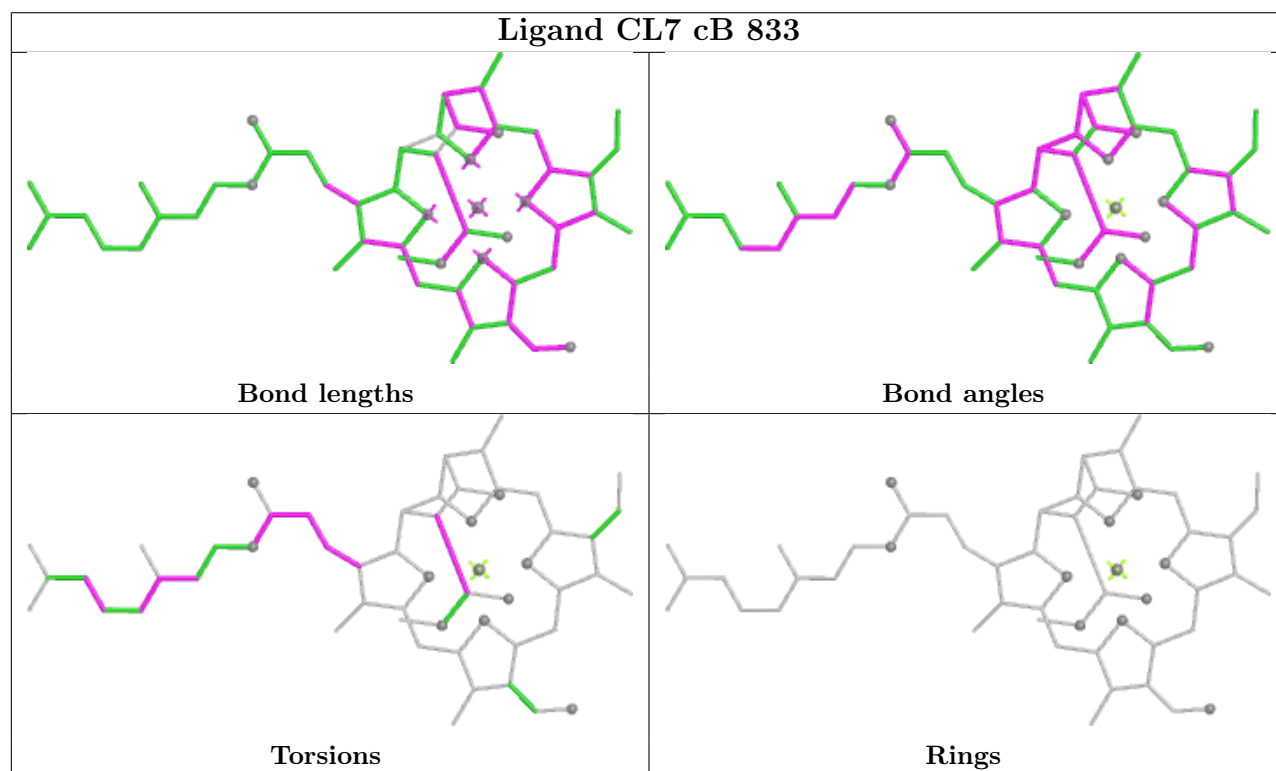
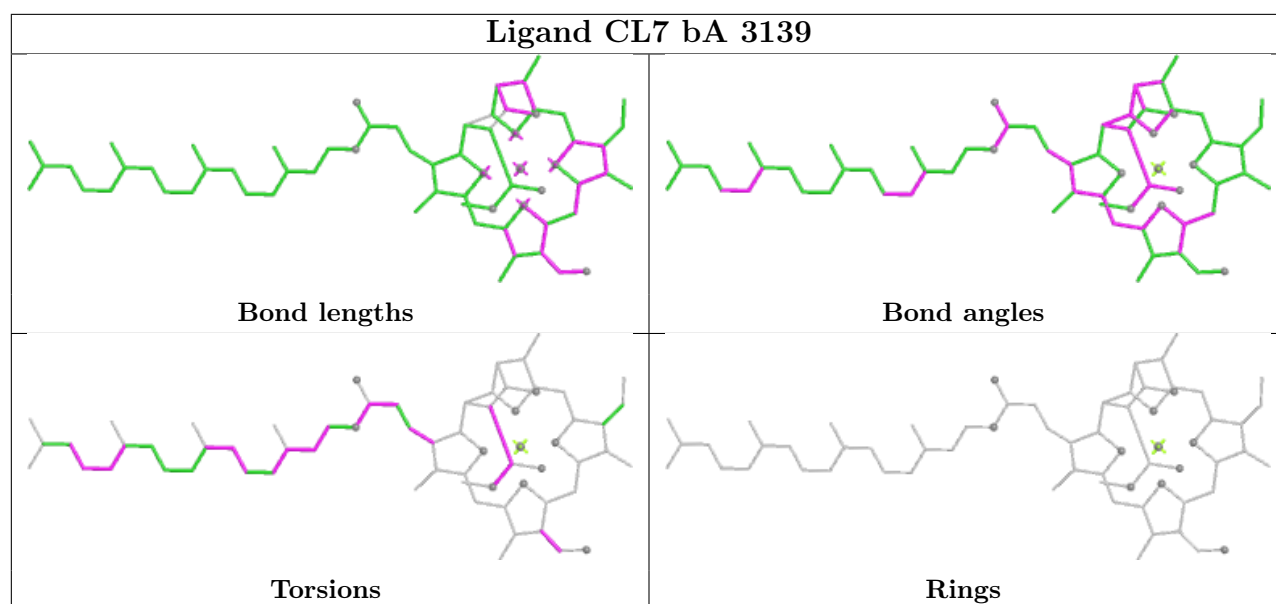


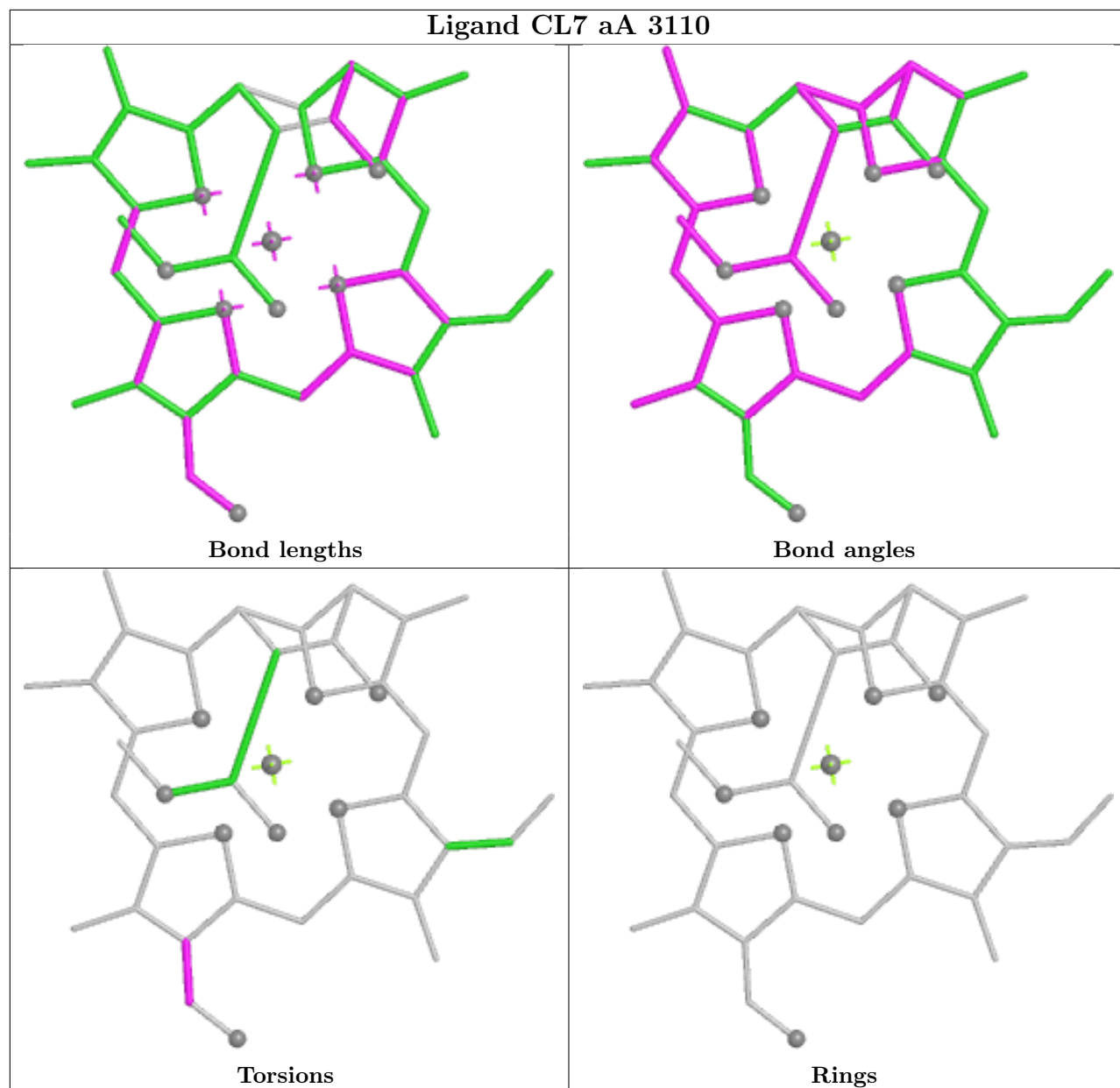


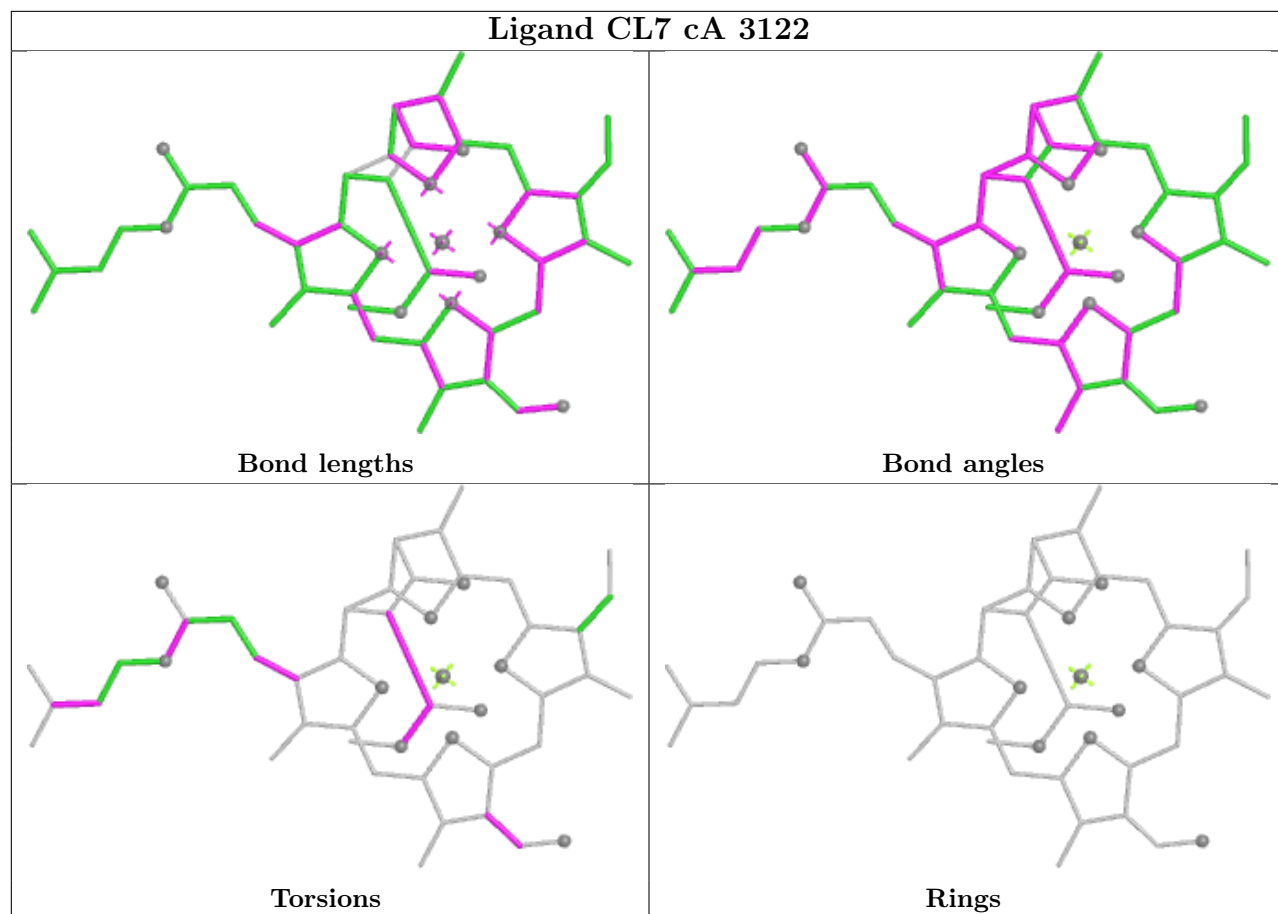




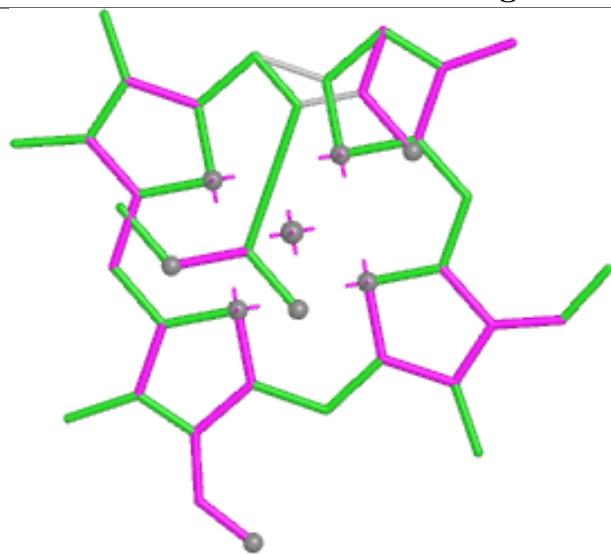




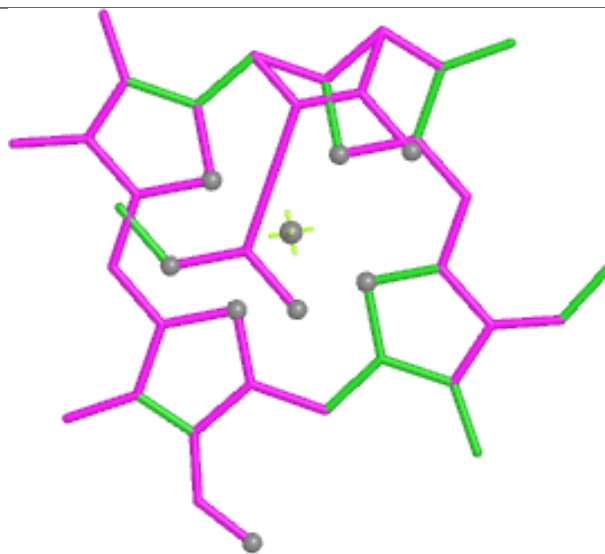




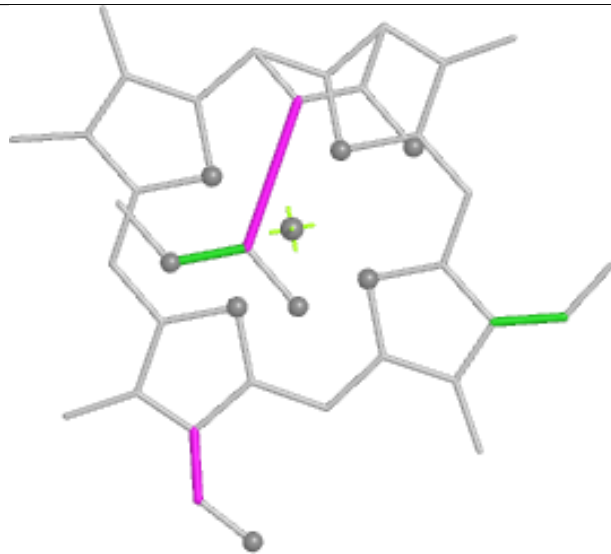
## Ligand CL7 bA 3105



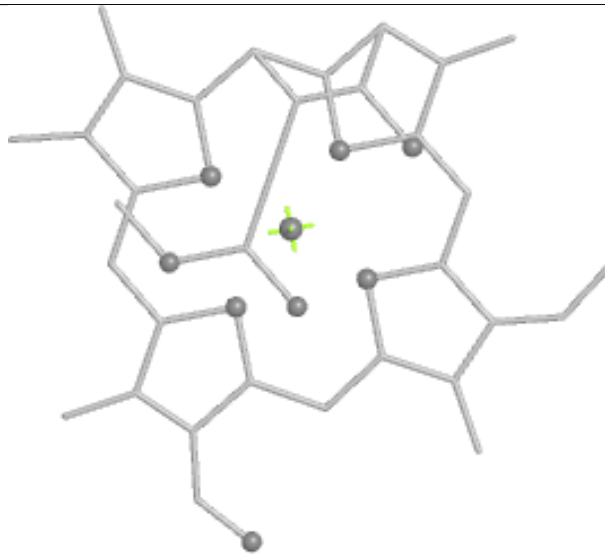
Bond lengths



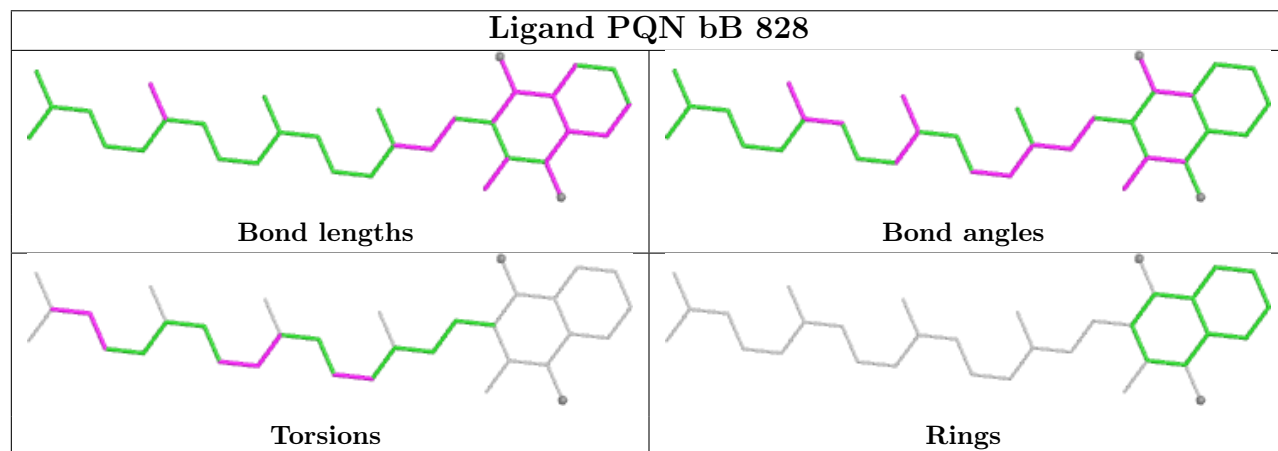
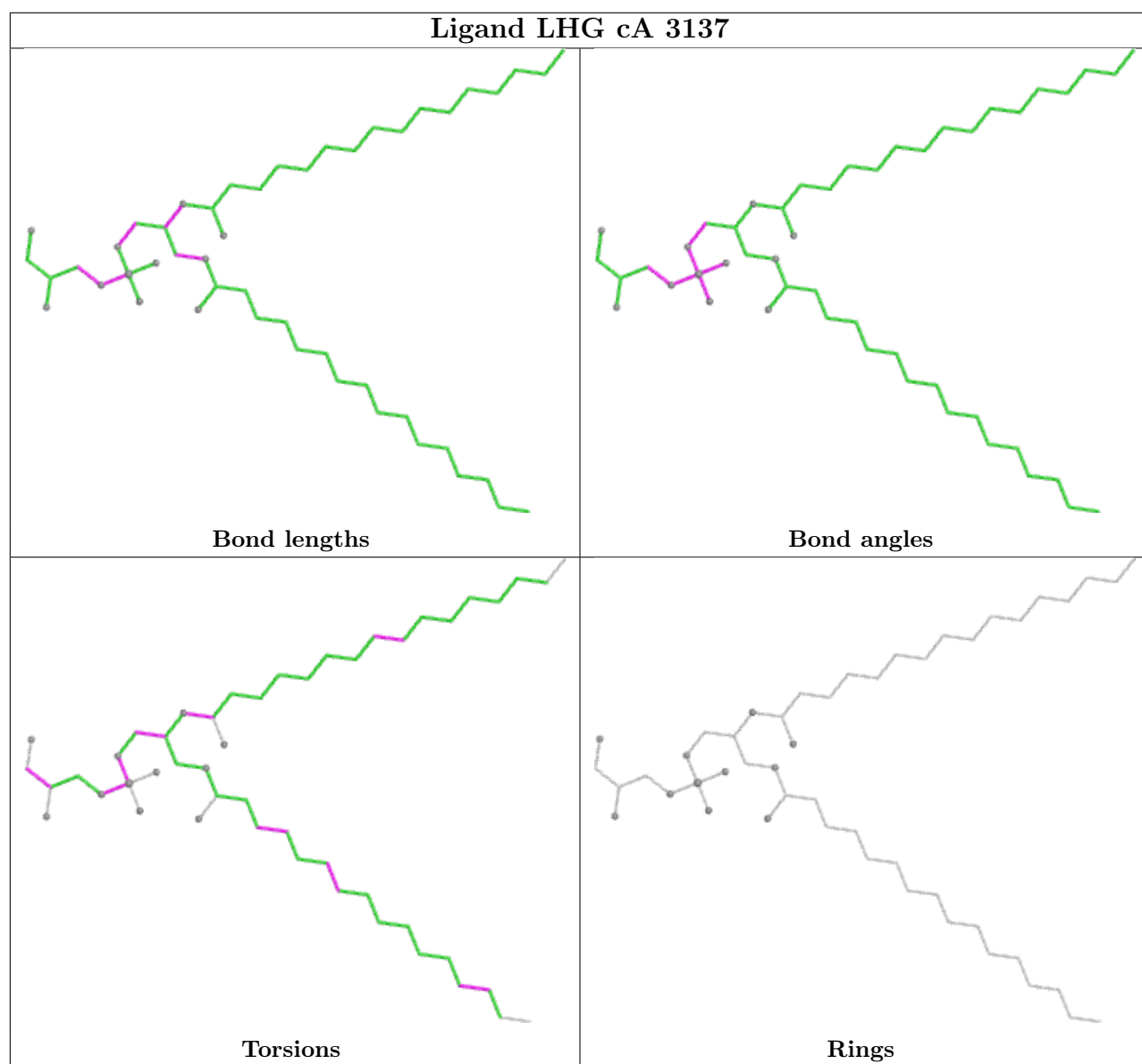
Bond angles

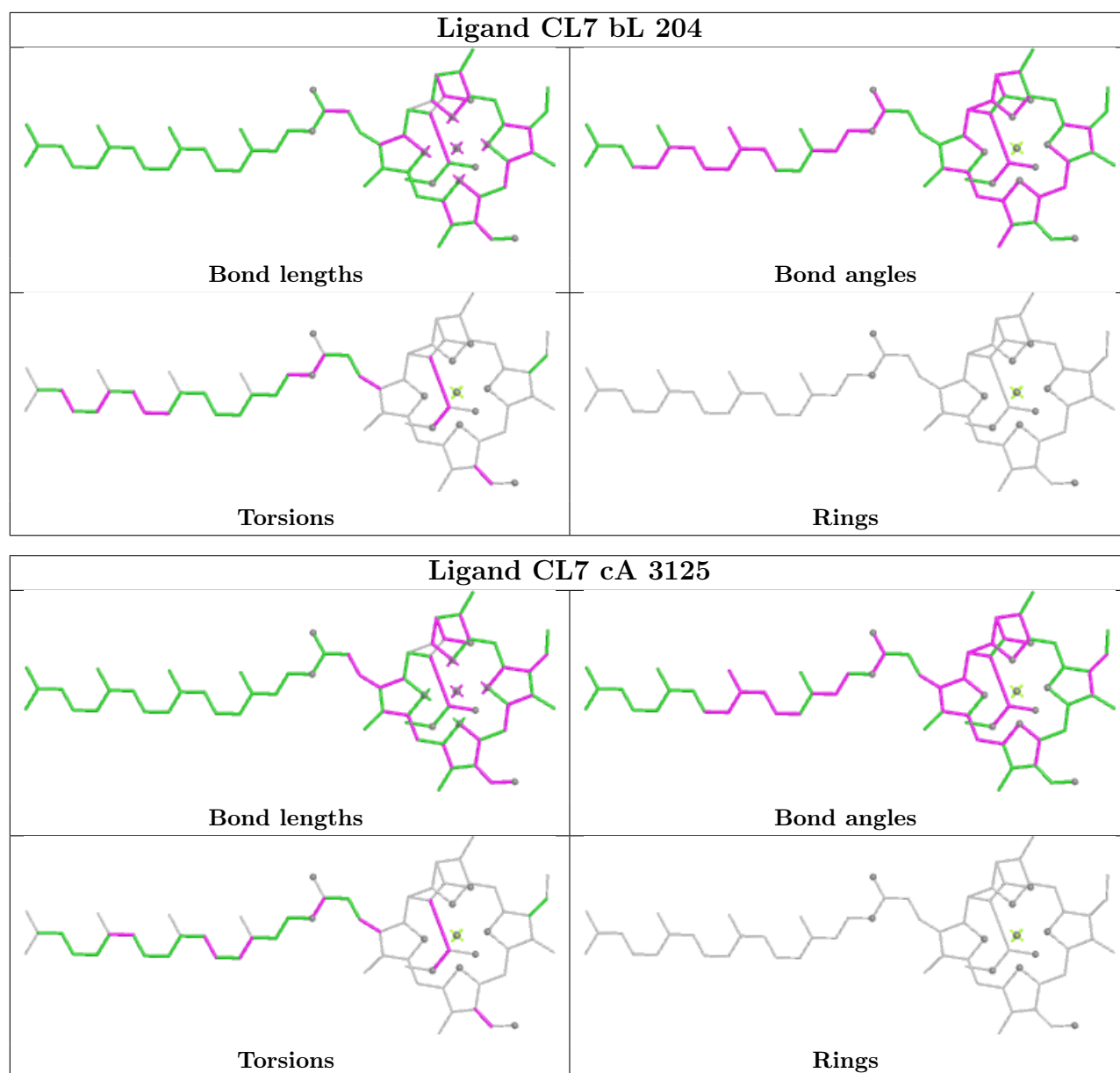


Torsions

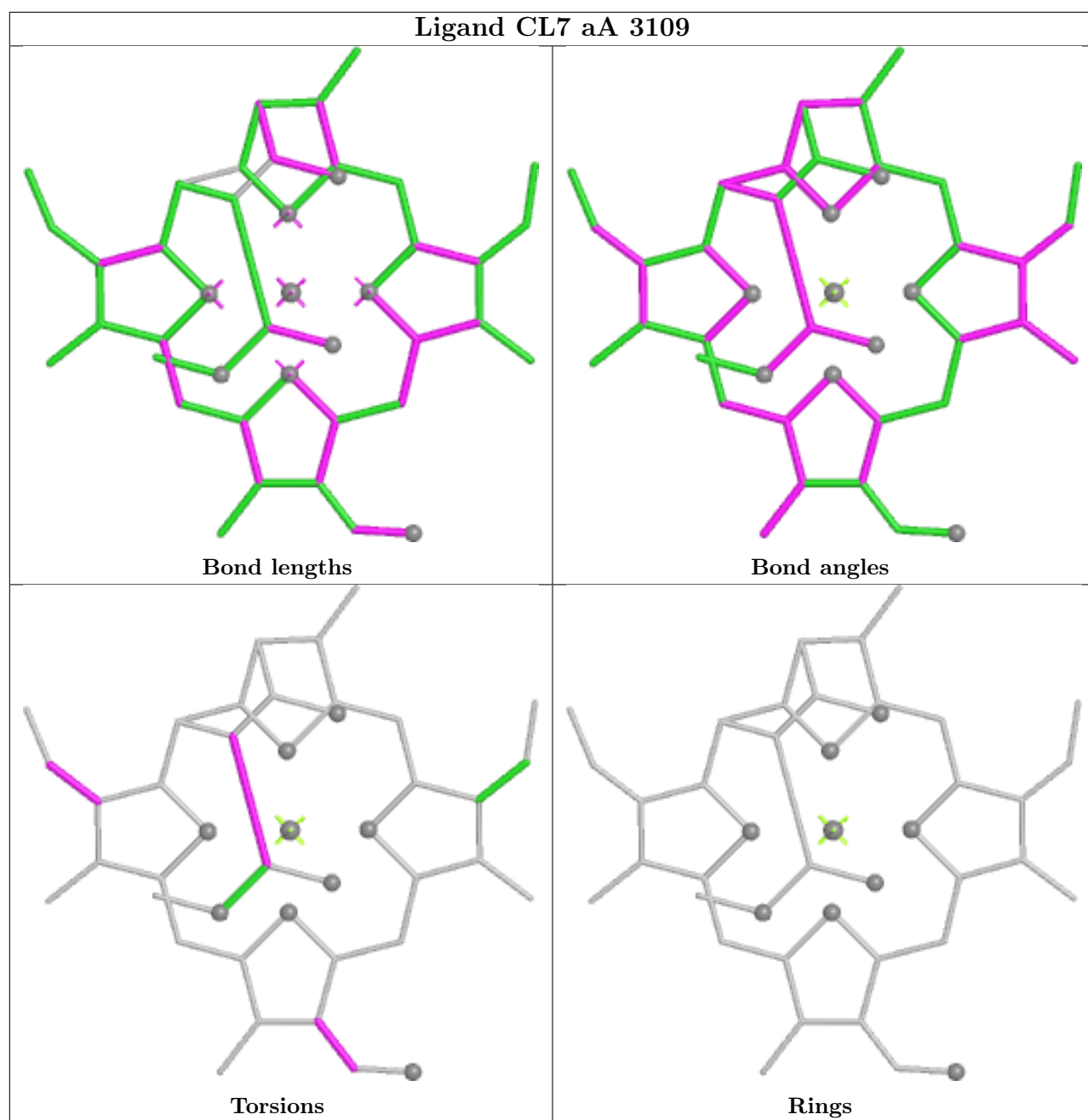


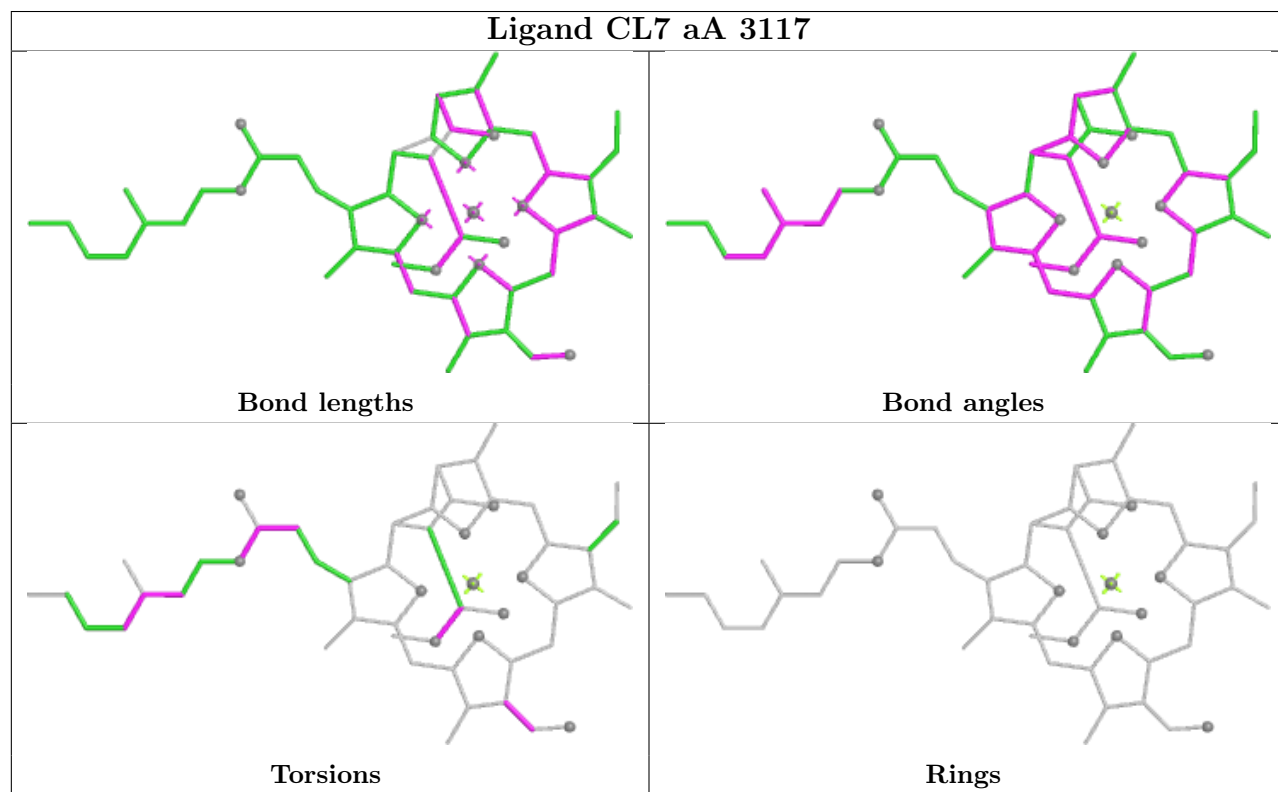
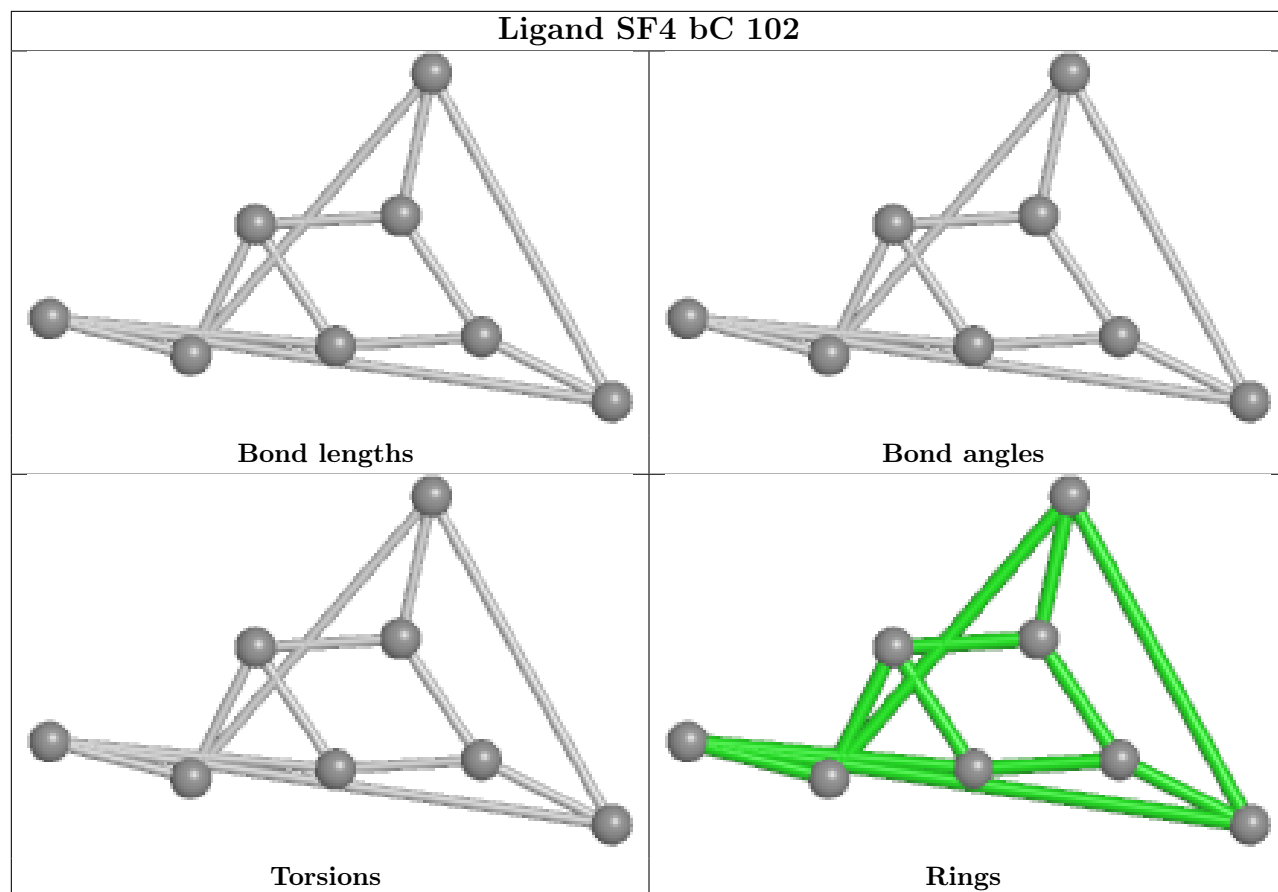
Rings

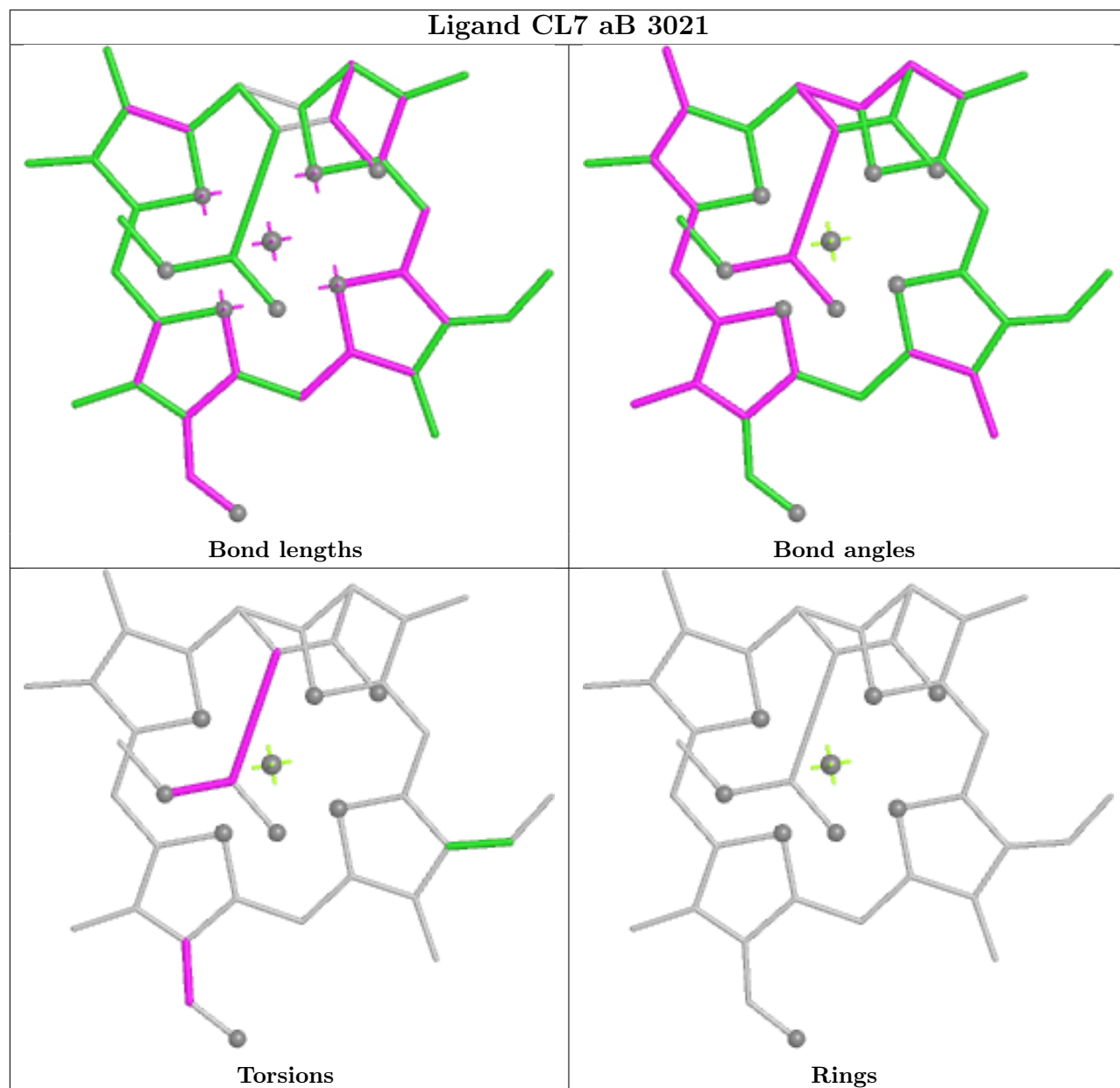


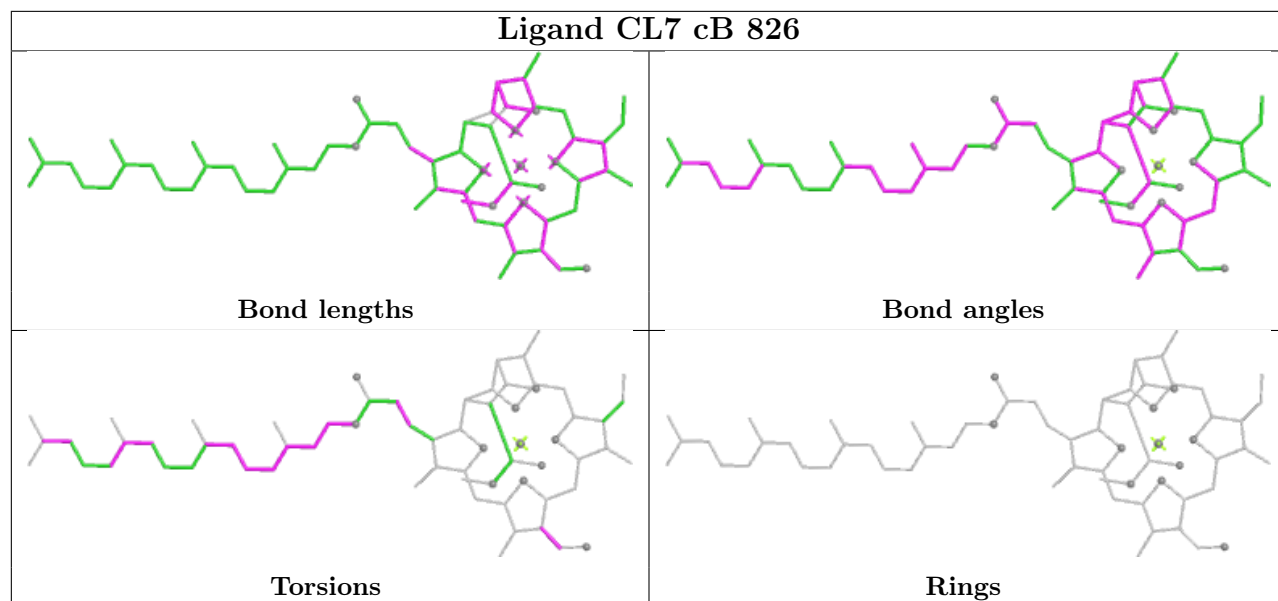


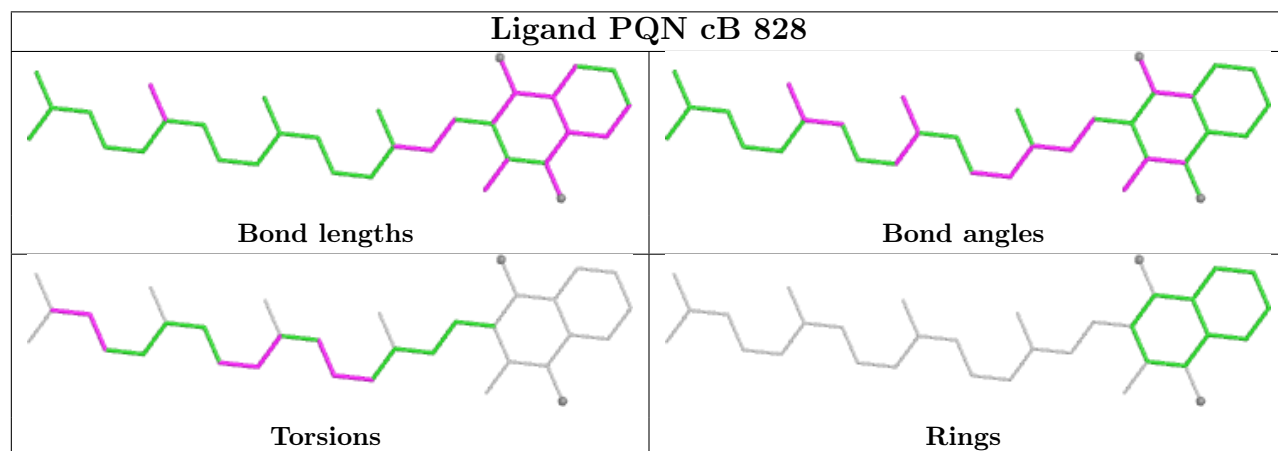
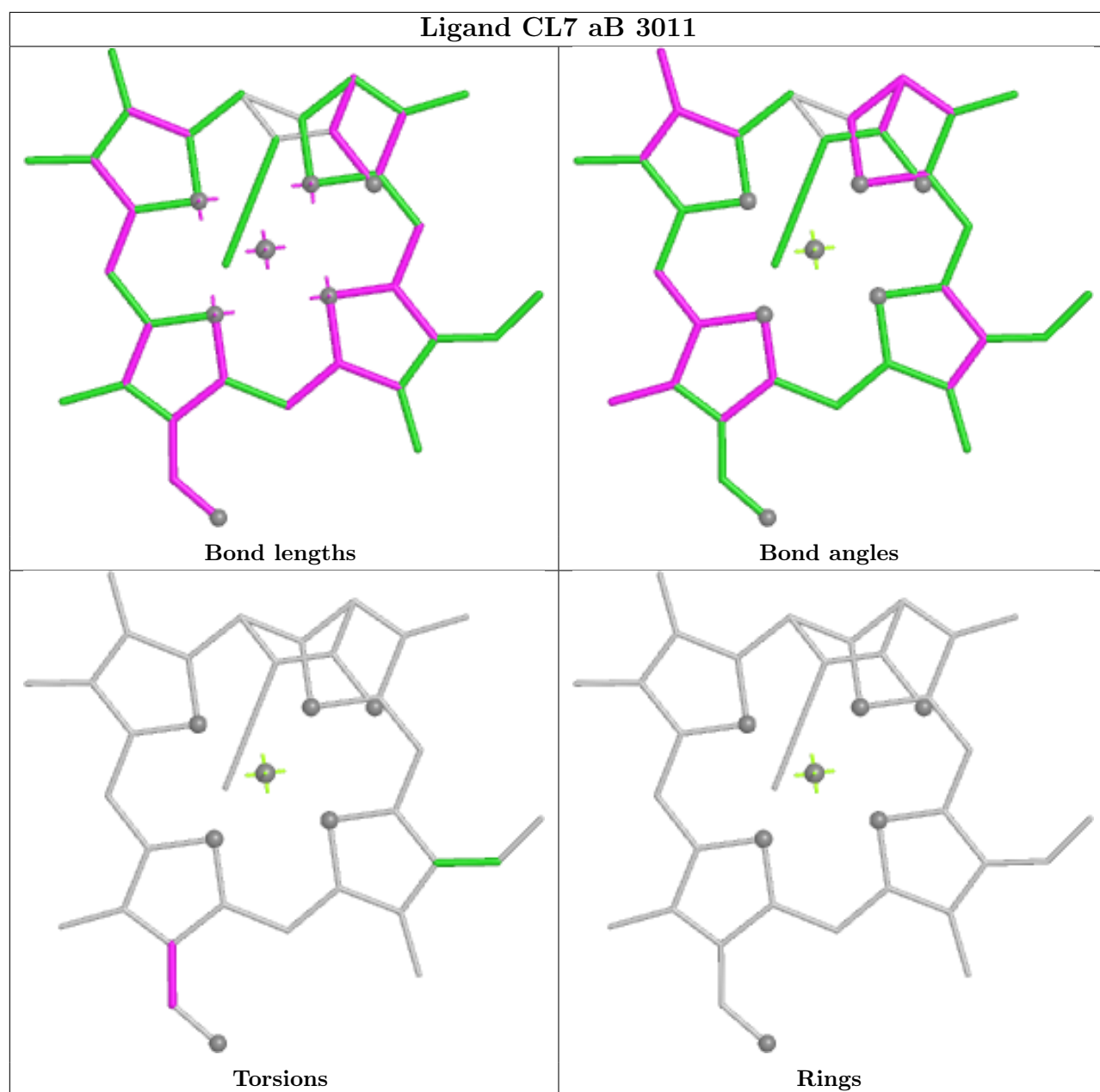


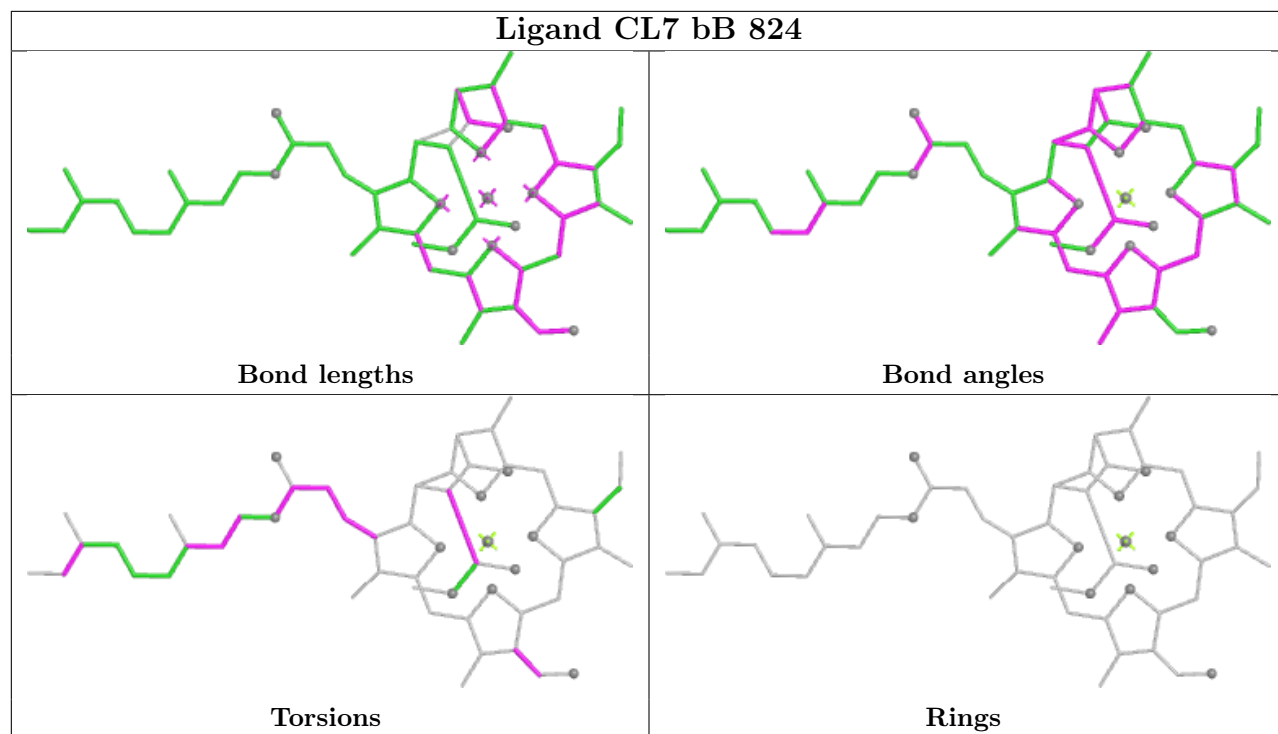


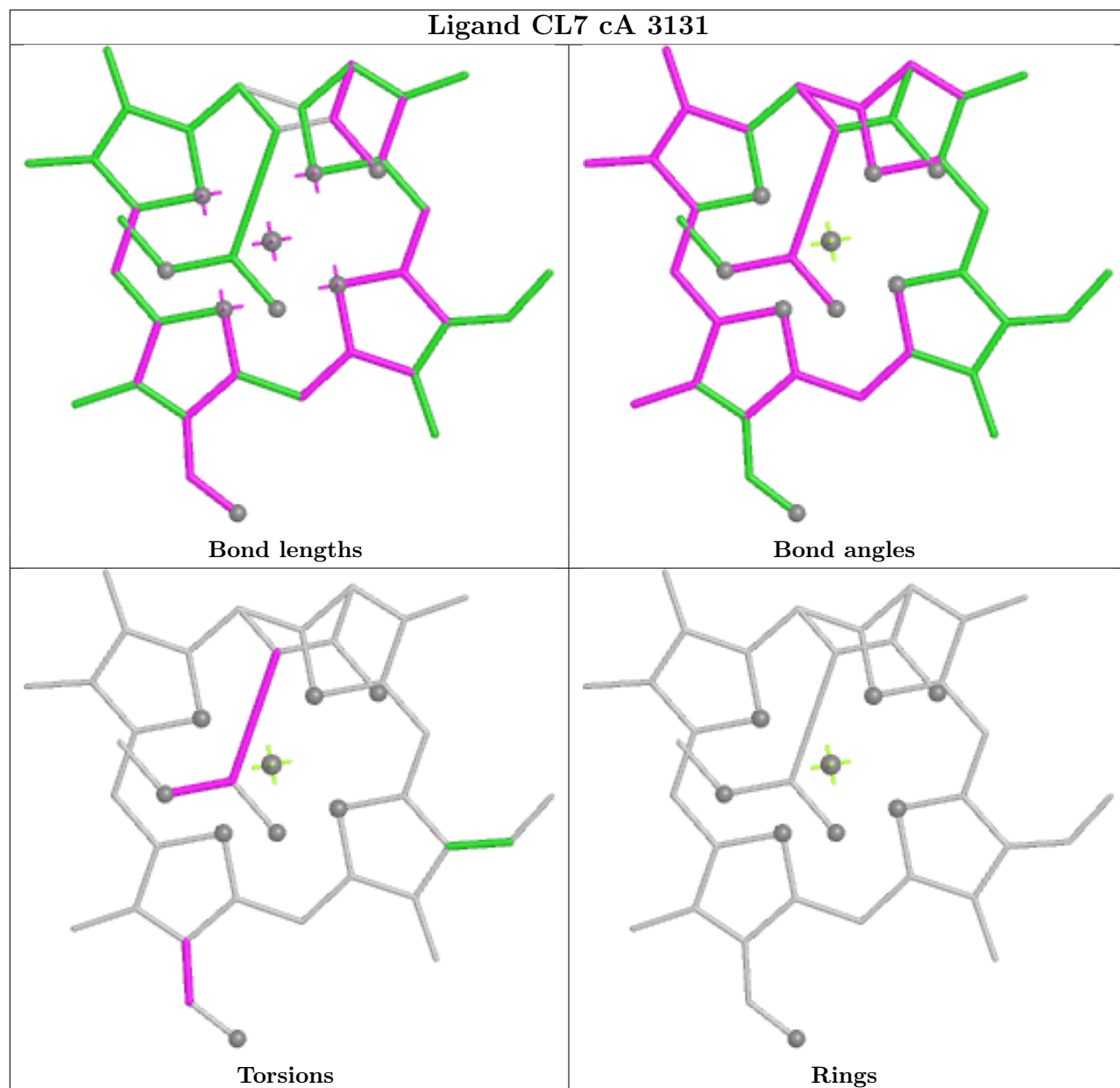




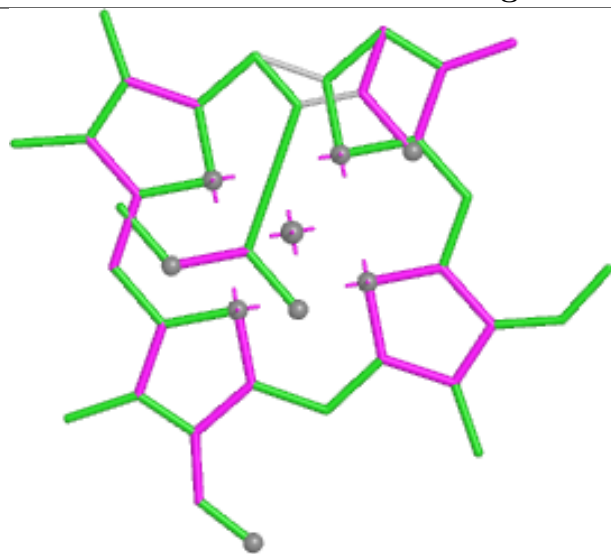




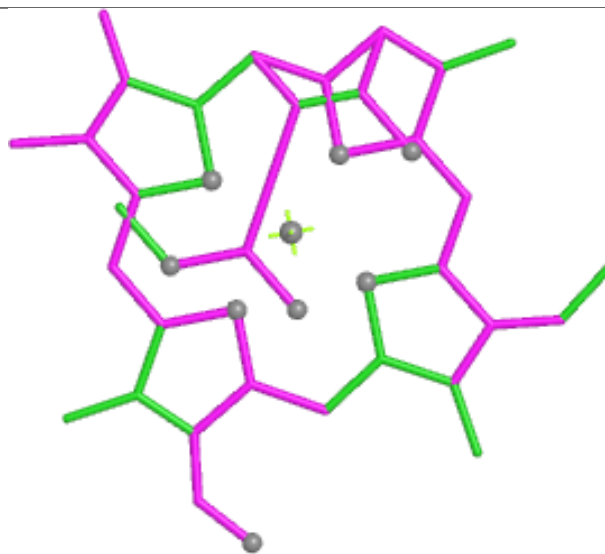




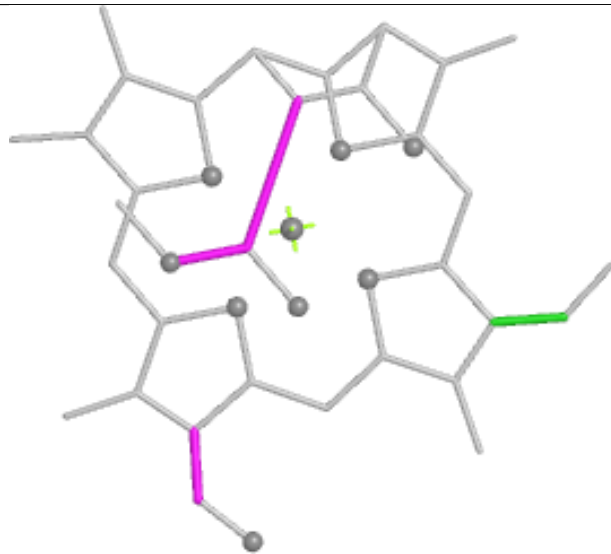
## Ligand CL7 aA 3106



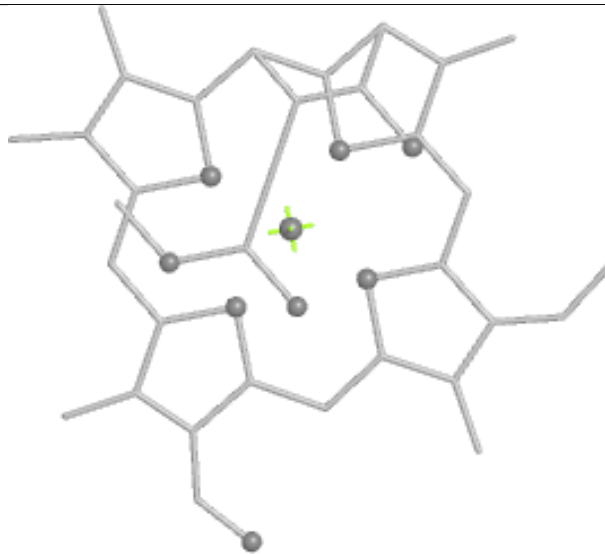
Bond lengths



Bond angles

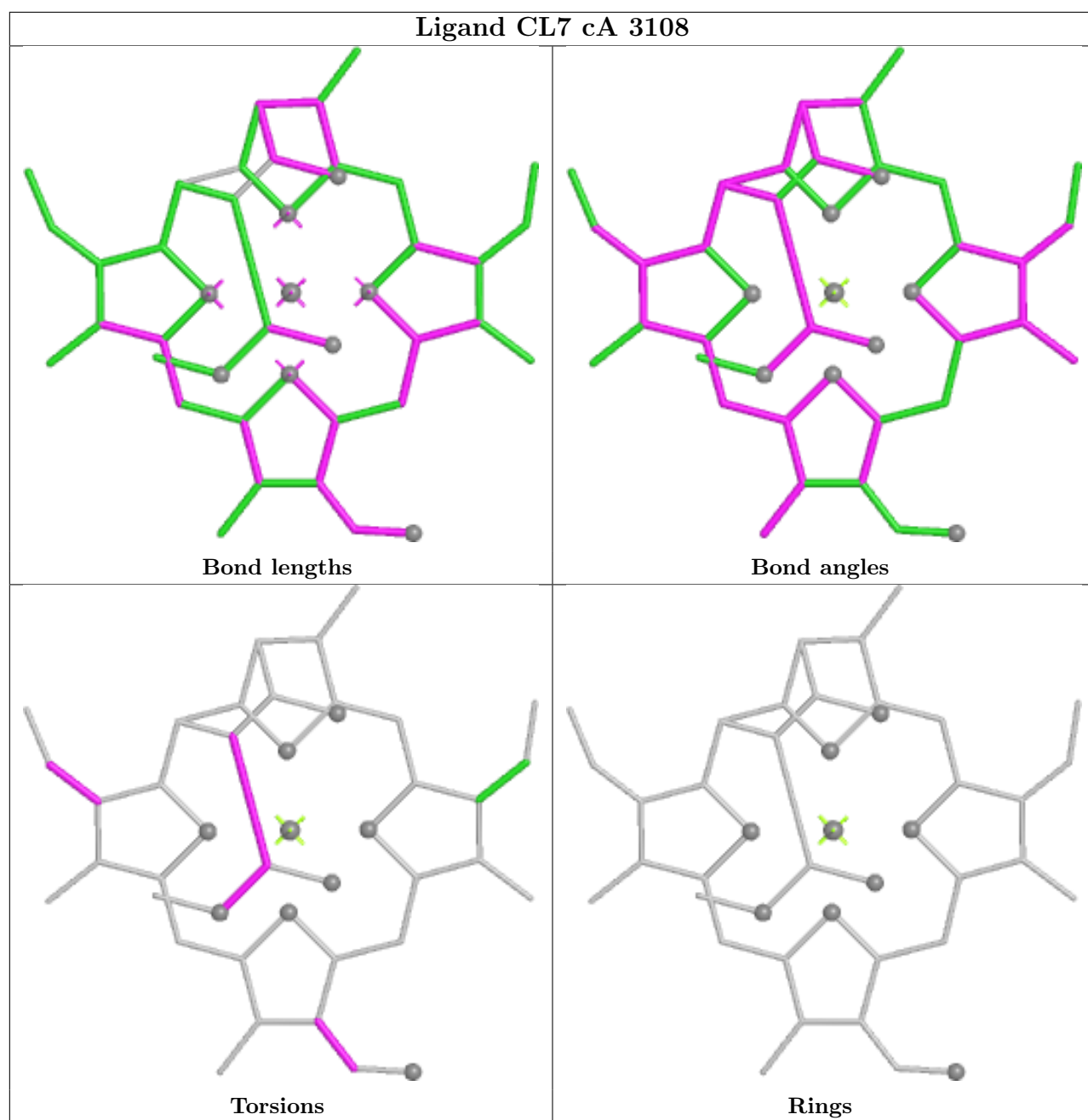


Torsions

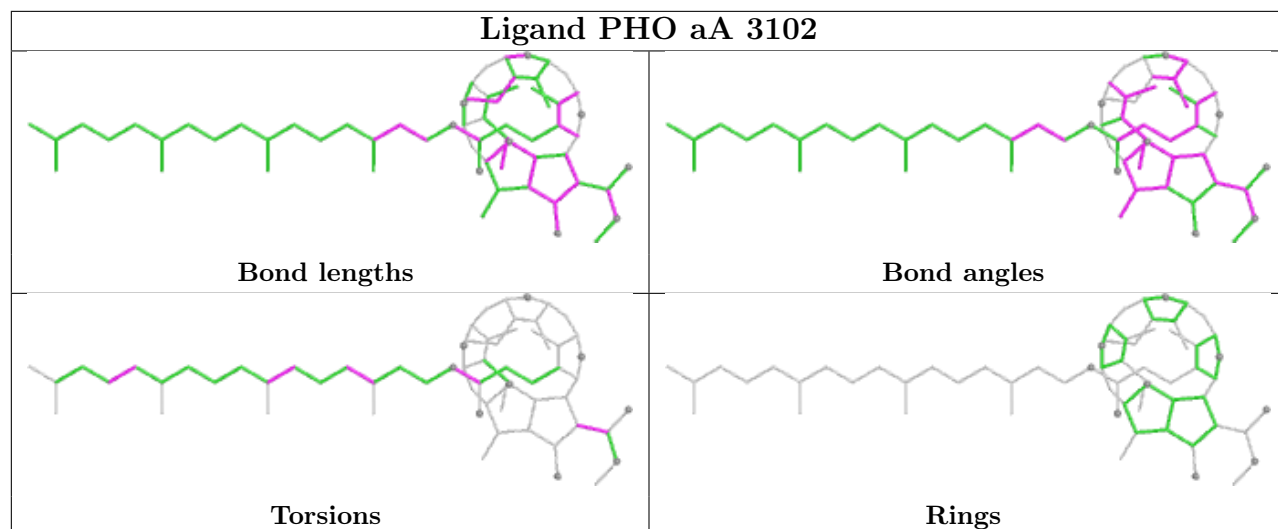


Rings

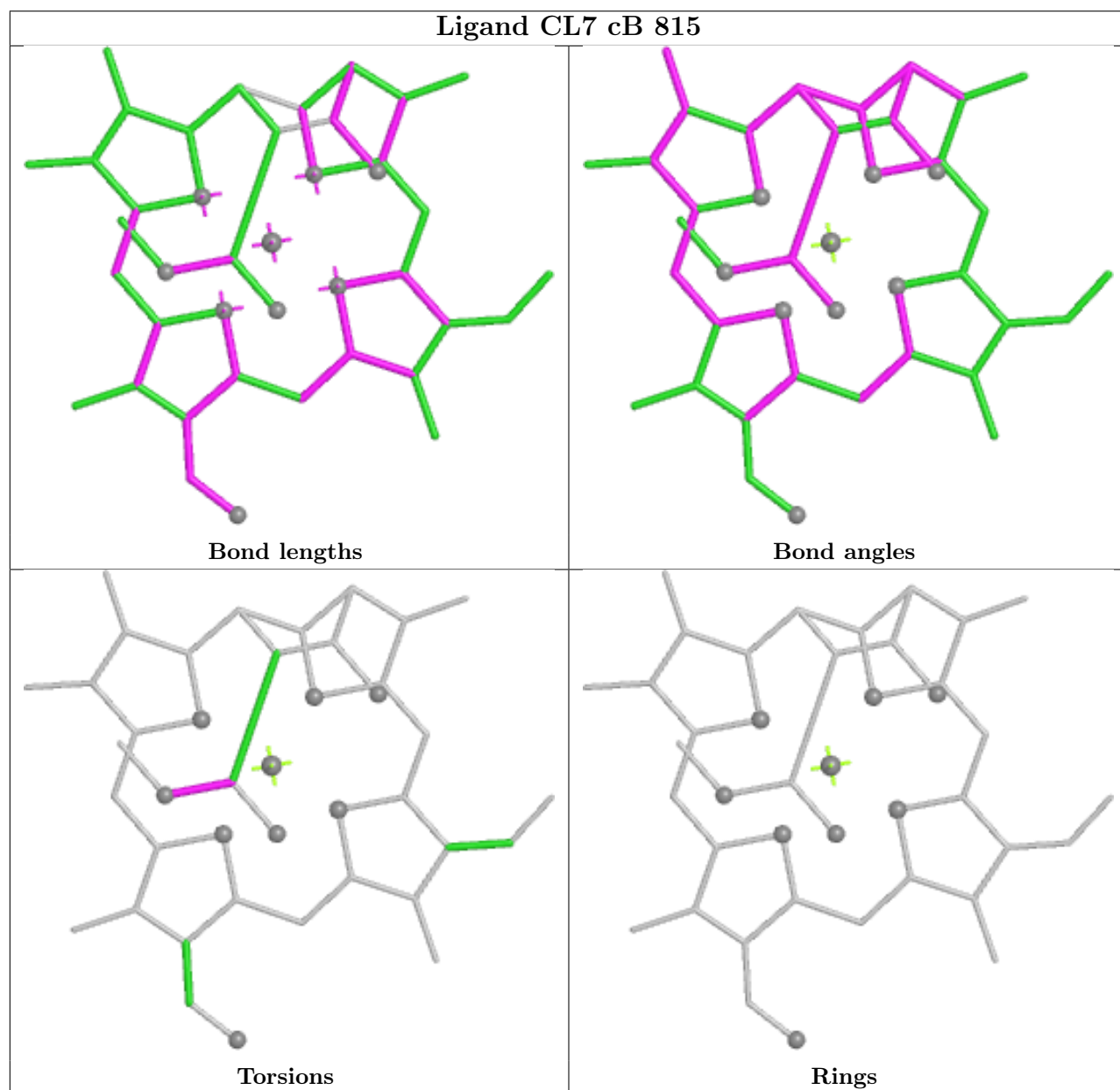


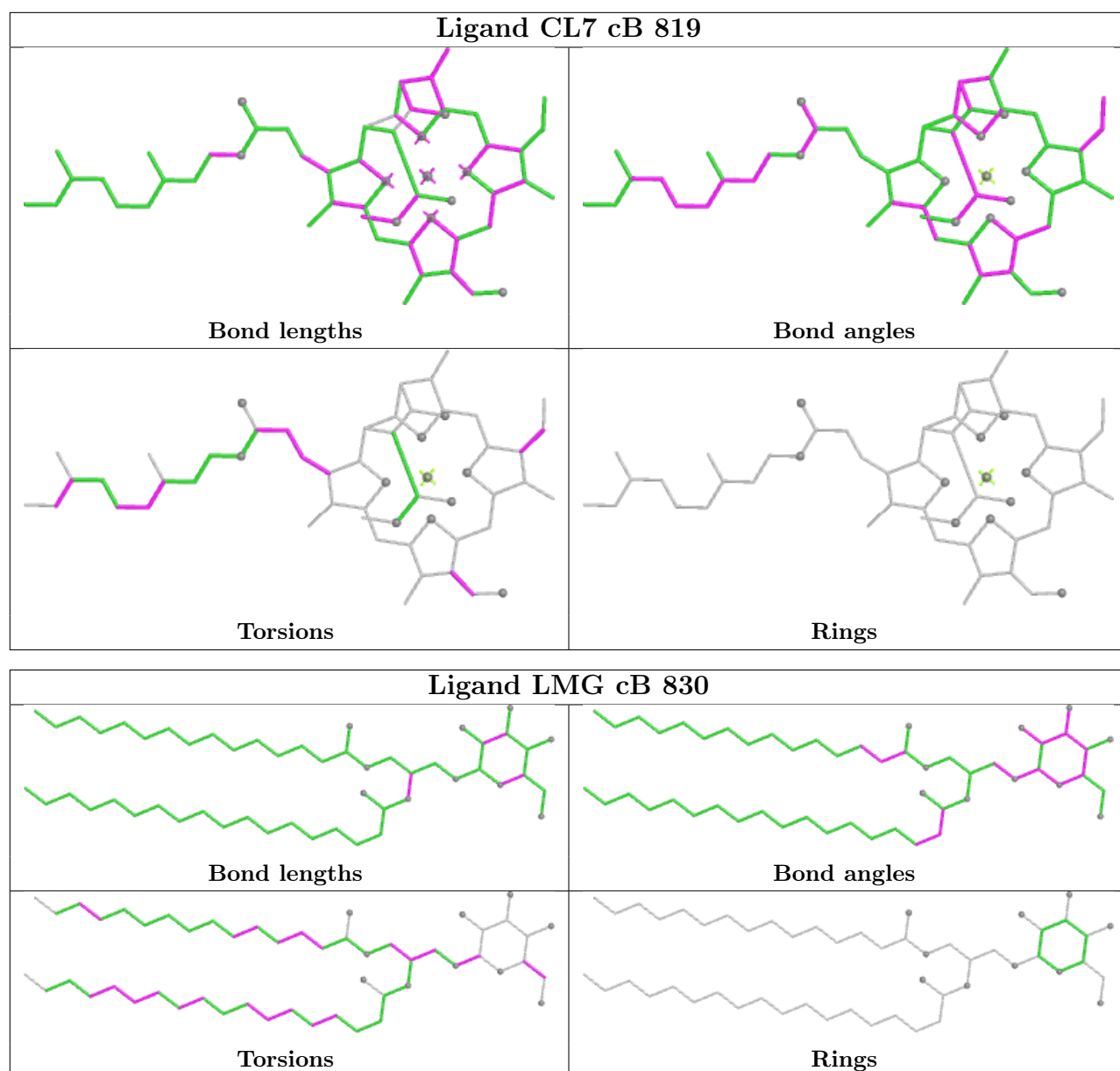


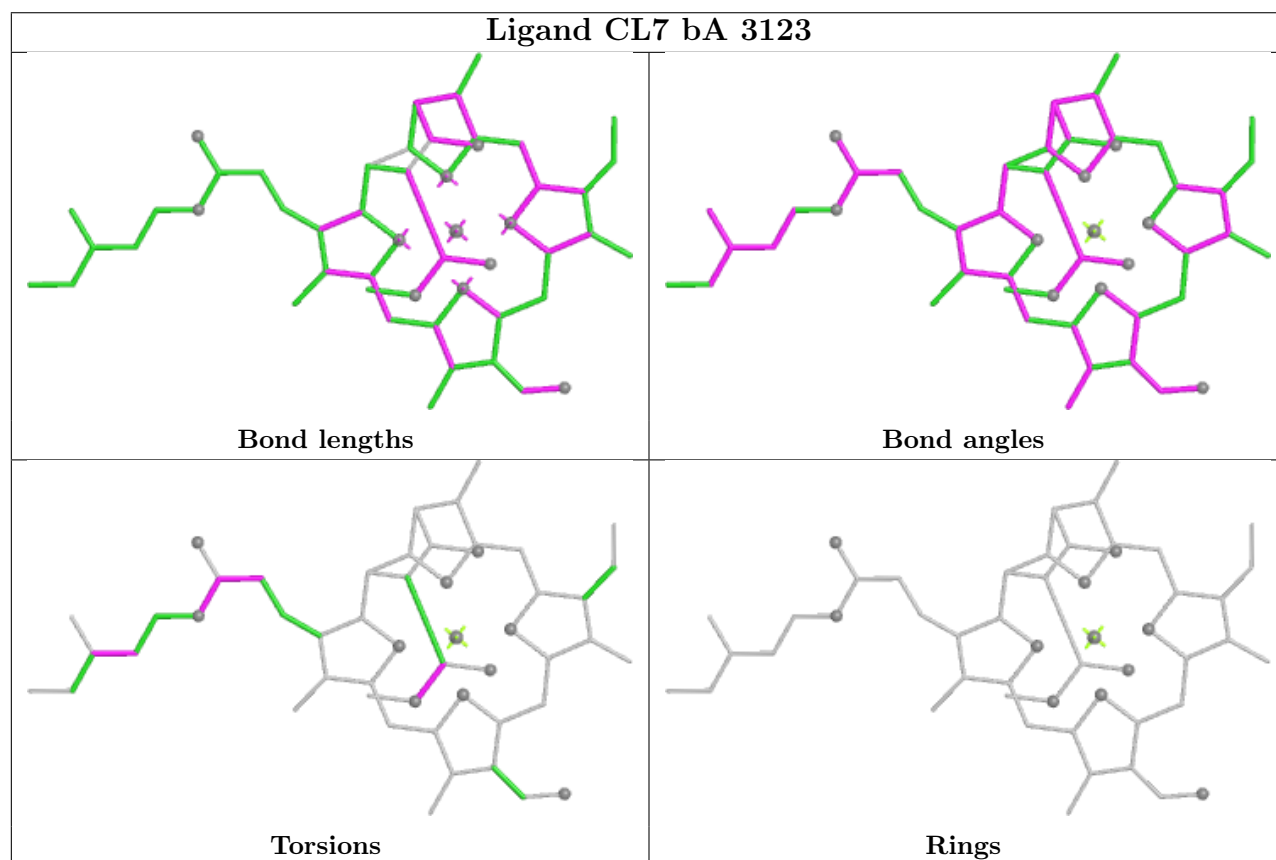
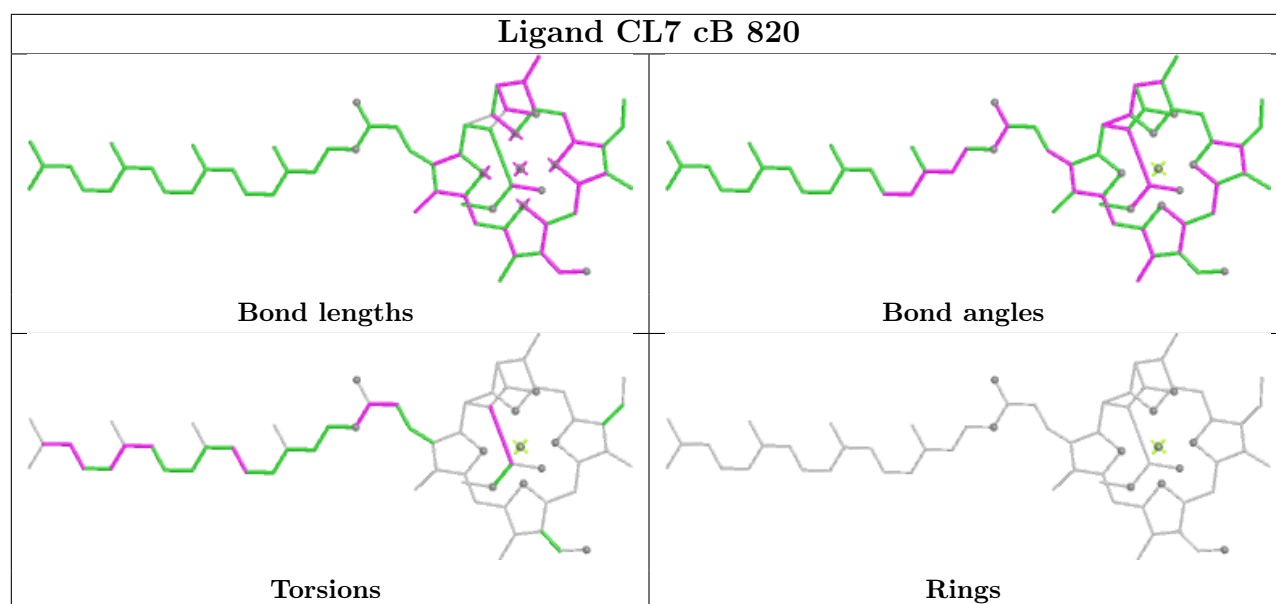
## Ligand PHO aA 3102

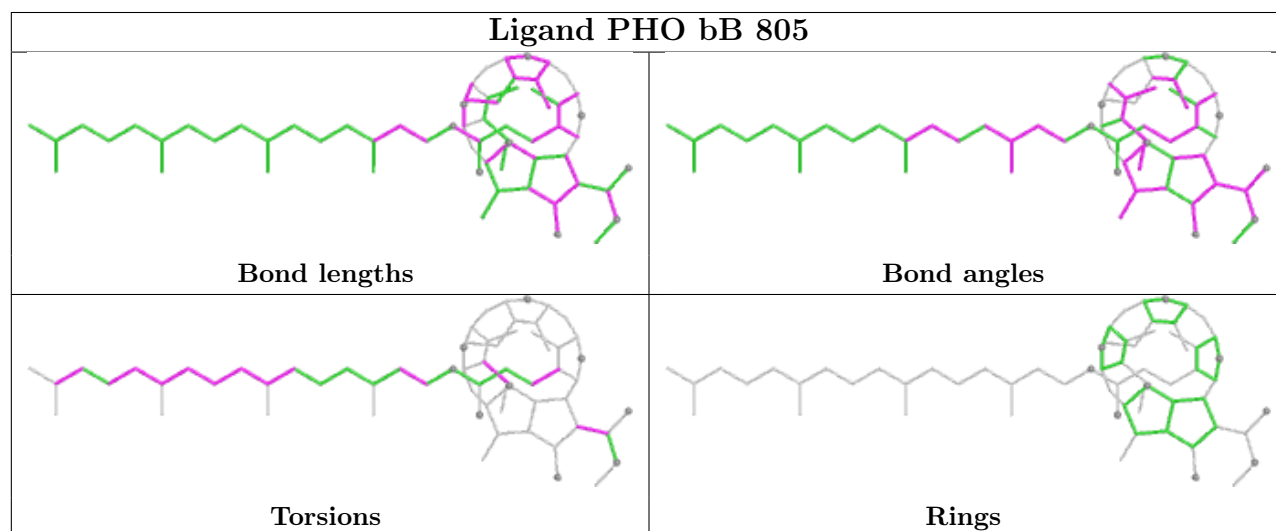
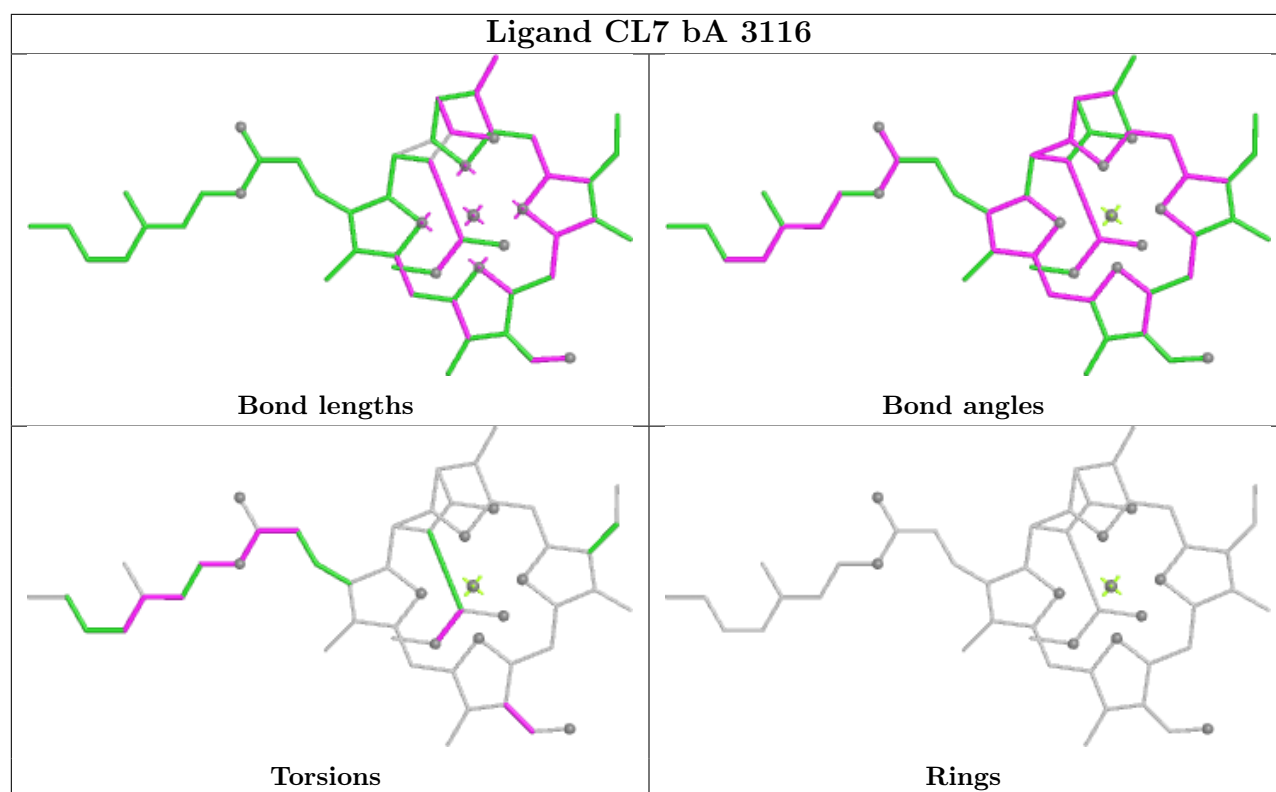


## Ligand CL7 cB 815

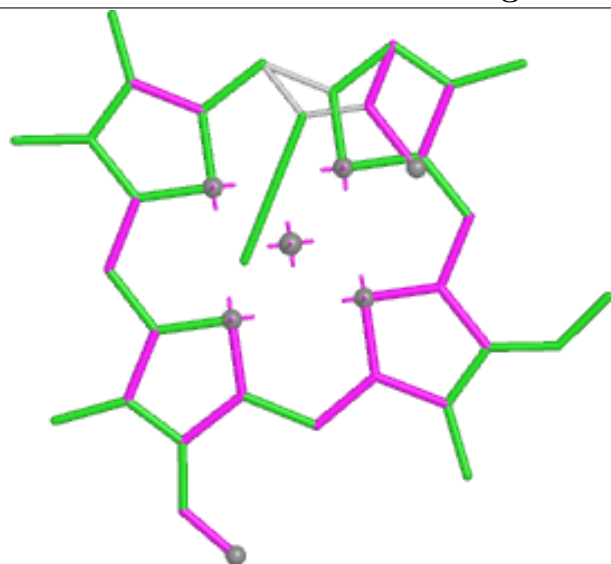




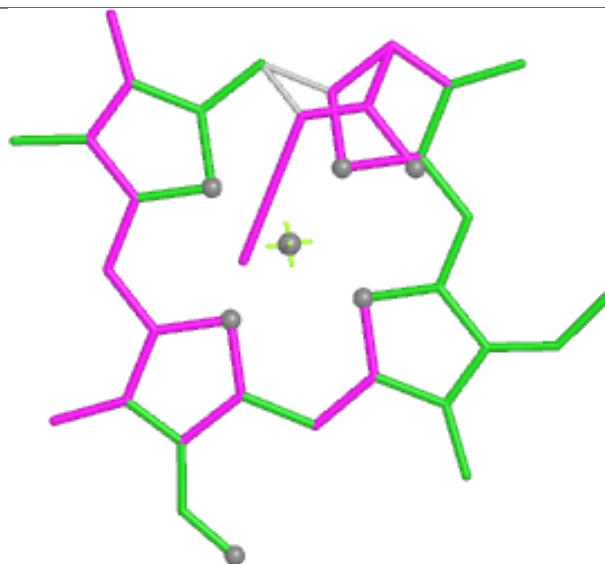




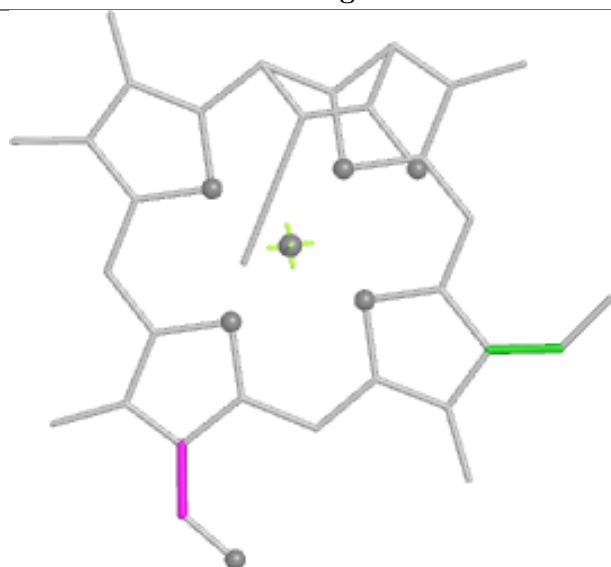
## Ligand CL7 cA 3117



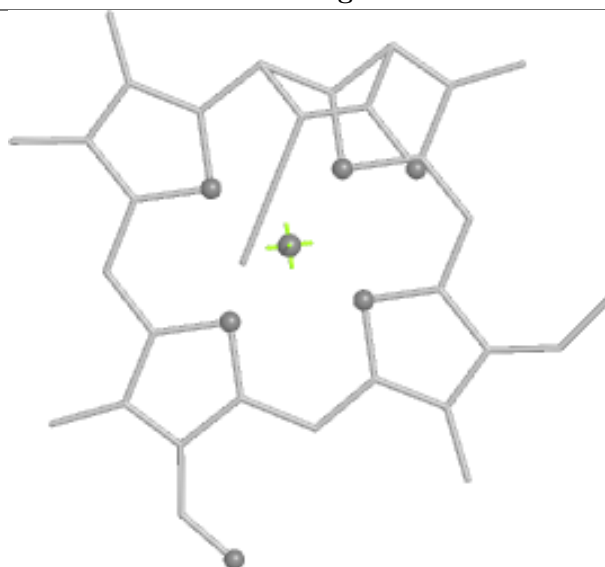
Bond lengths



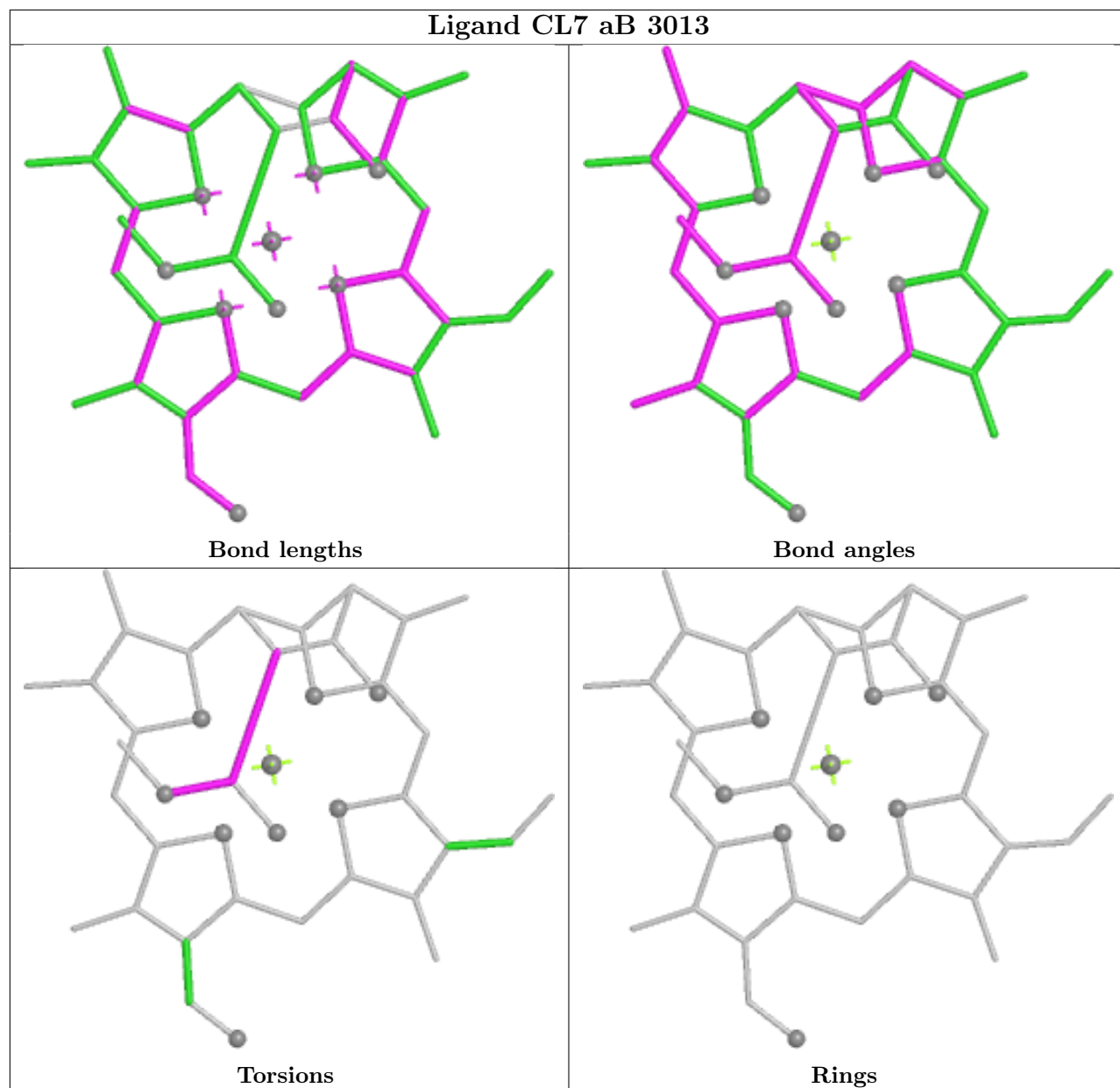
Bond angles

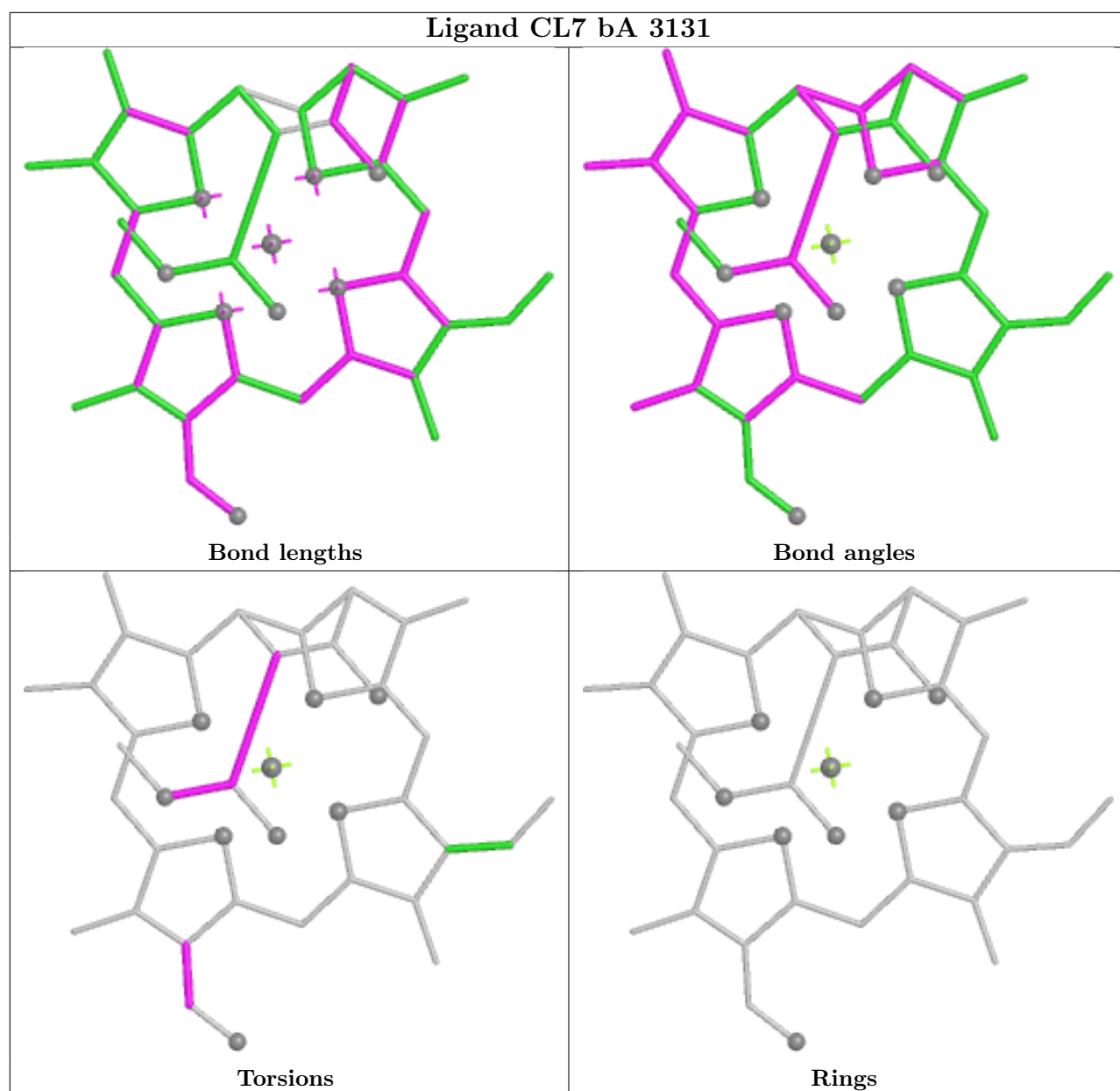


Torsions

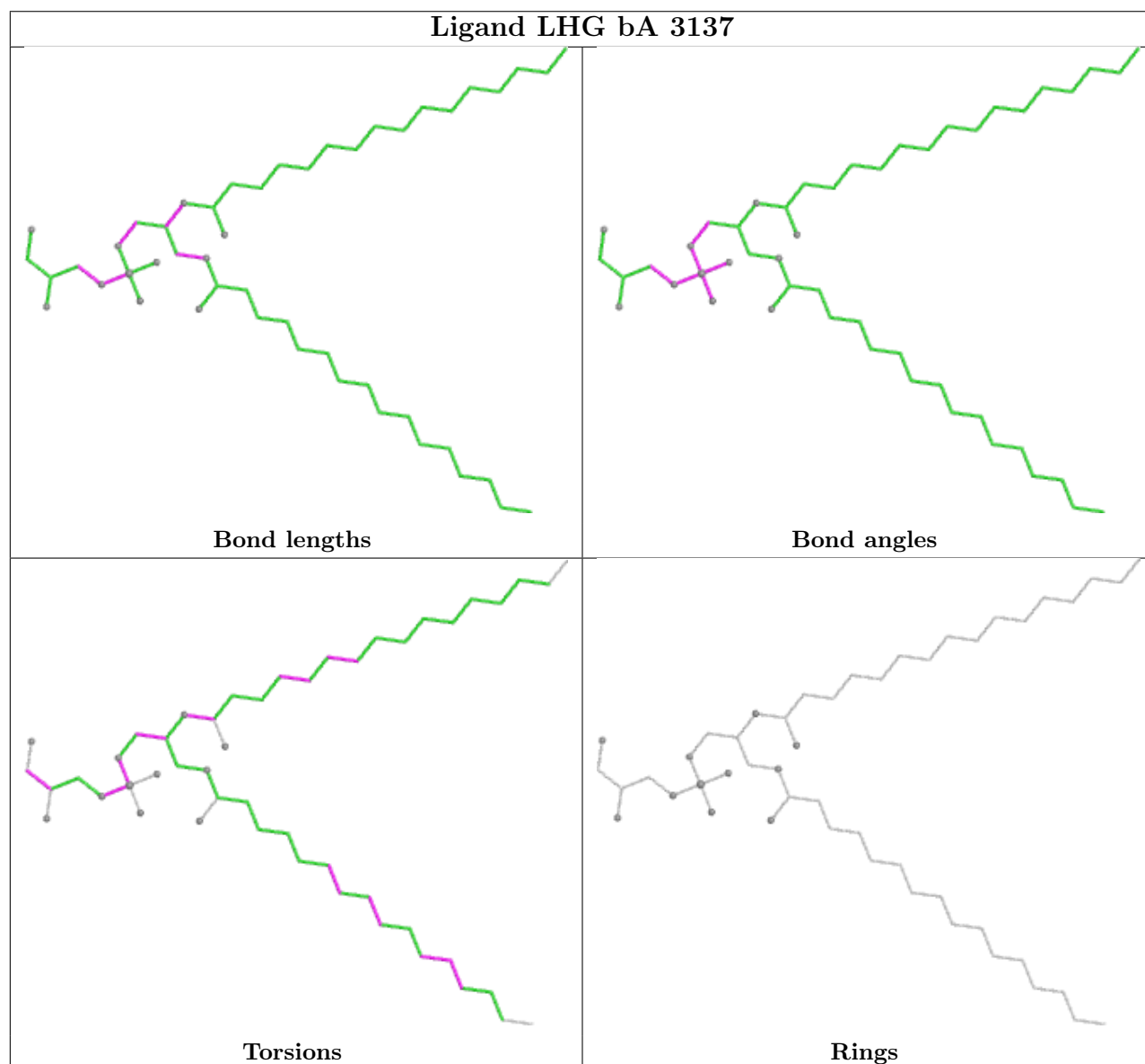
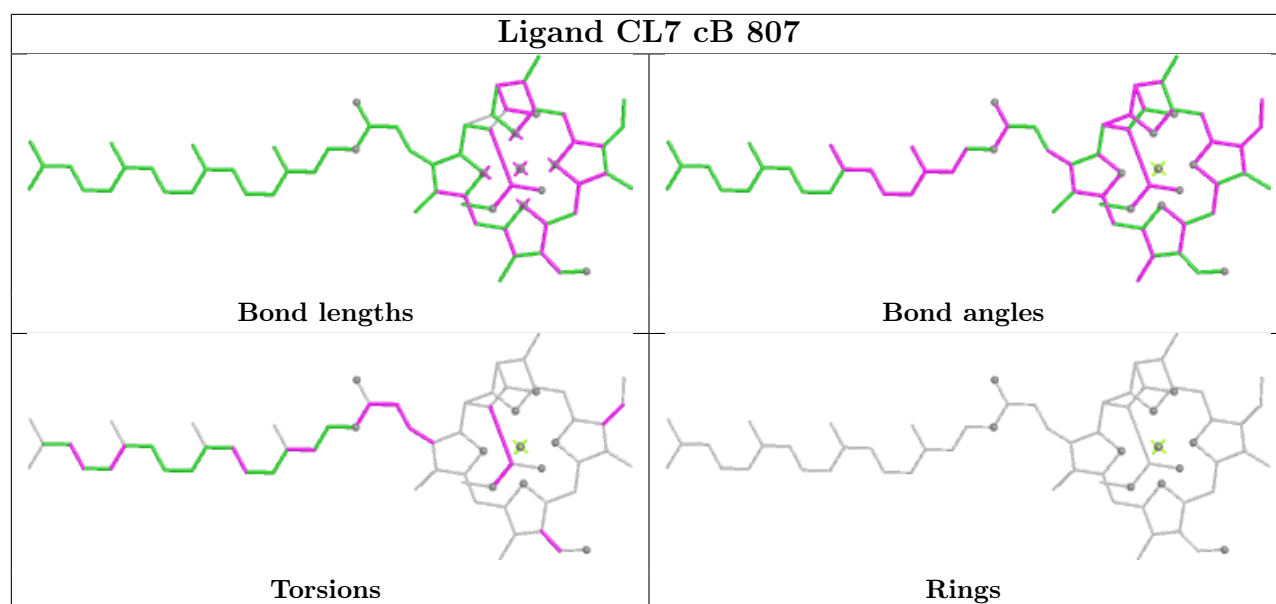


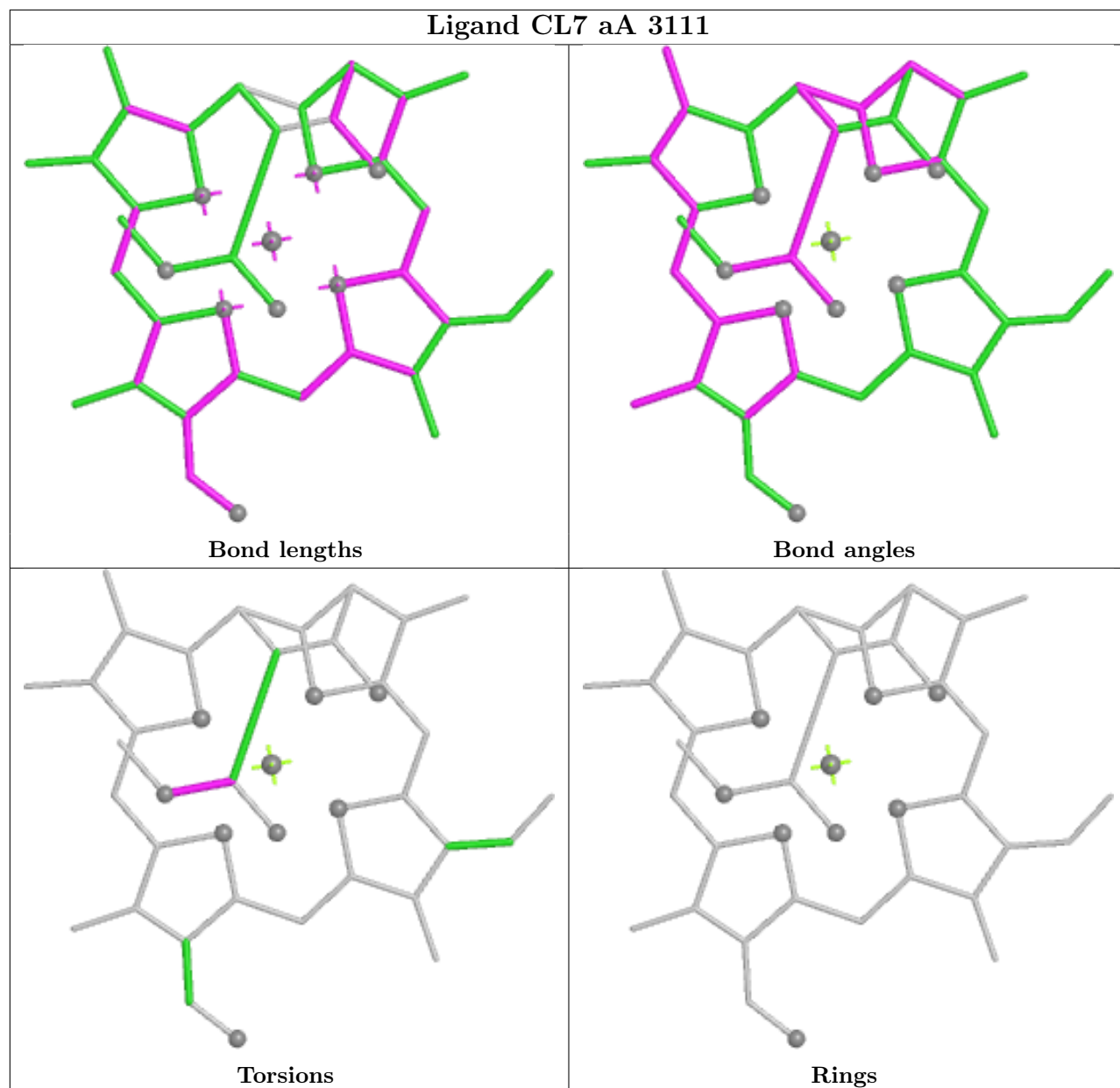
Rings



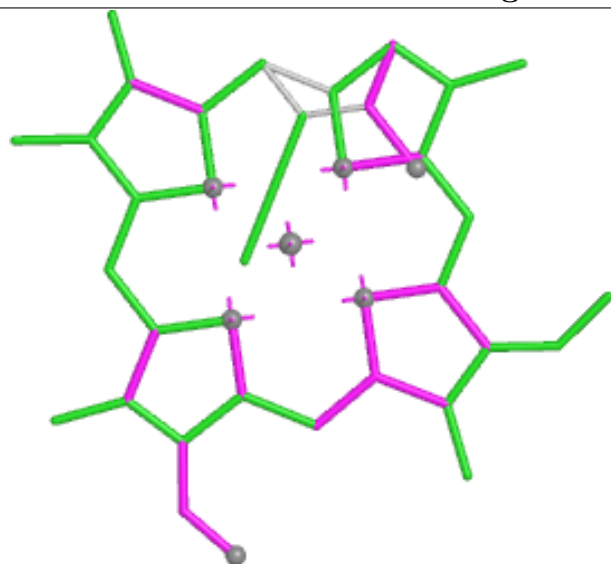




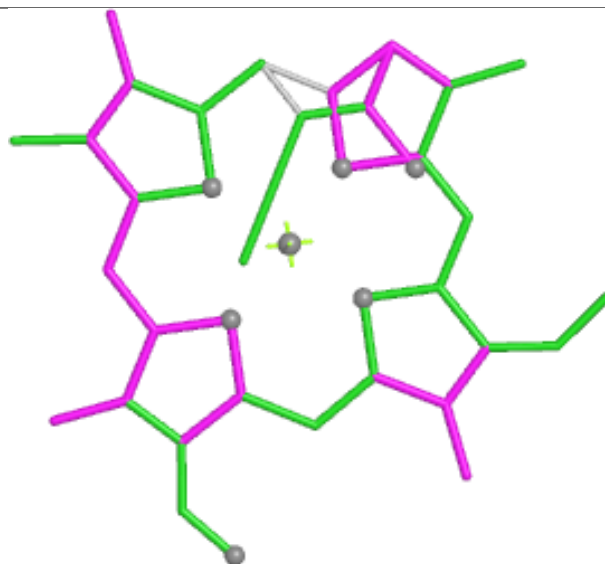




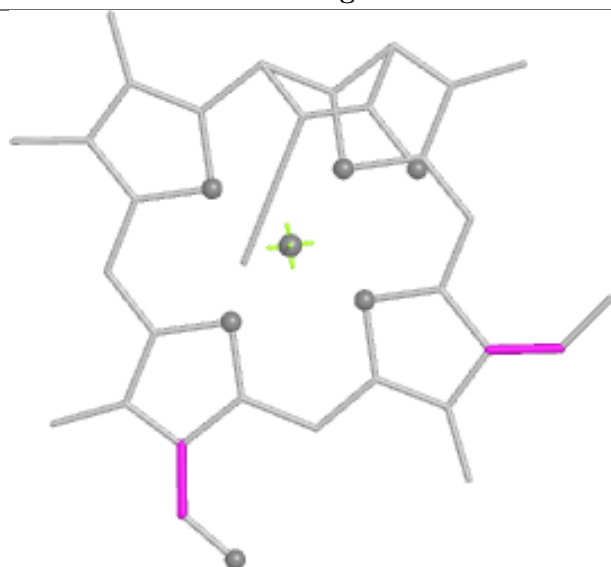
## Ligand CL7 cA 3115



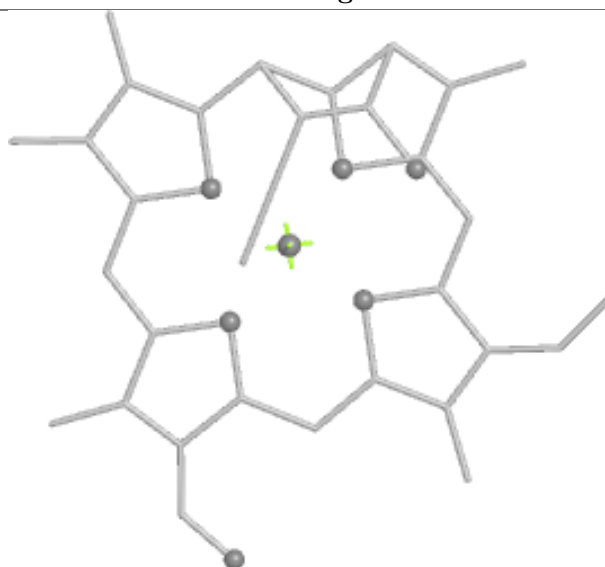
Bond lengths



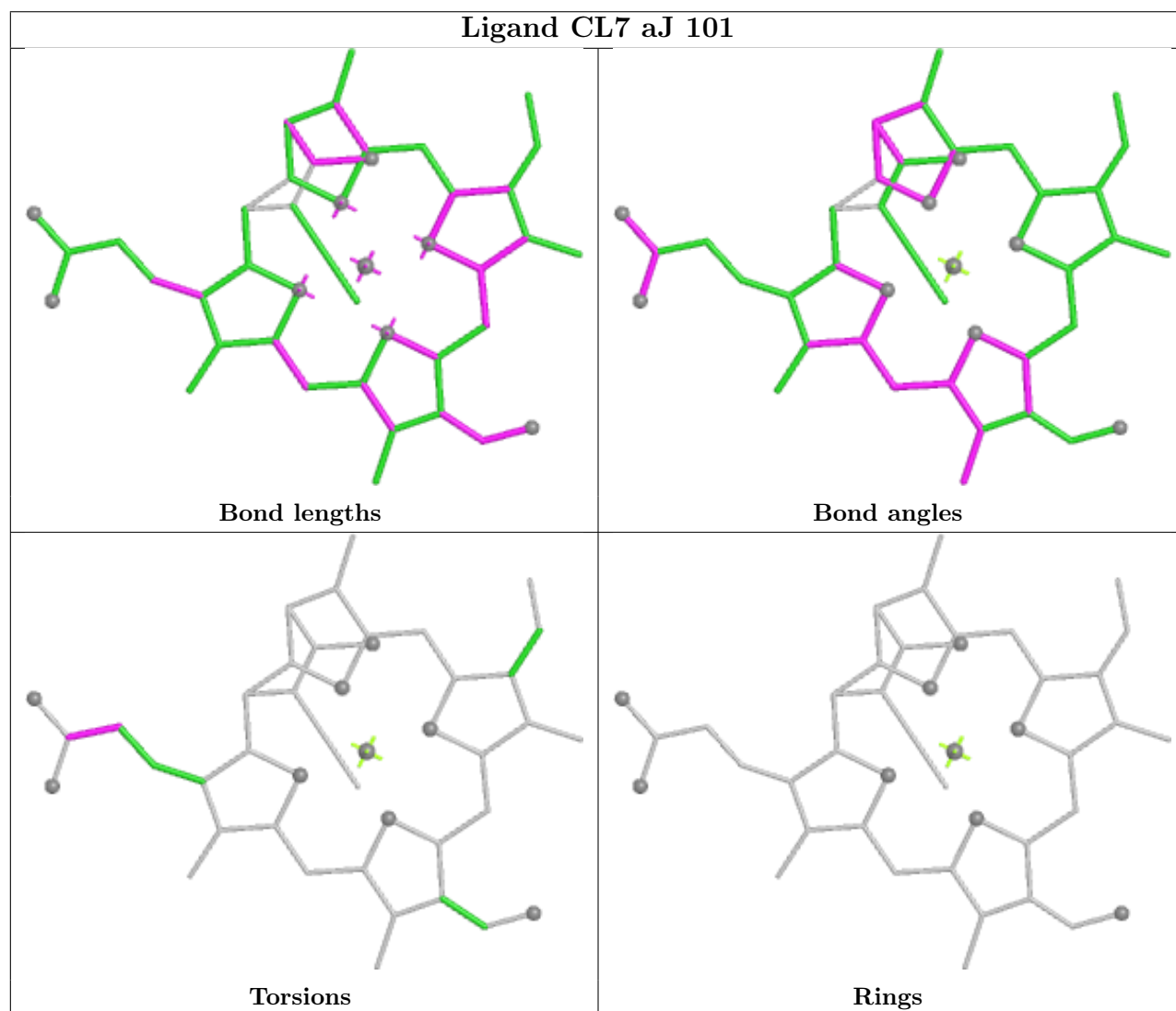
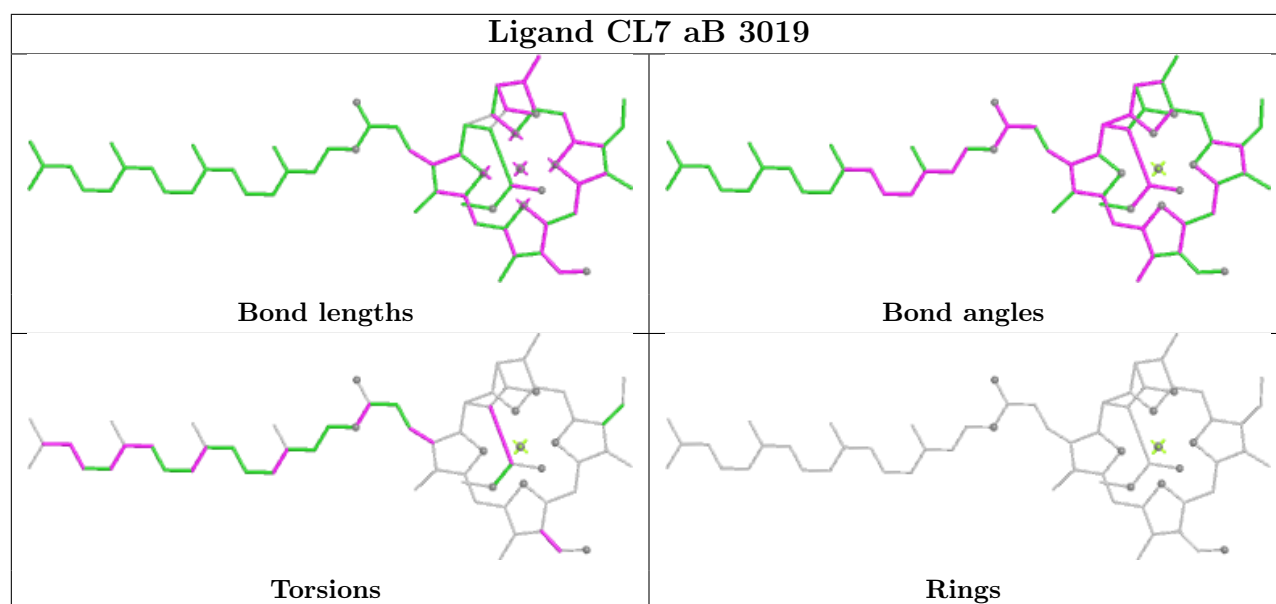
Bond angles

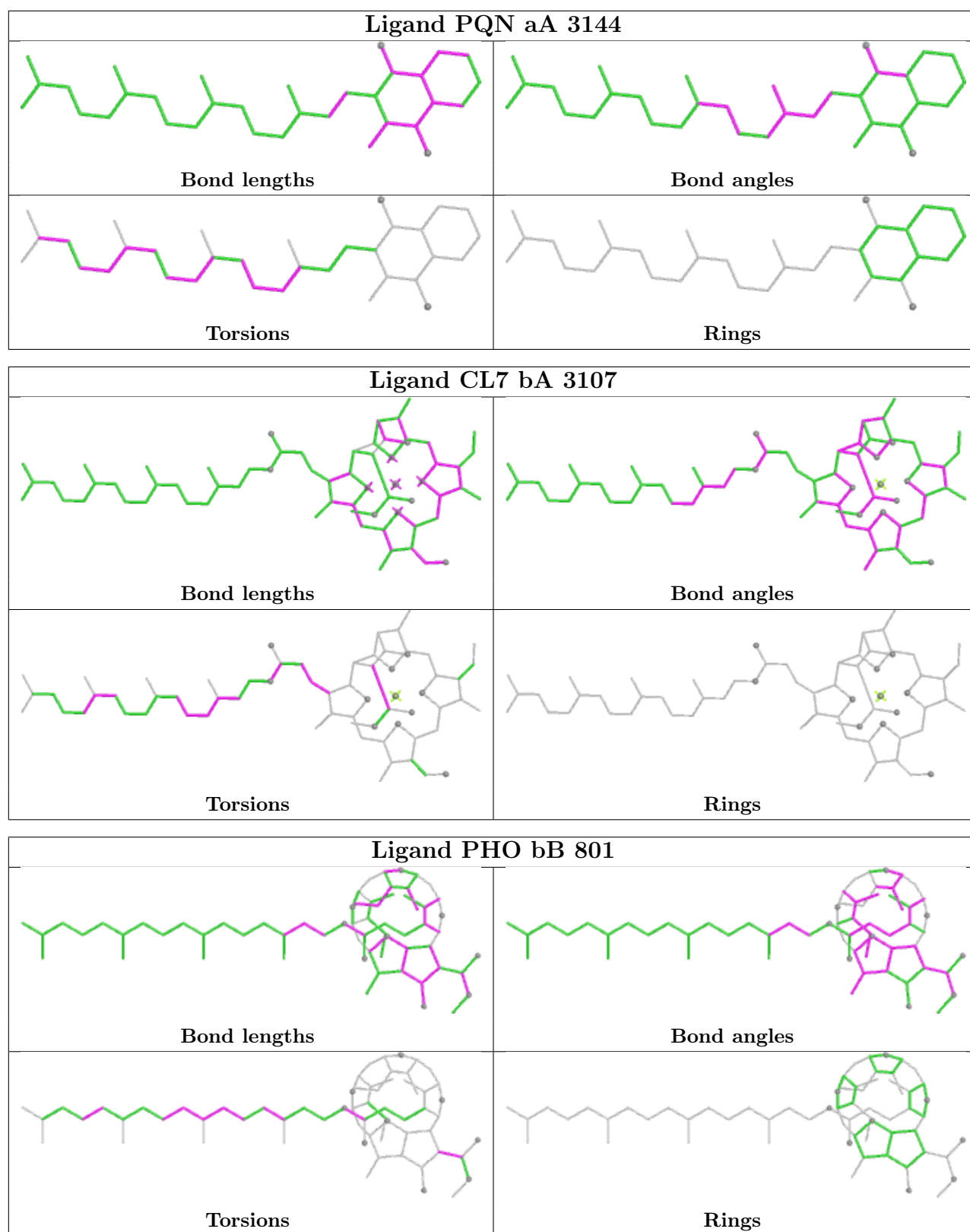


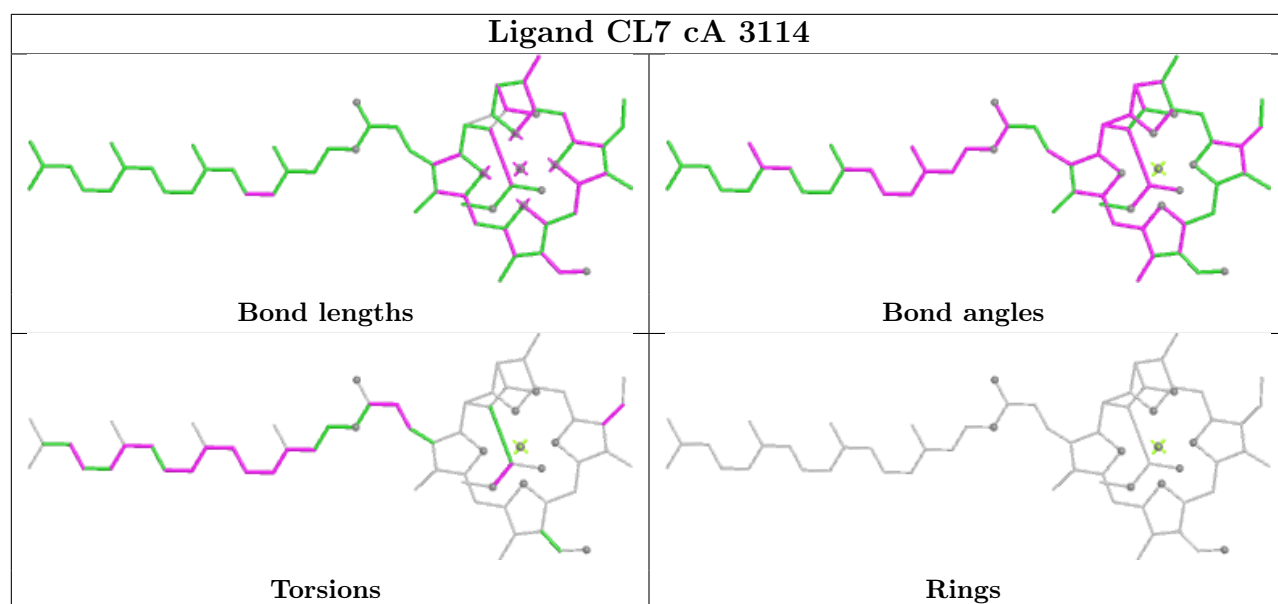
Torsions

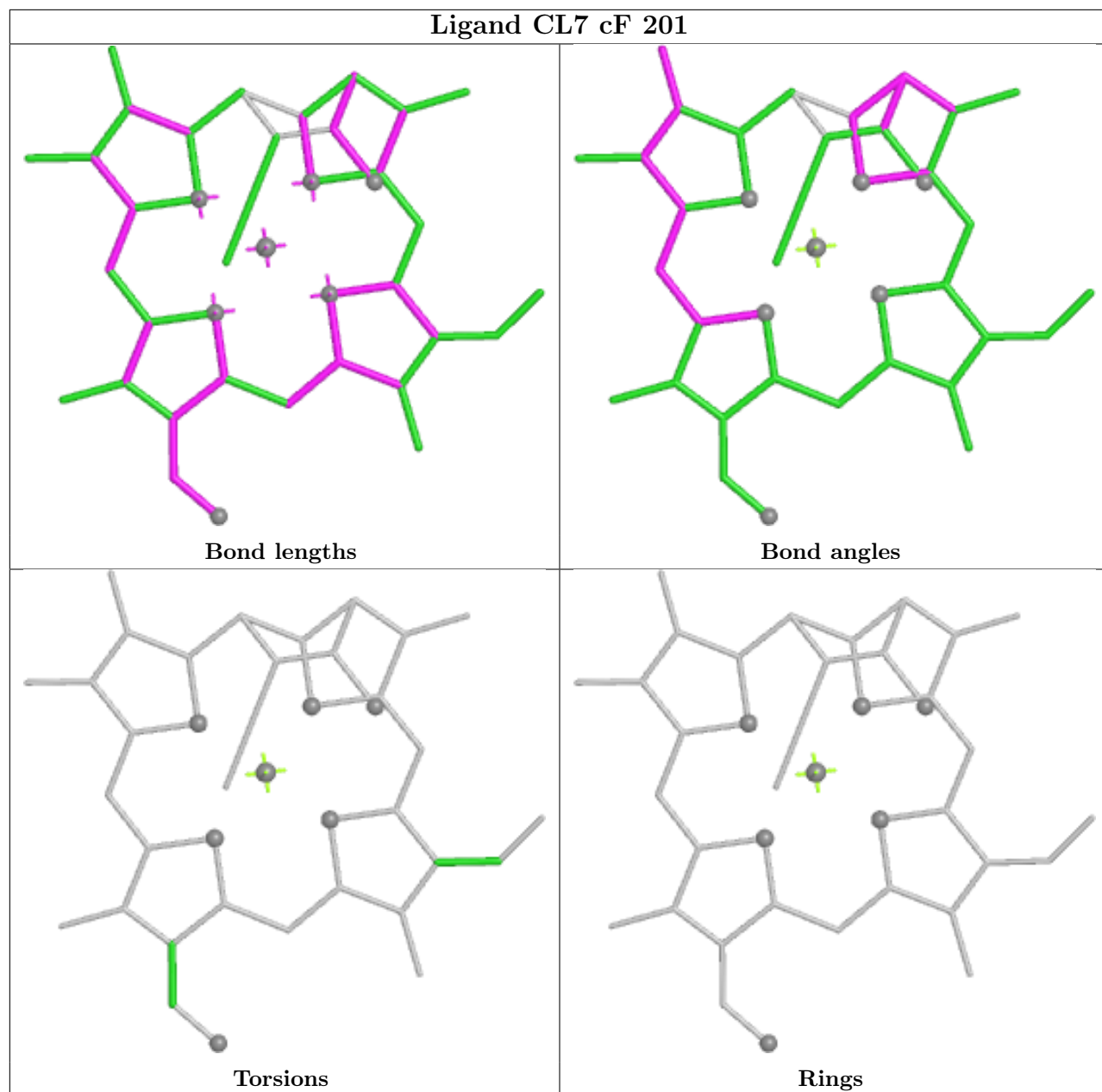


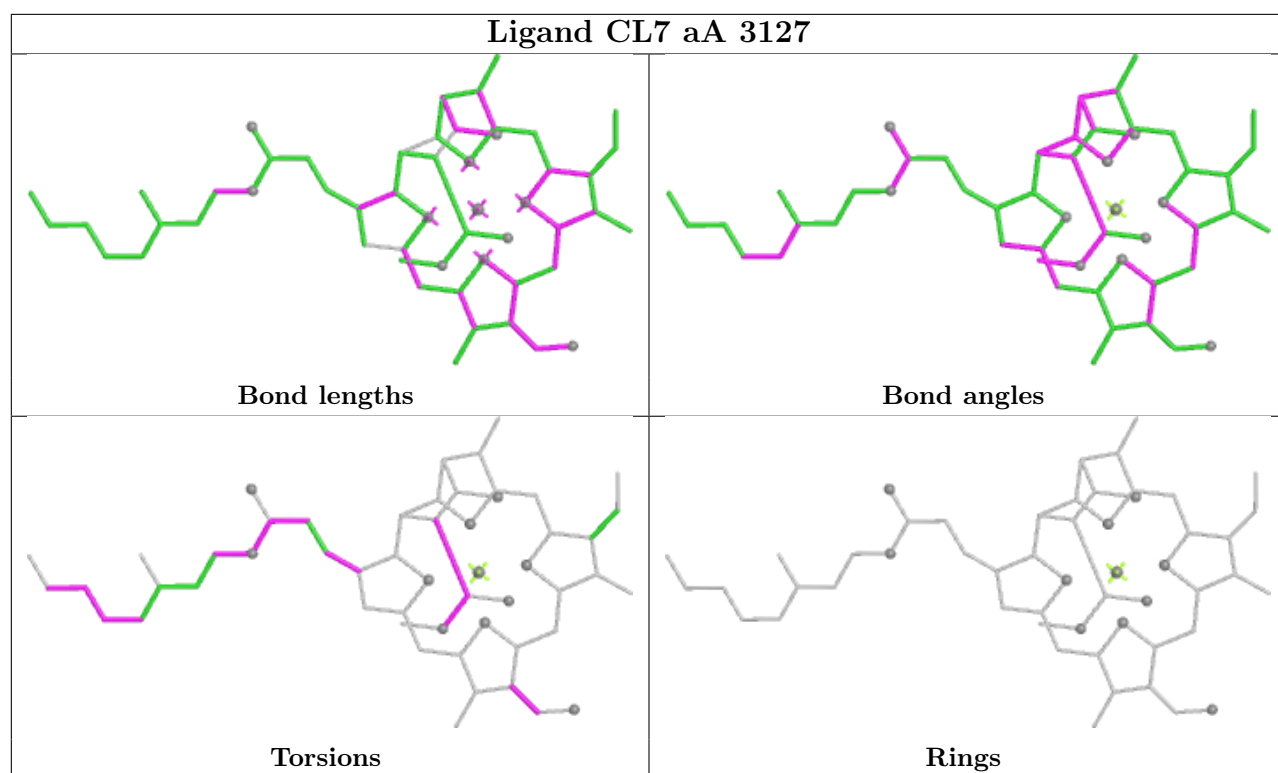
Rings





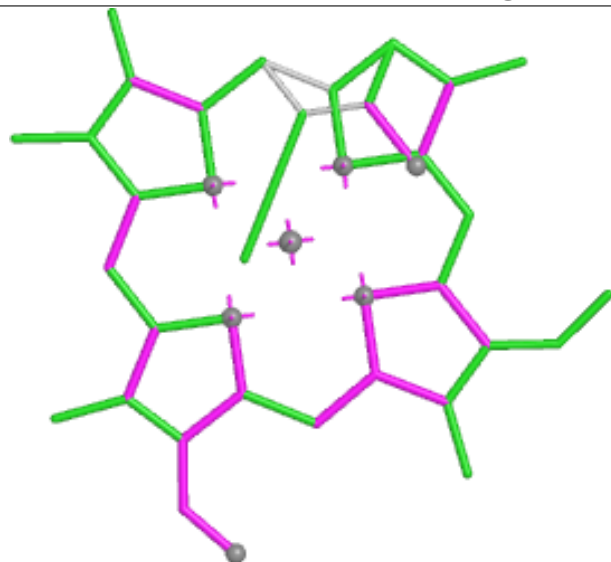




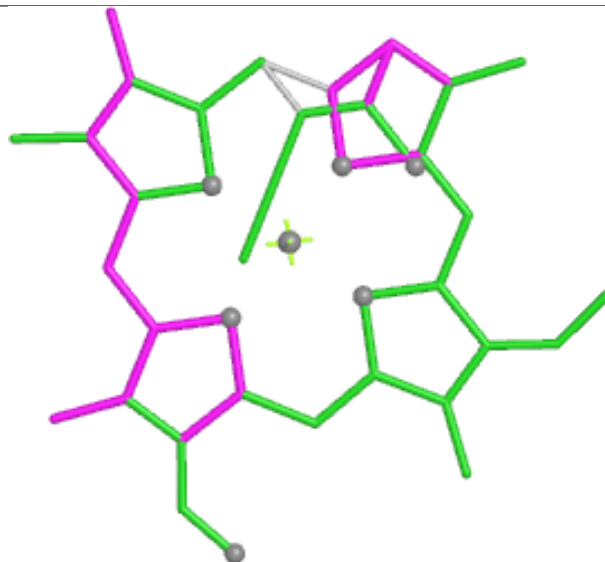




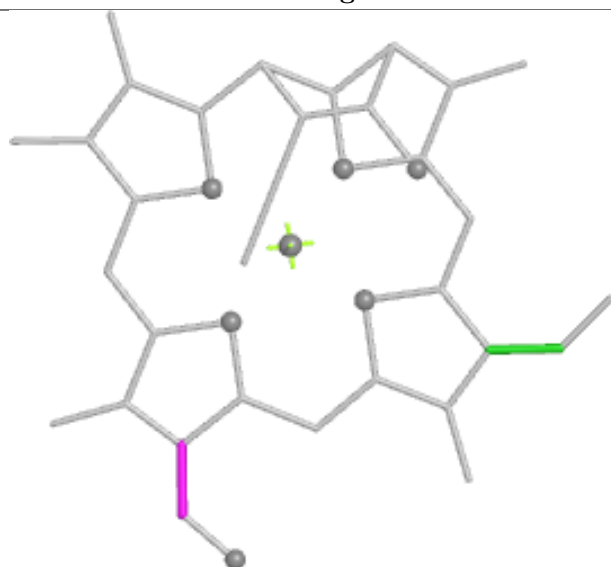
## Ligand CL7 bA 3111



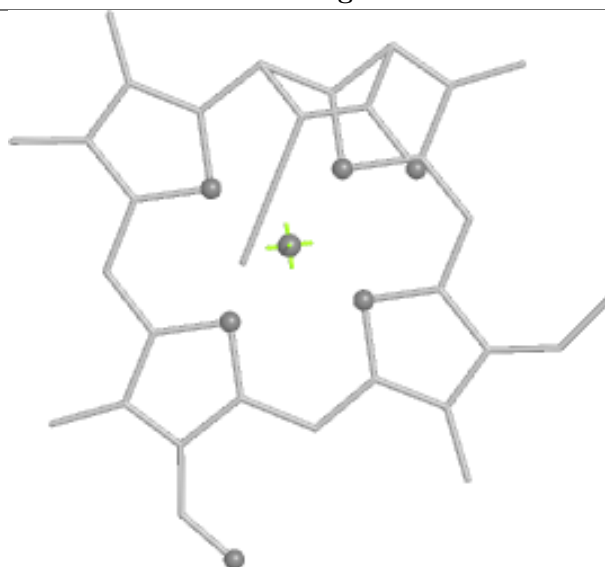
Bond lengths



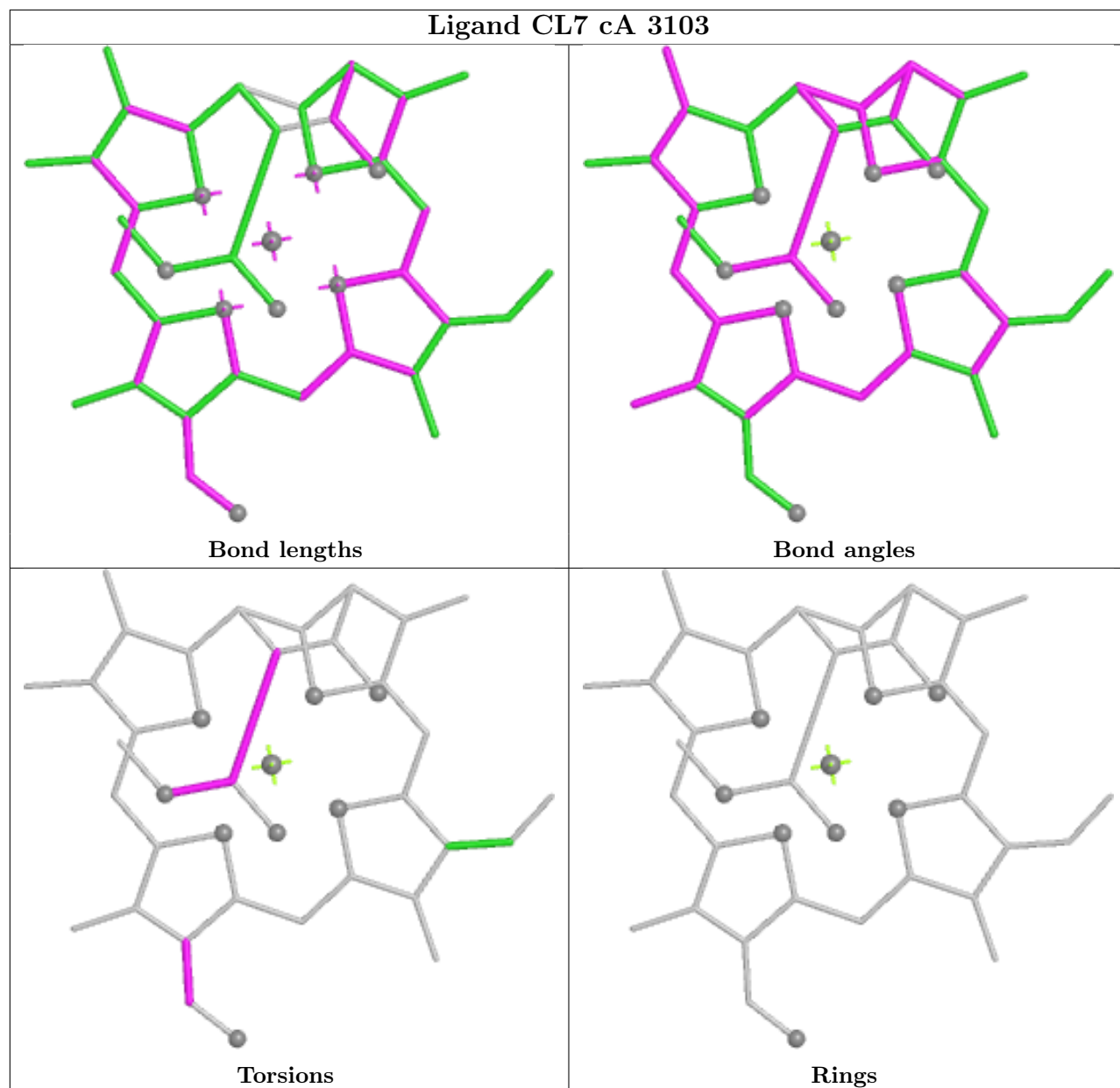
Bond angles

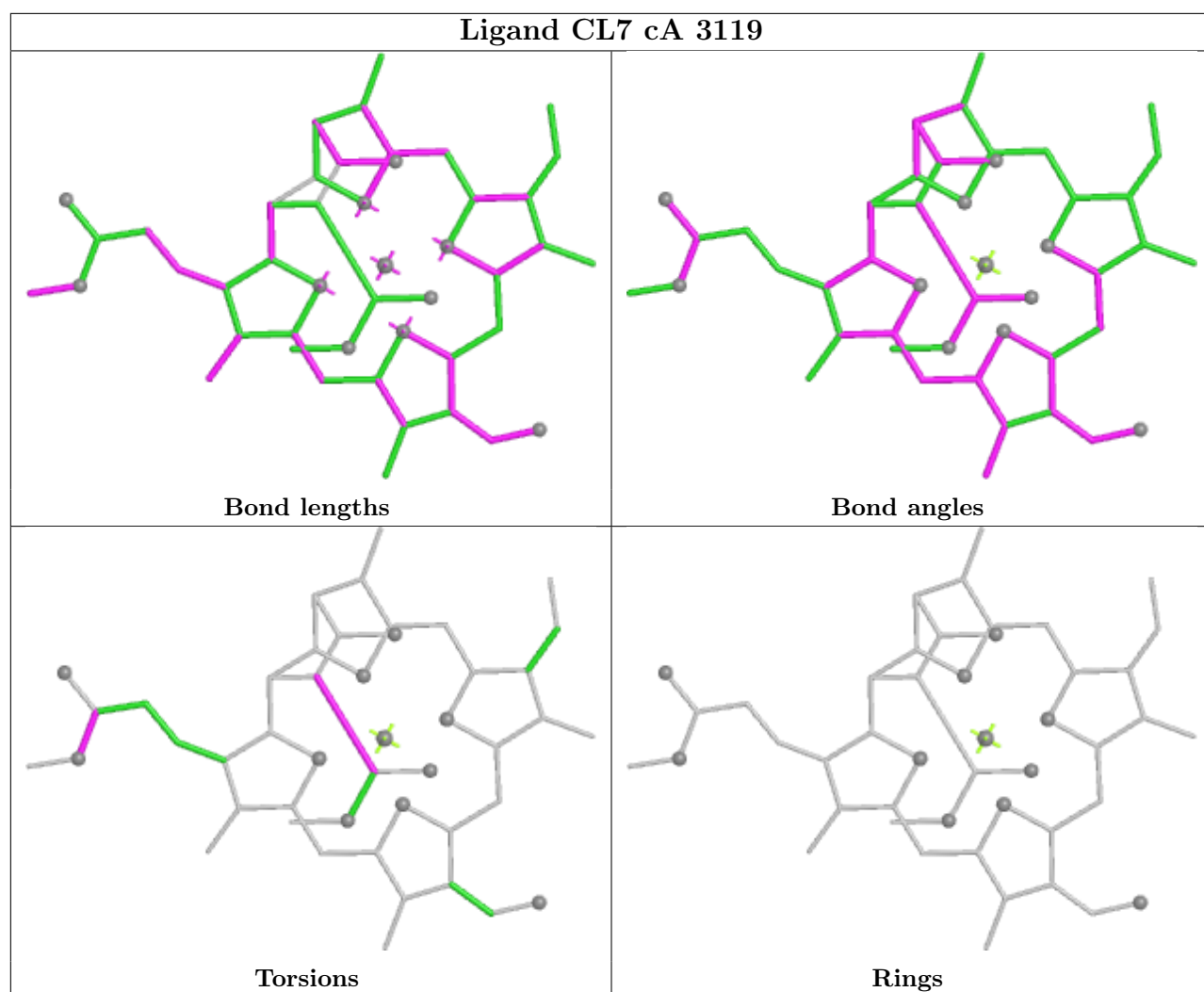


Torsions

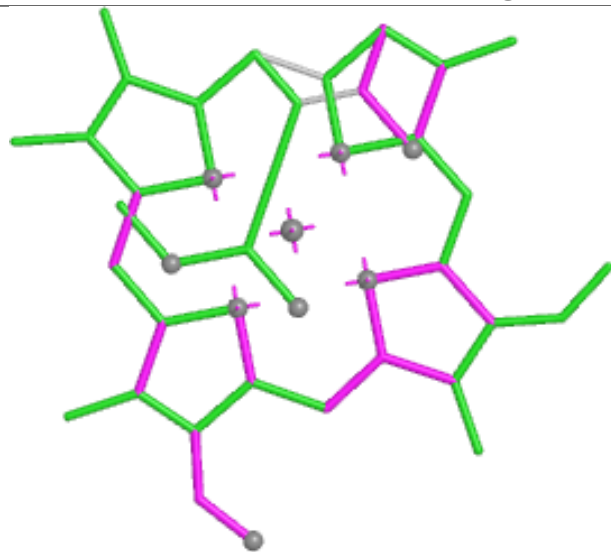


Rings

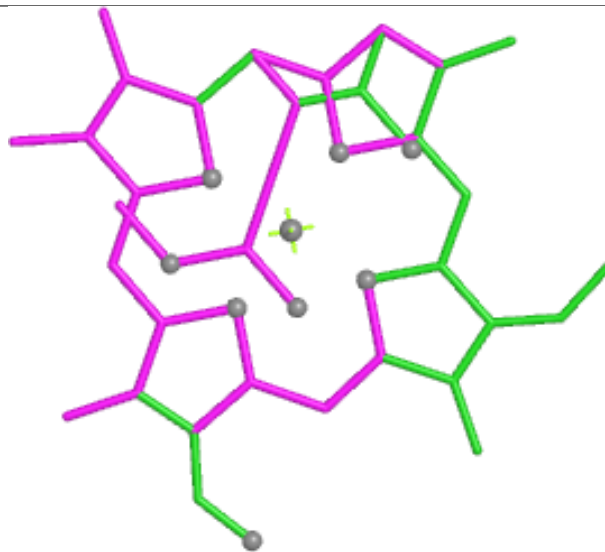




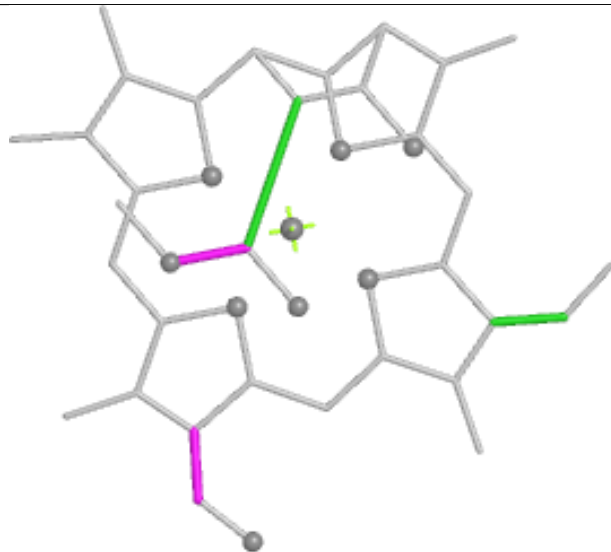
## Ligand CL7 bA 3109



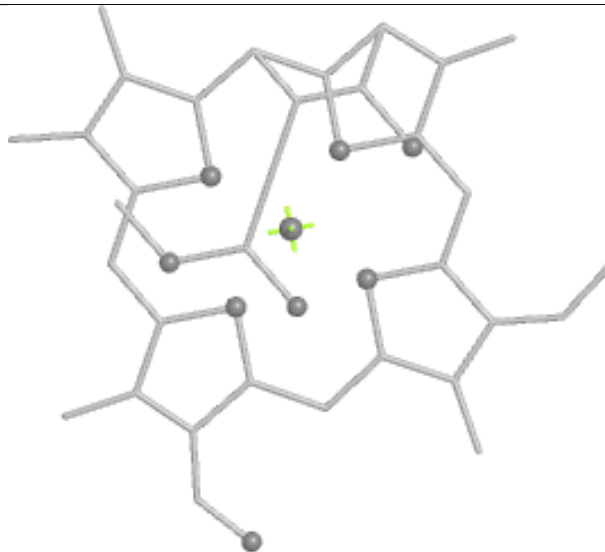
Bond lengths



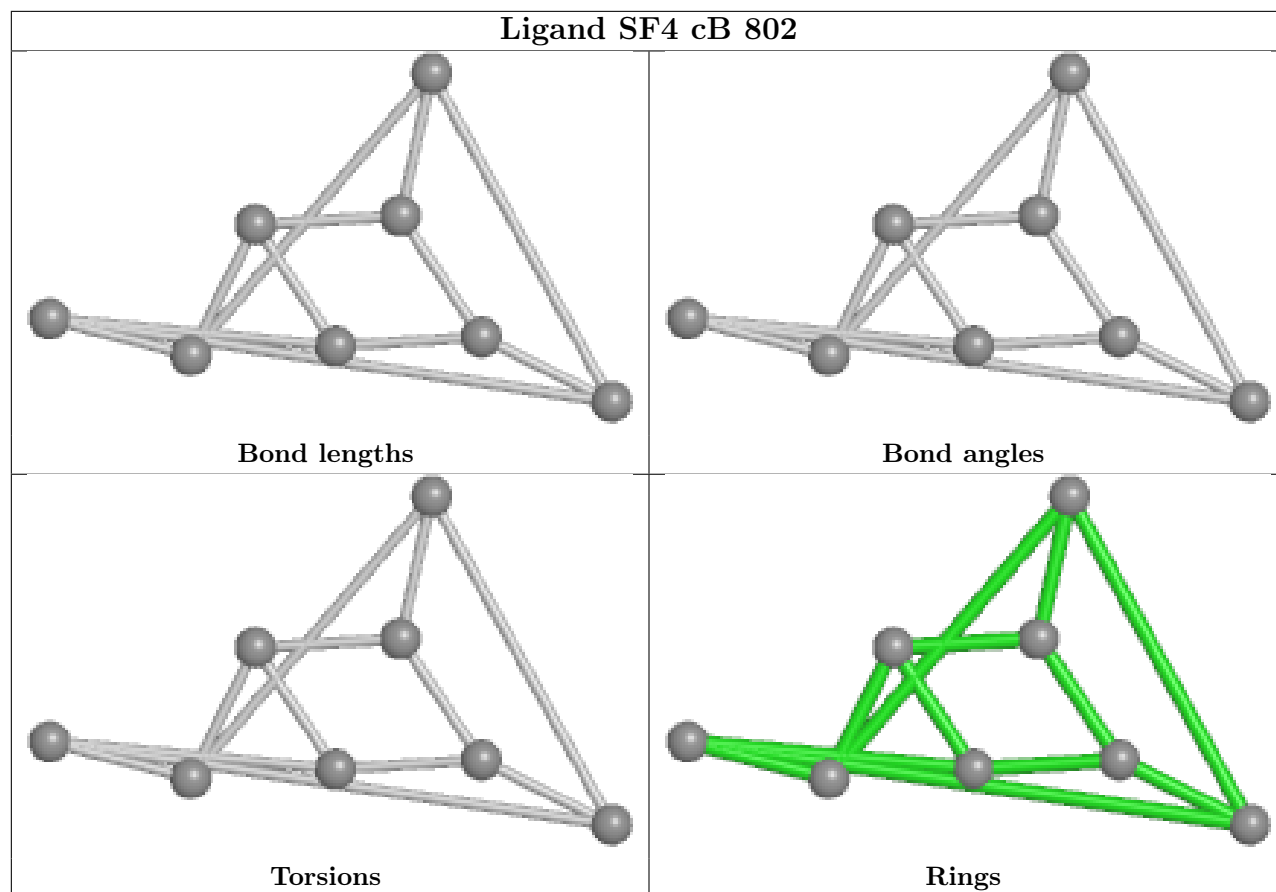
Bond angles

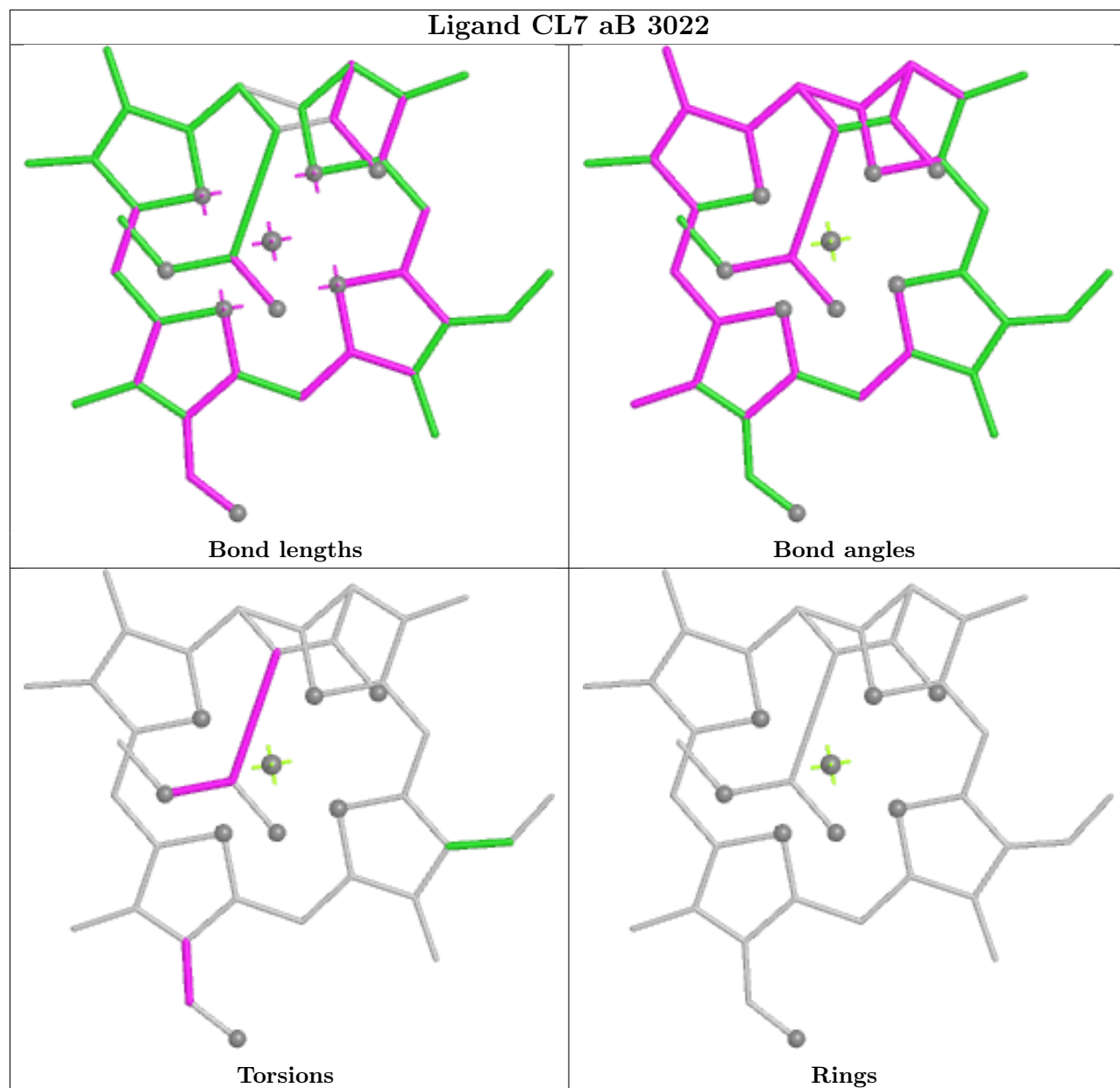


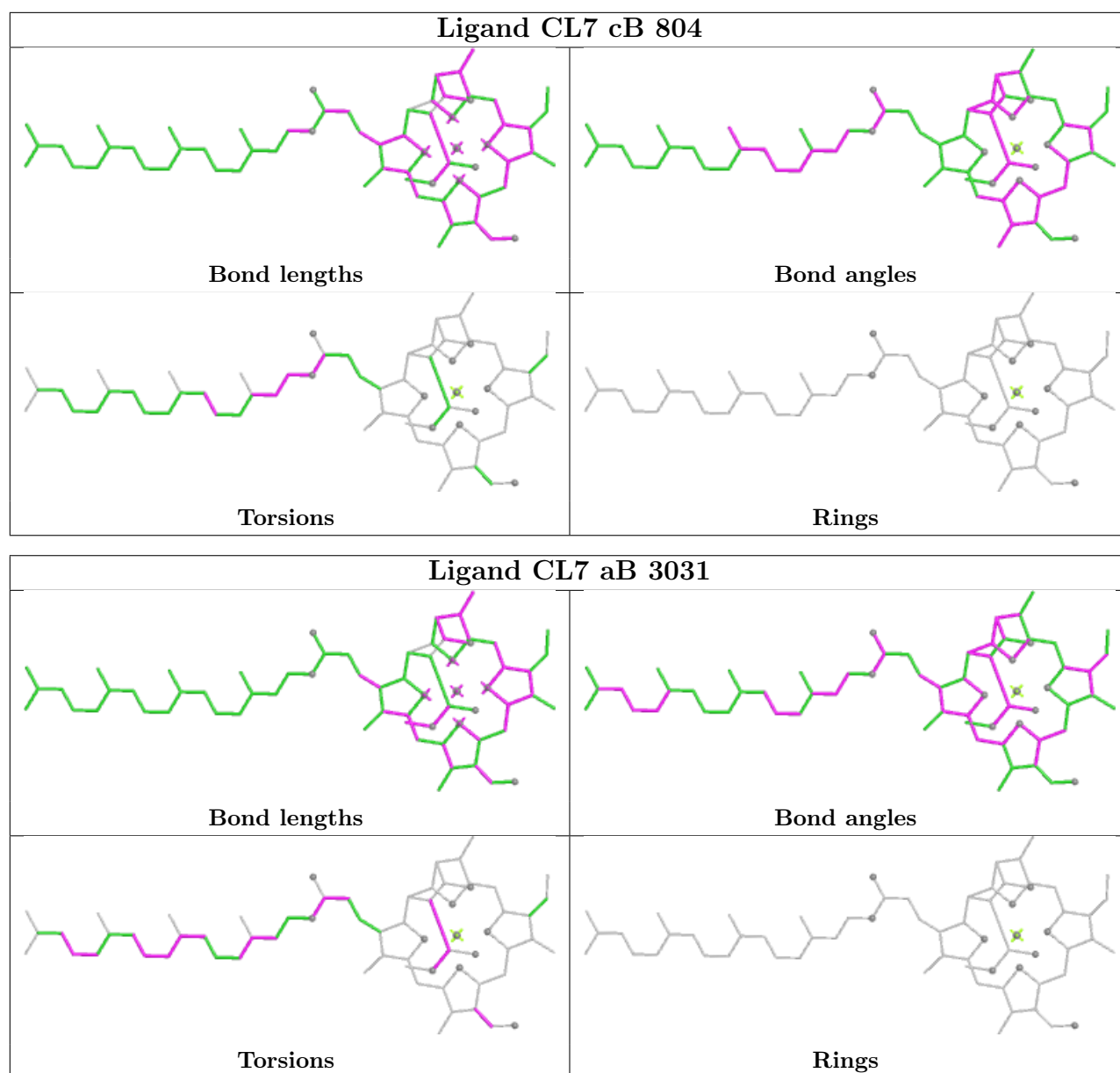
Torsions

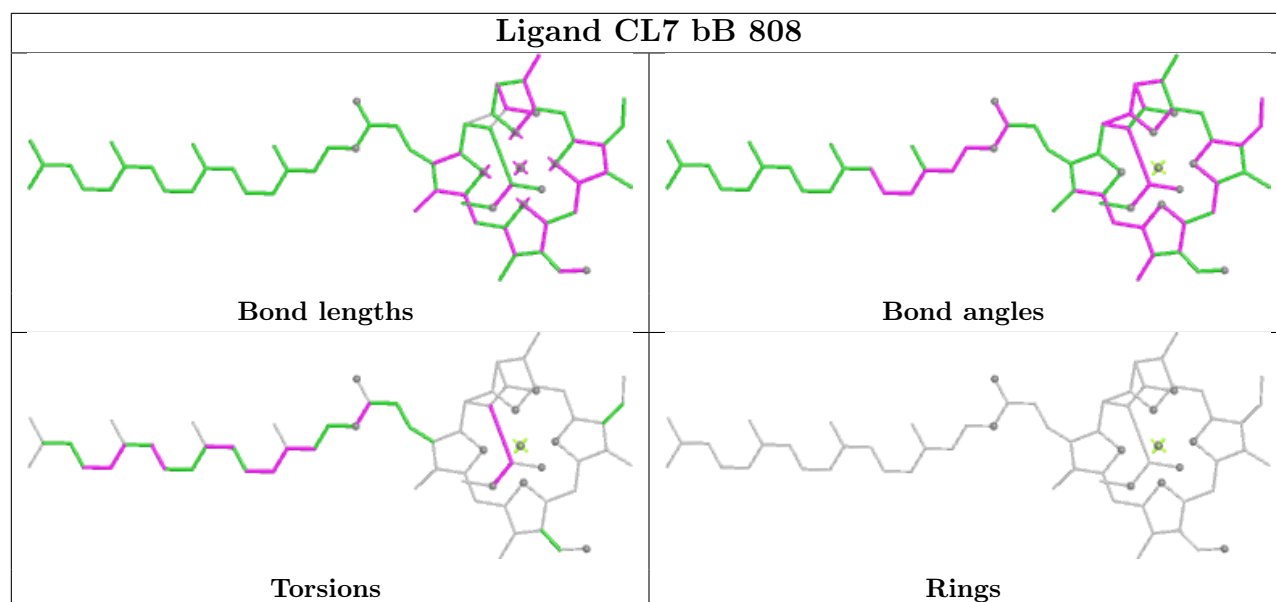
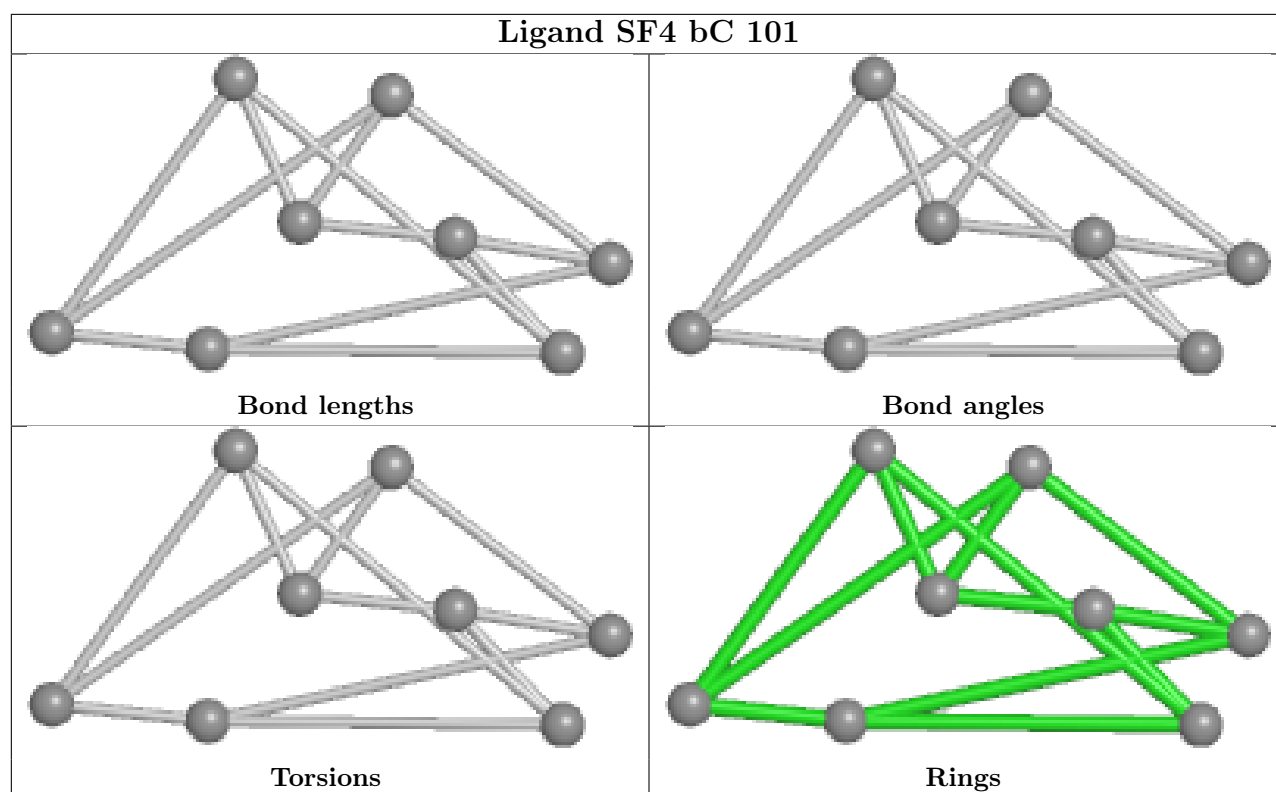


Rings

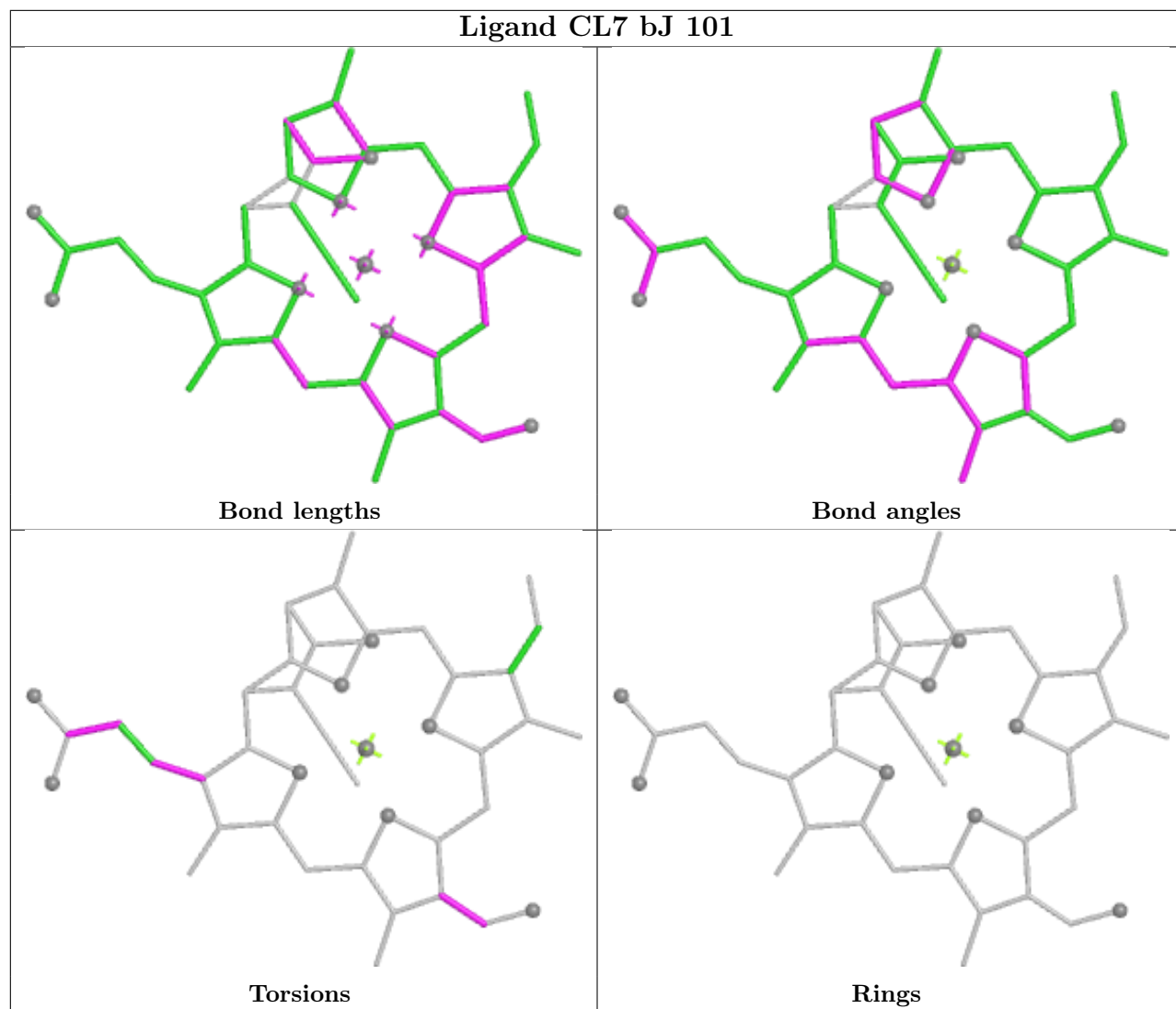


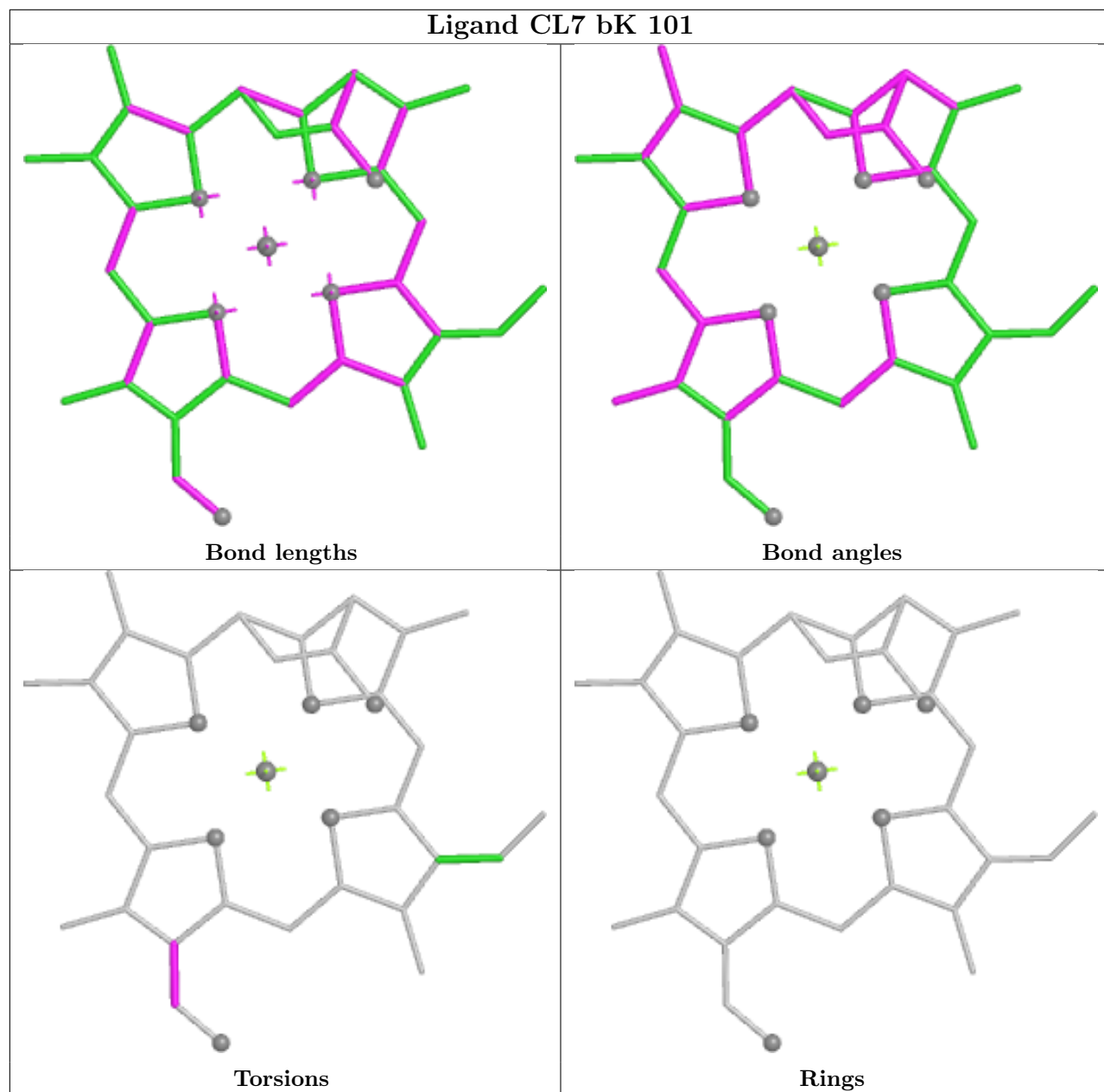




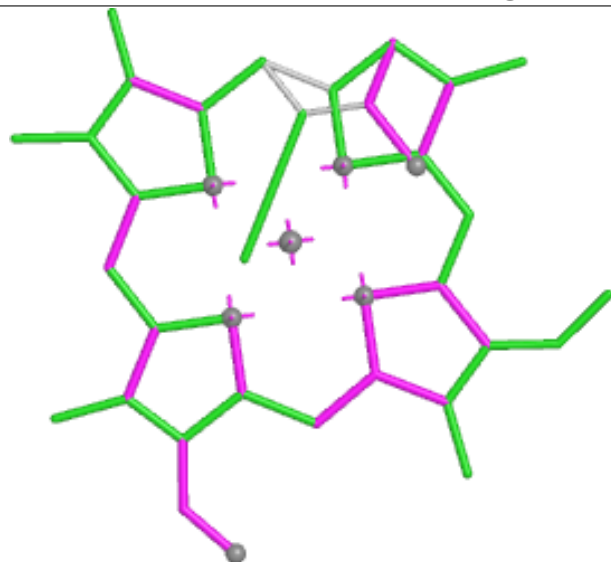




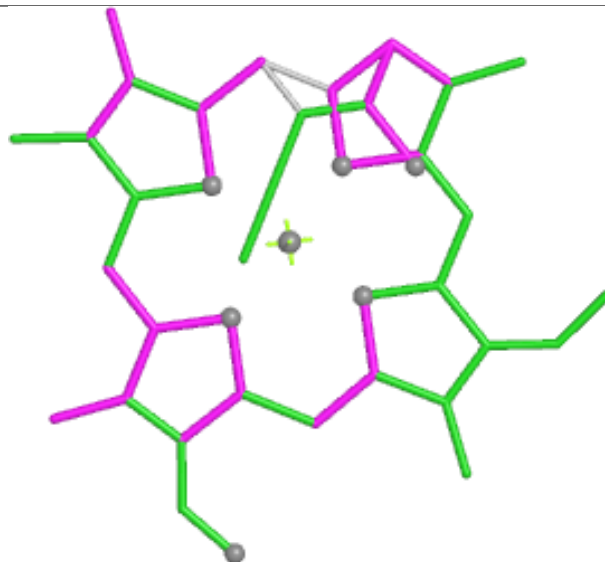




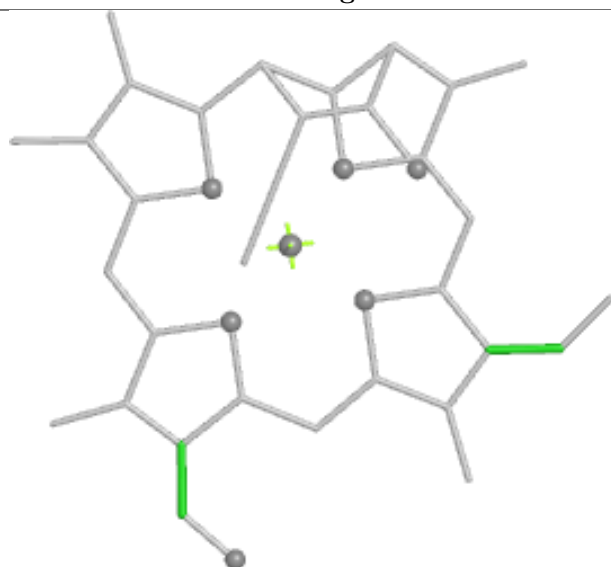
## Ligand CL7 aB 3012



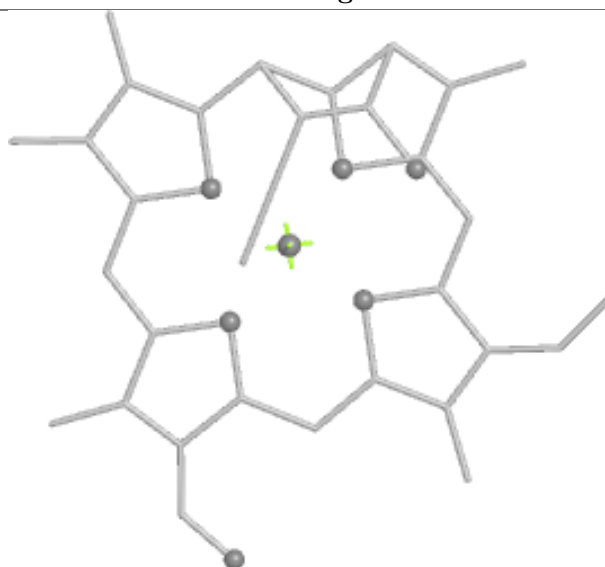
Bond lengths



Bond angles

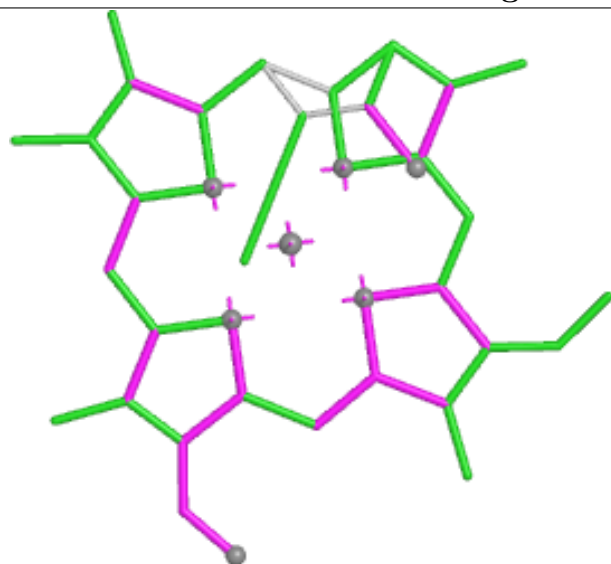


Torsions

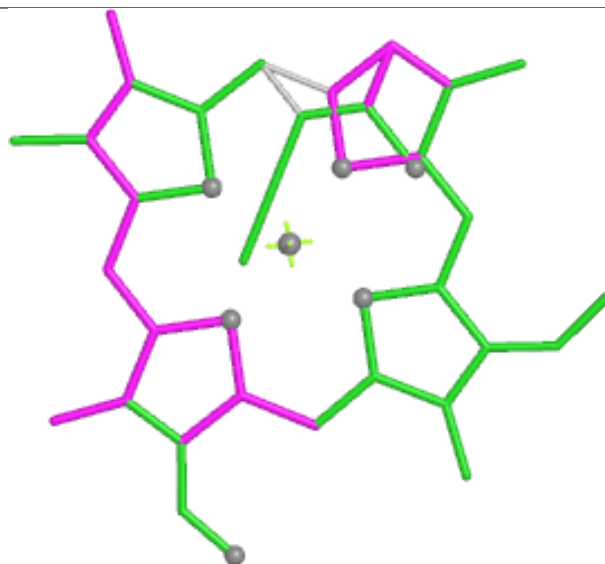


Rings

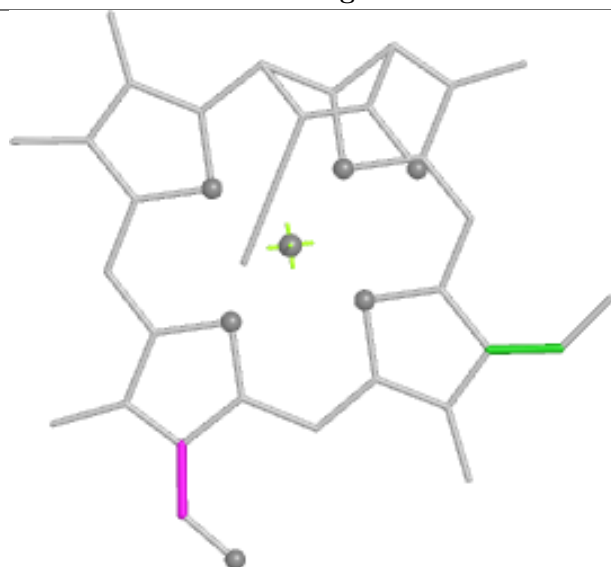
## Ligand CL7 cA 3111



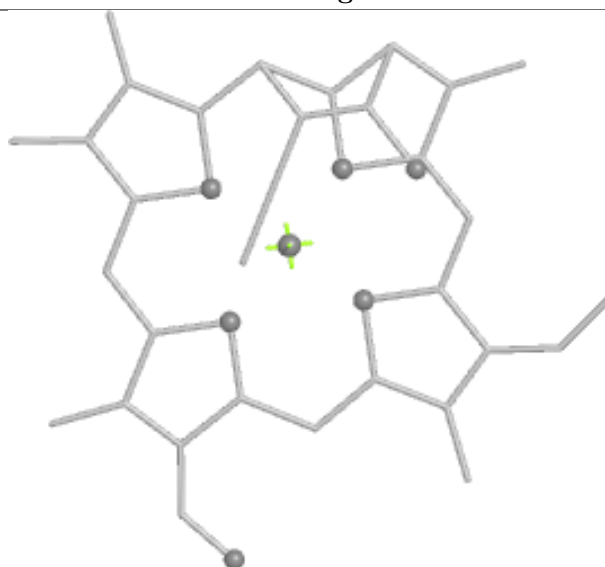
Bond lengths



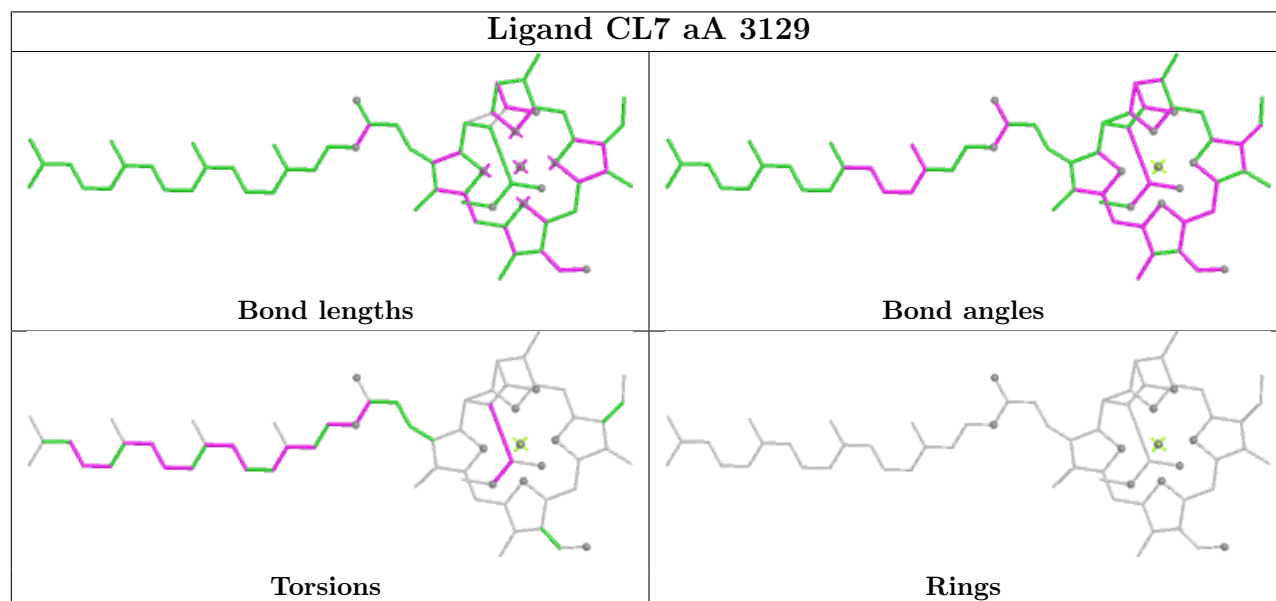
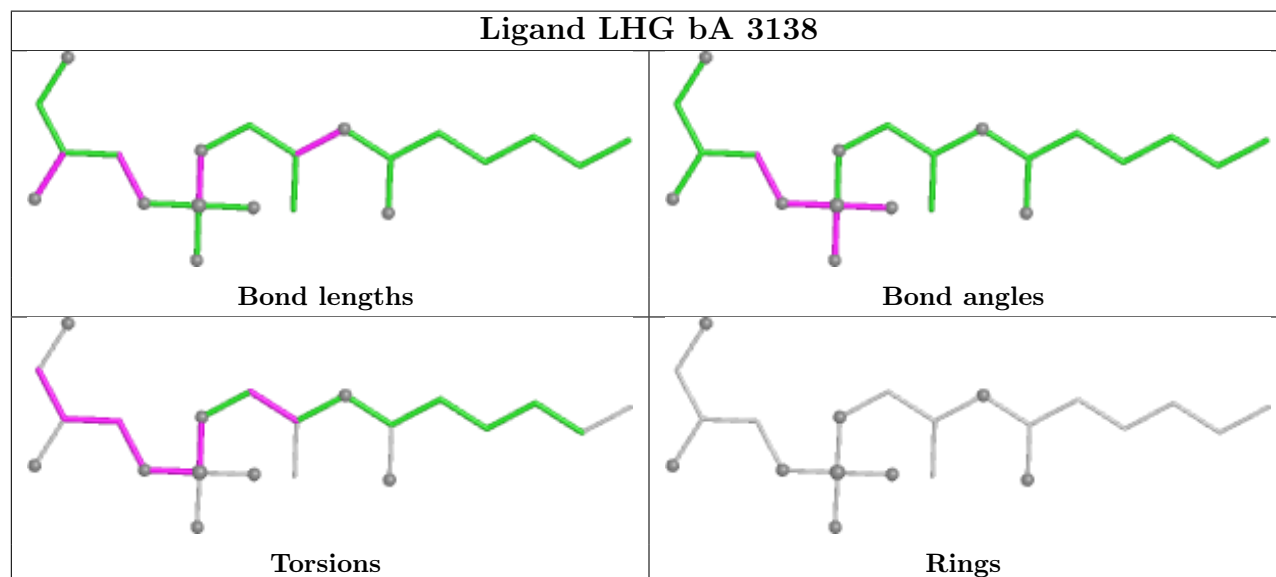
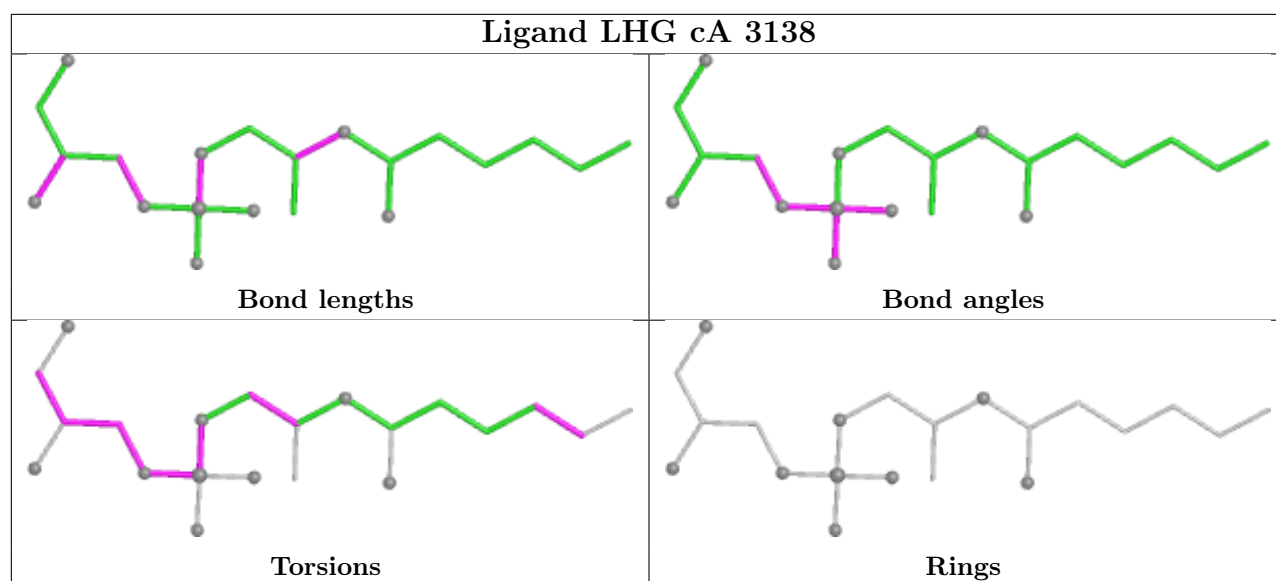
Bond angles

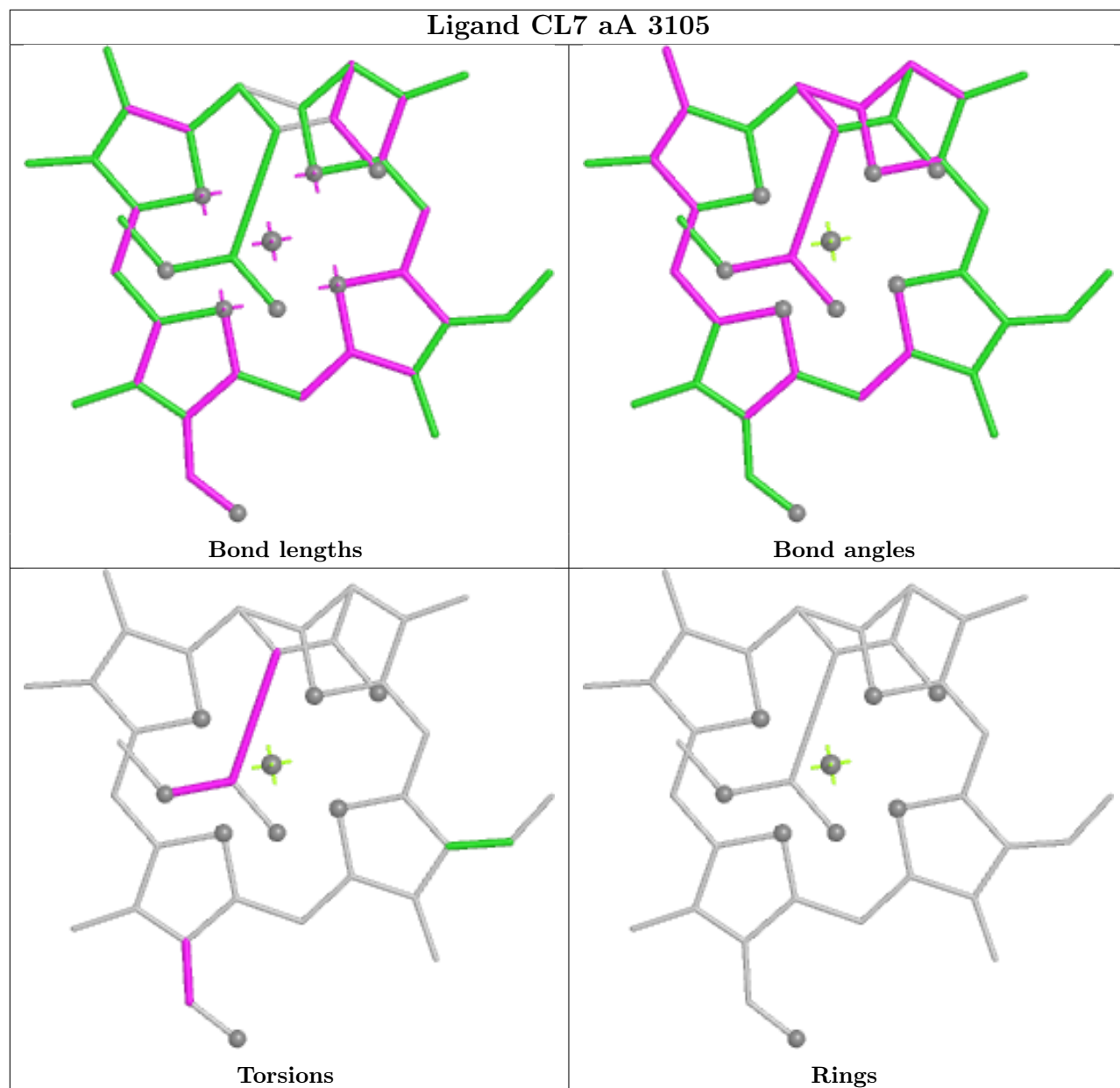


Torsions

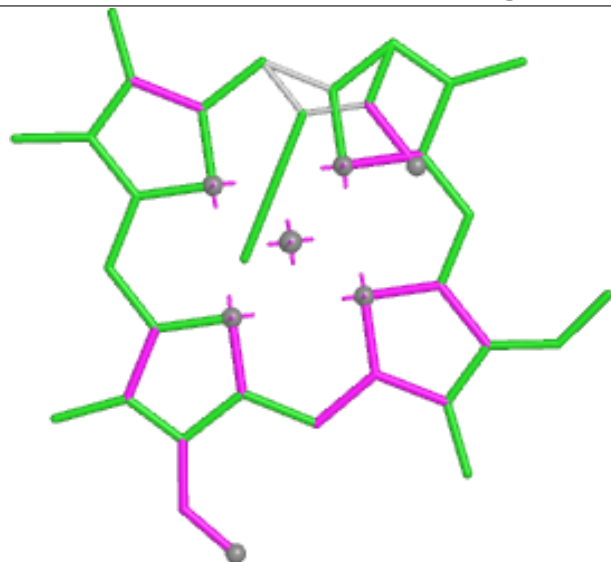


Rings

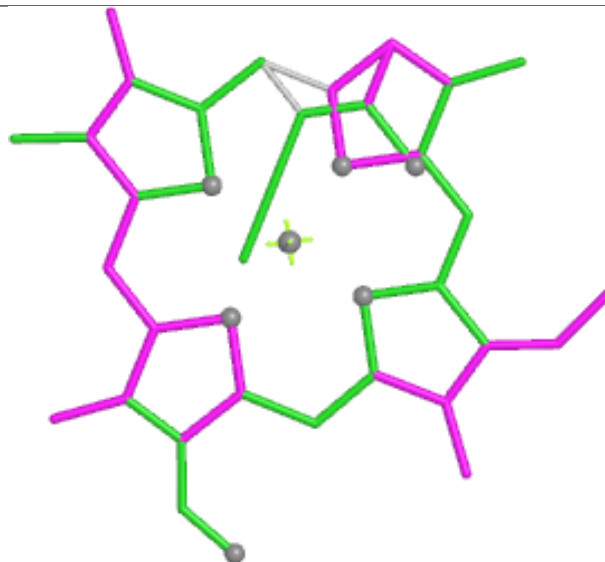




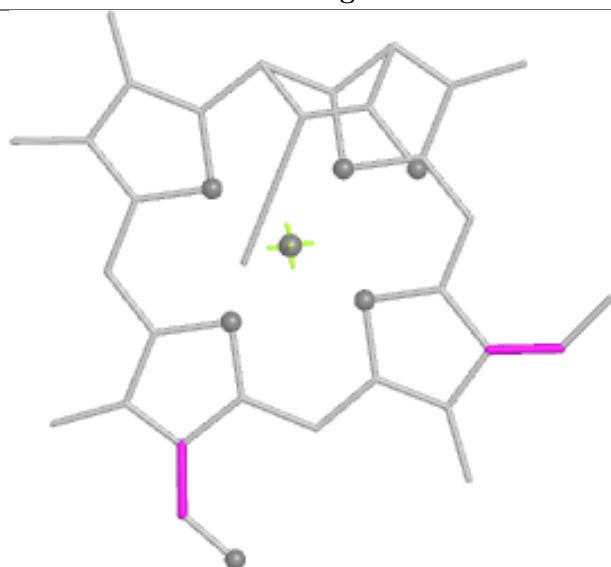
## Ligand CL7 aA 3116



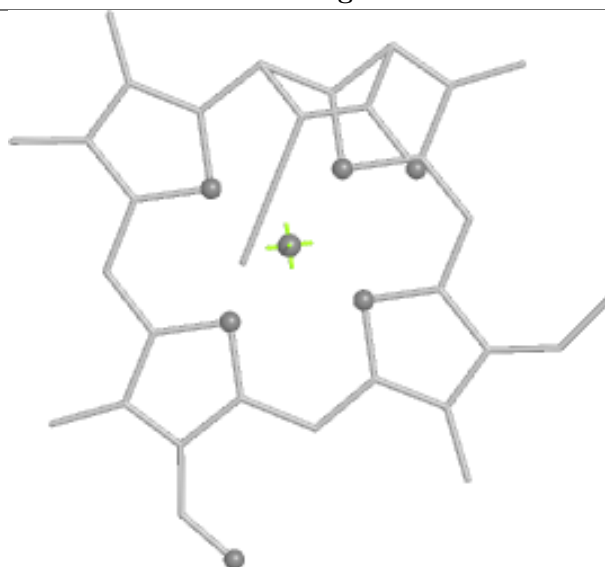
Bond lengths



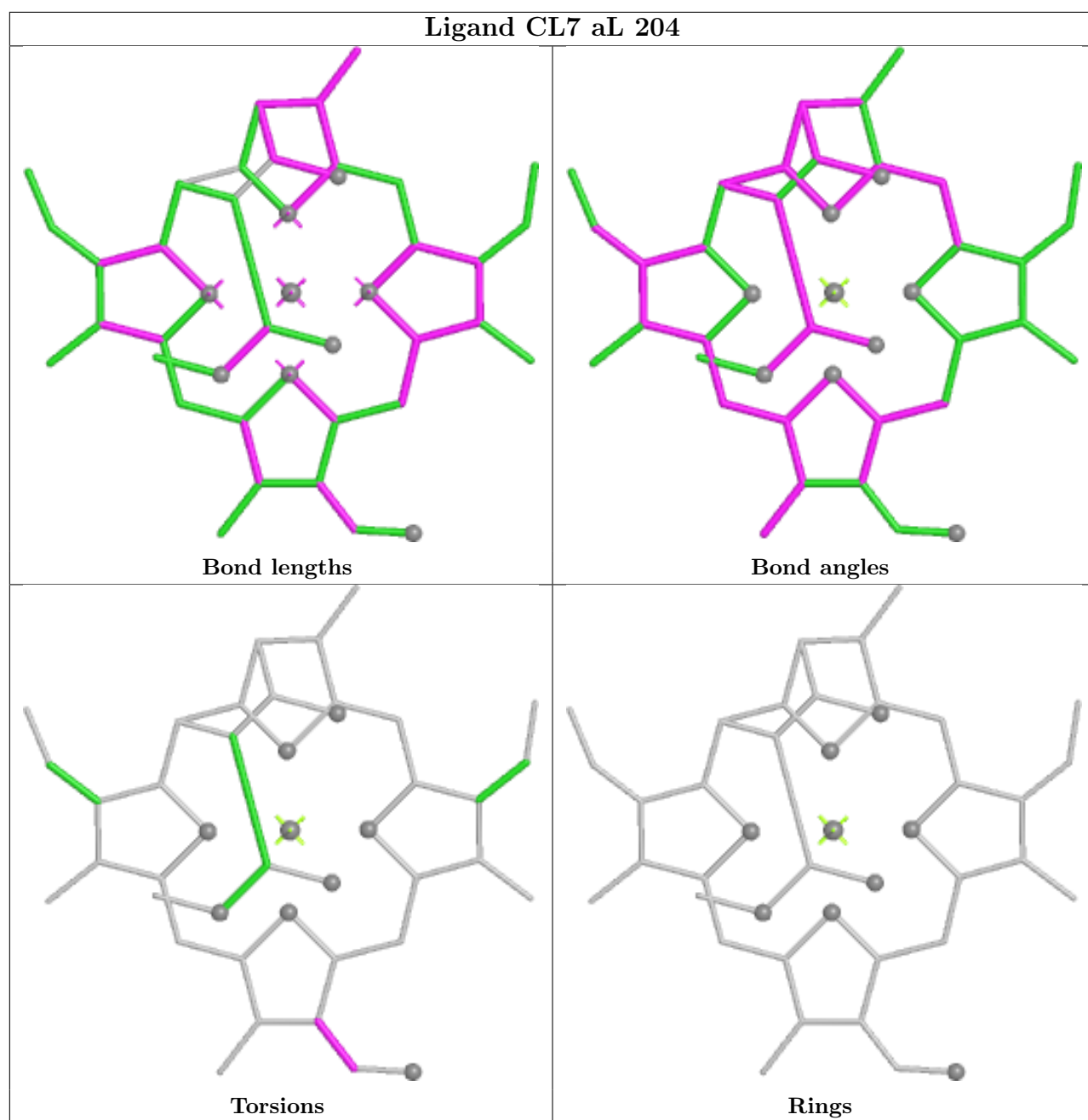
Bond angles



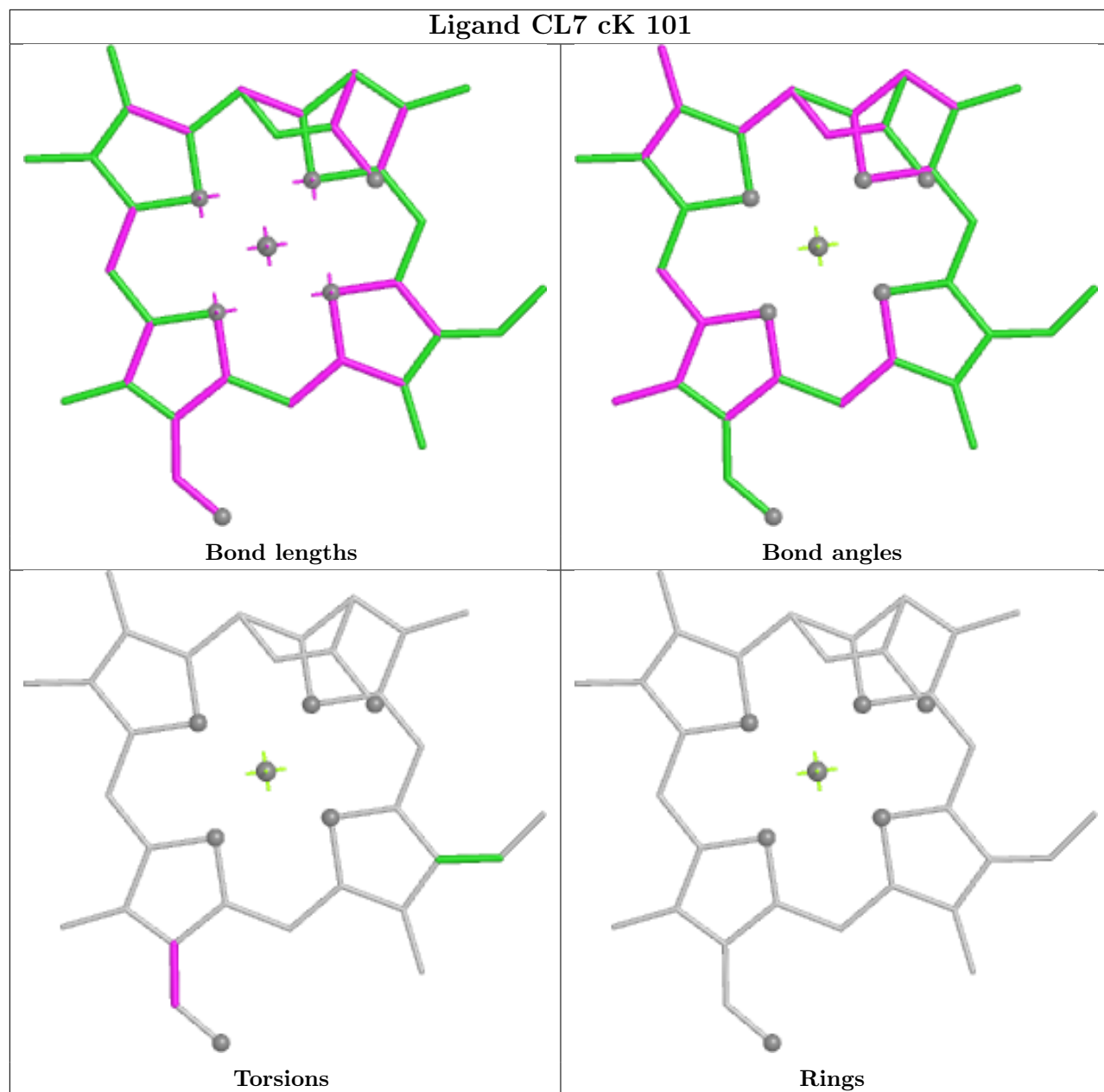
Torsions

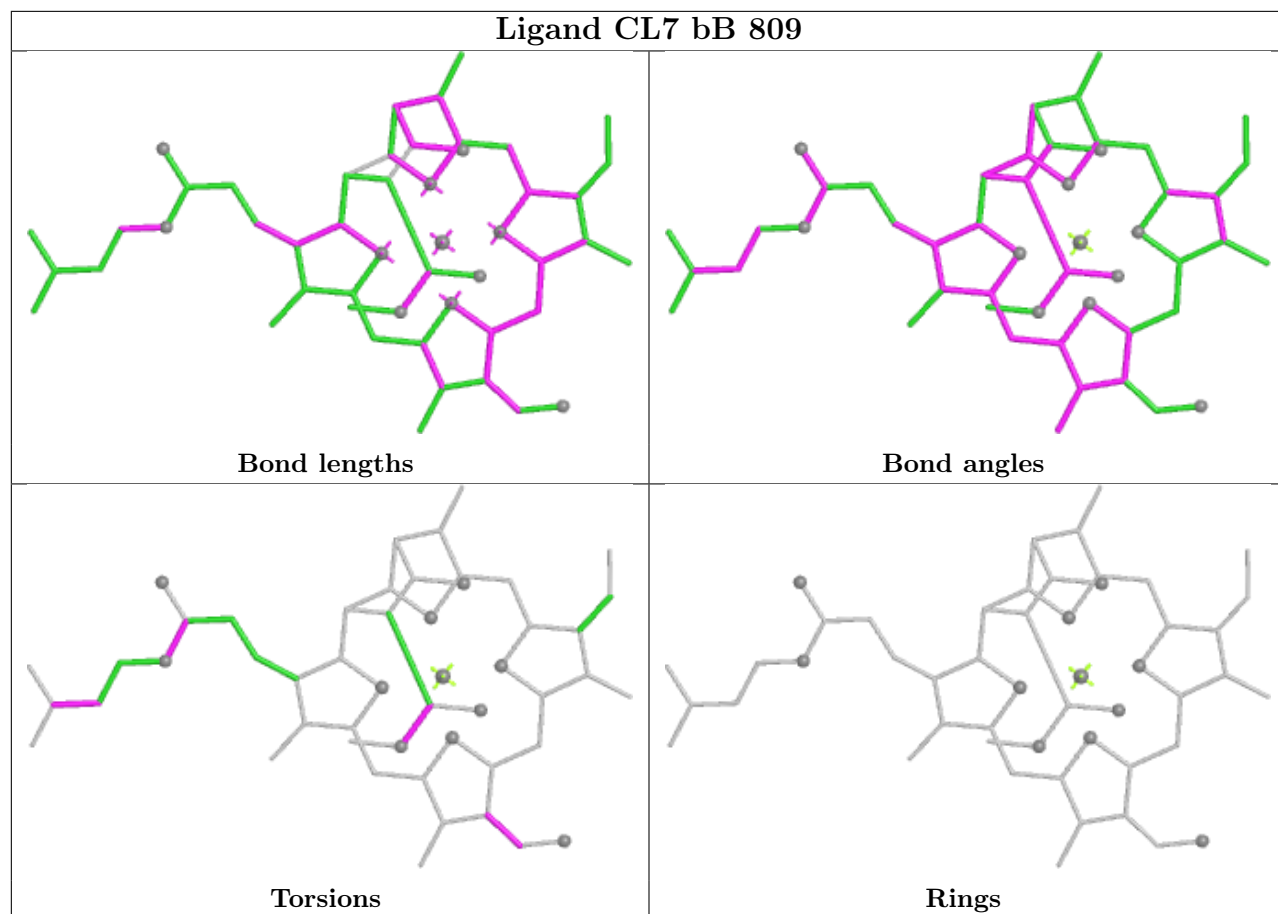


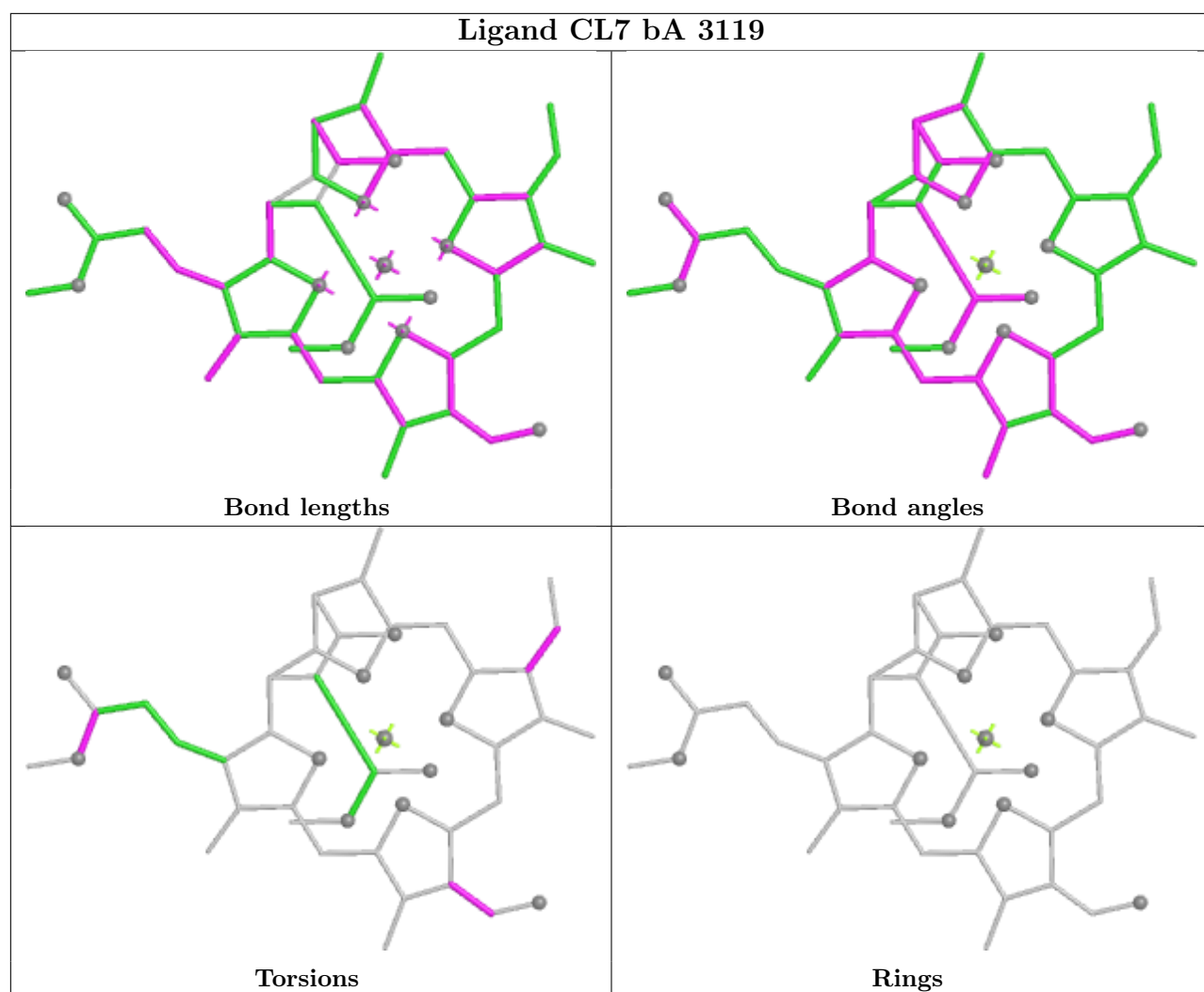
Rings

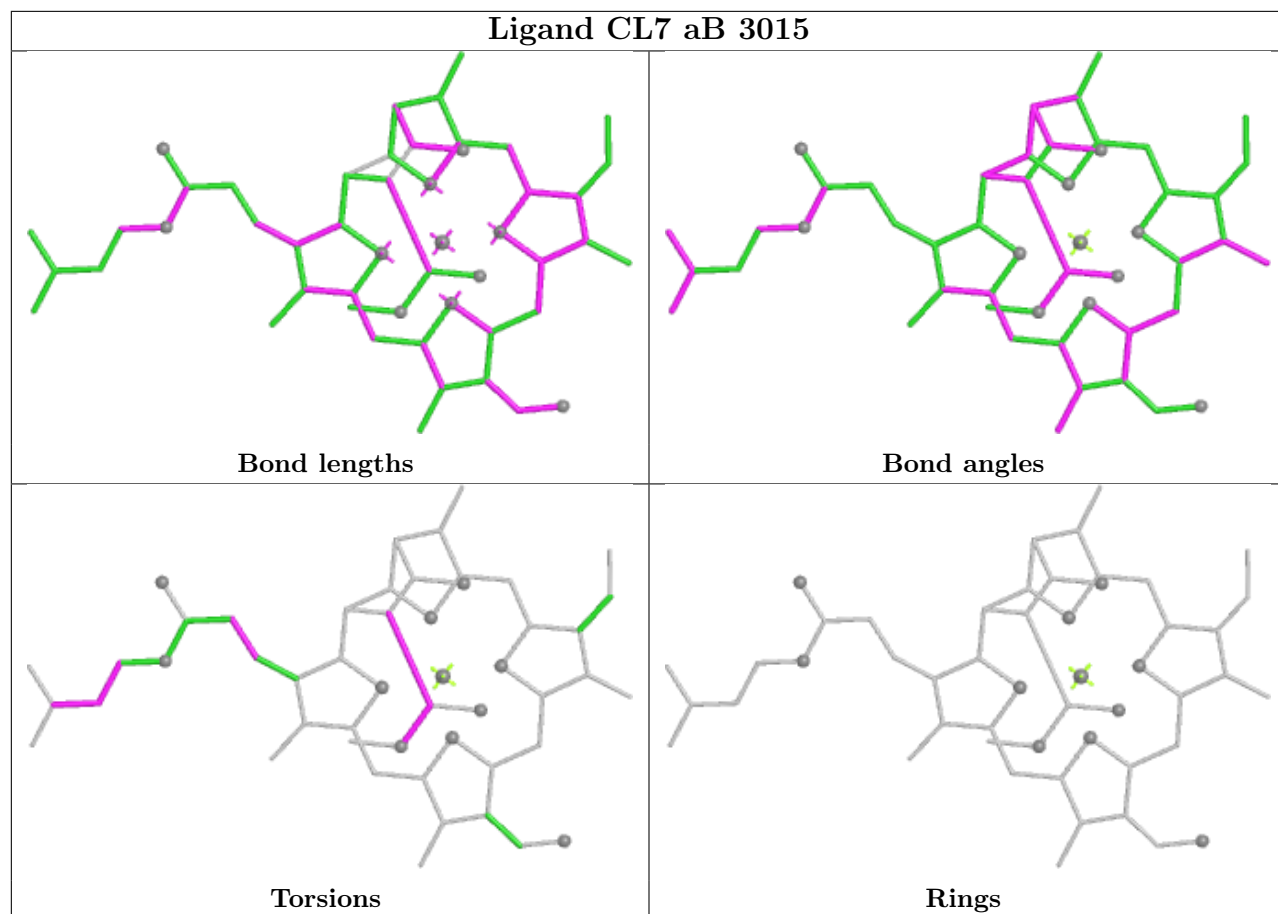


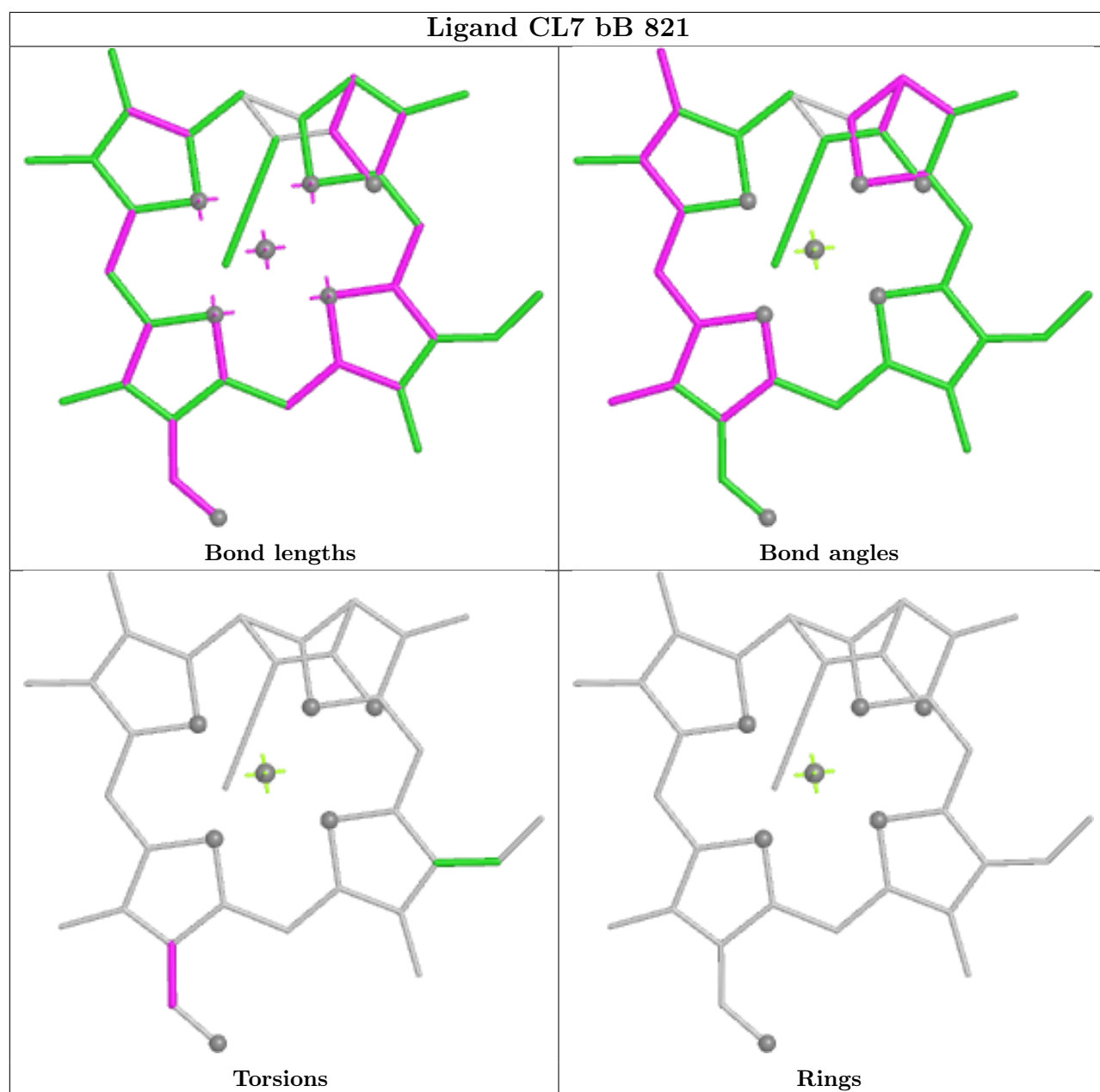


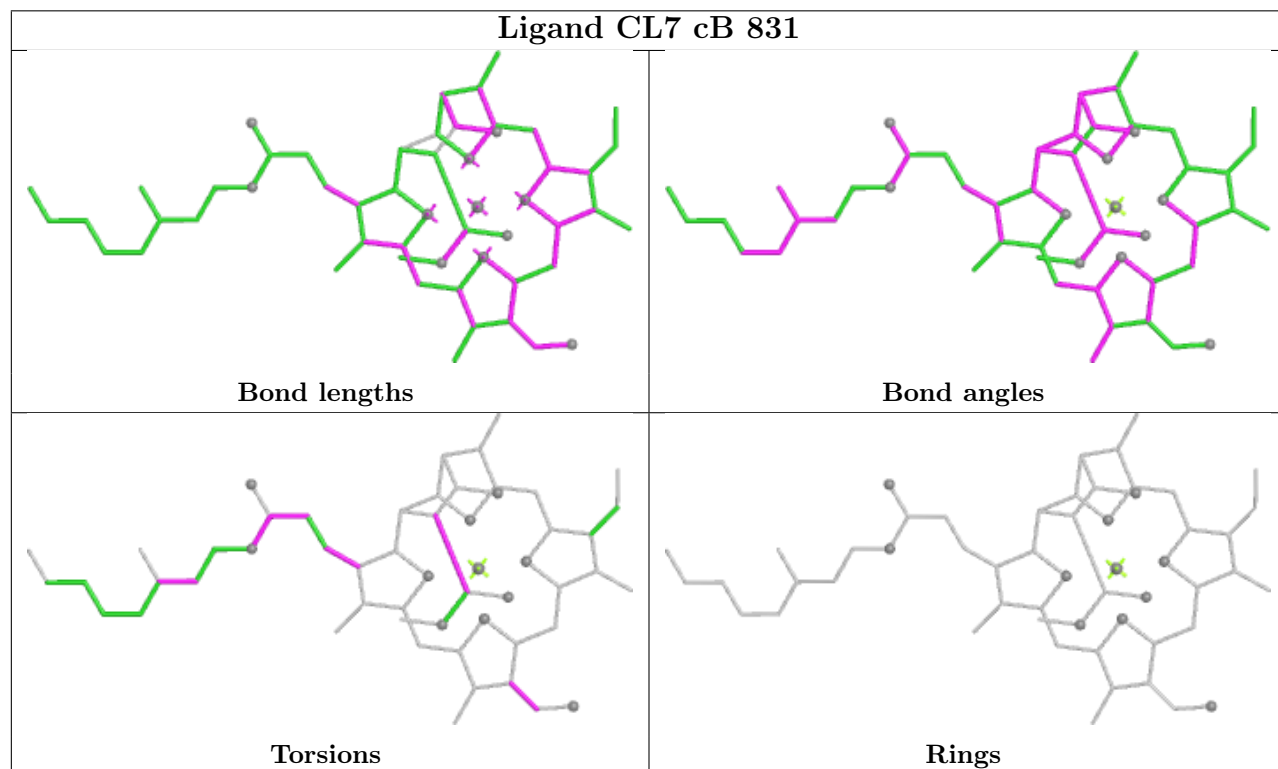
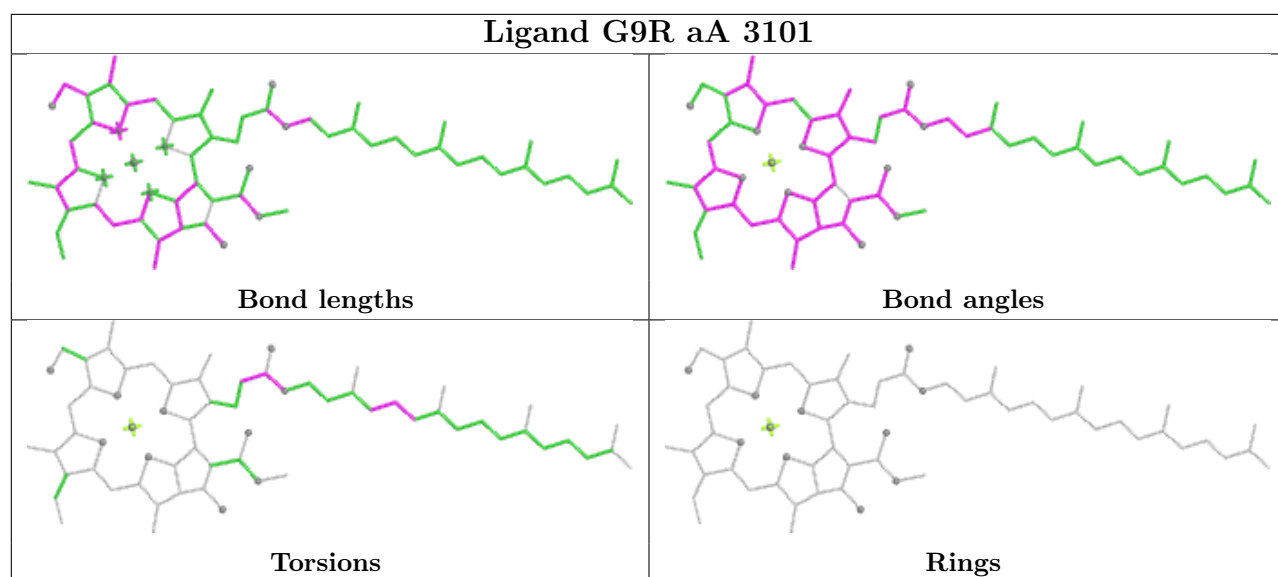




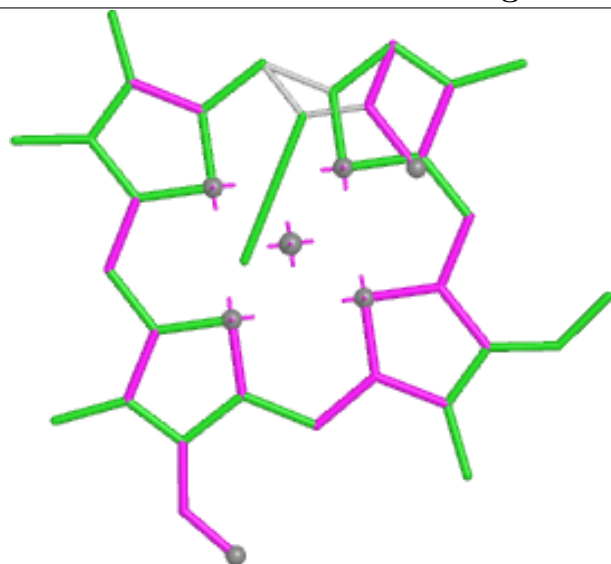




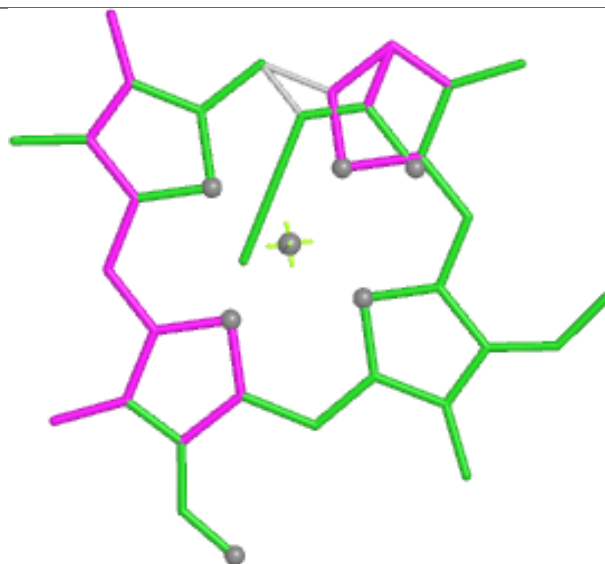




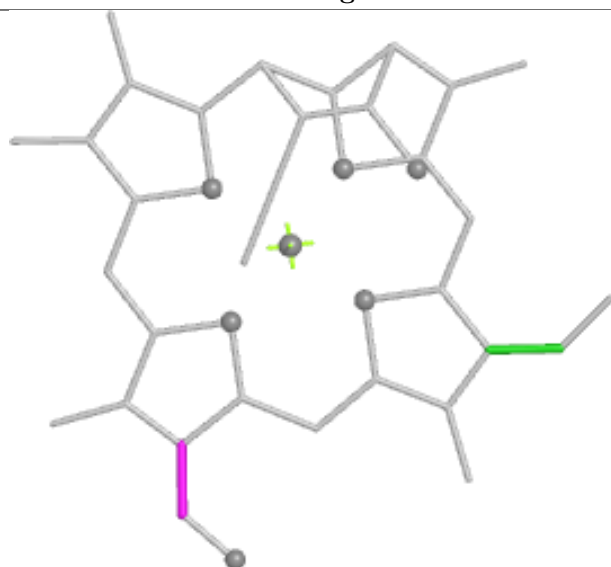
## Ligand CL7 aB 3020



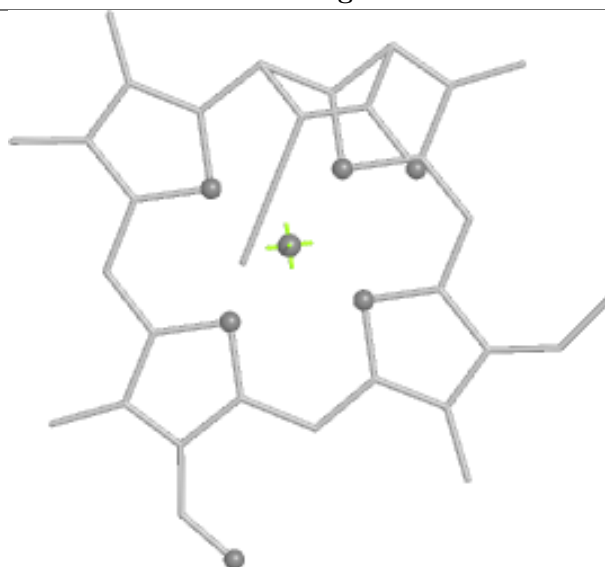
Bond lengths



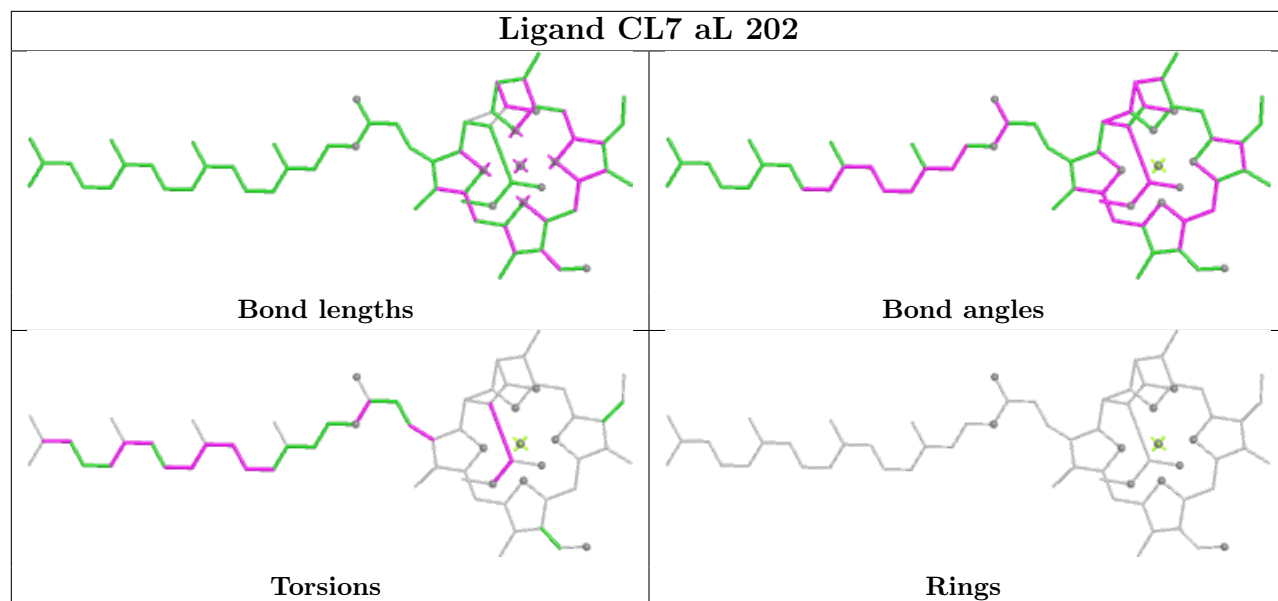
Bond angles



Torsions

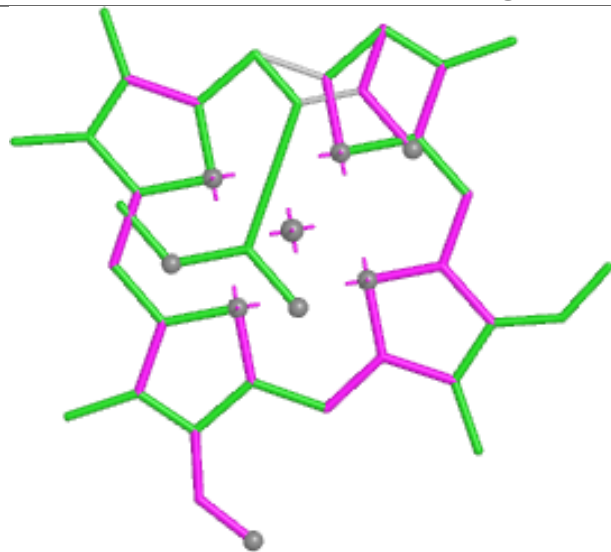


Rings

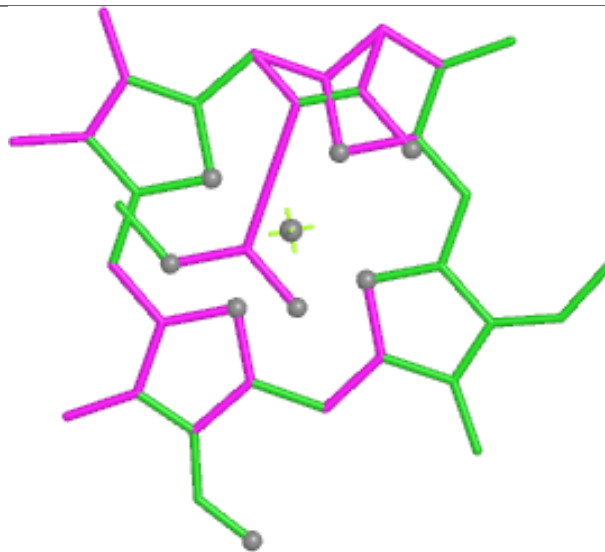




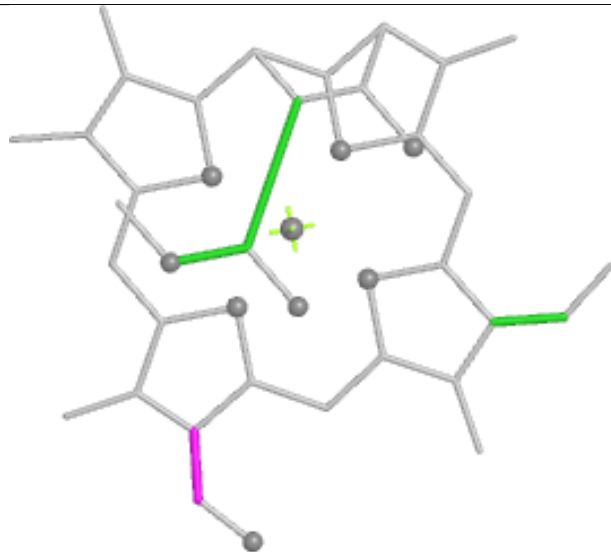
## Ligand CL7 bA 3113



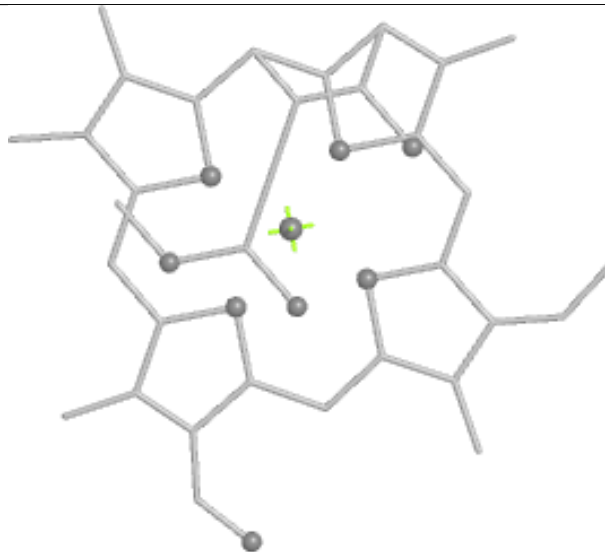
Bond lengths



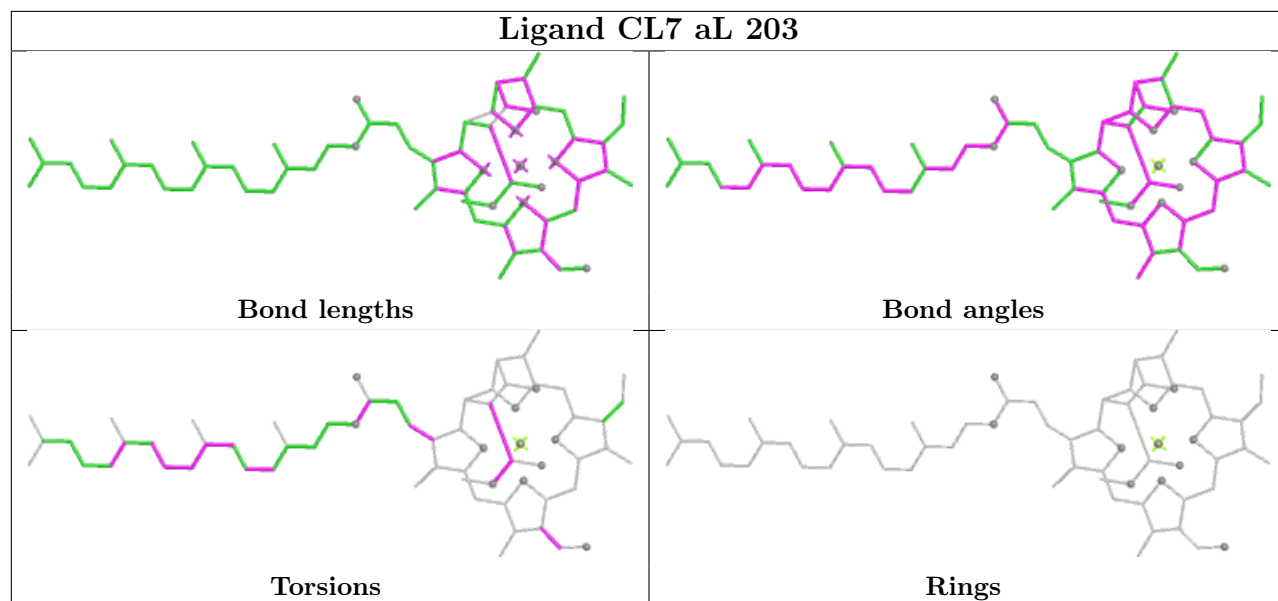
Bond angles

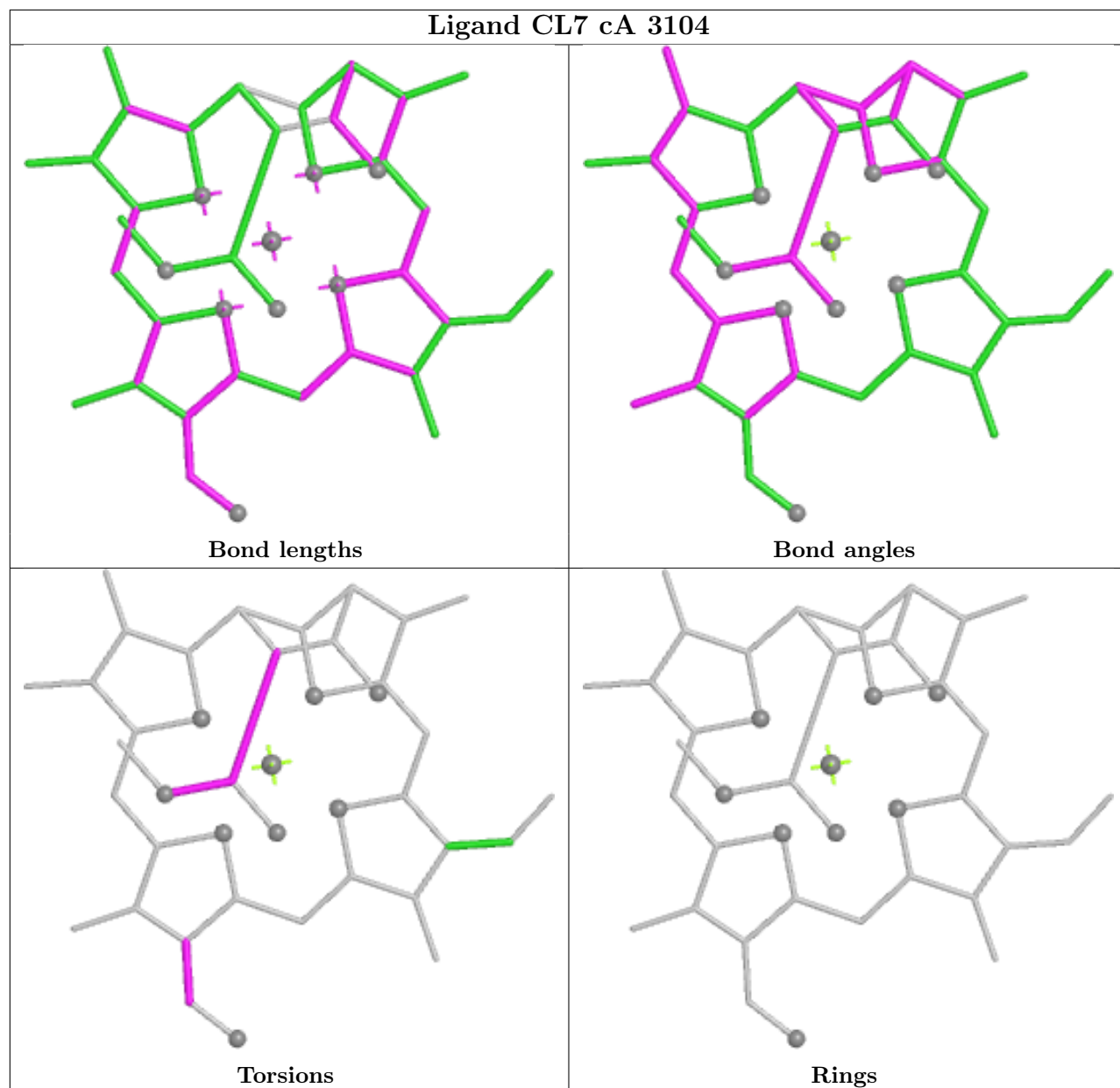


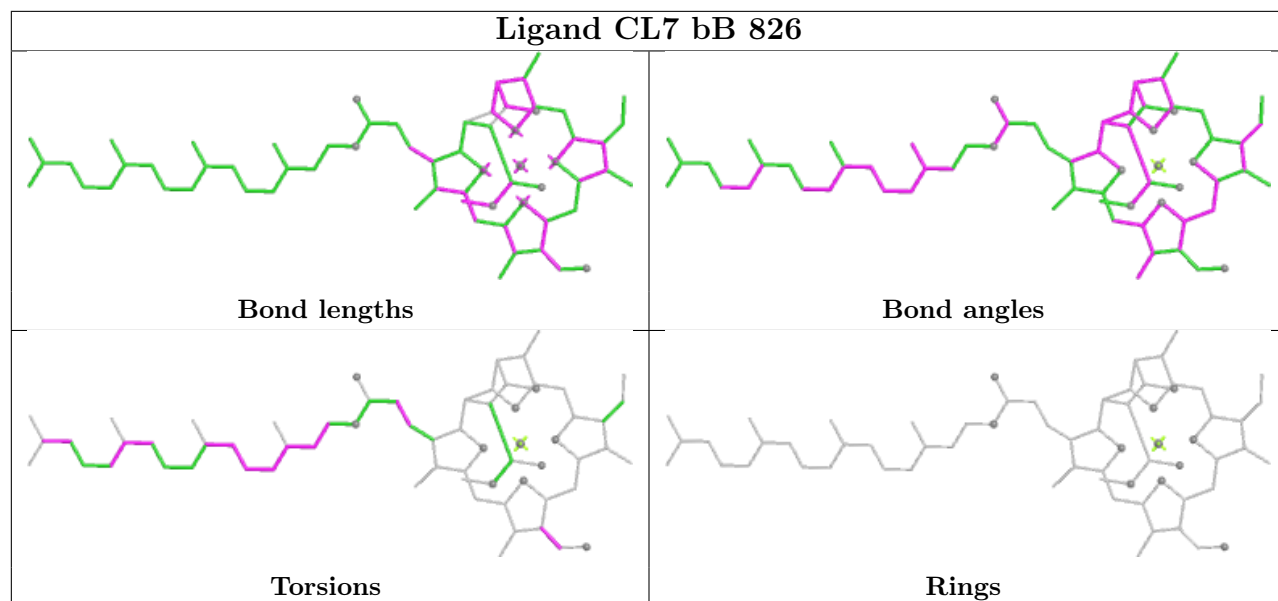
Torsions

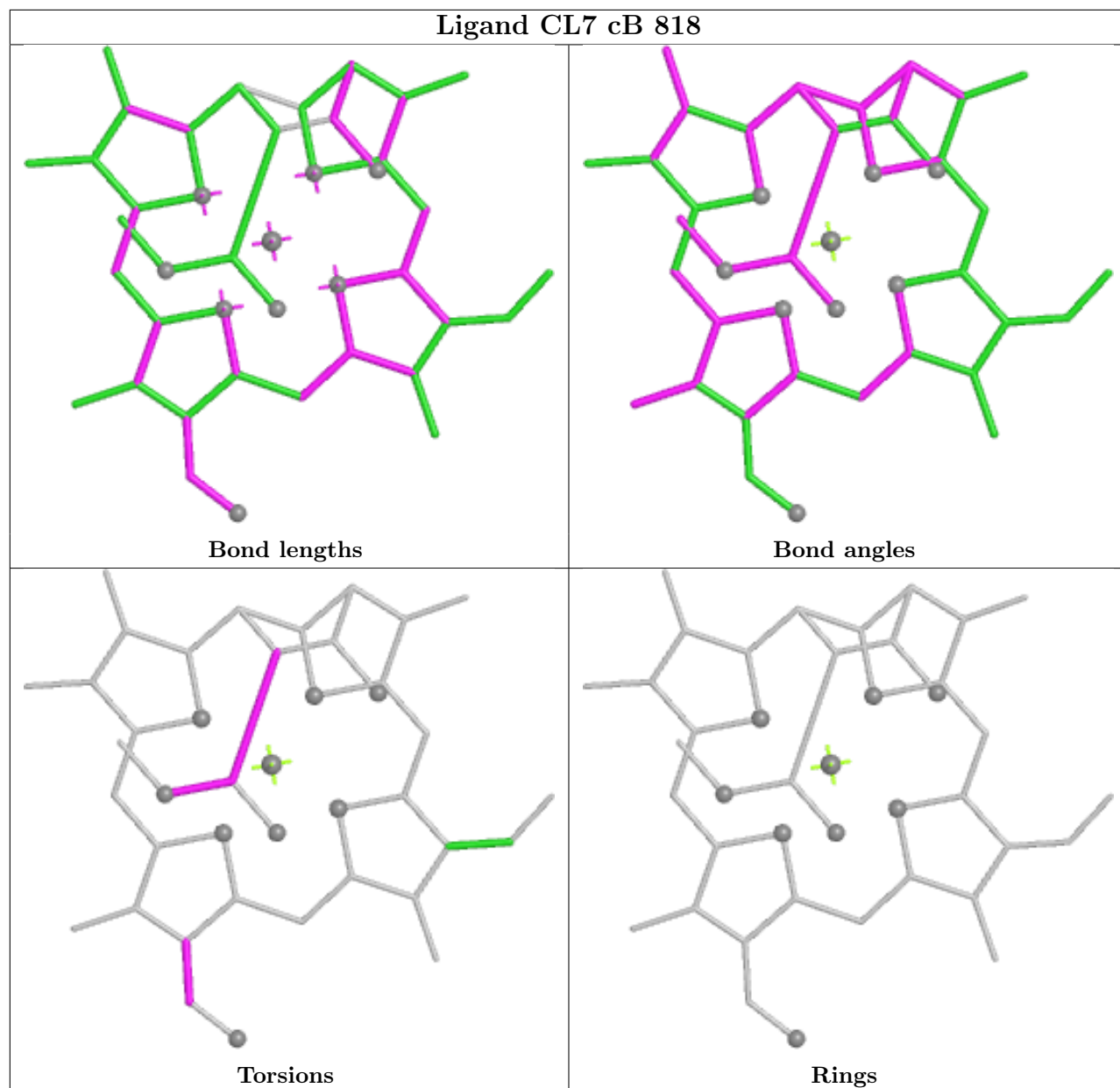


Rings

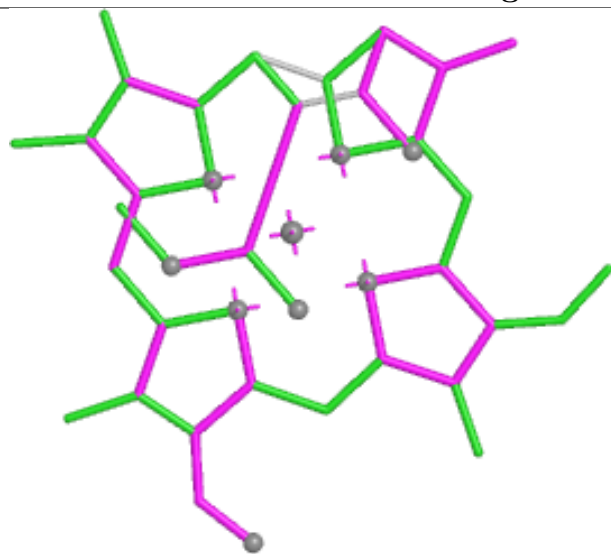




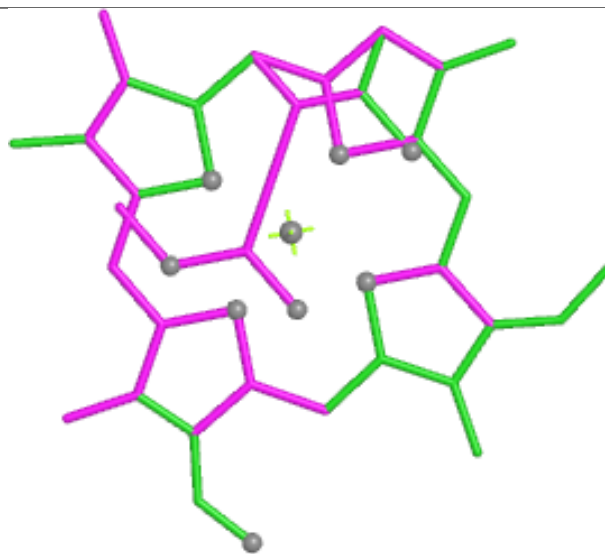




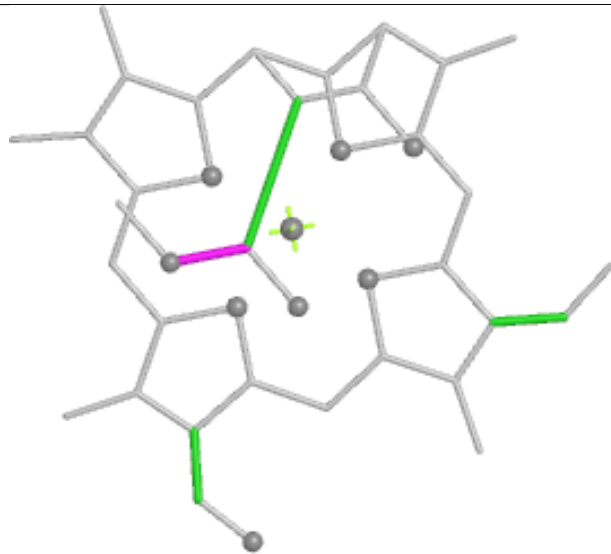
## Ligand CL7 cA 3121



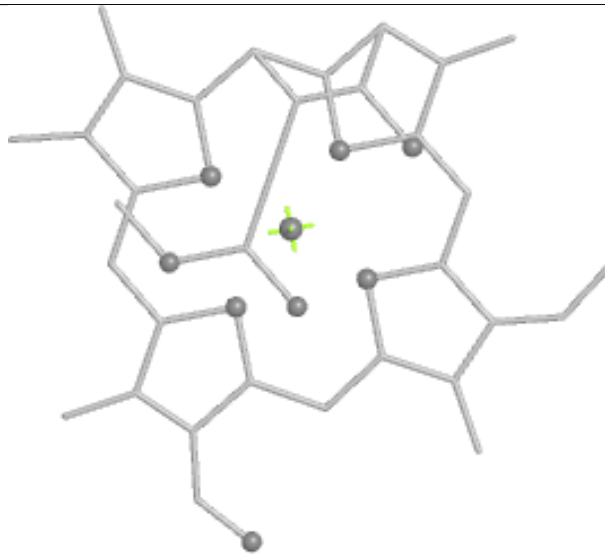
Bond lengths



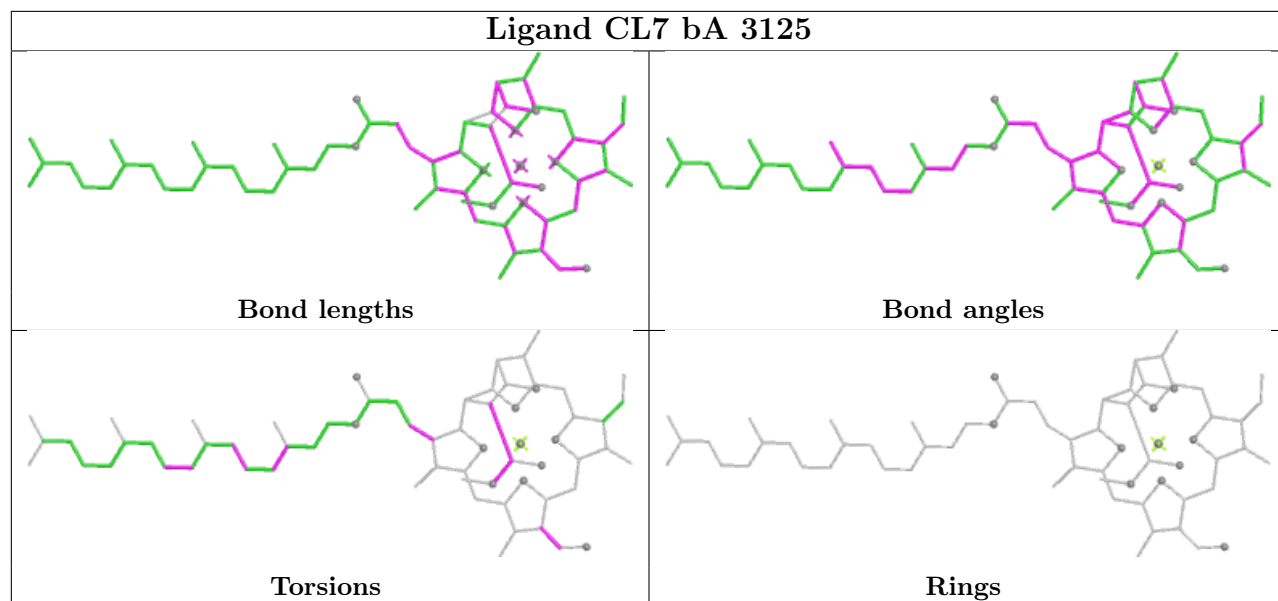
Bond angles

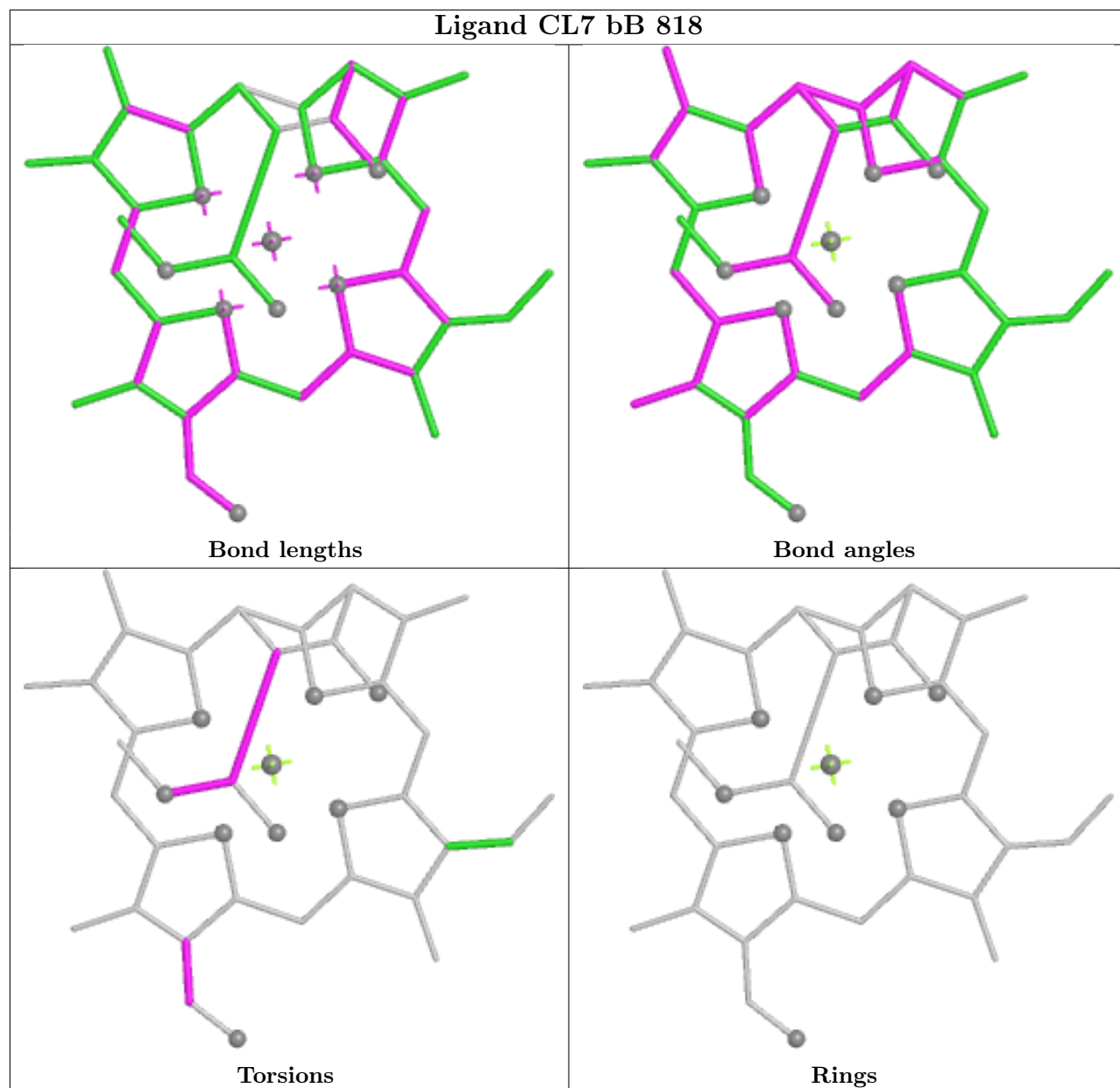


Torsions

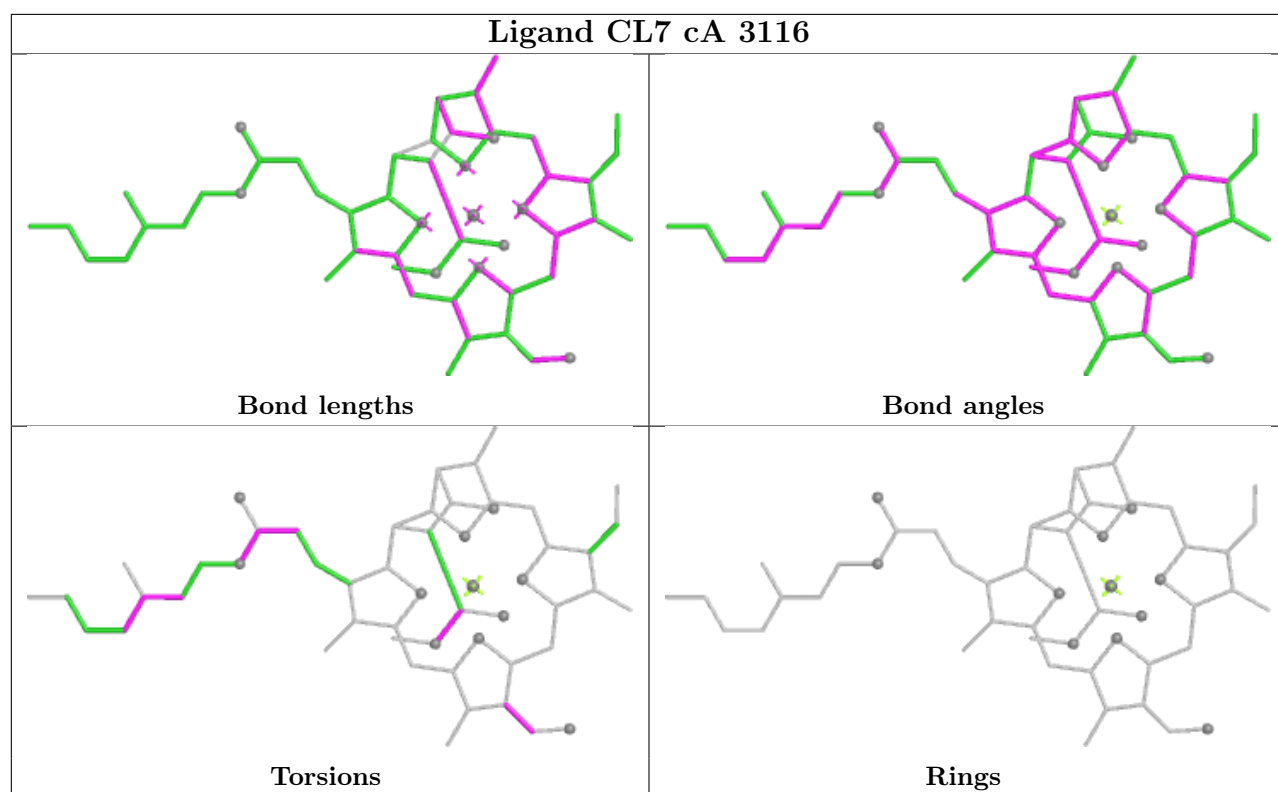


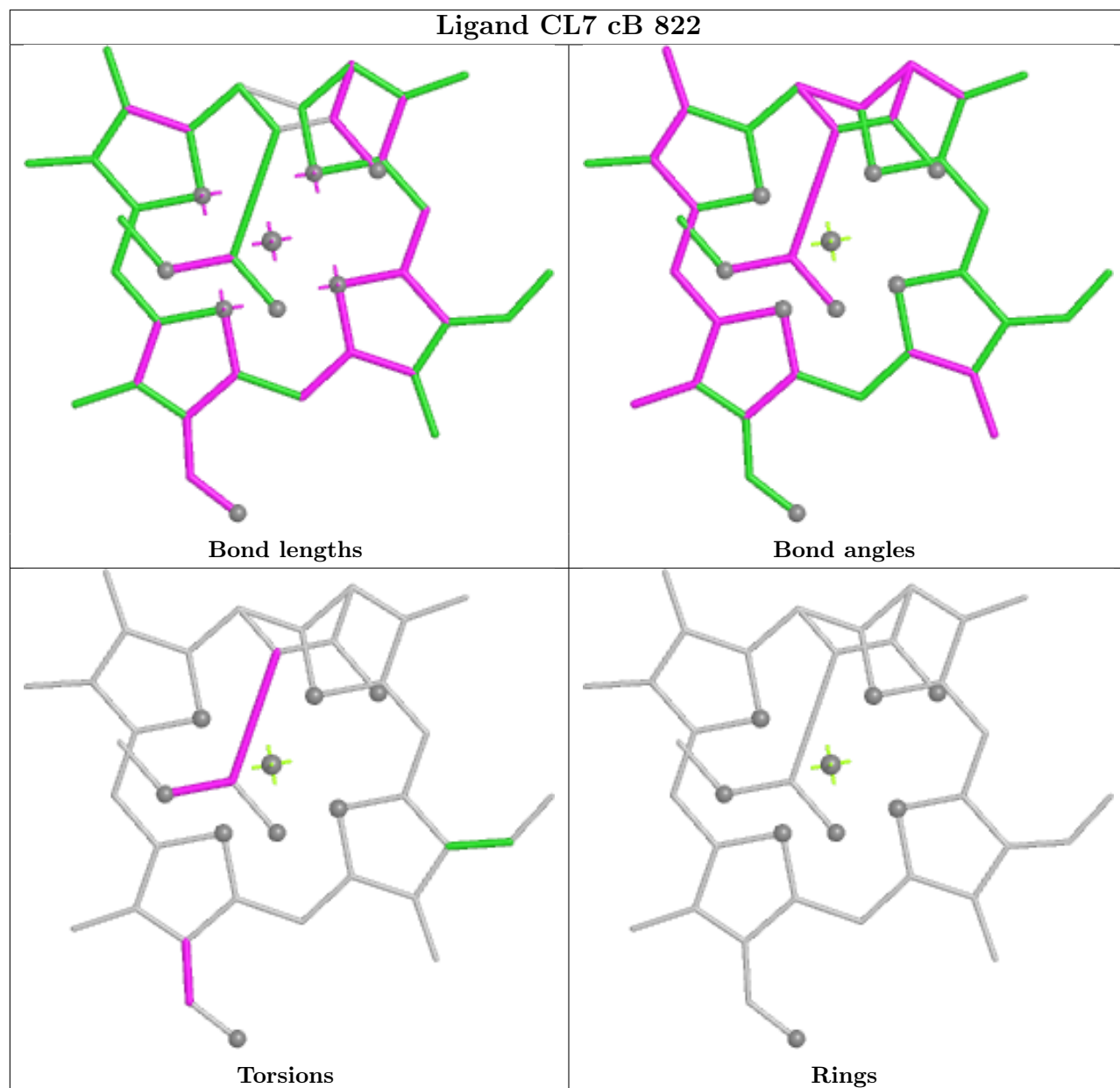
Rings

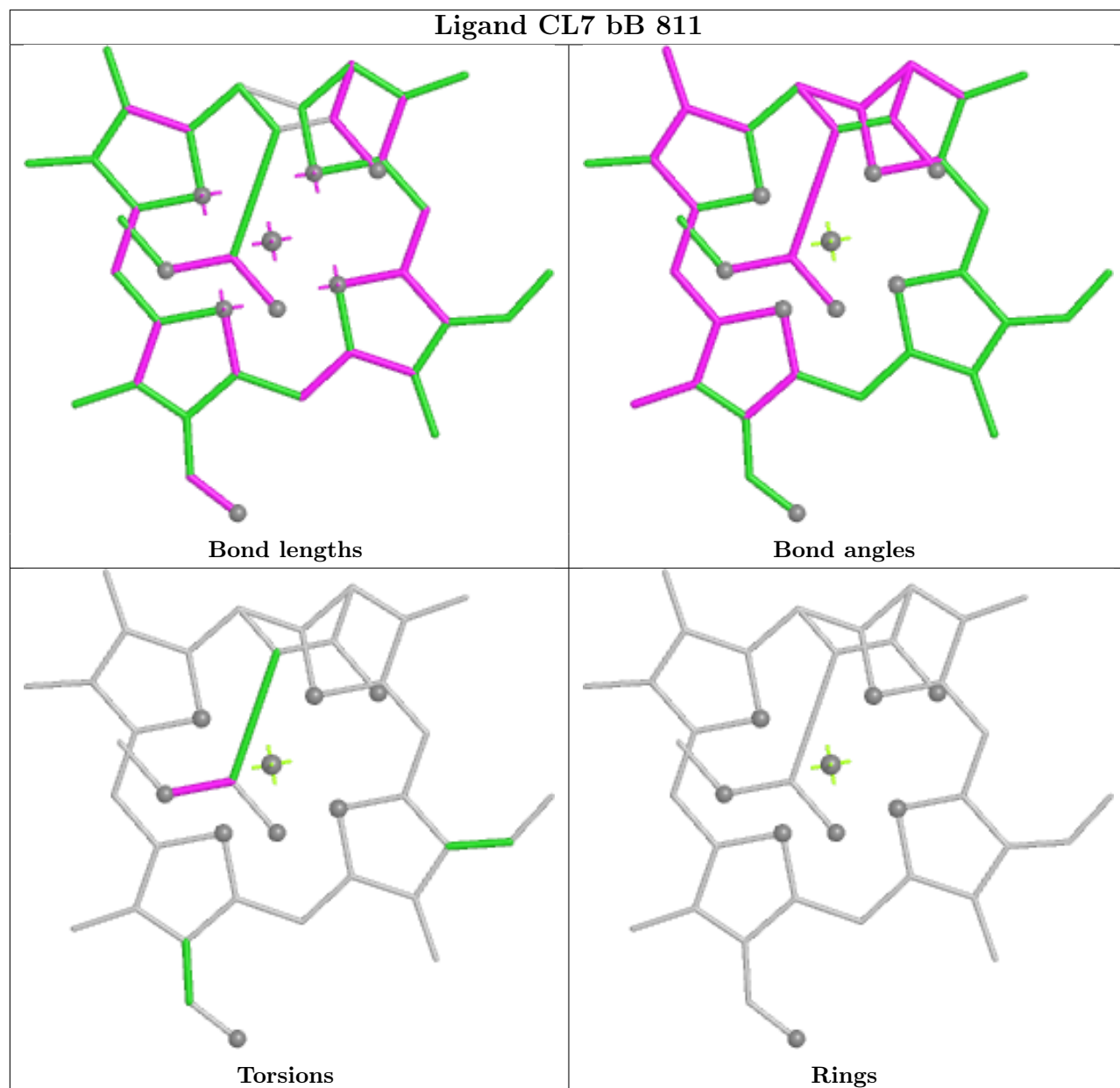


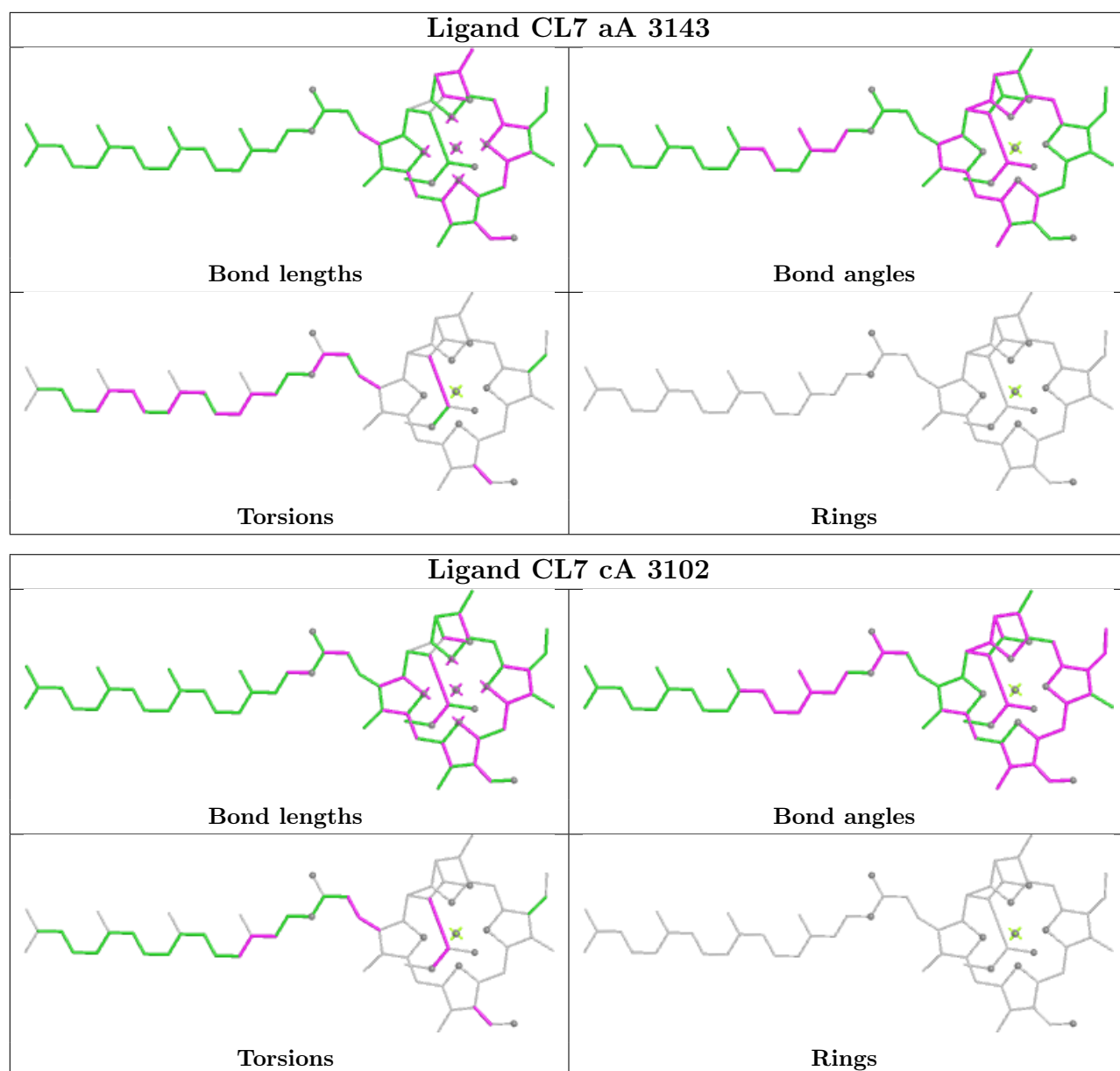


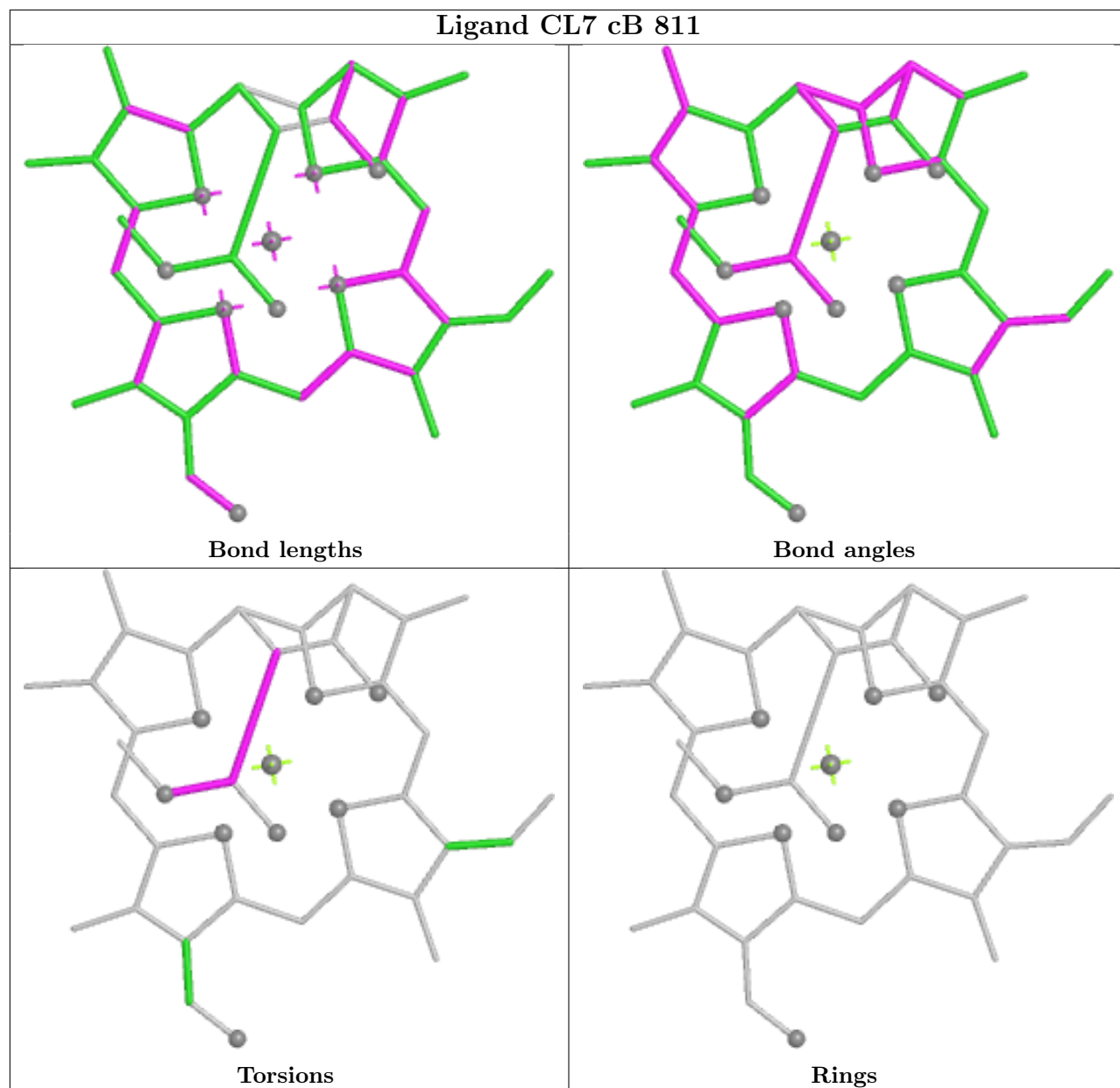


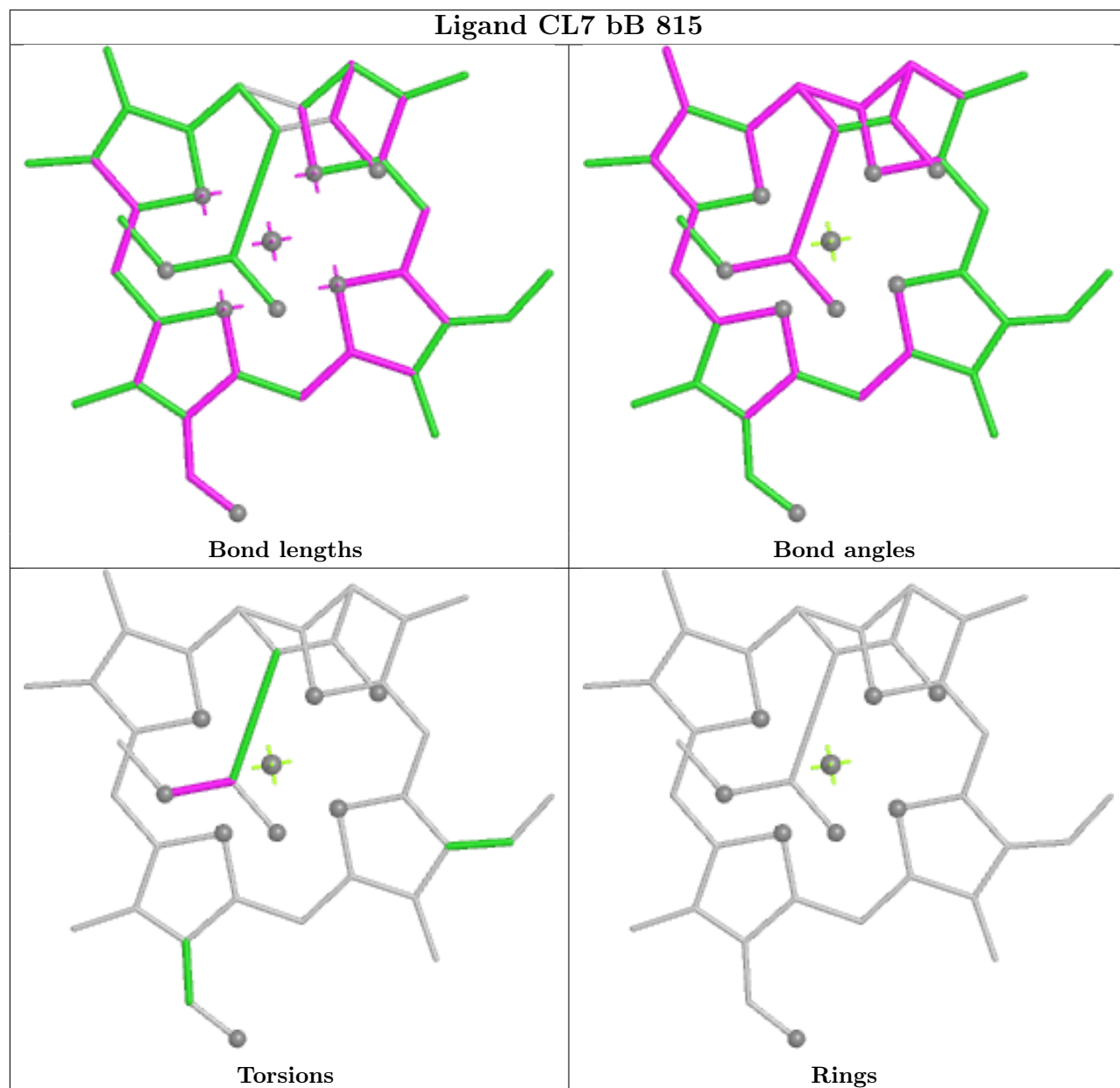


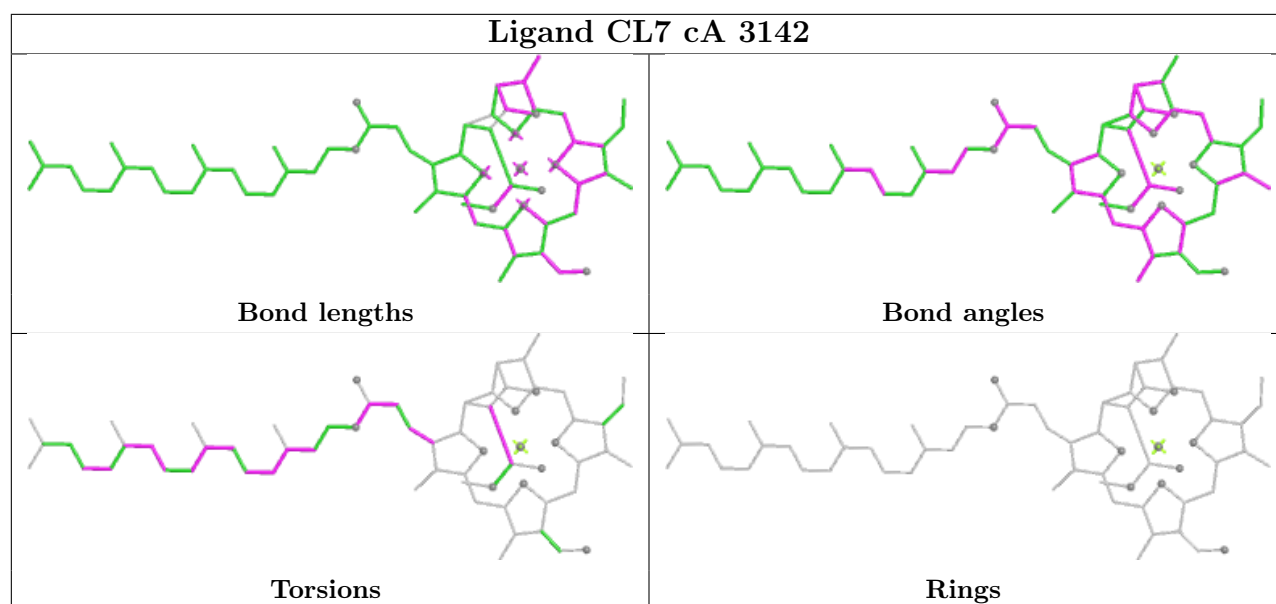




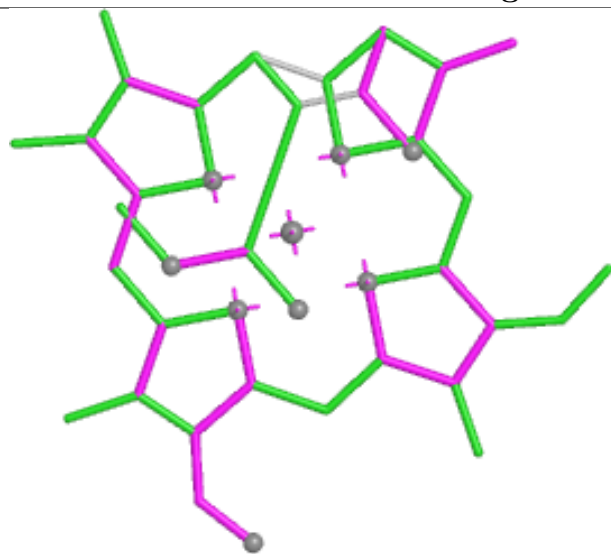




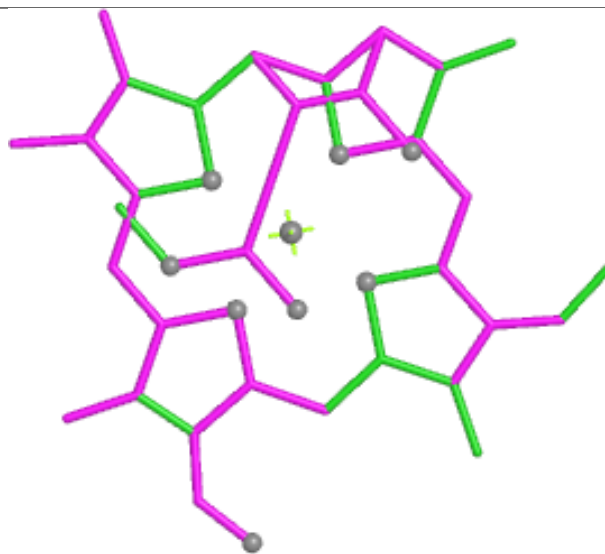




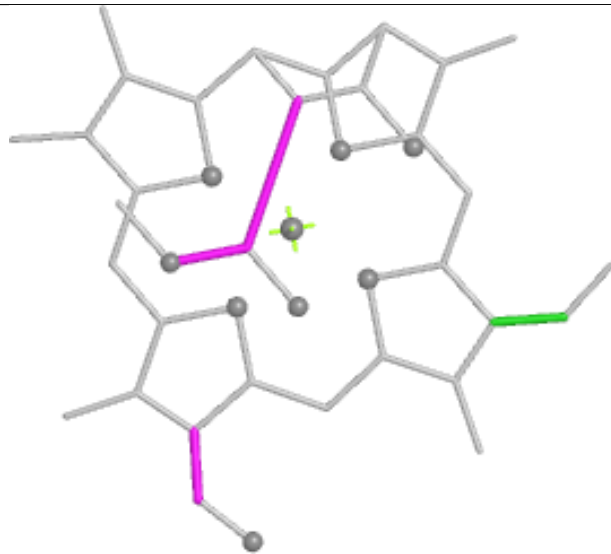
## Ligand CL7 cA 3105



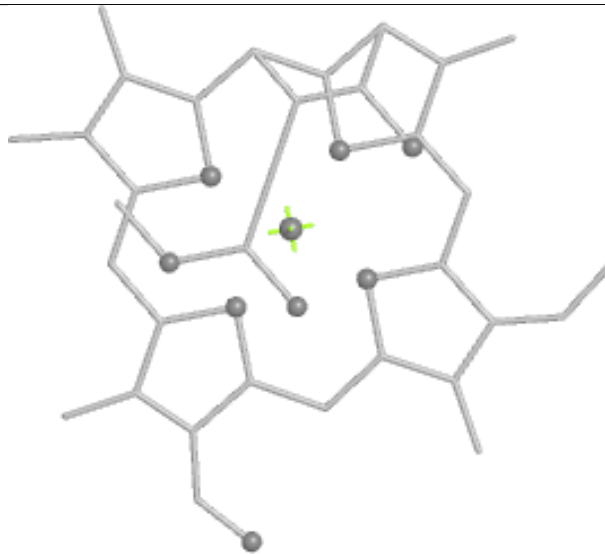
Bond lengths



Bond angles

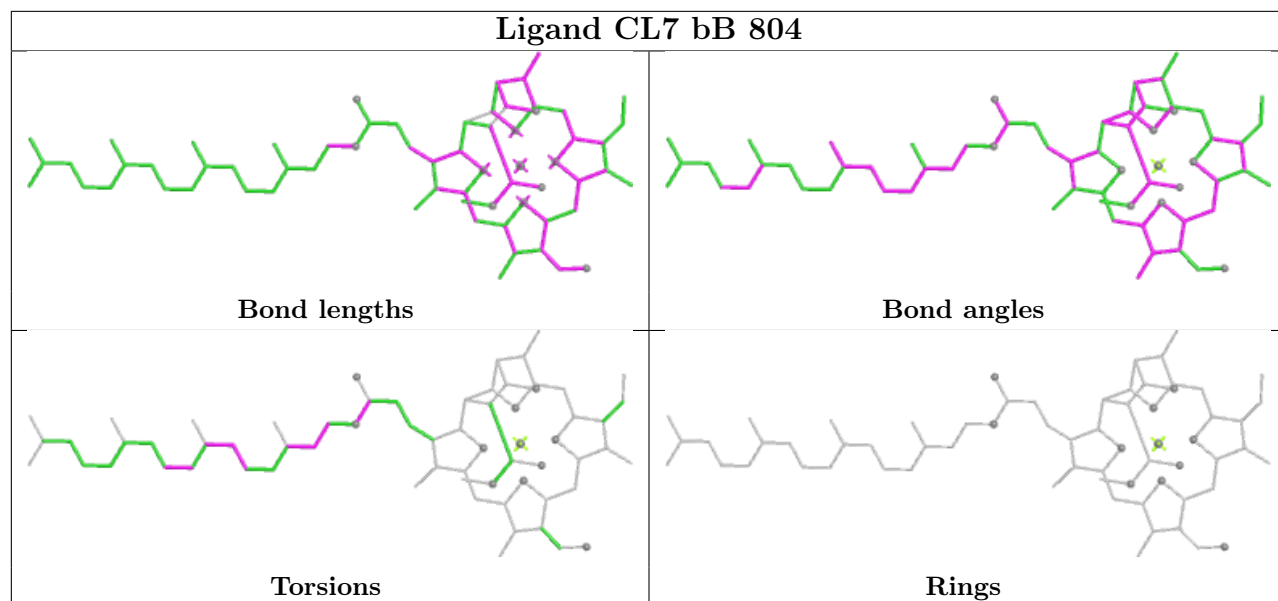


Torsions

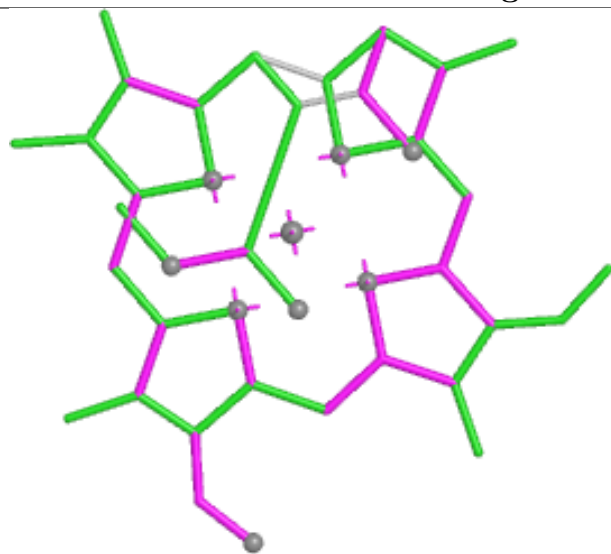


Rings

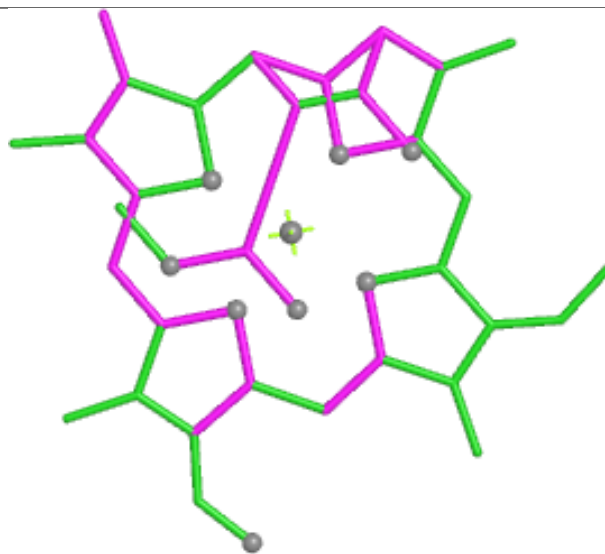




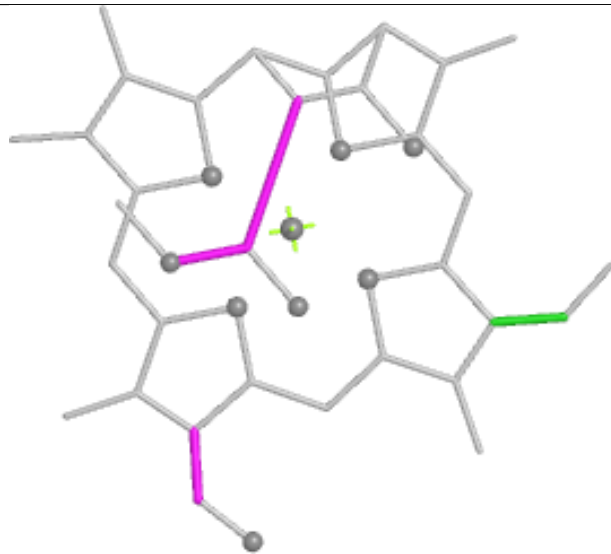
## Ligand CL7 aB 3016



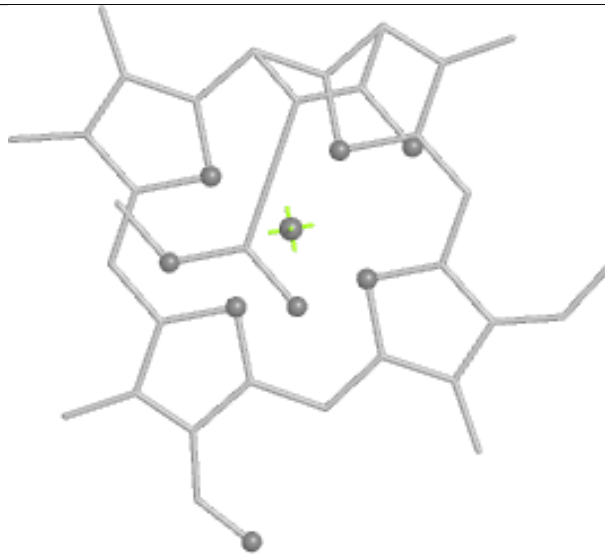
Bond lengths



Bond angles

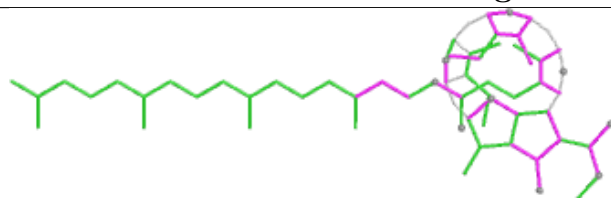


Torsions

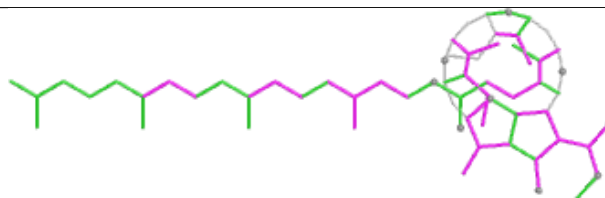


Rings

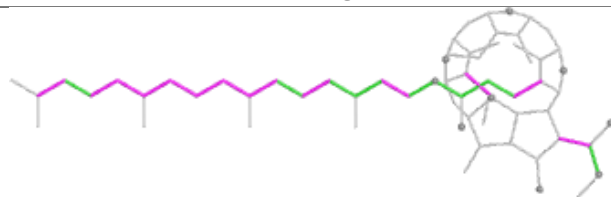
## Ligand PHO aB 3004



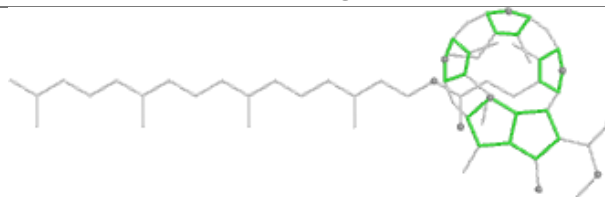
Bond lengths



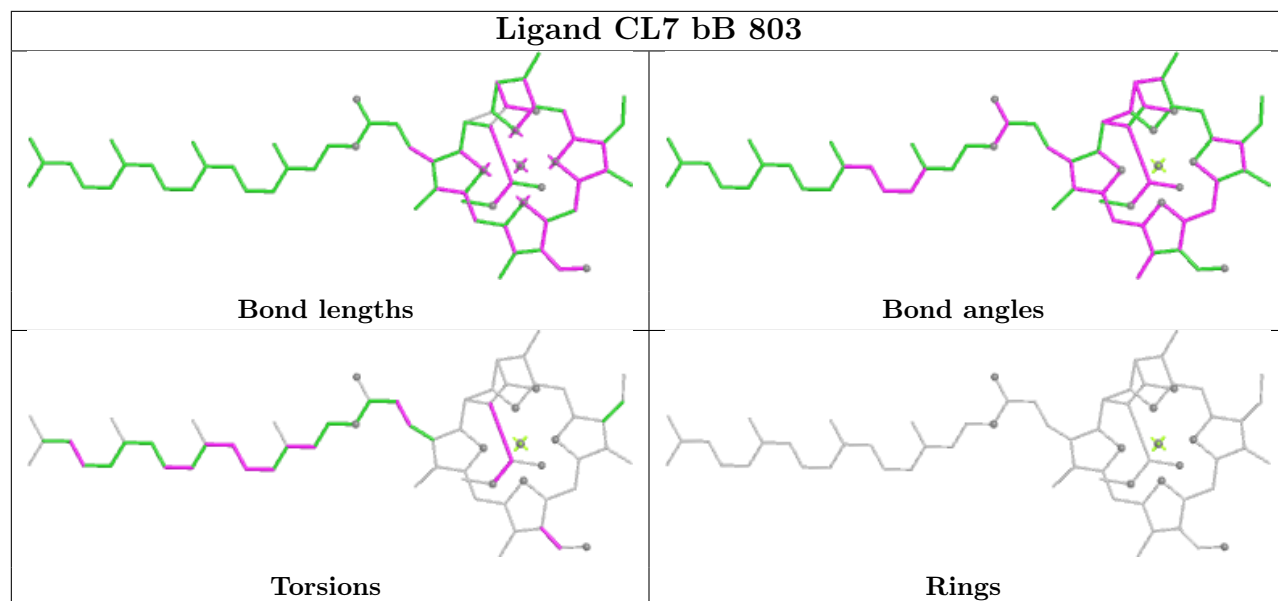
Bond angles

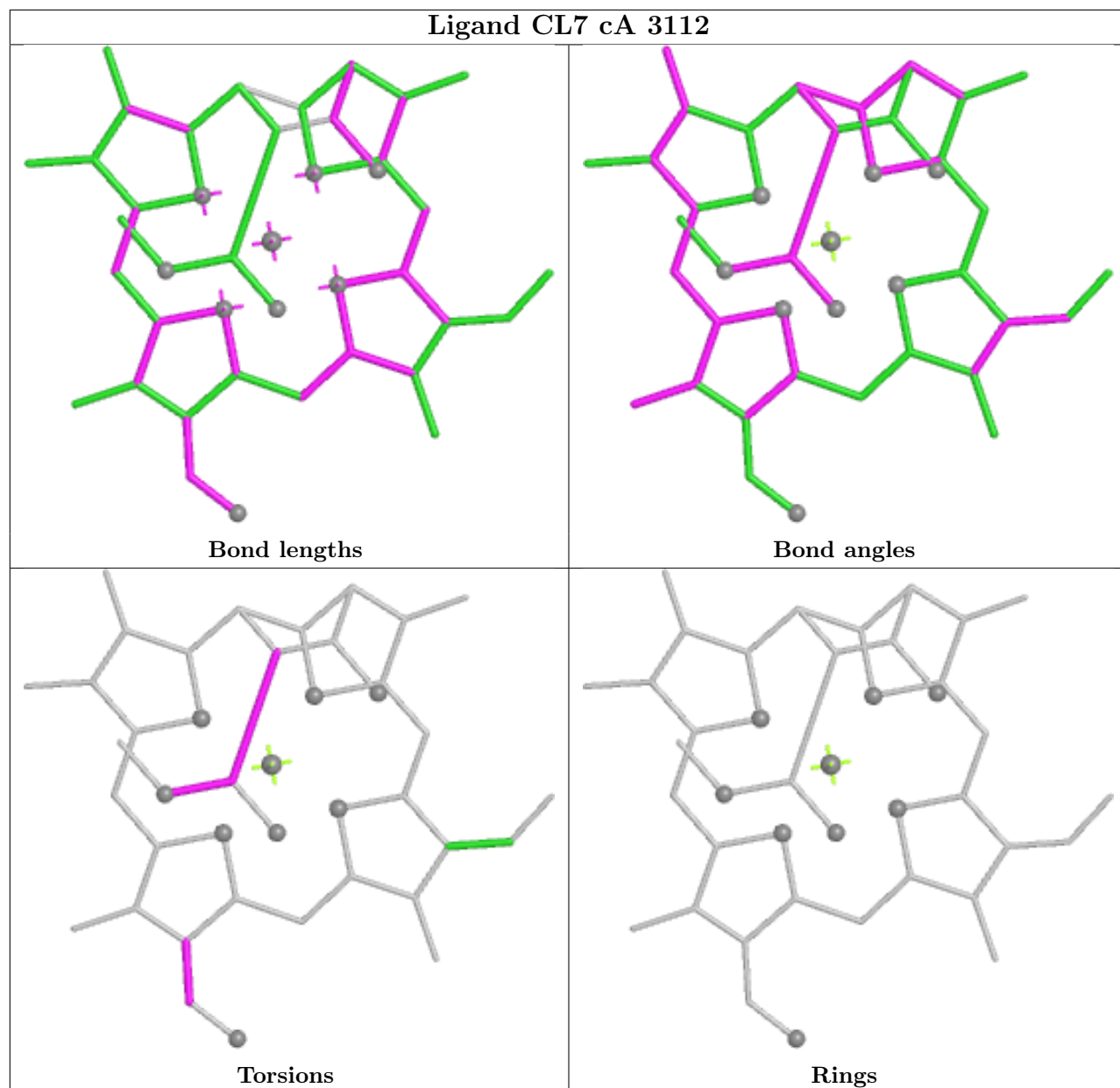


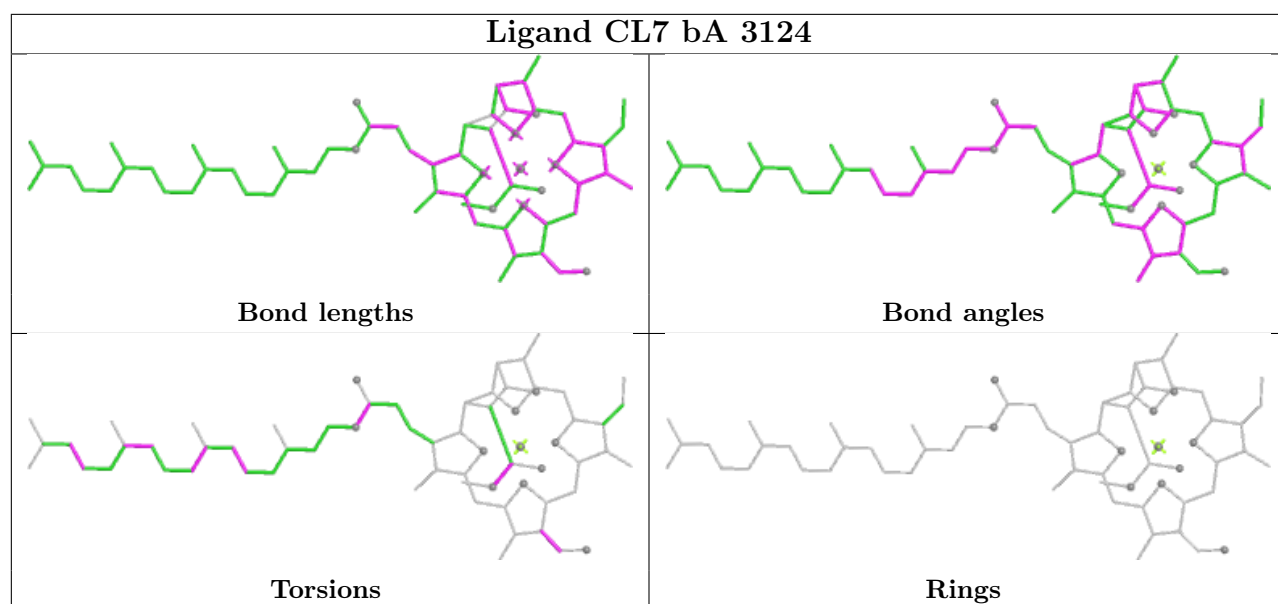
Torsions

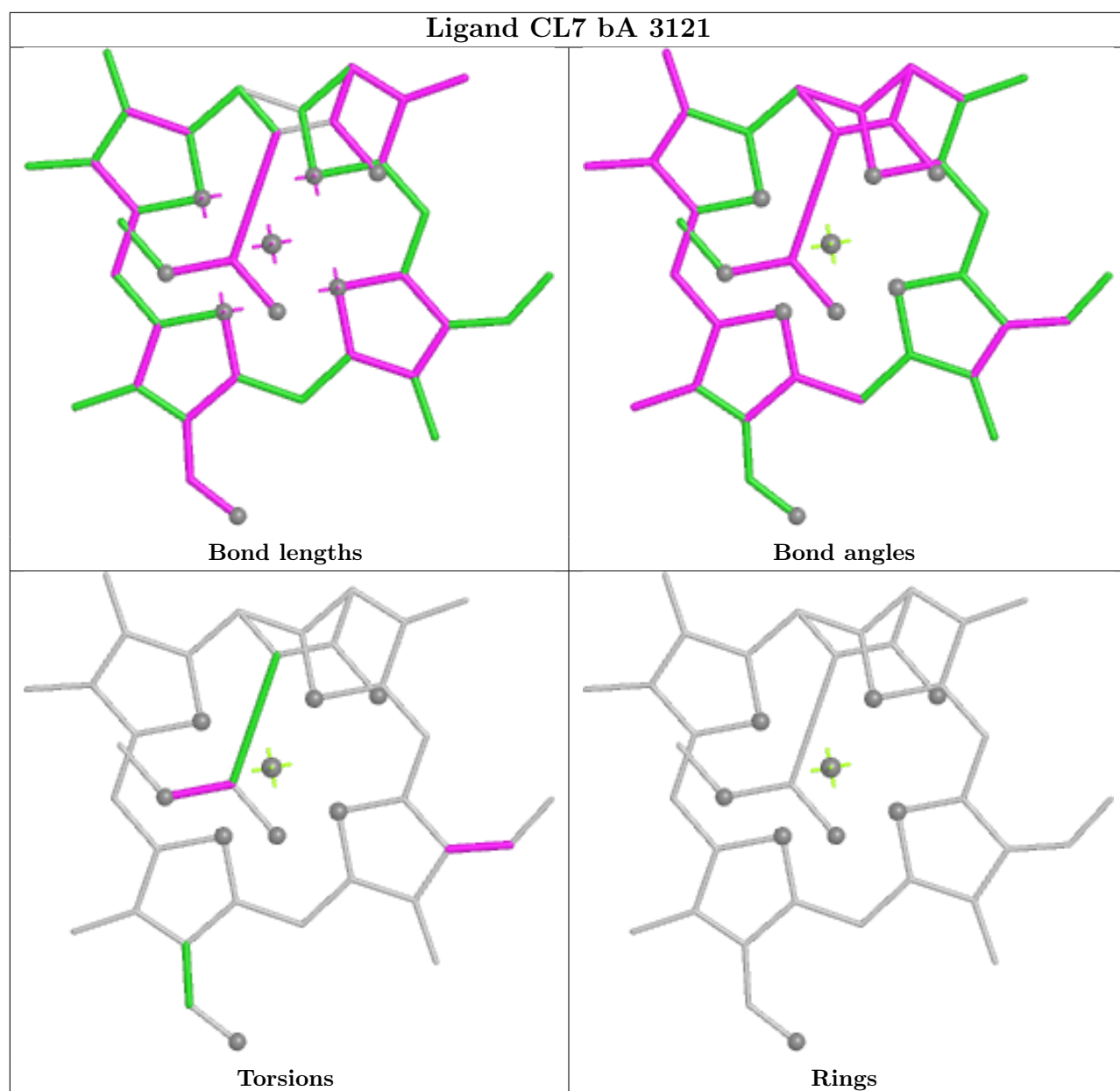


Rings

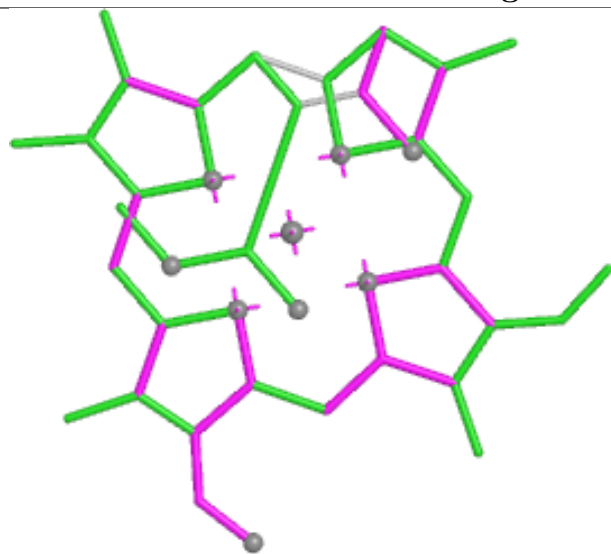




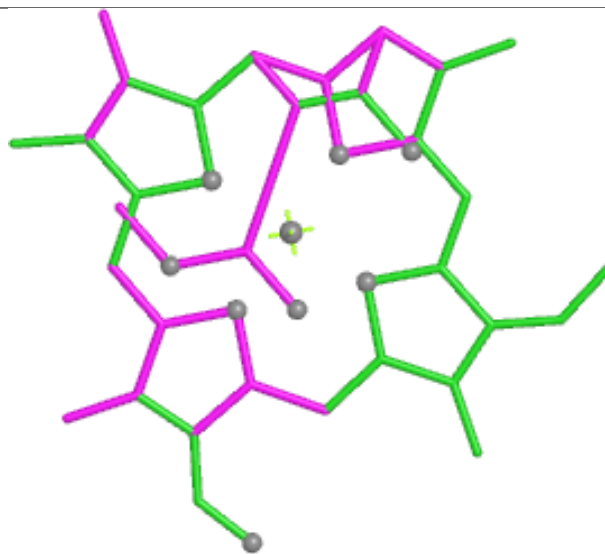




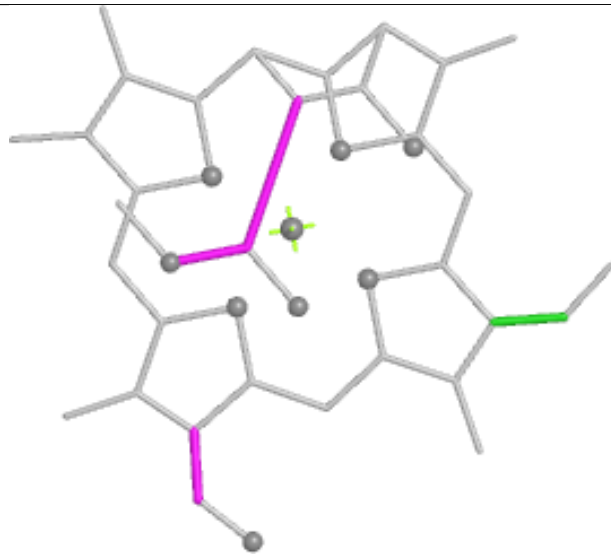
## Ligand CL7 cA 3144



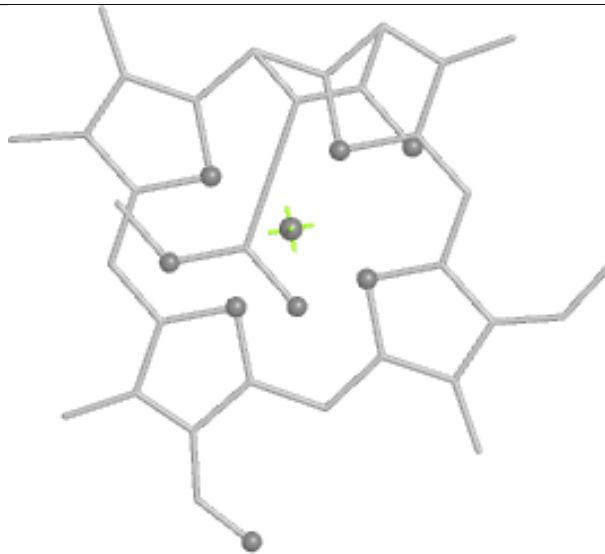
Bond lengths



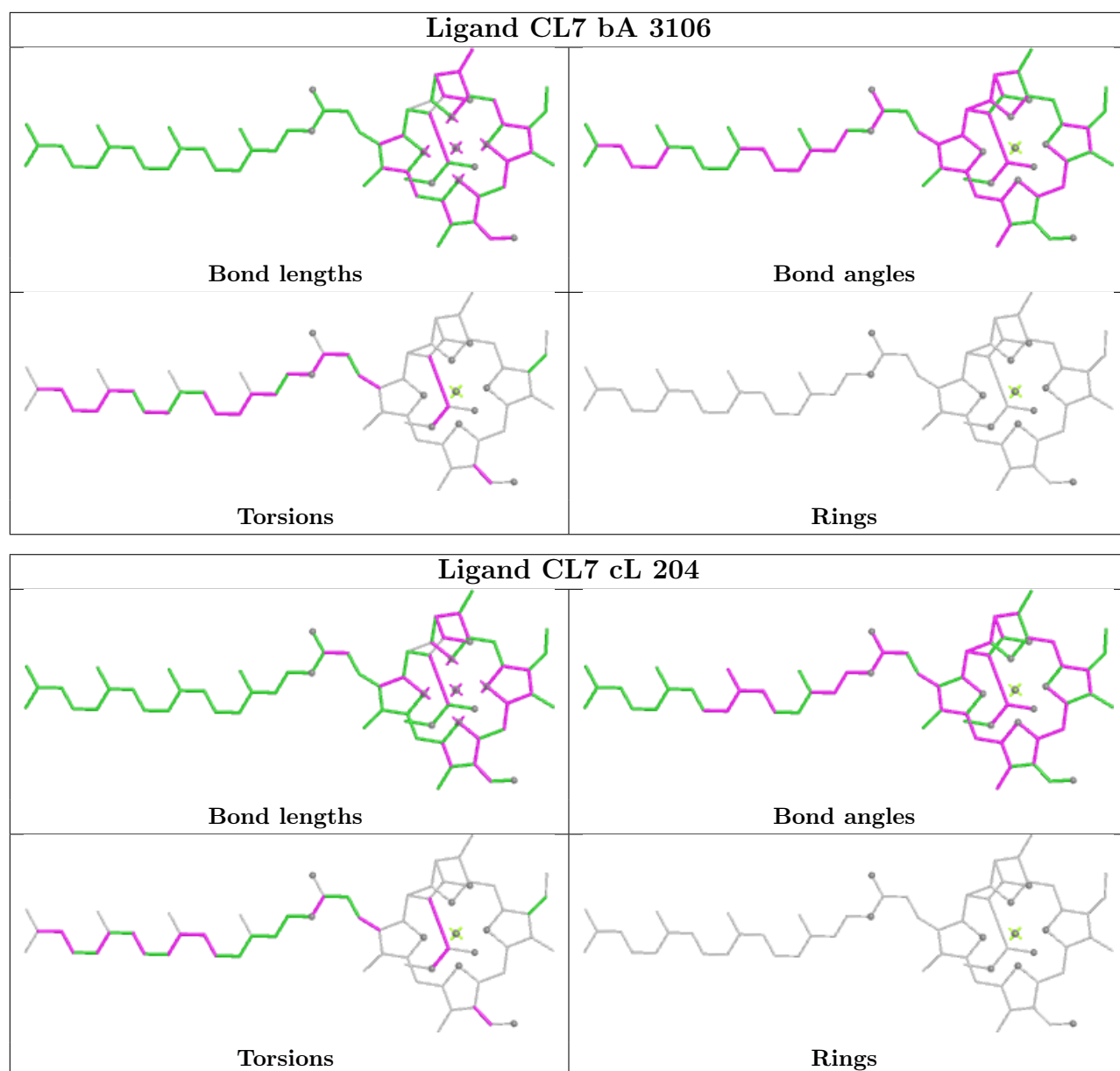
Bond angles



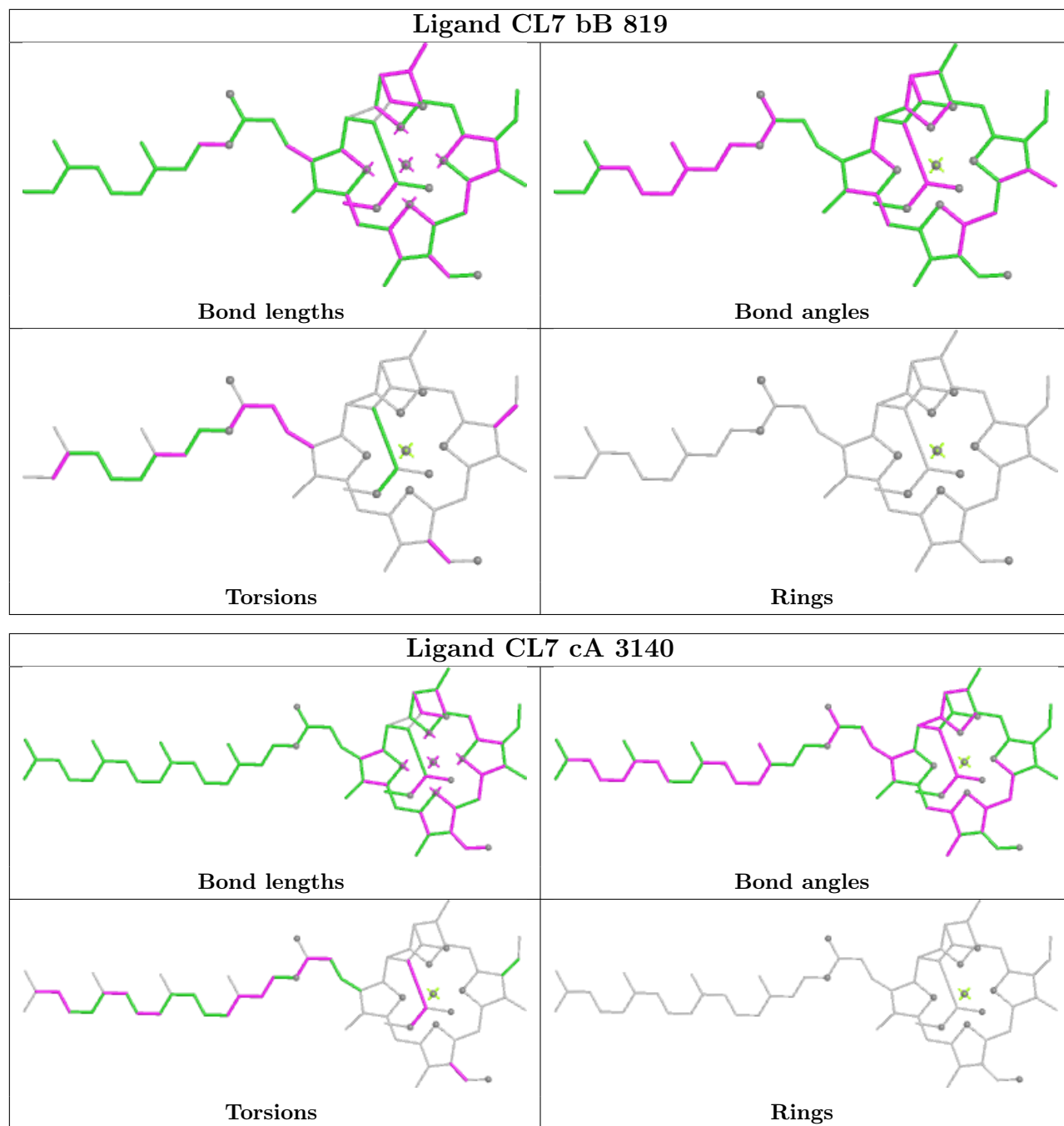
Torsions

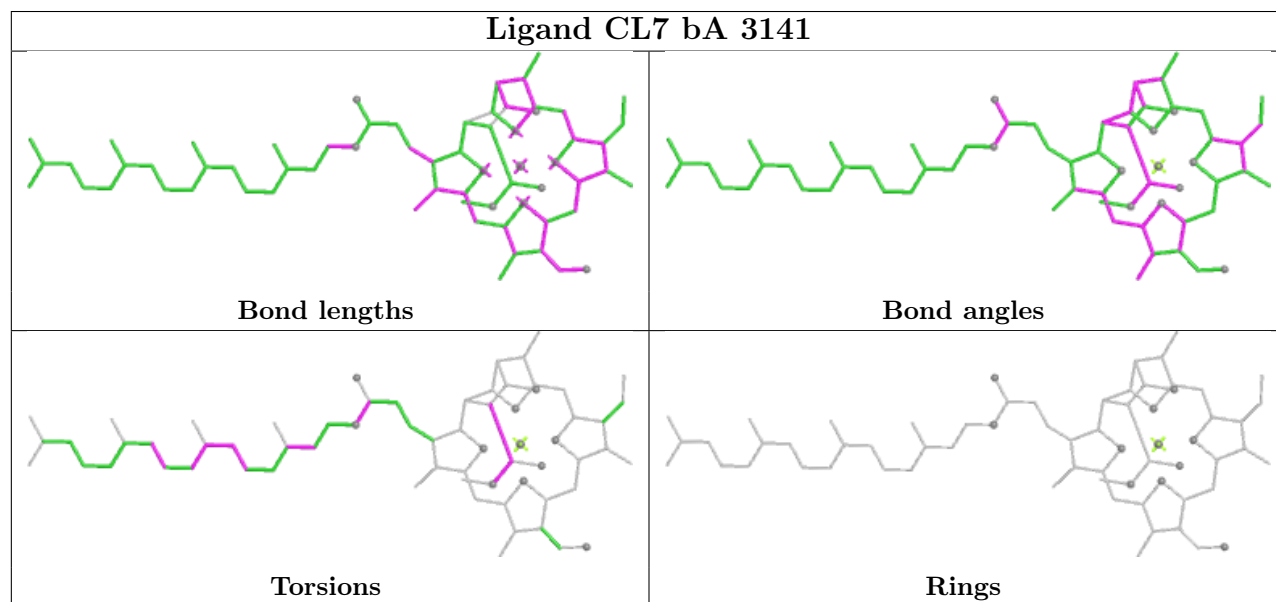
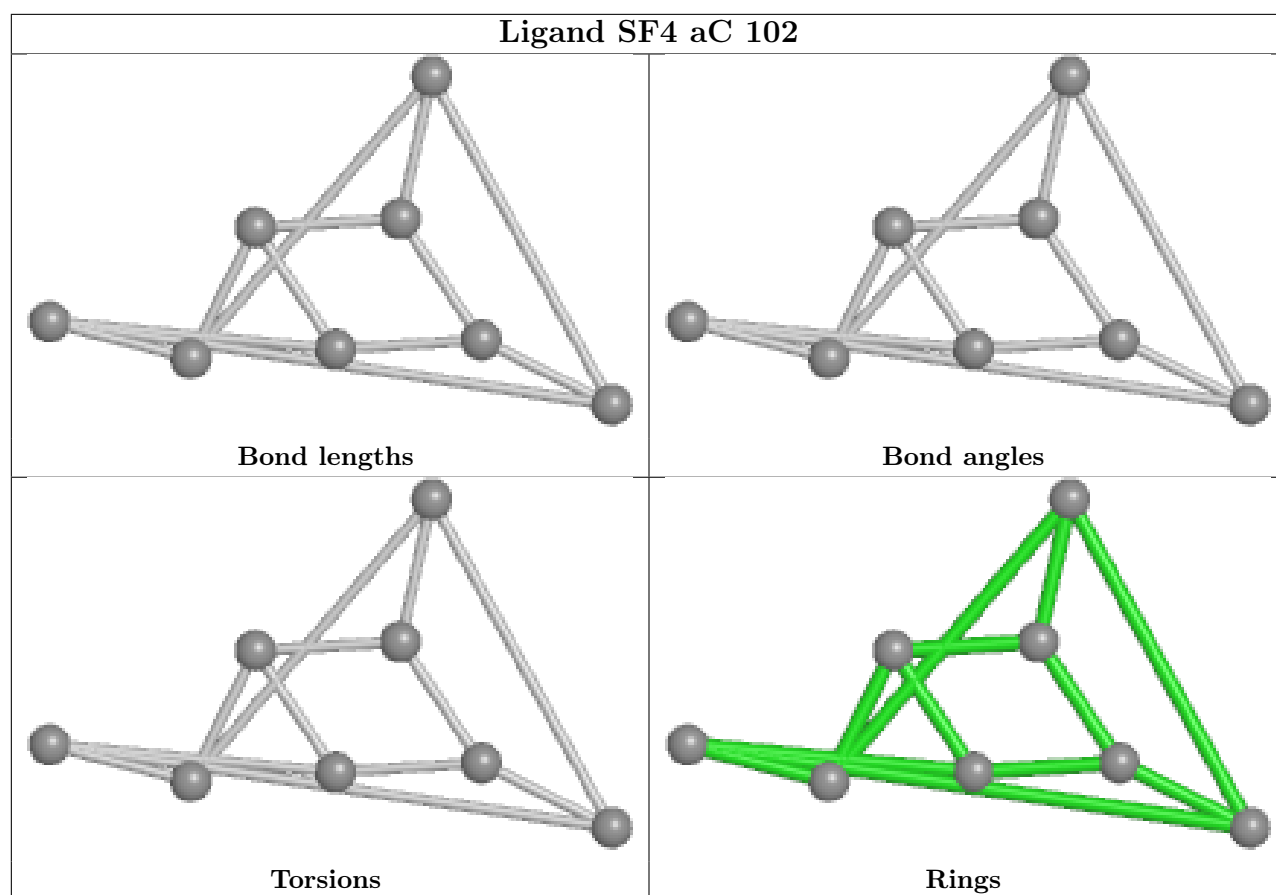


Rings

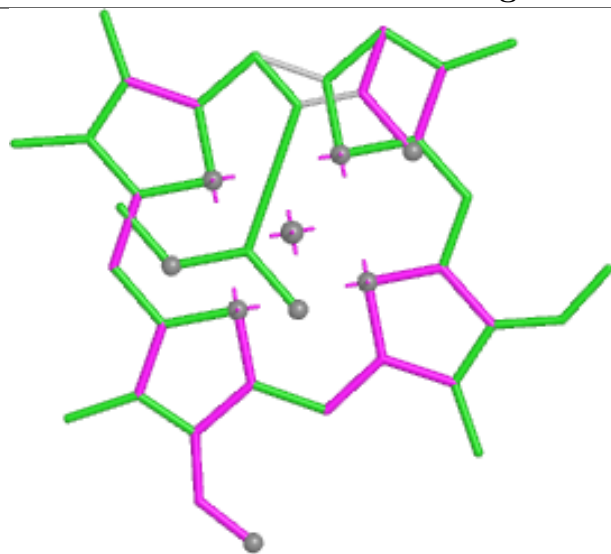




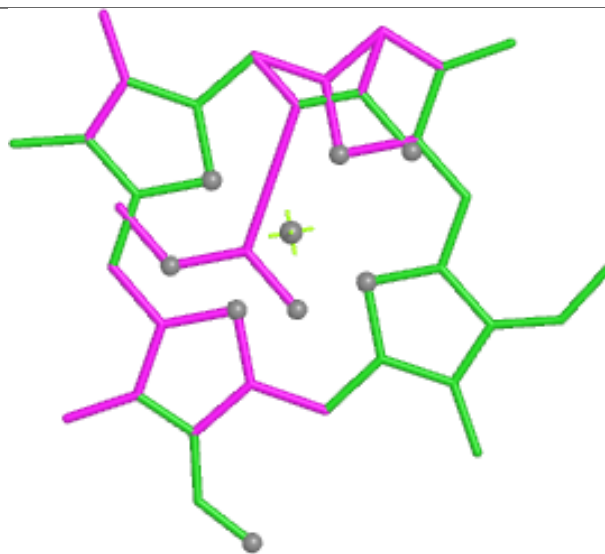




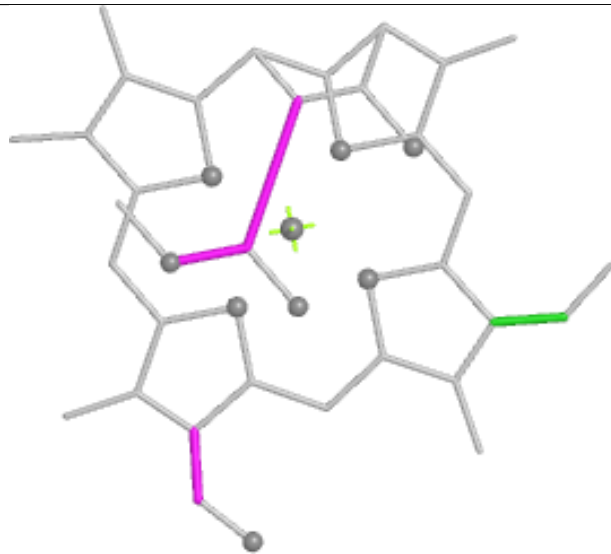
## Ligand CL7 bA 3145



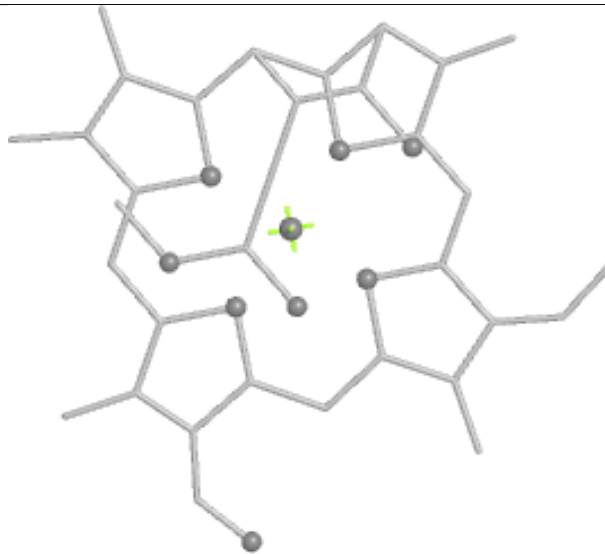
Bond lengths



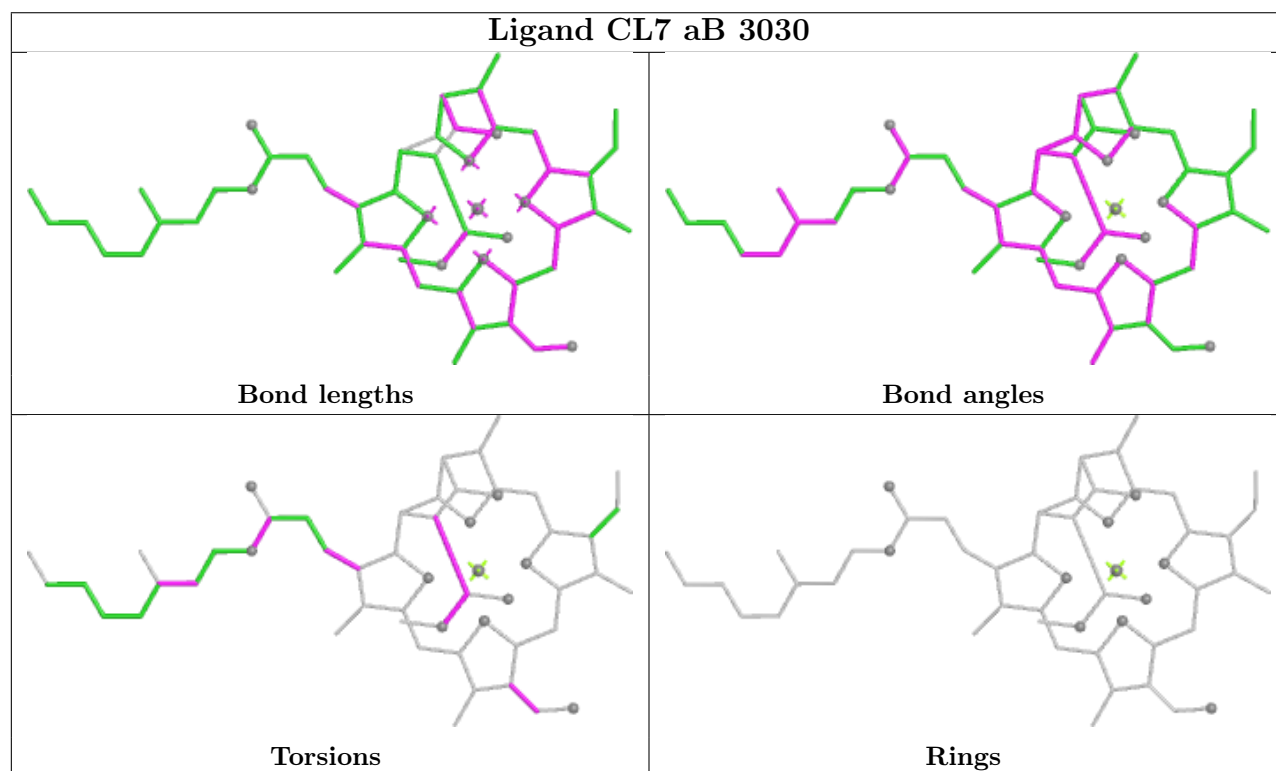
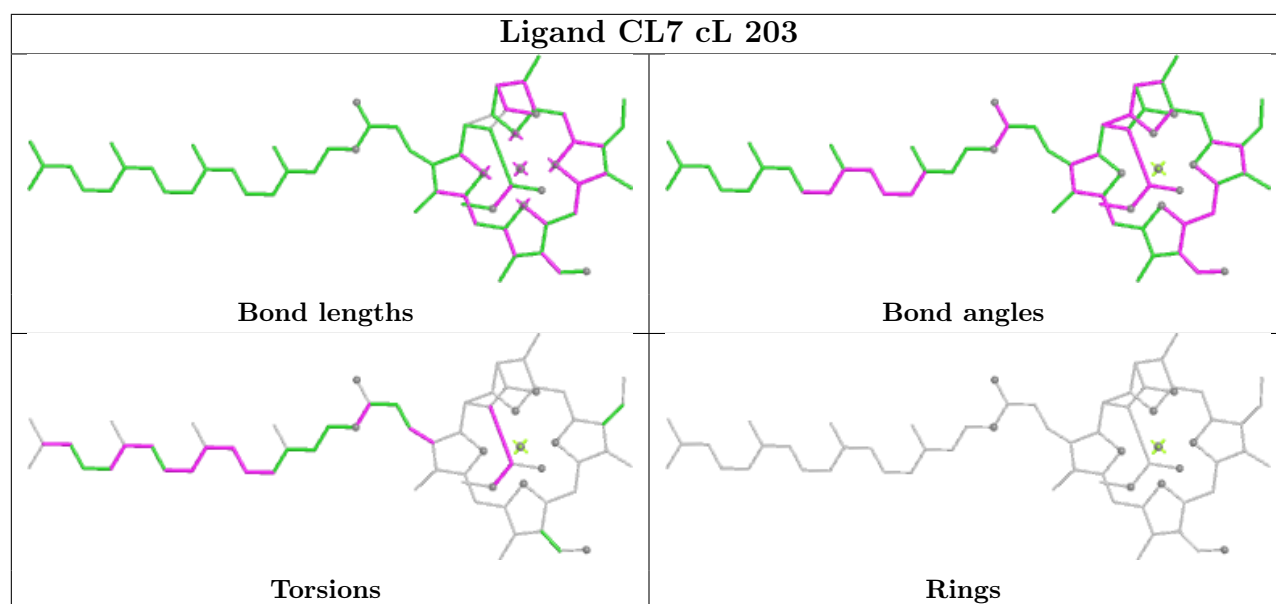
Bond angles

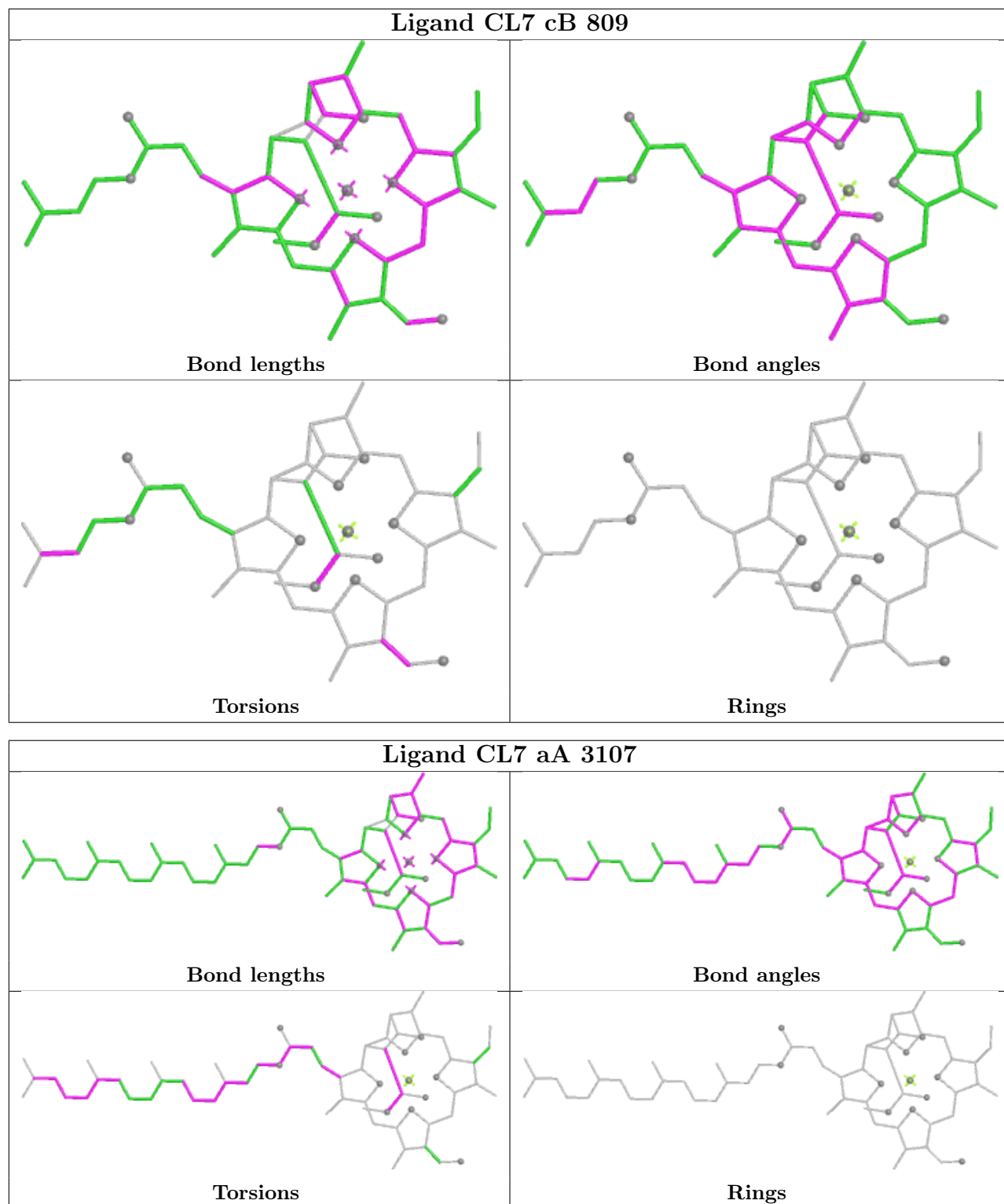


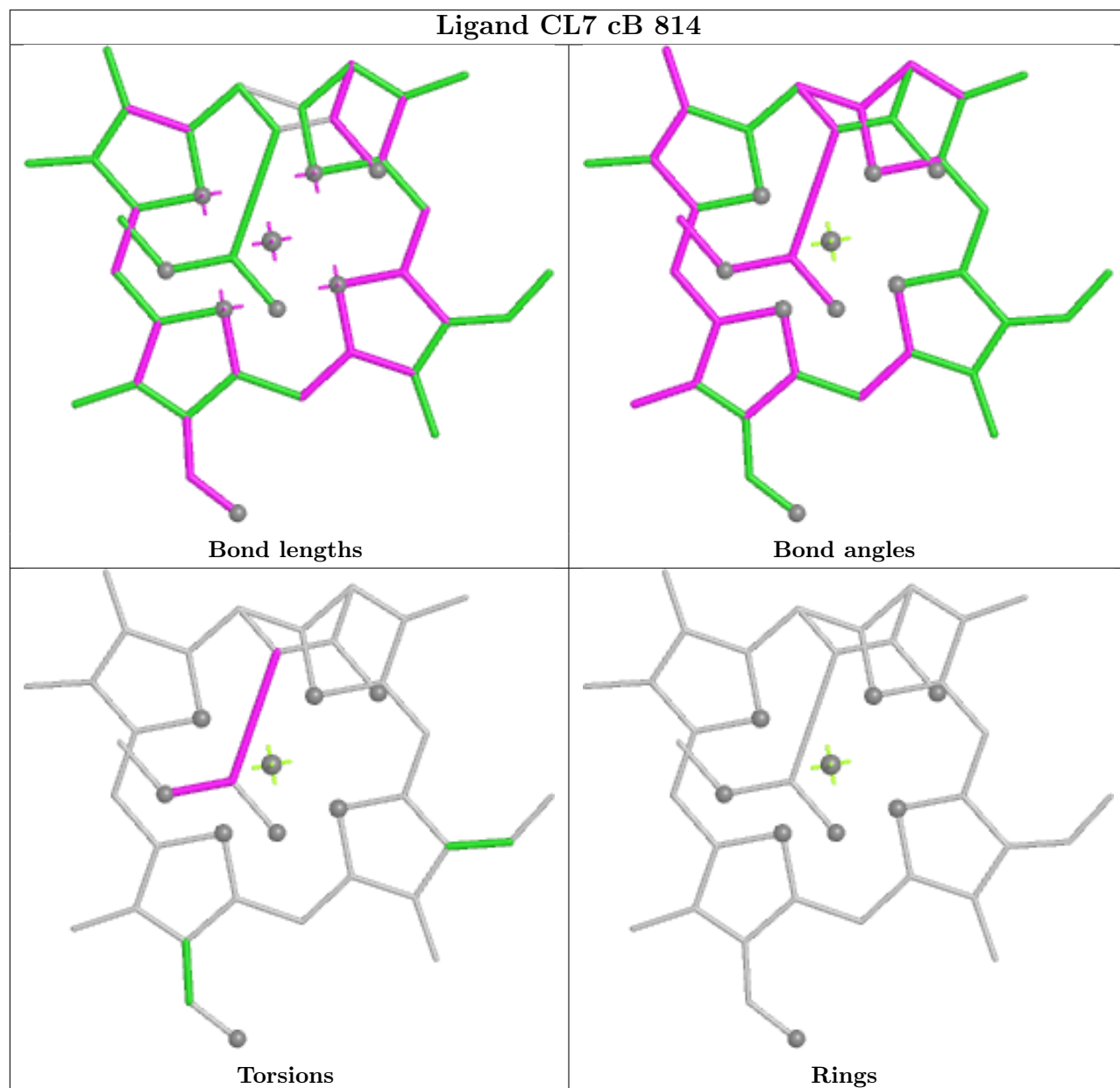
Torsions



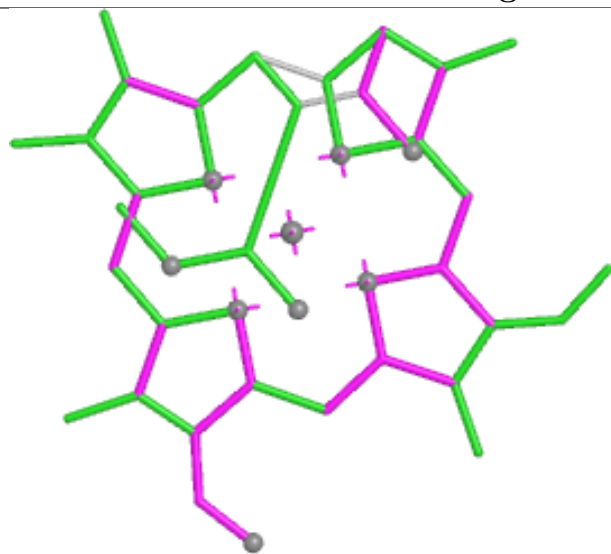
Rings



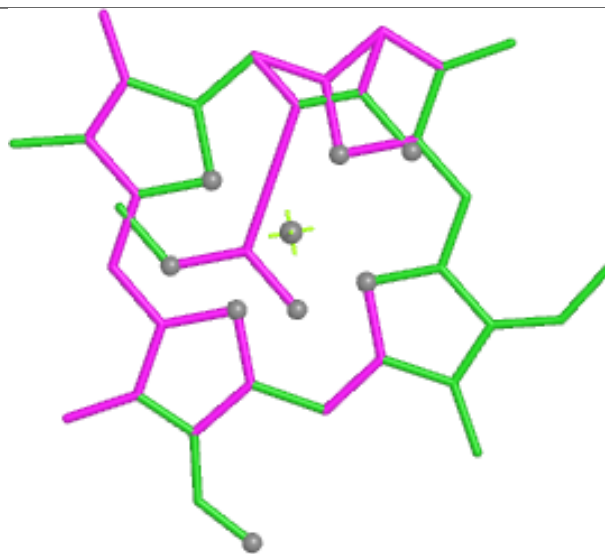




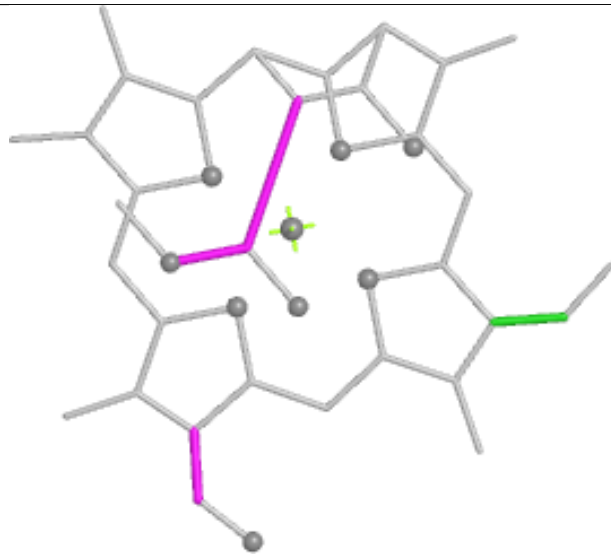
## Ligand CL7 bA 3104



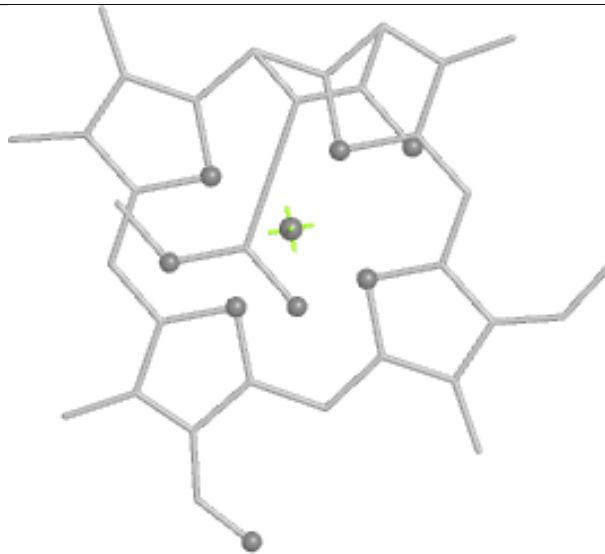
Bond lengths



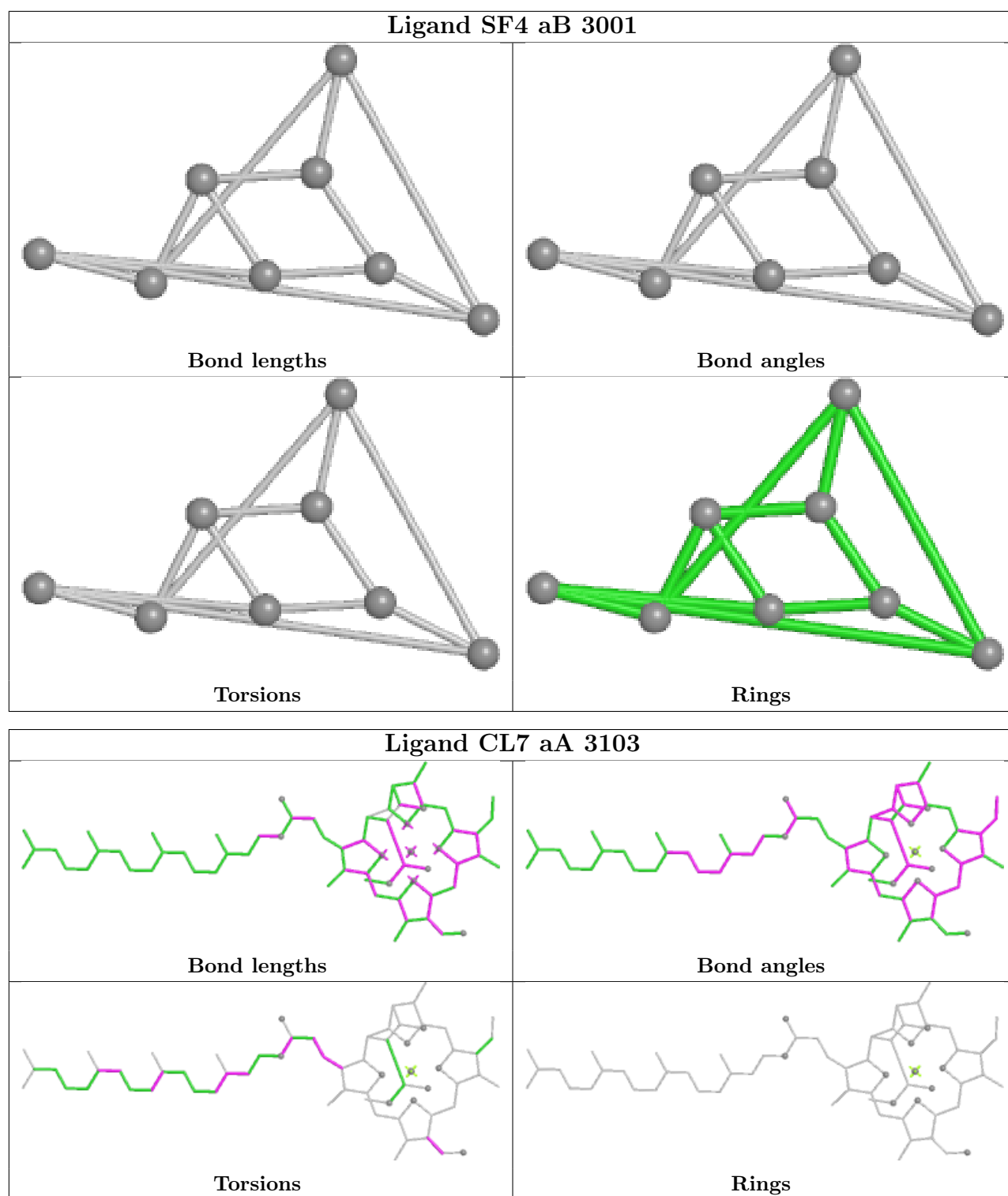
Bond angles



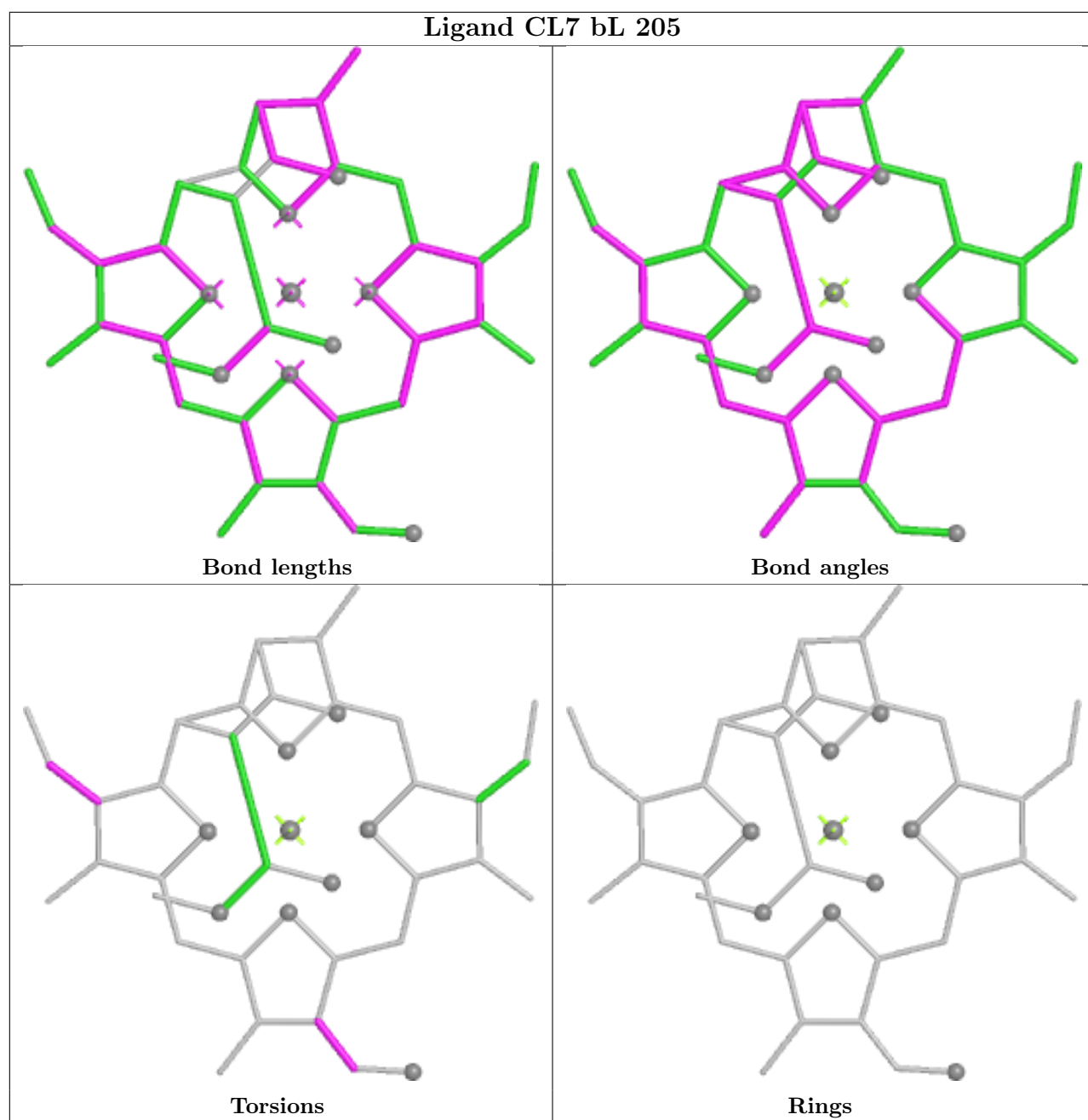
Torsions

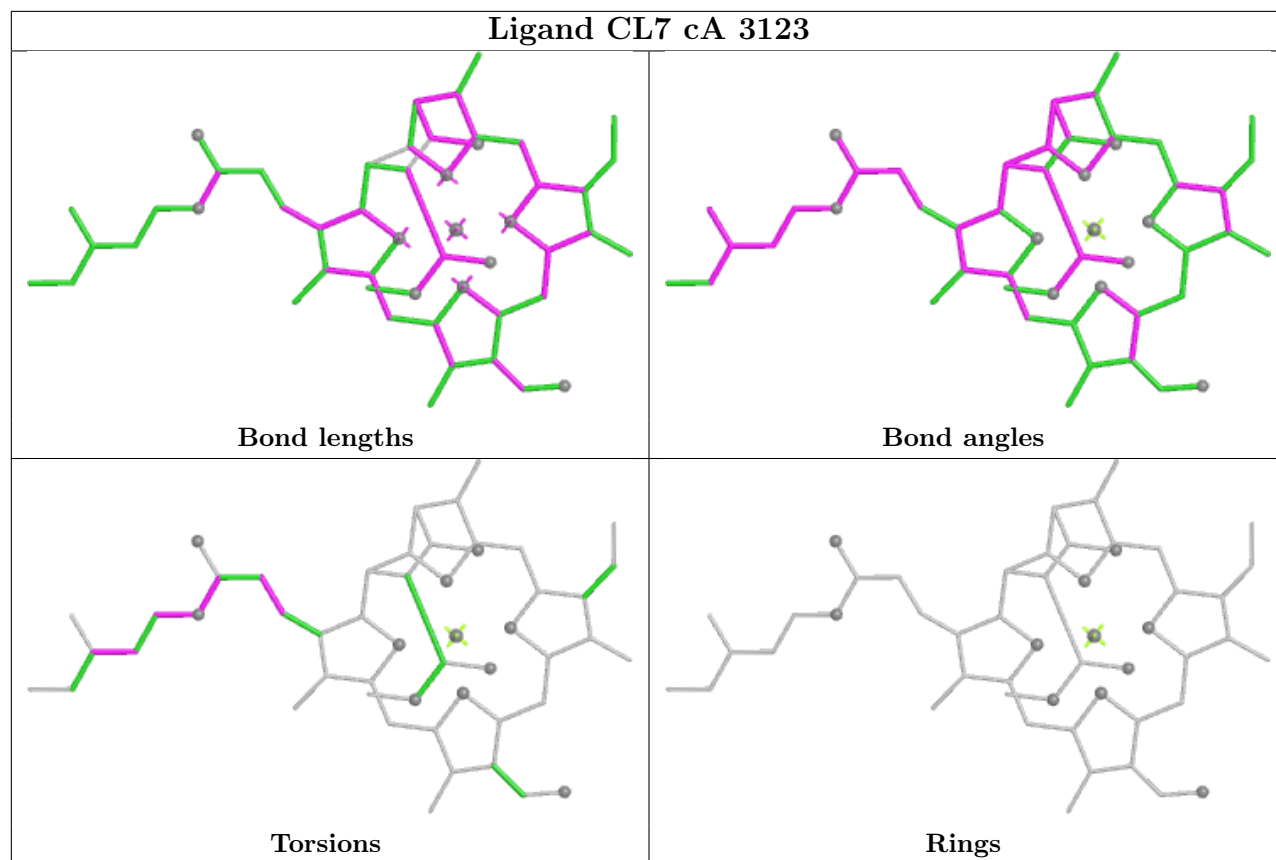


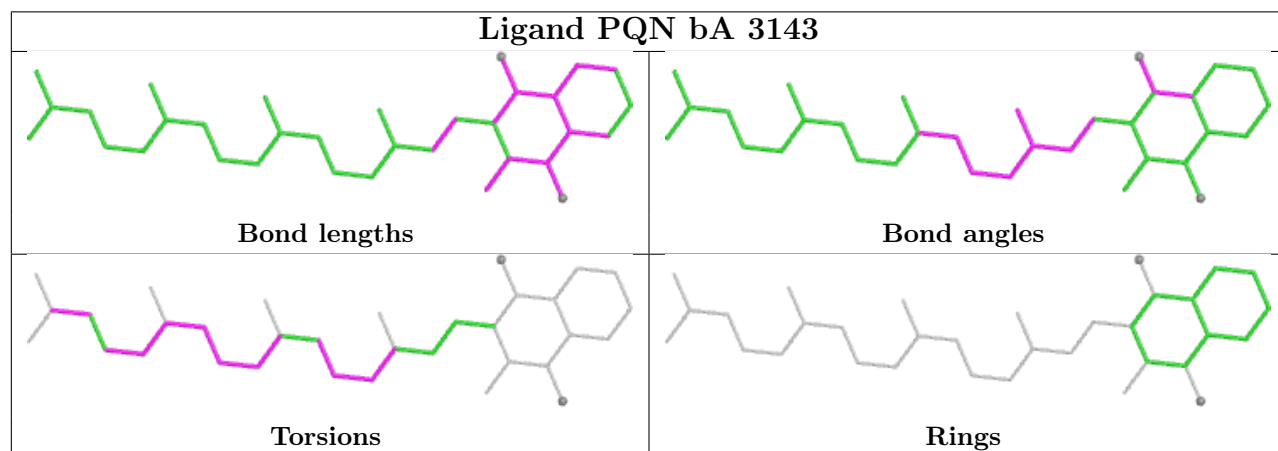
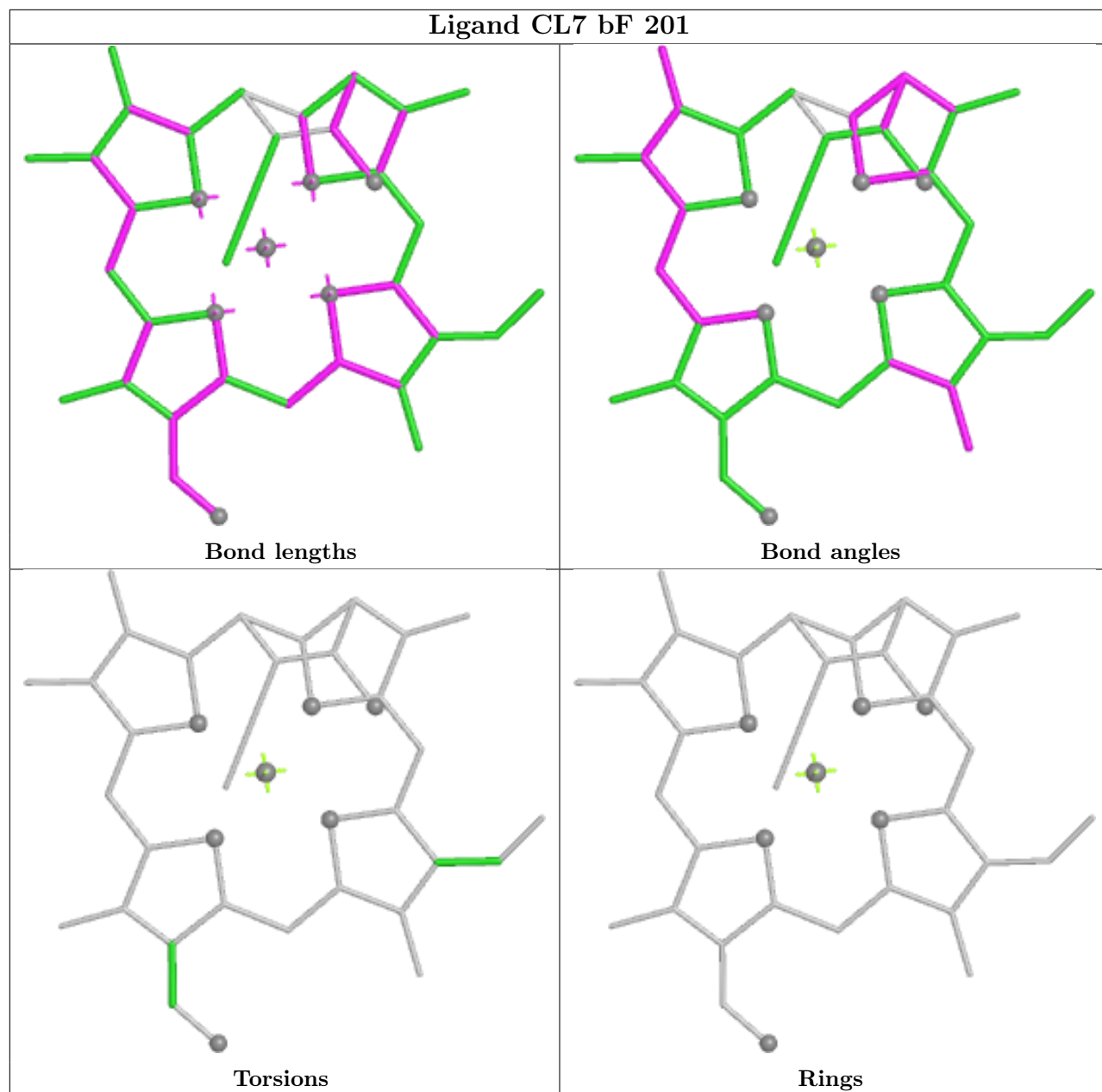
Rings

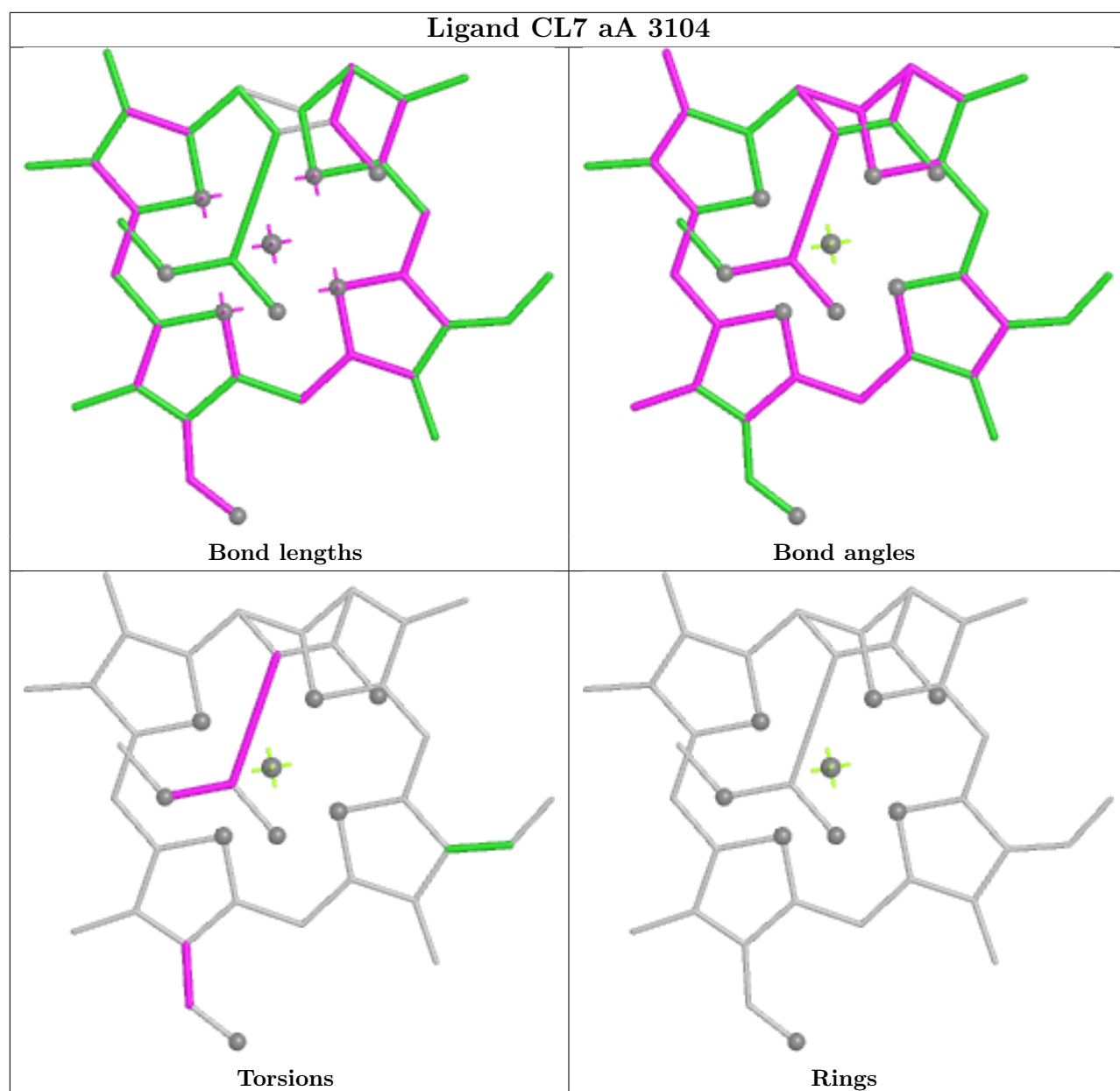


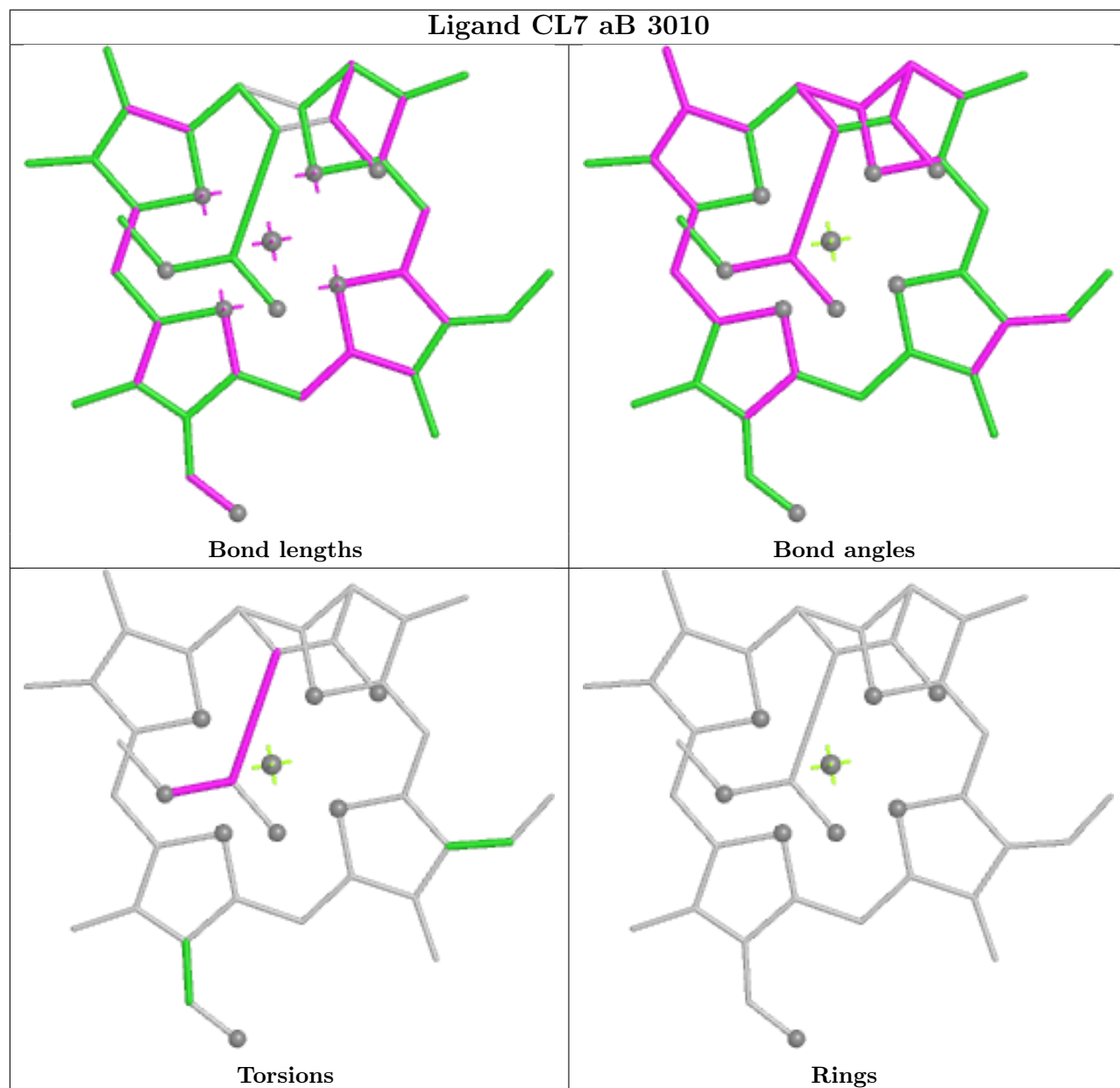


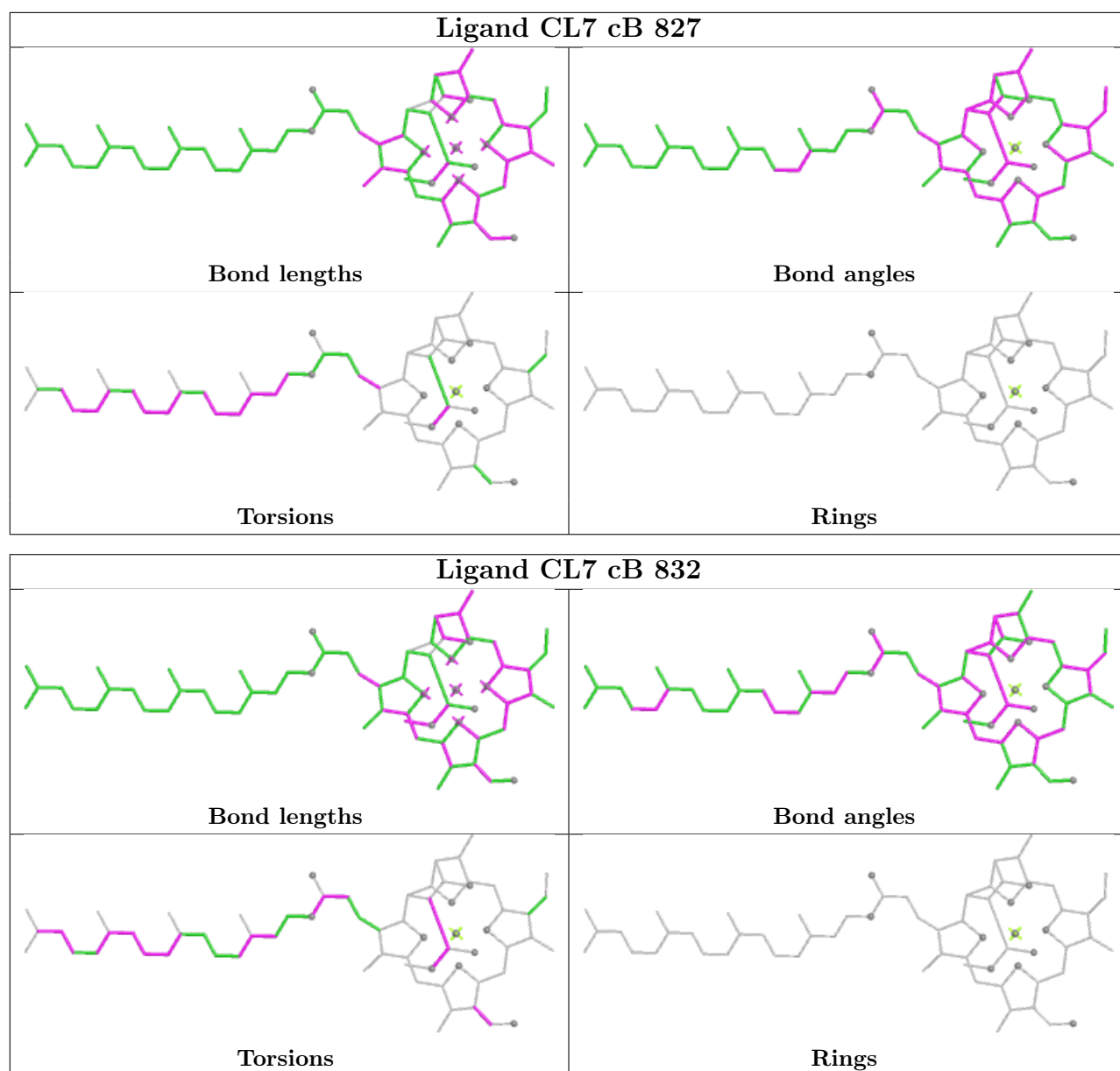


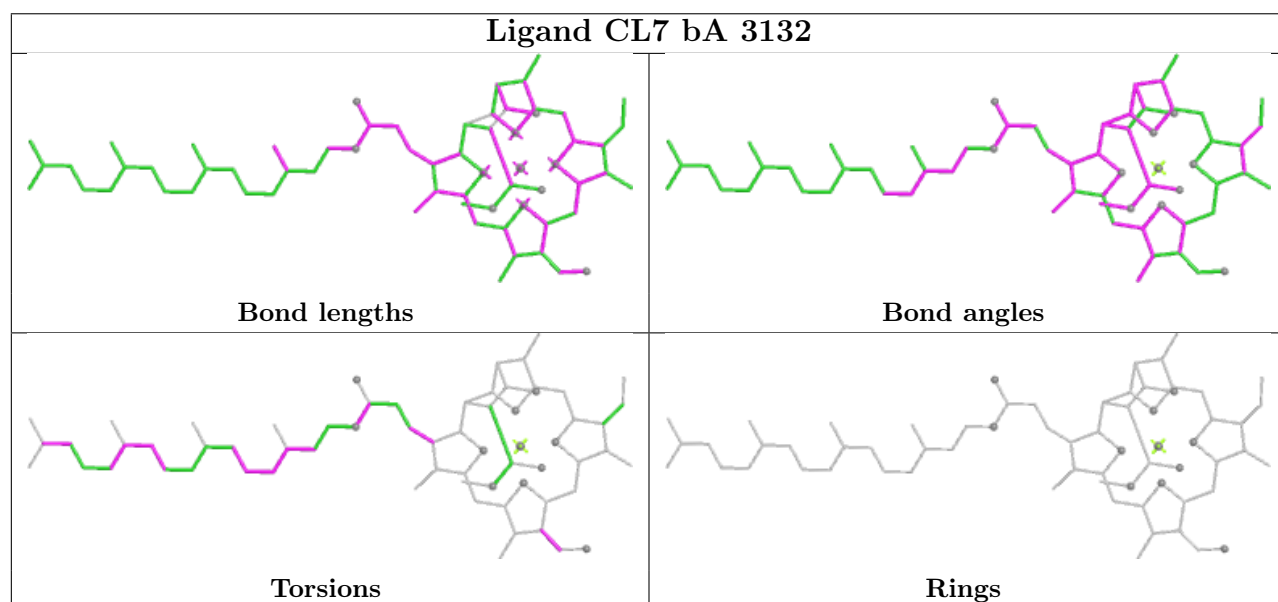
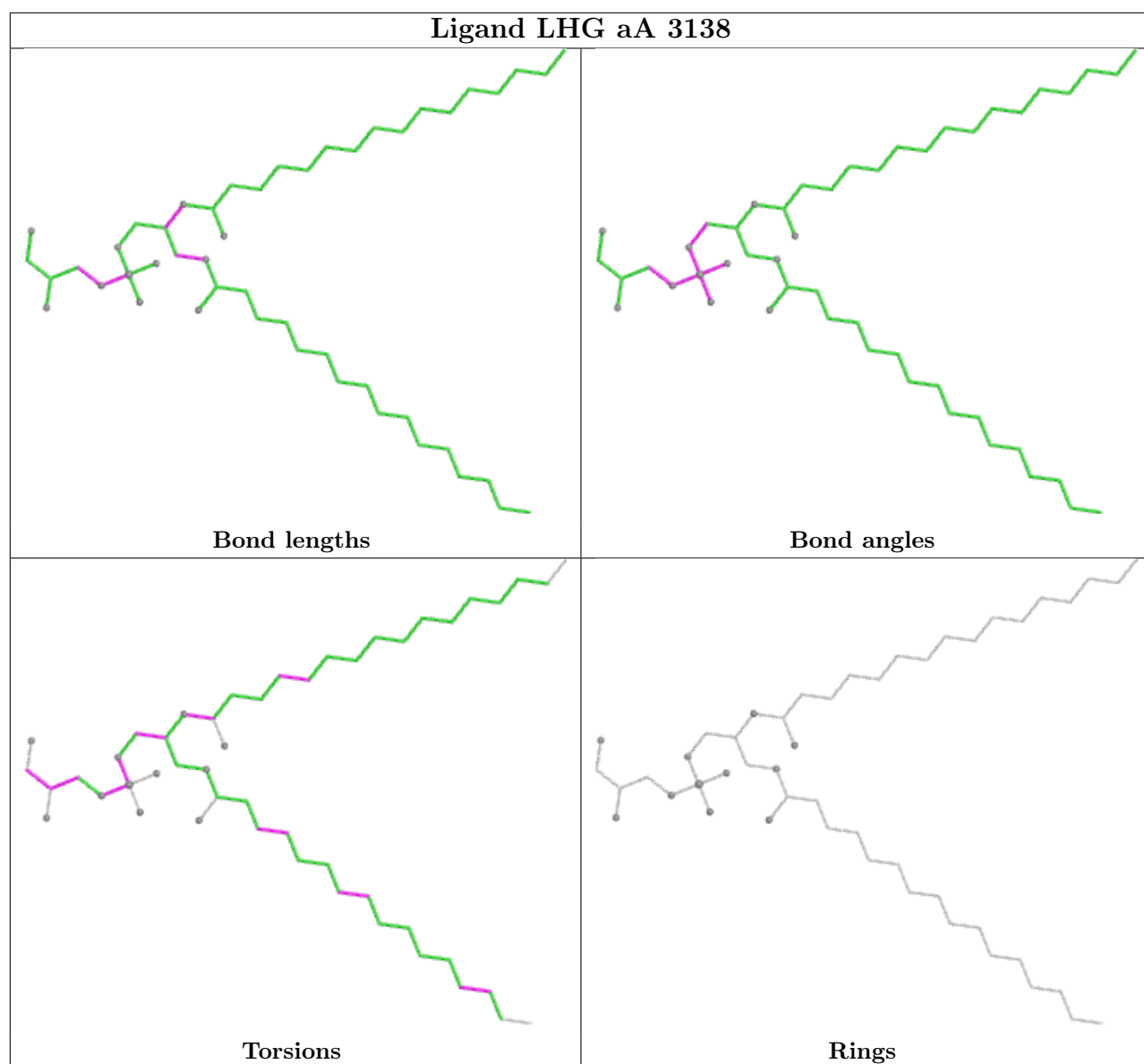


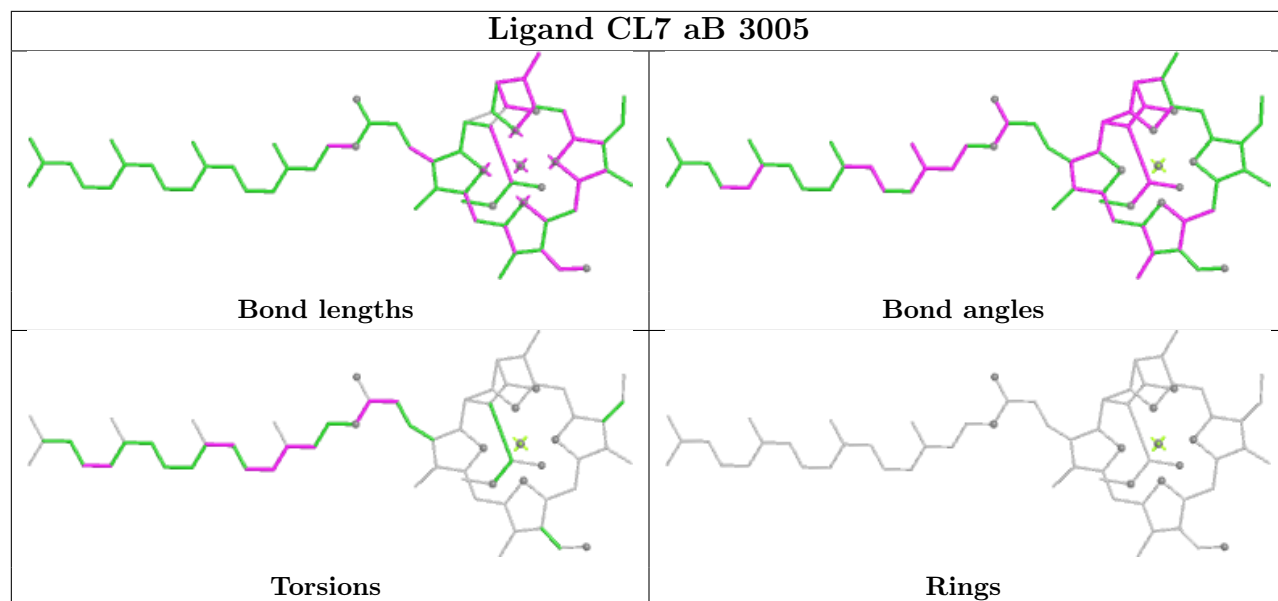




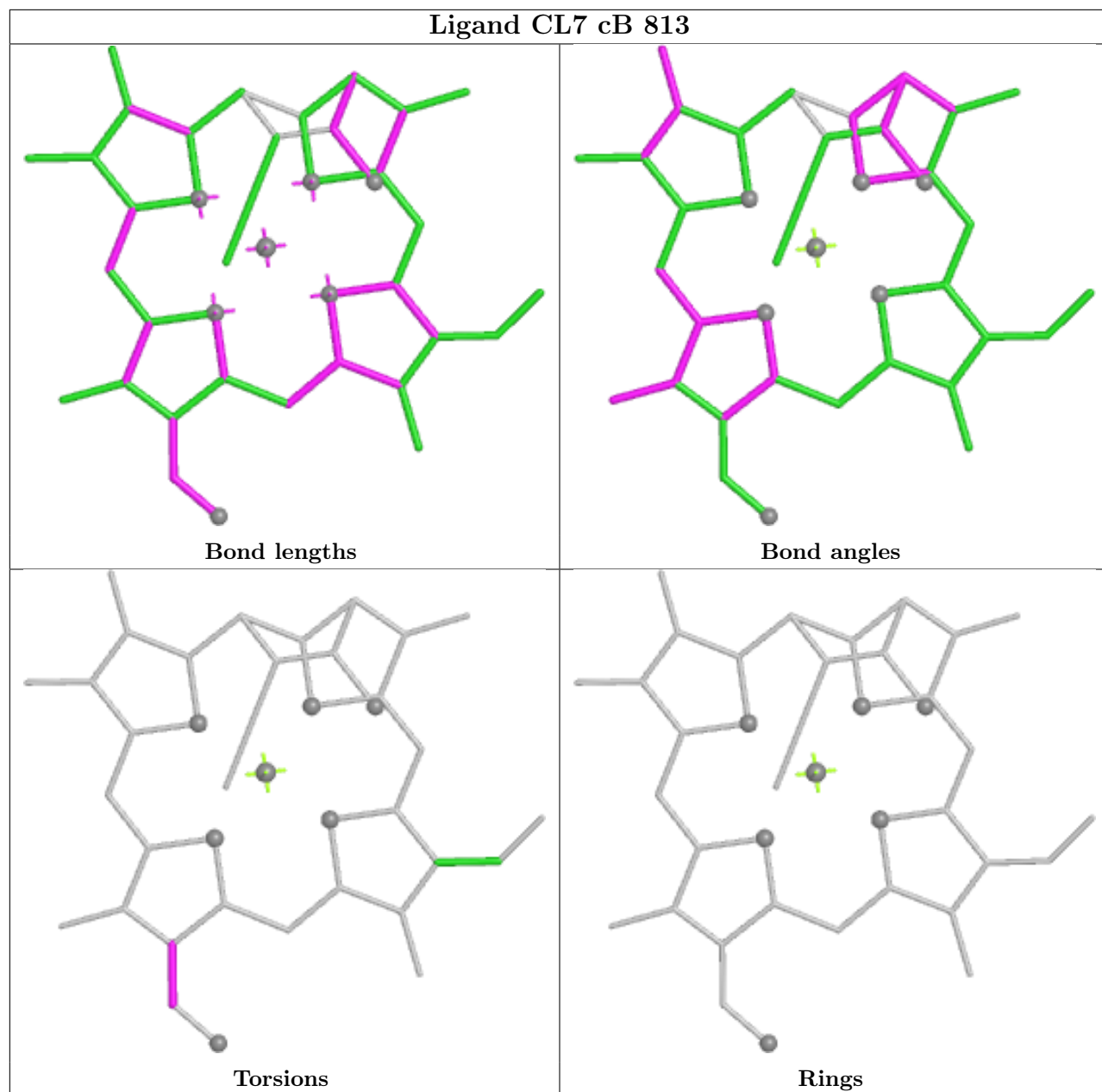


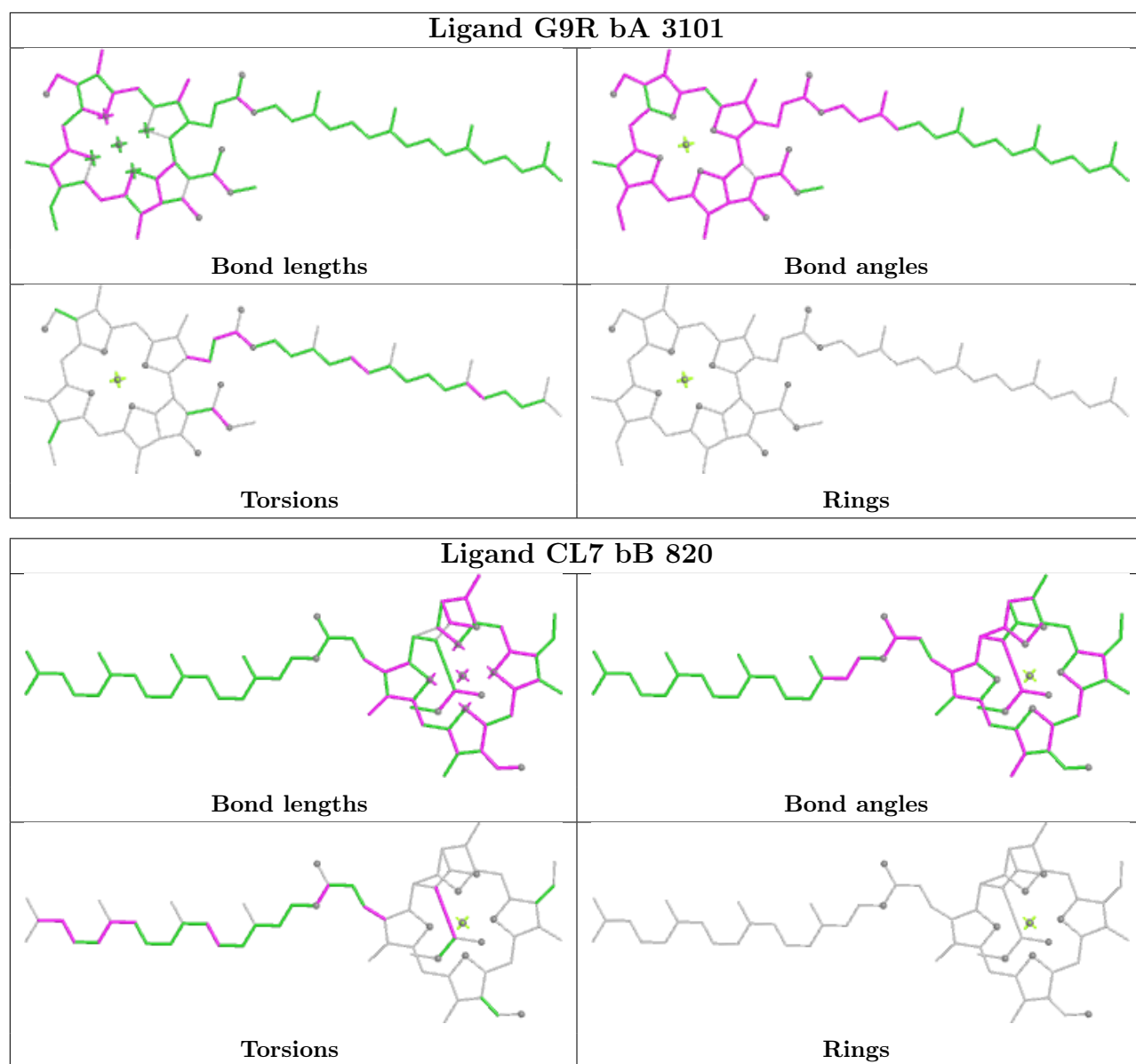


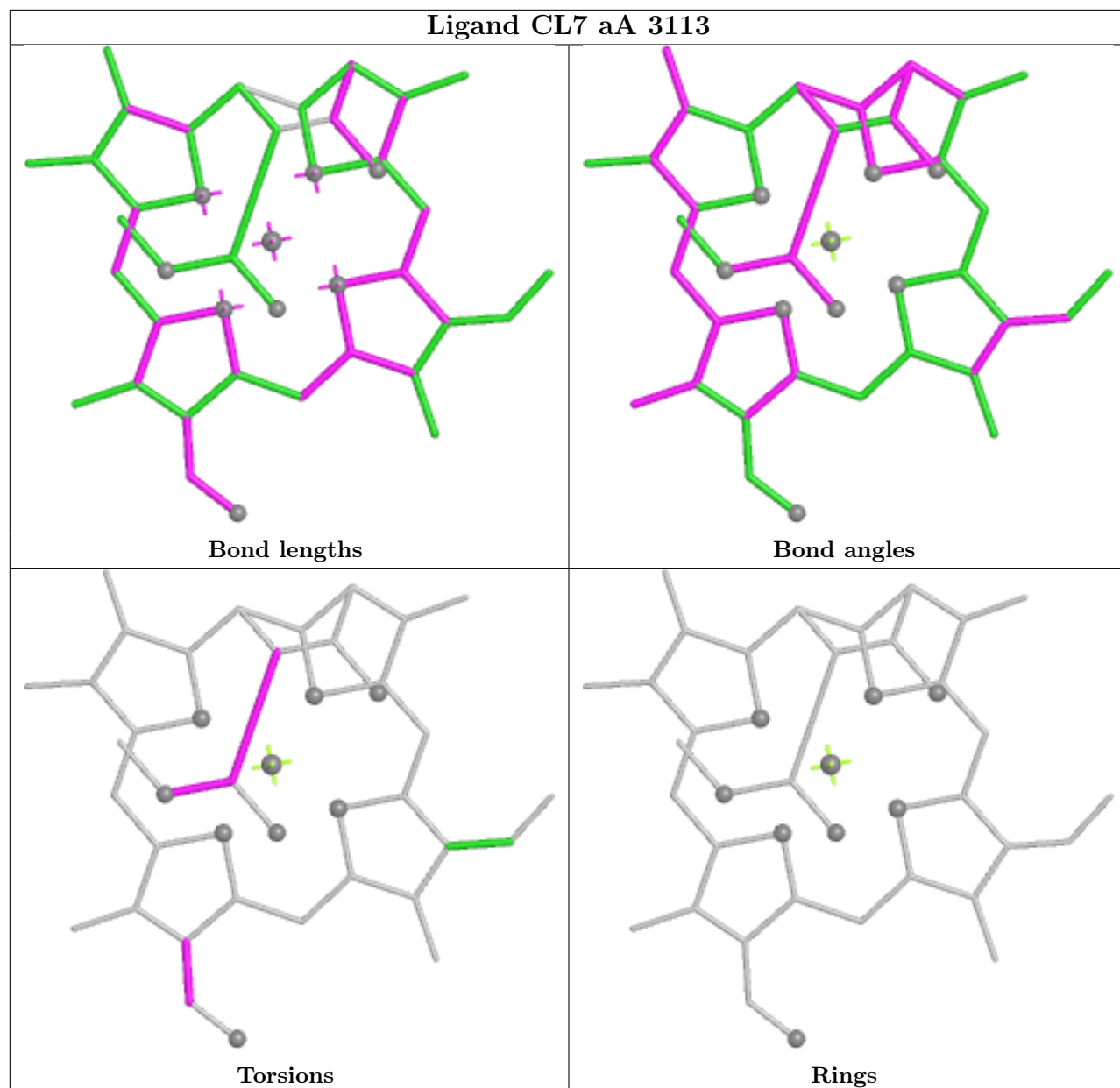


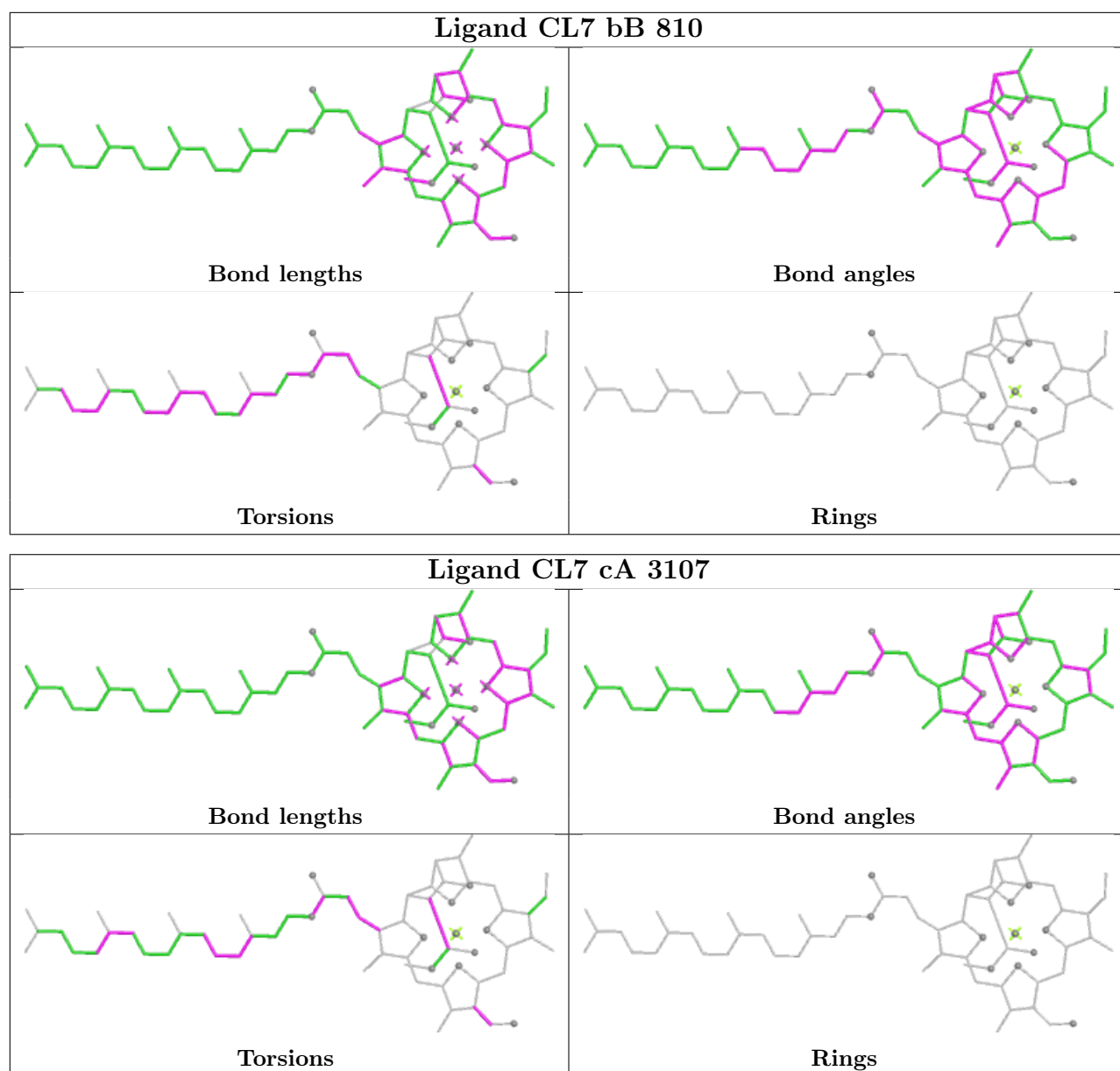




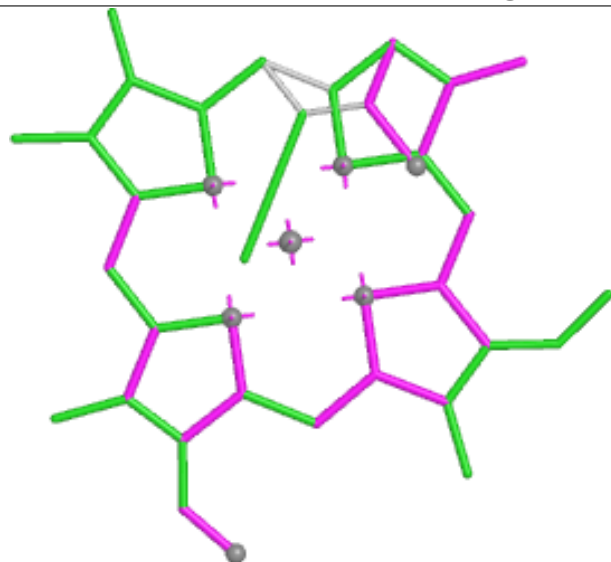




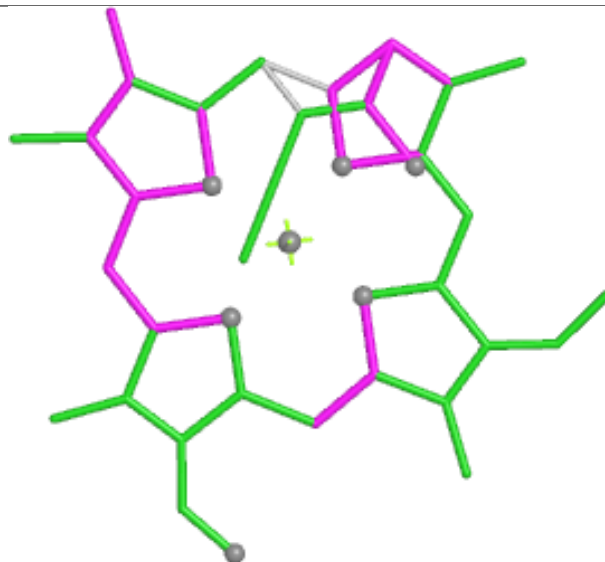




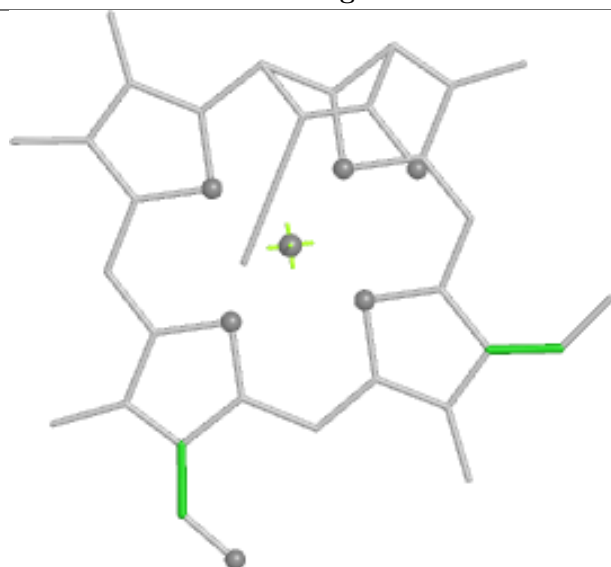
## Ligand CL7 cA 3118



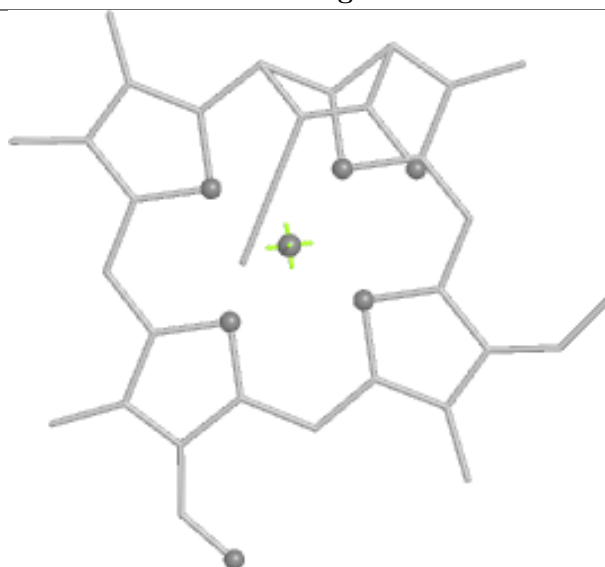
Bond lengths



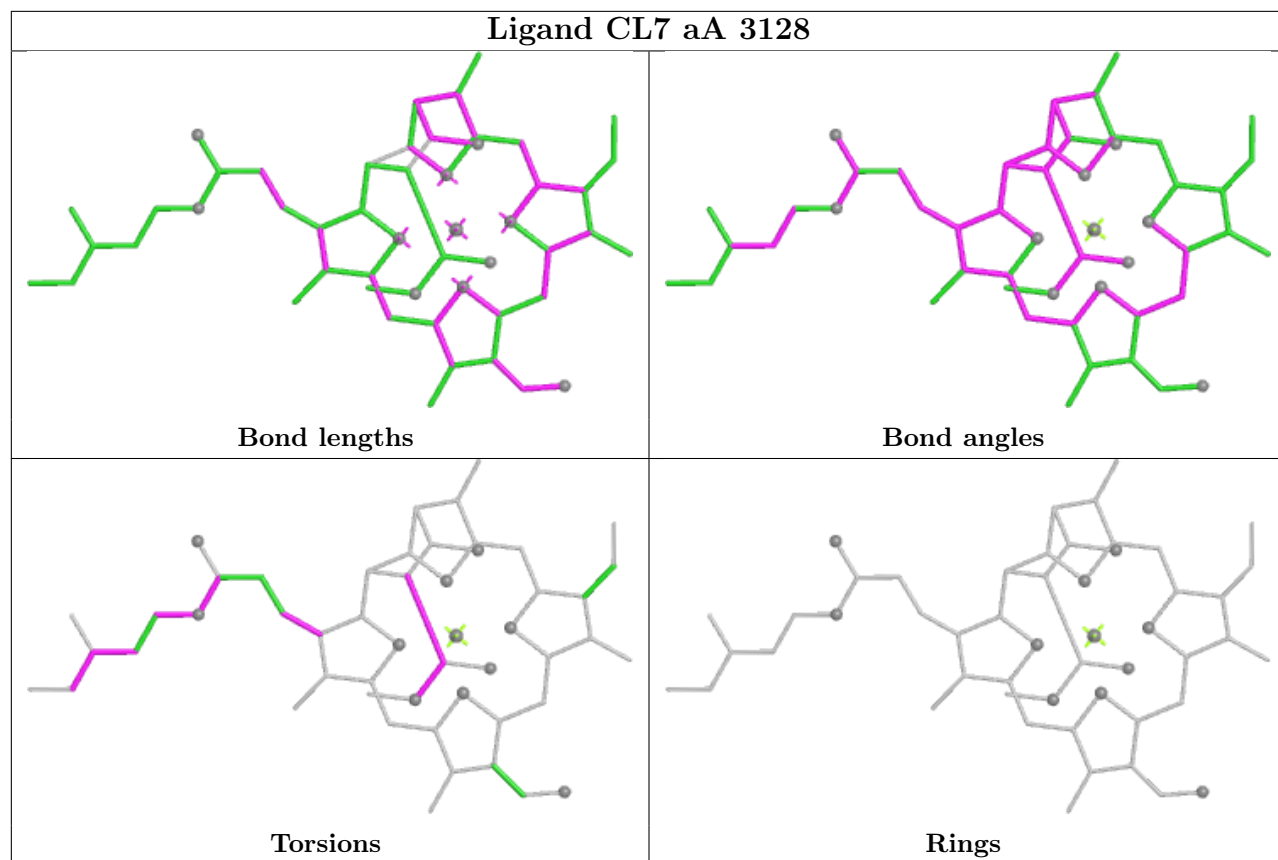
Bond angles

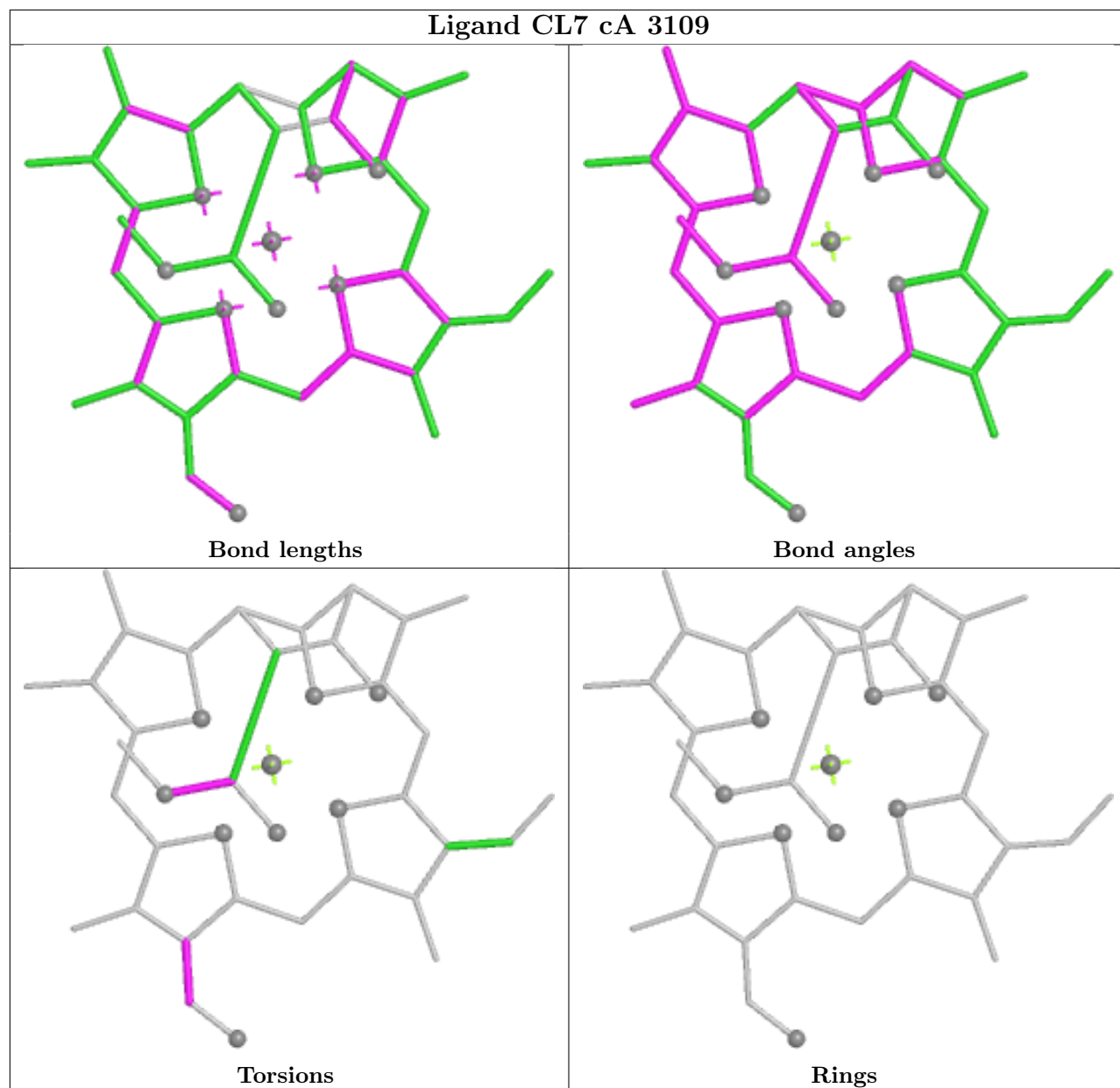


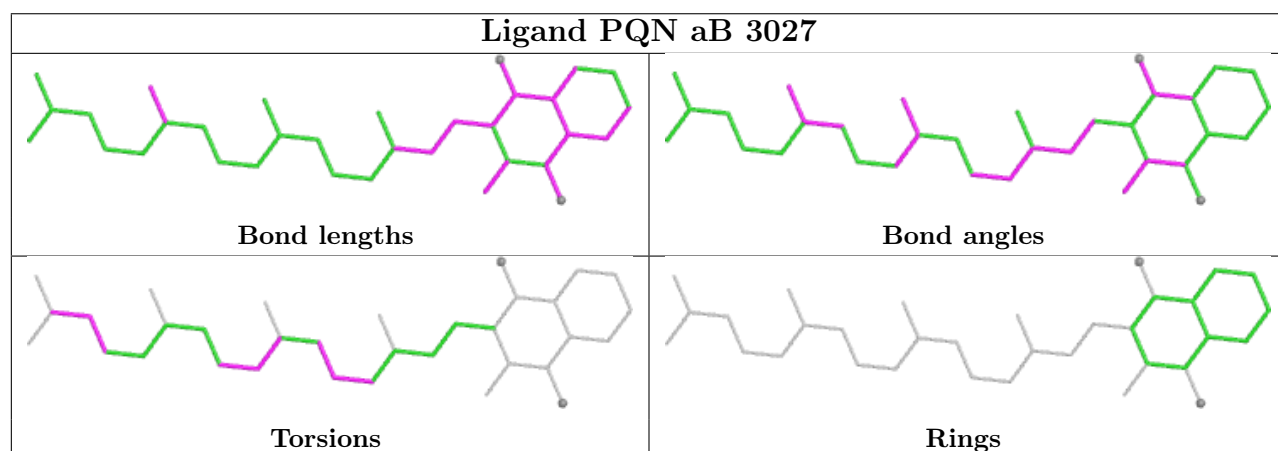
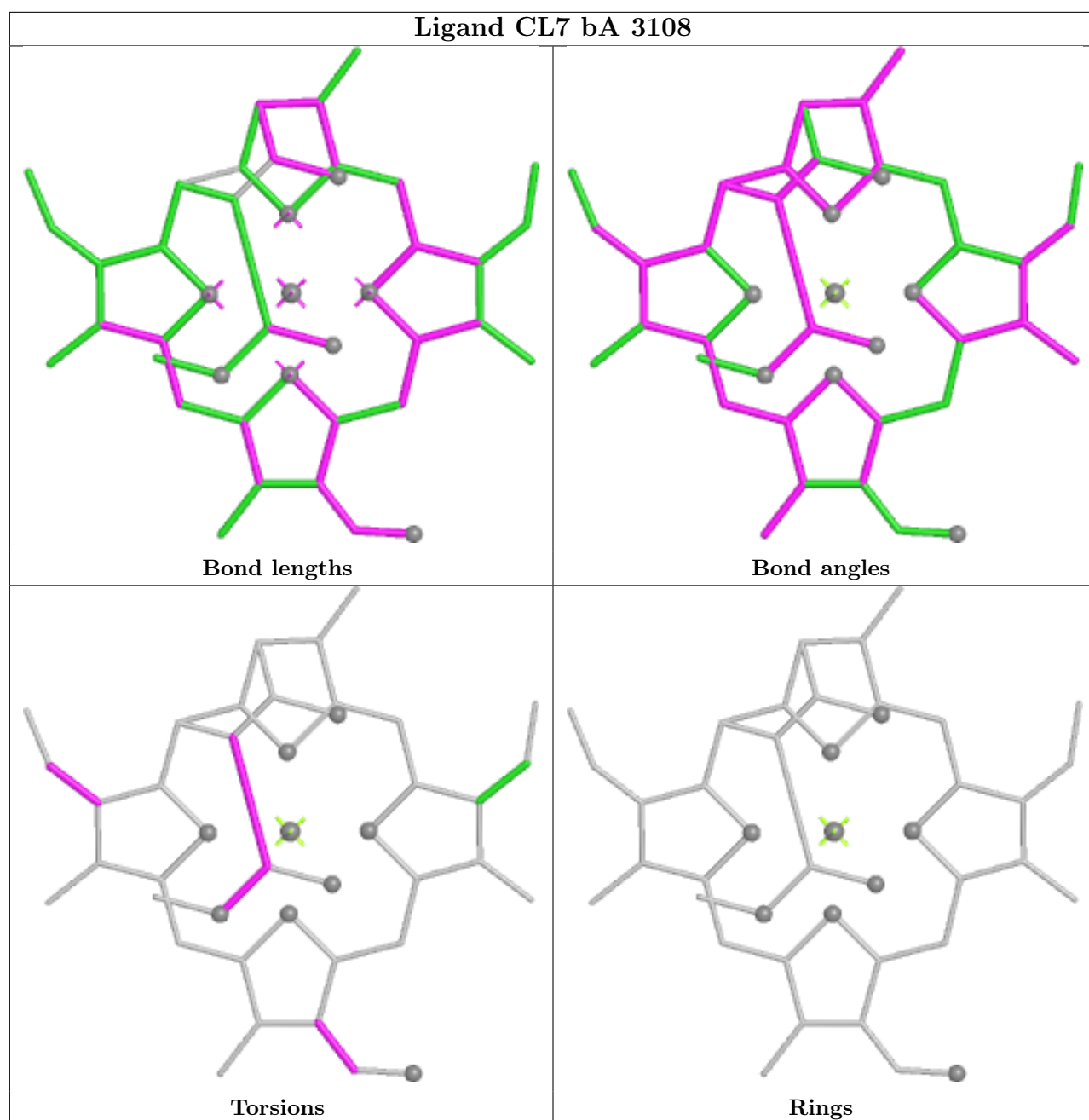
Torsions



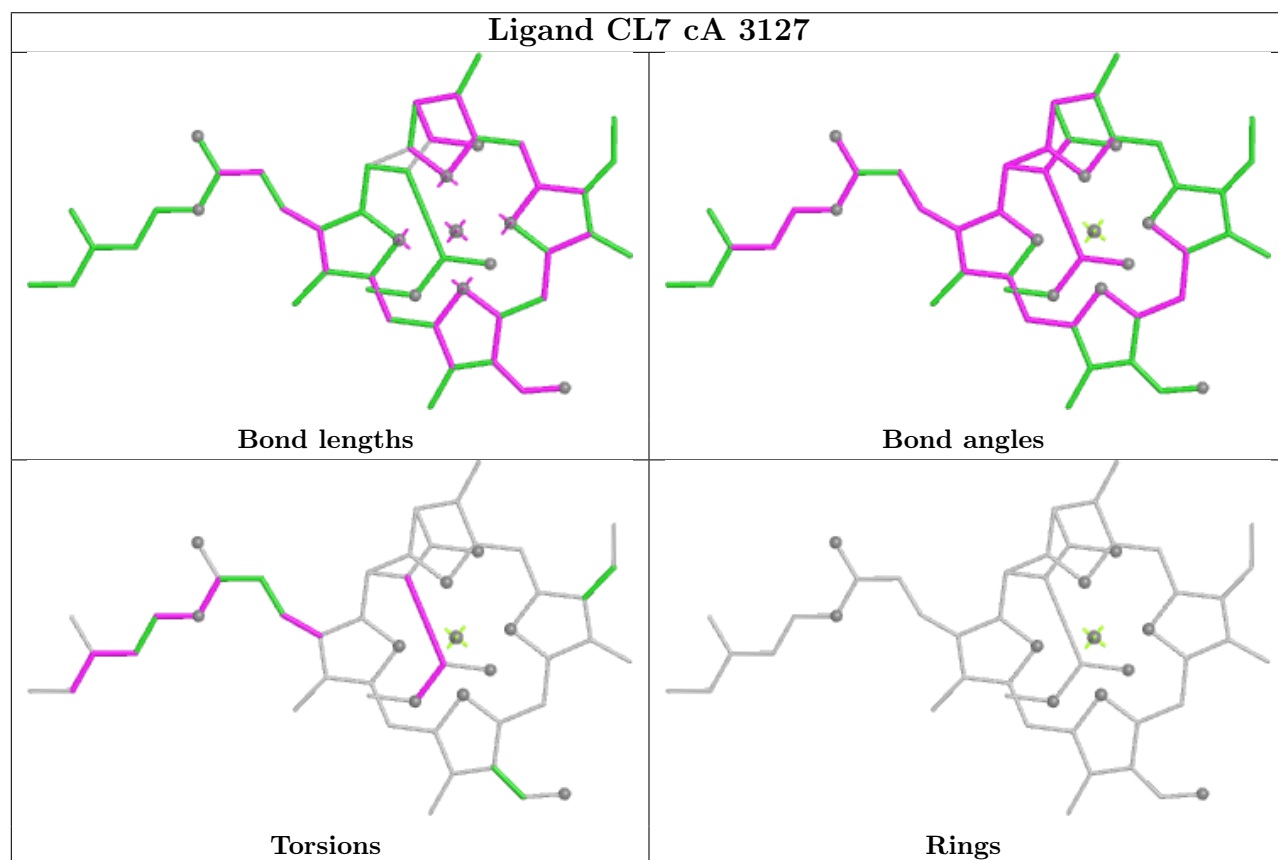
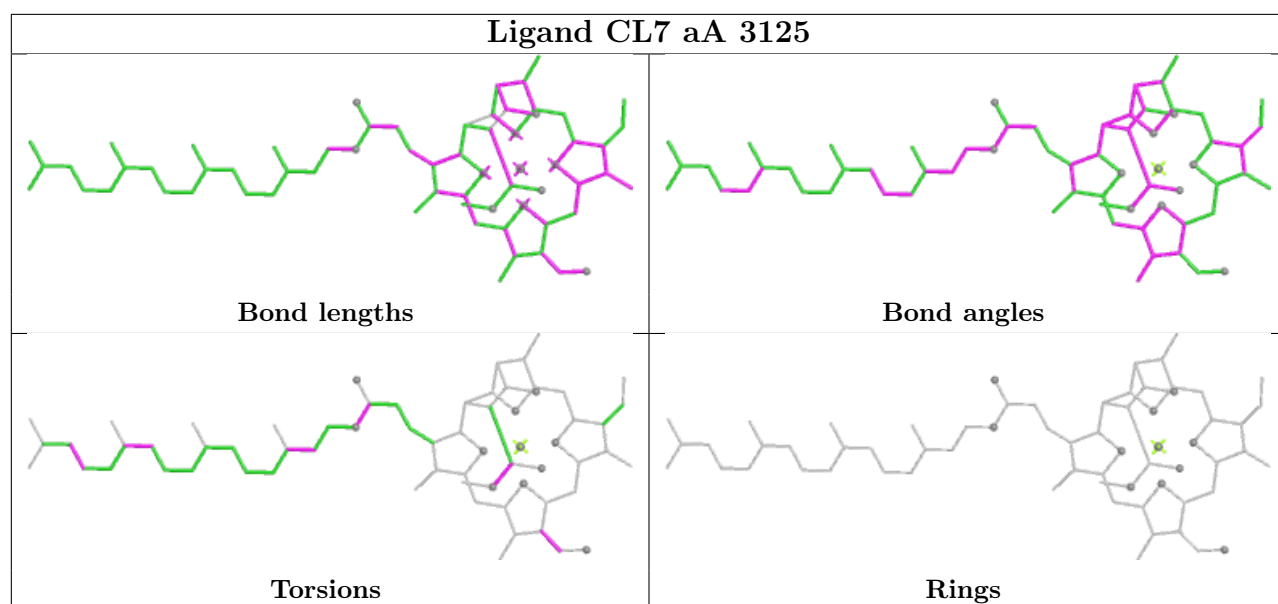
Rings

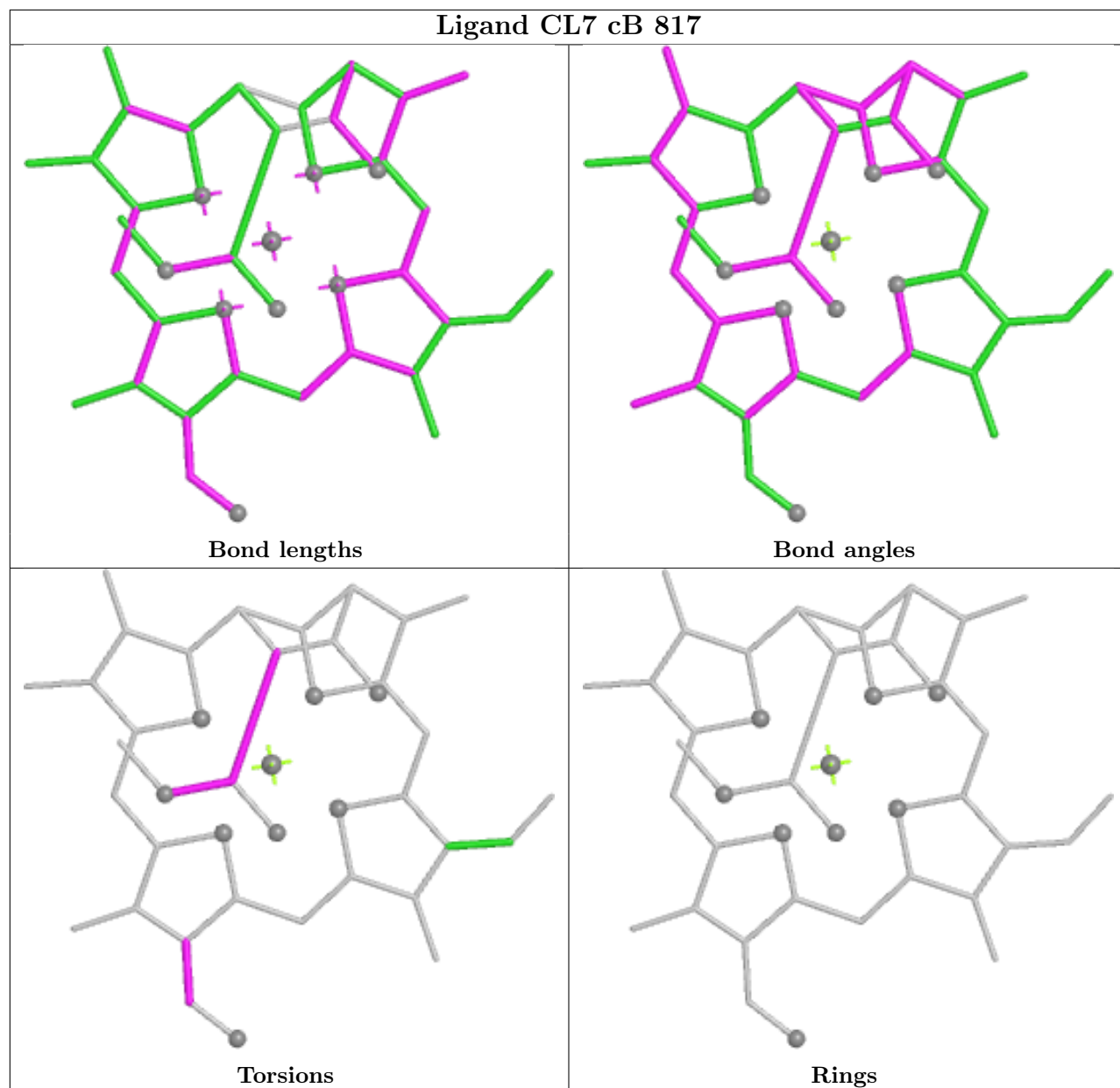


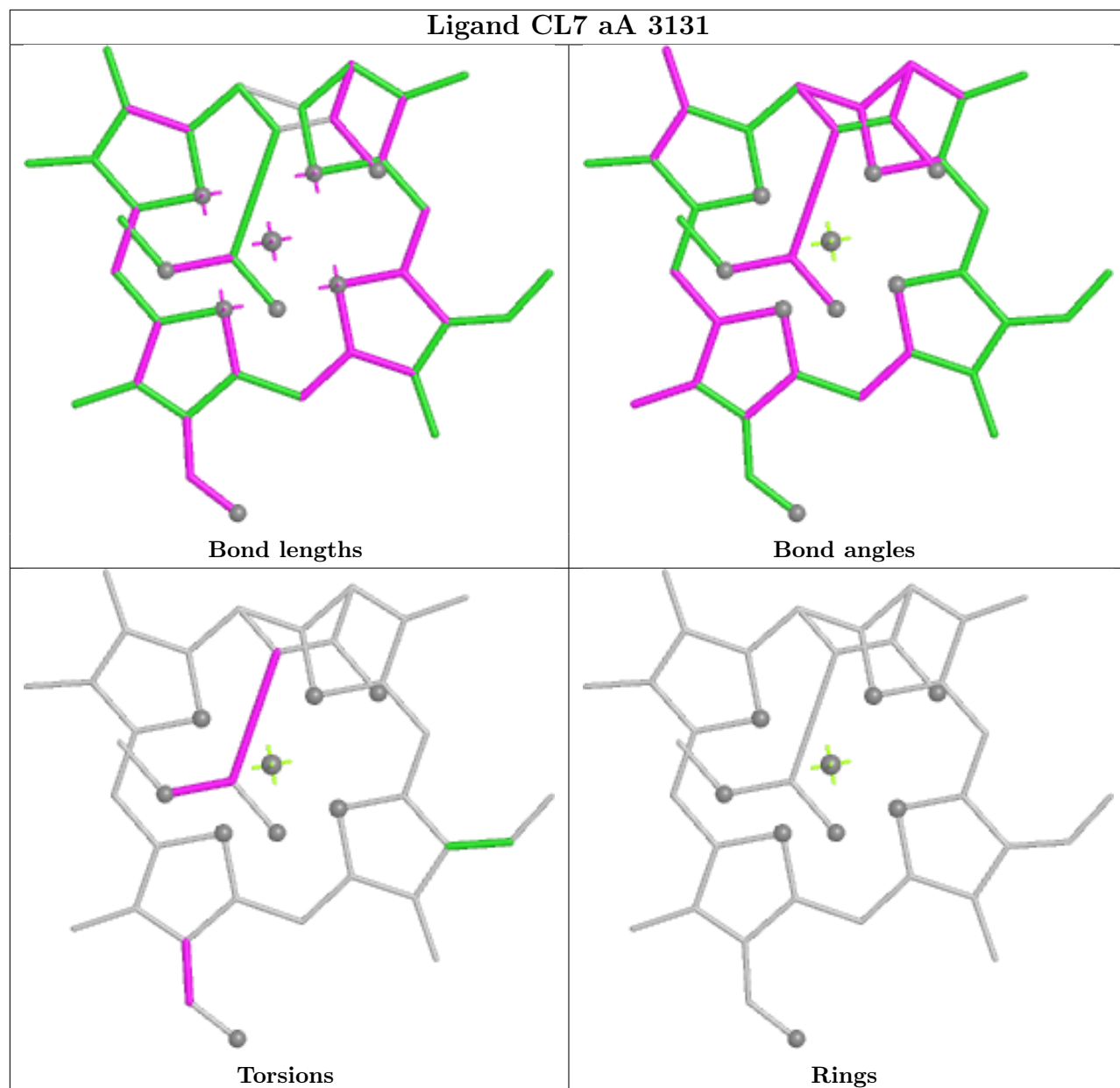


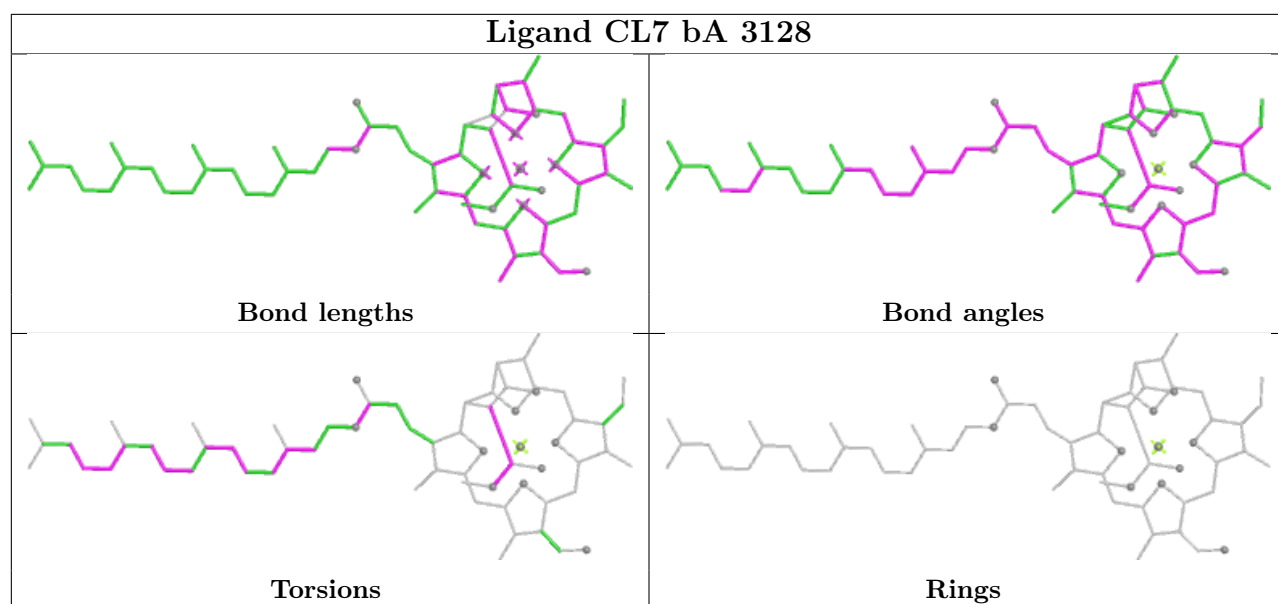




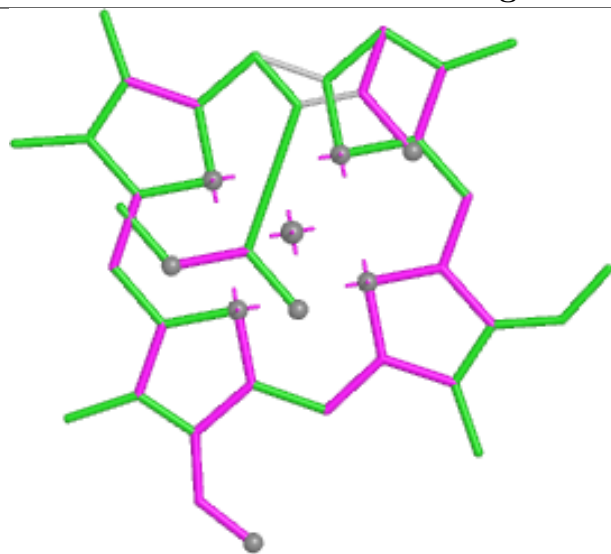




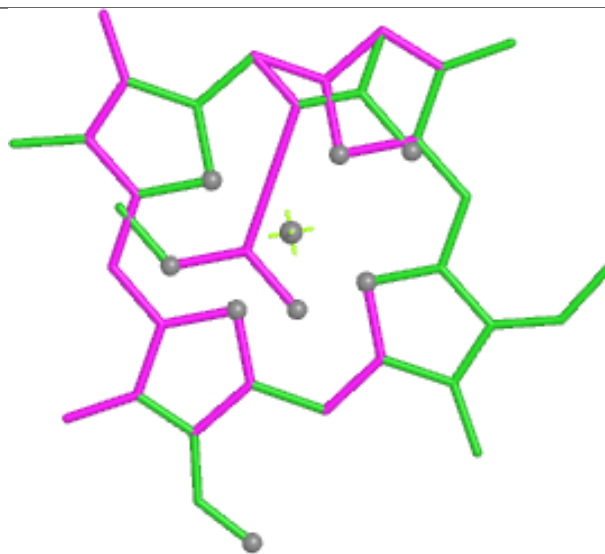




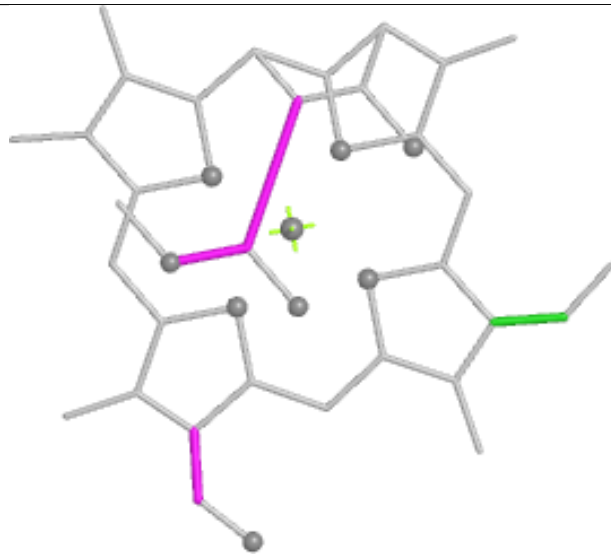
## Ligand CL7 bA 3130



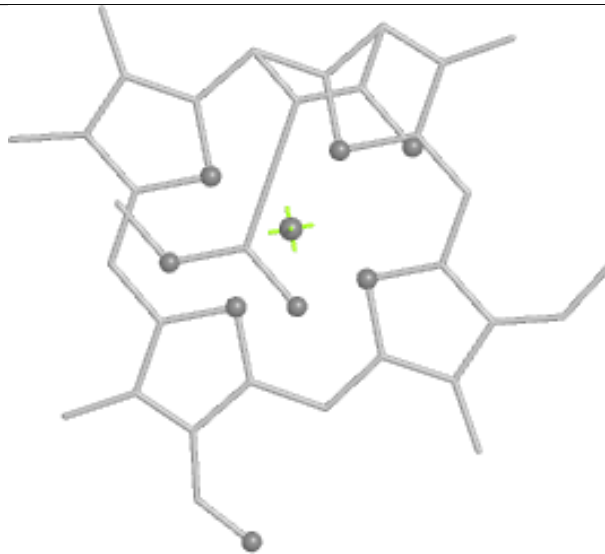
Bond lengths



Bond angles

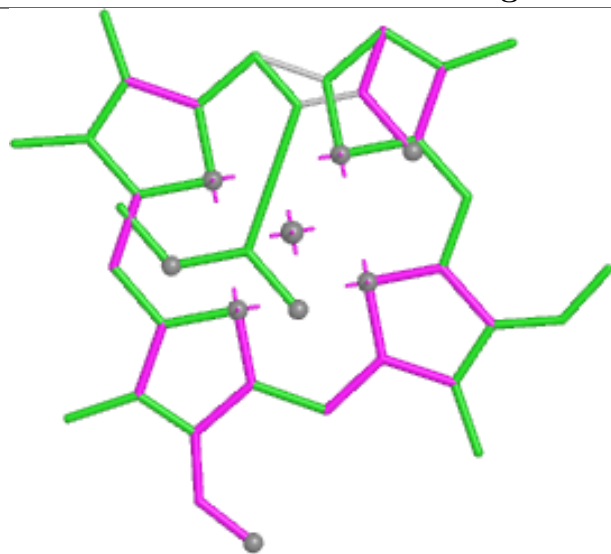


Torsions

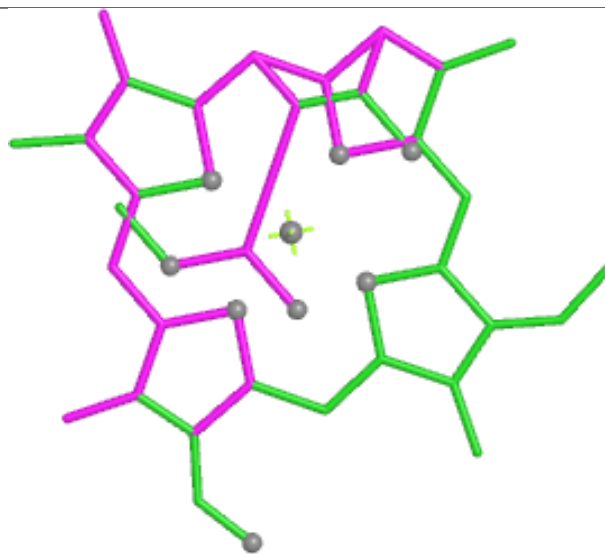


Rings

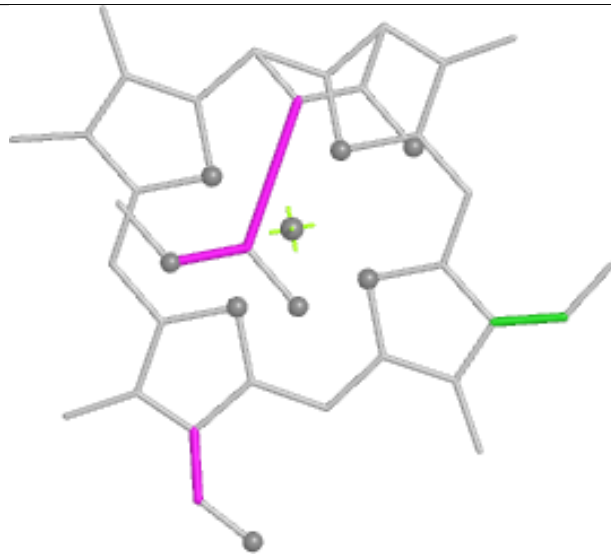
## Ligand CL7 aA 3146



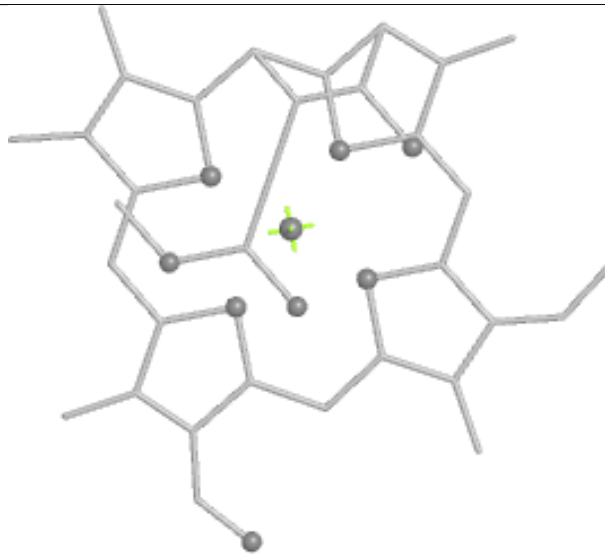
Bond lengths



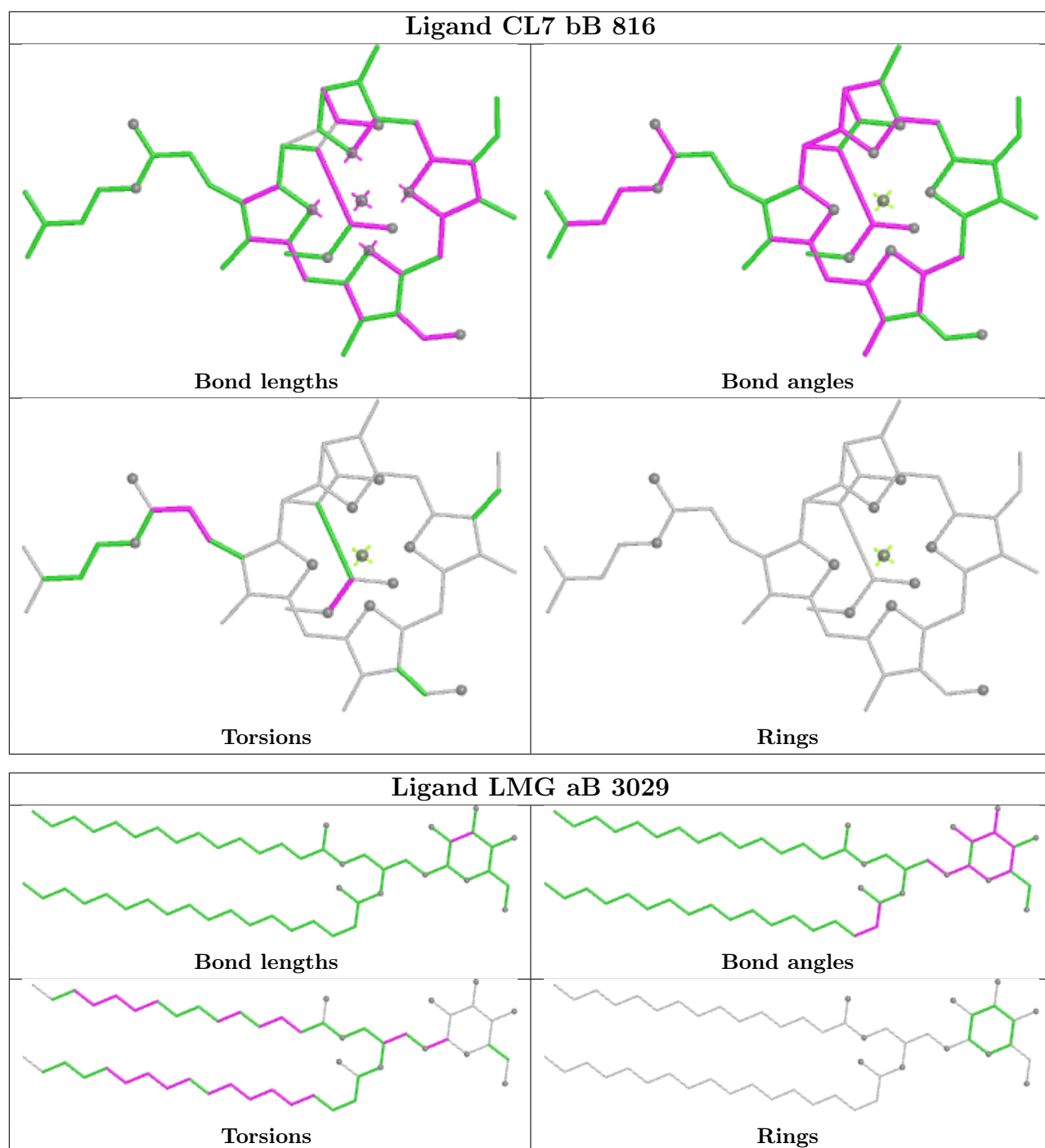
Bond angles

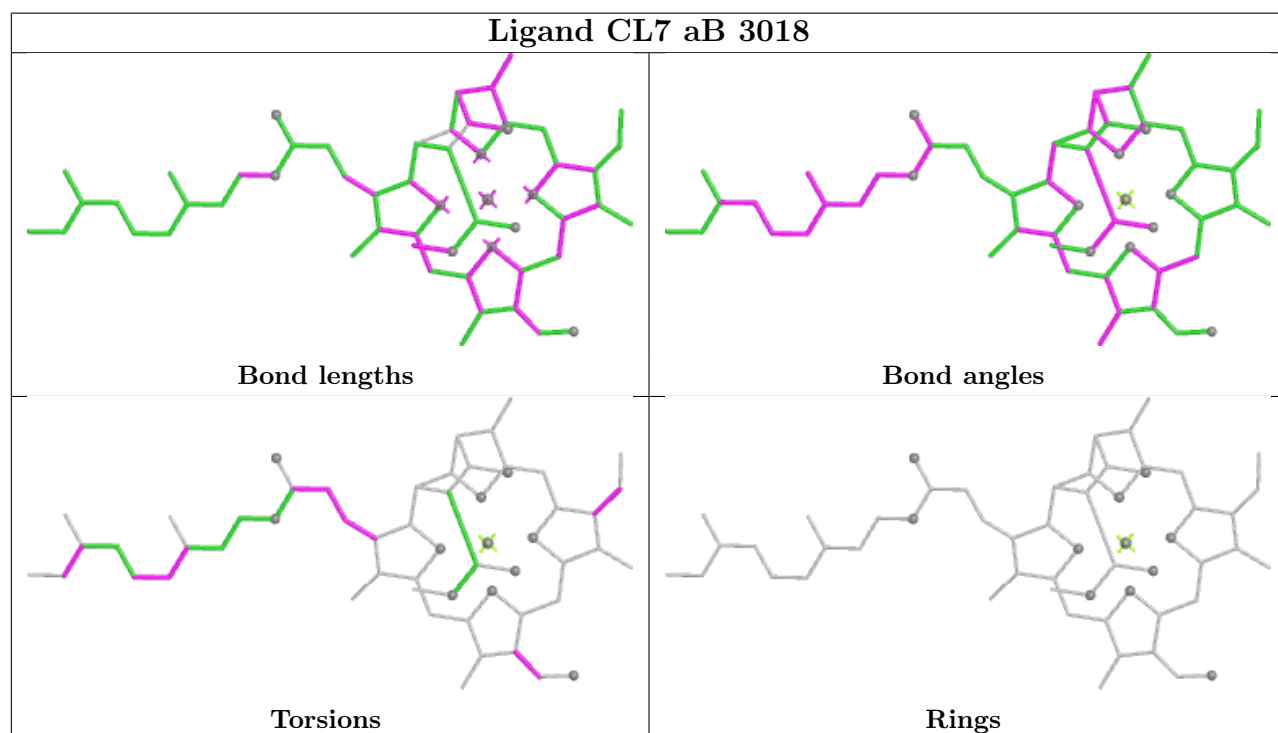
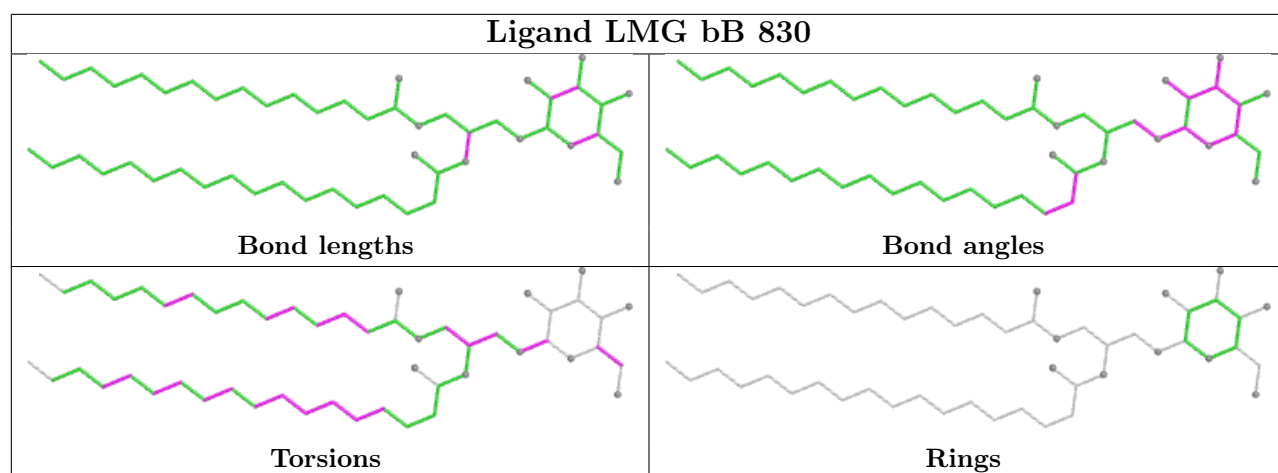


Torsions

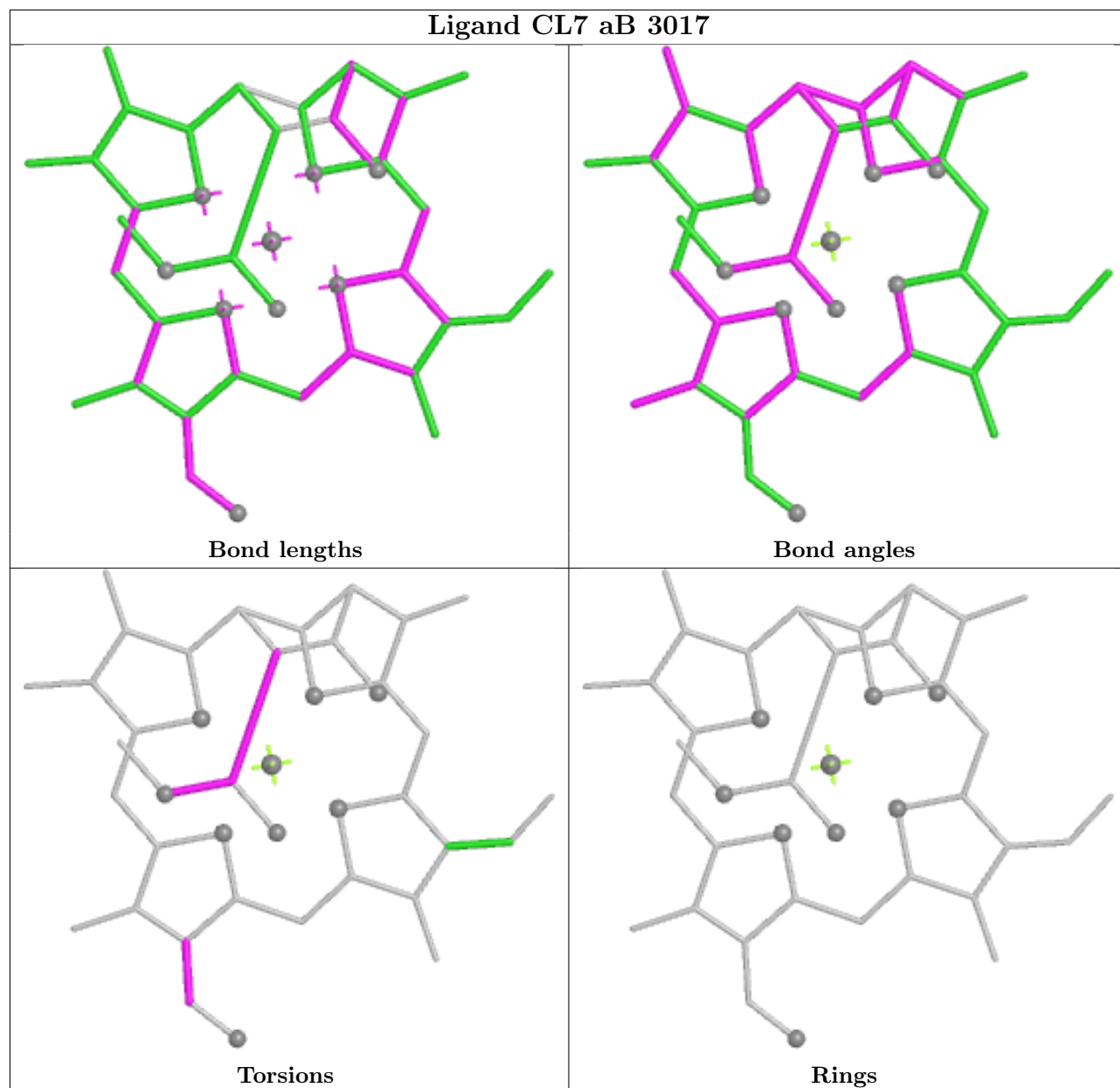


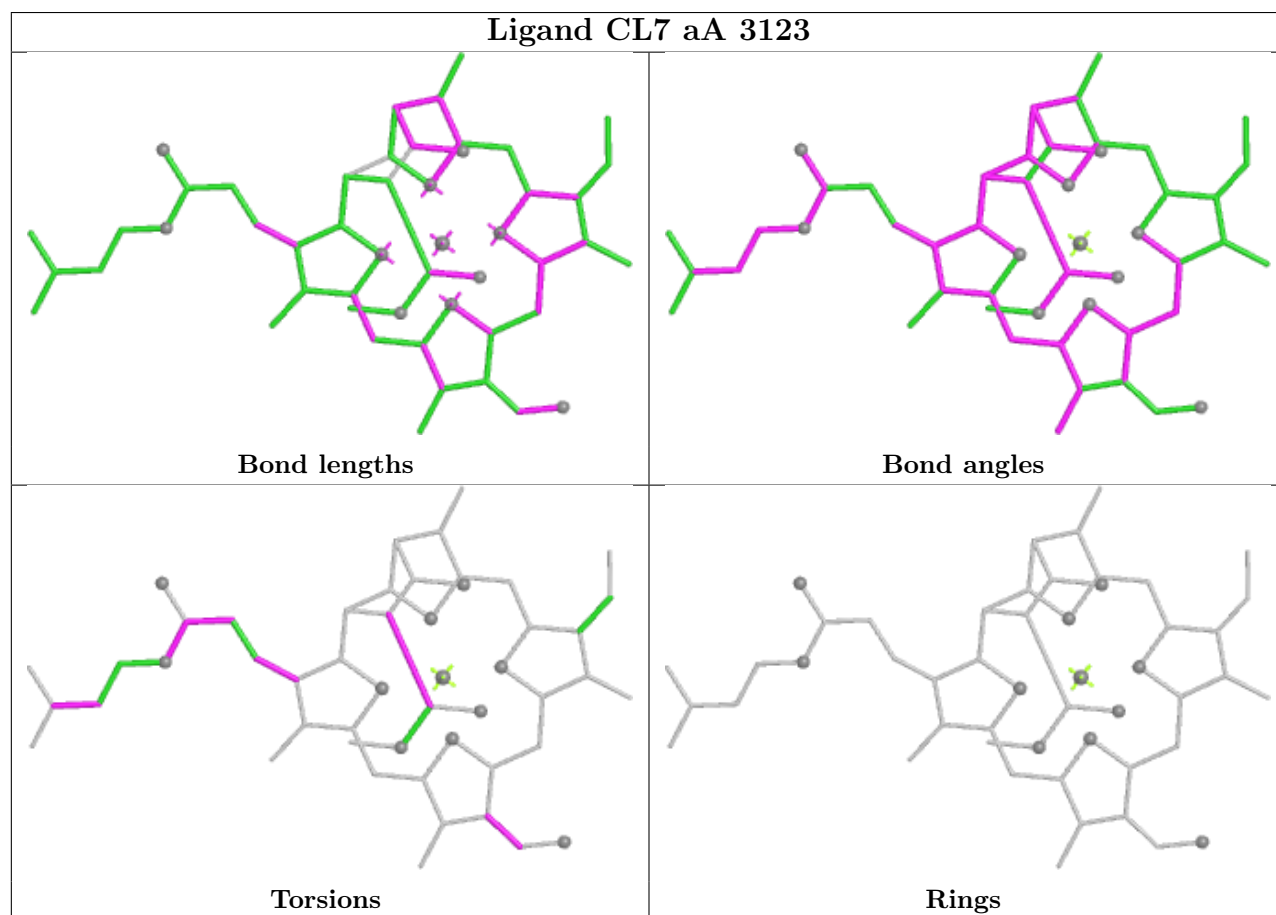
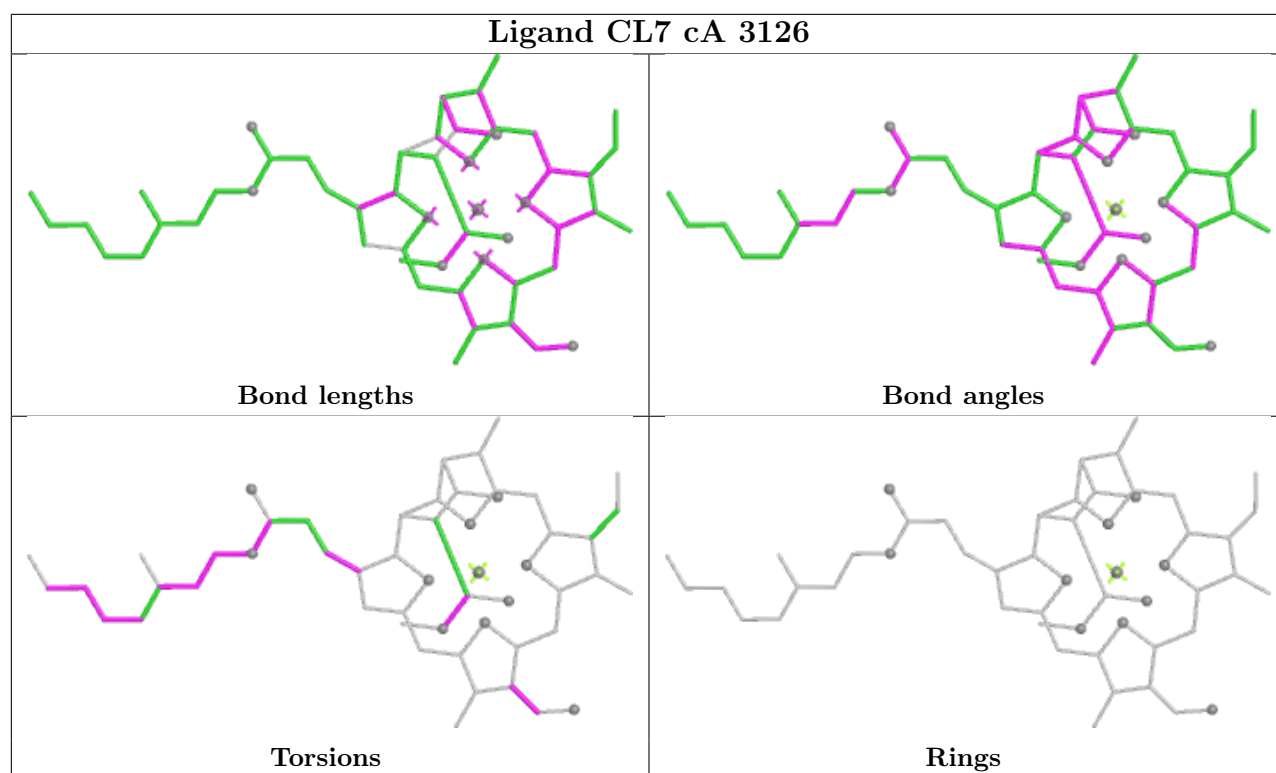
Rings



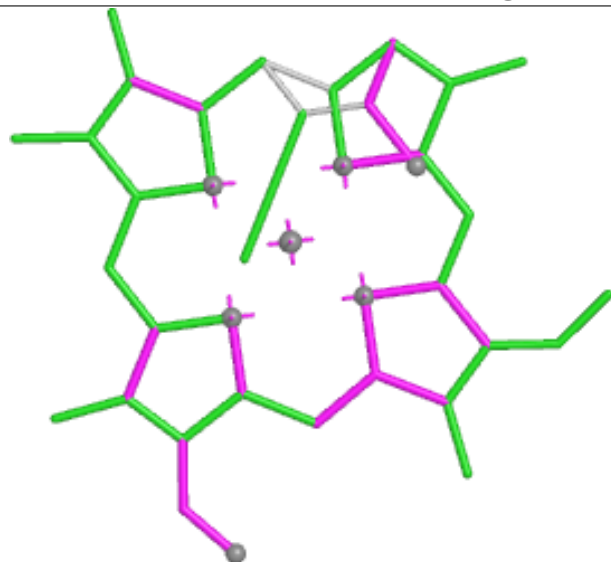




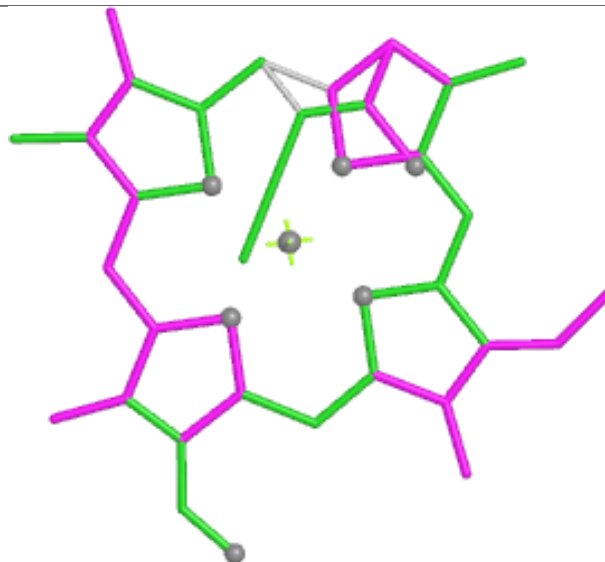




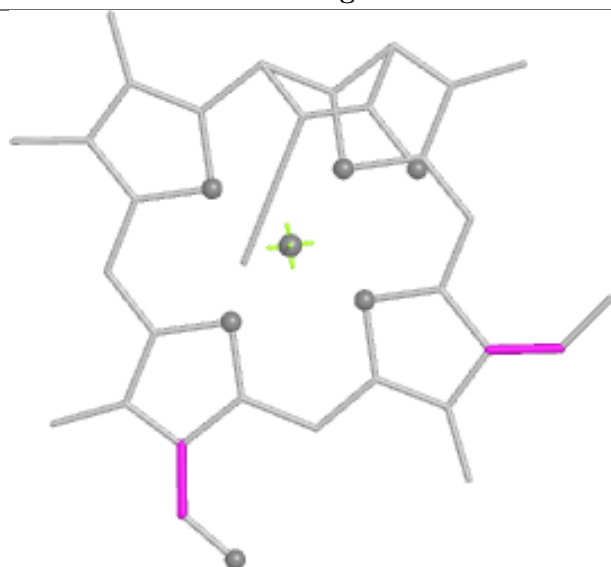
## Ligand CL7 bA 3115



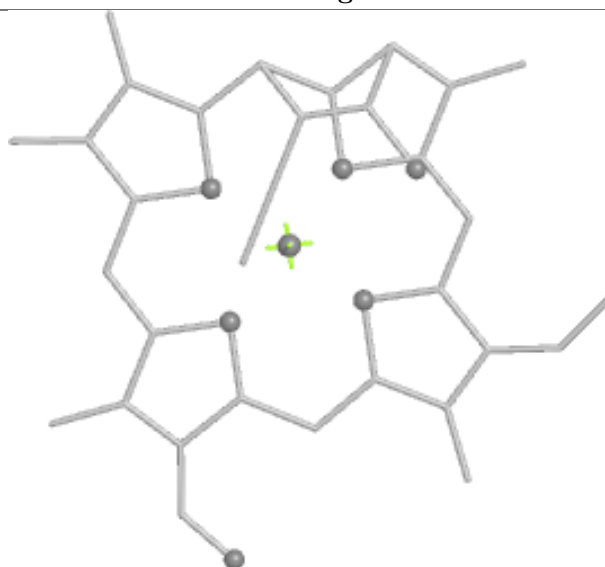
Bond lengths



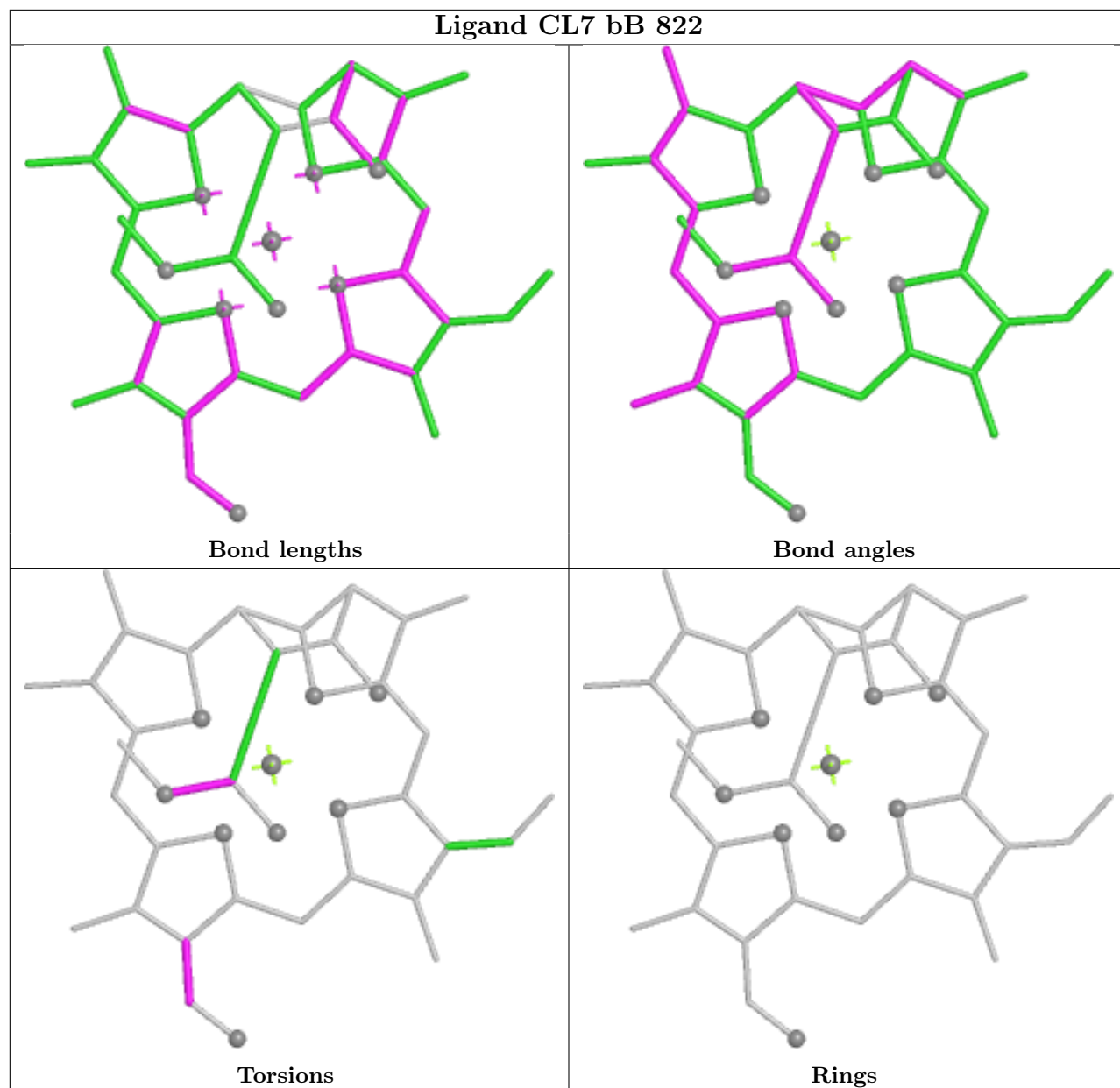
Bond angles



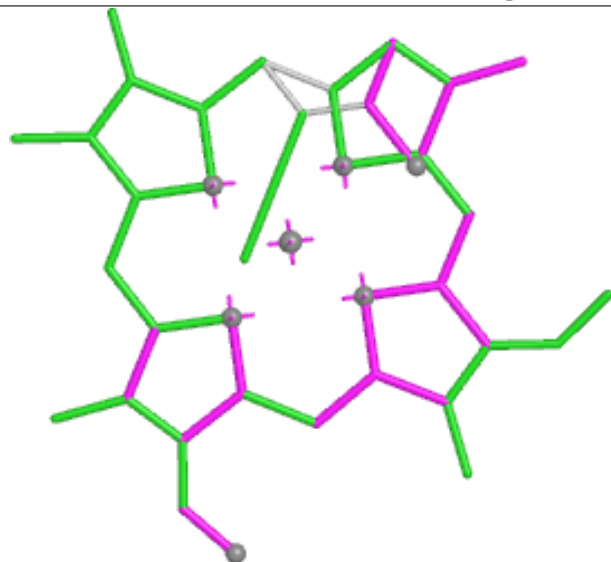
Torsions



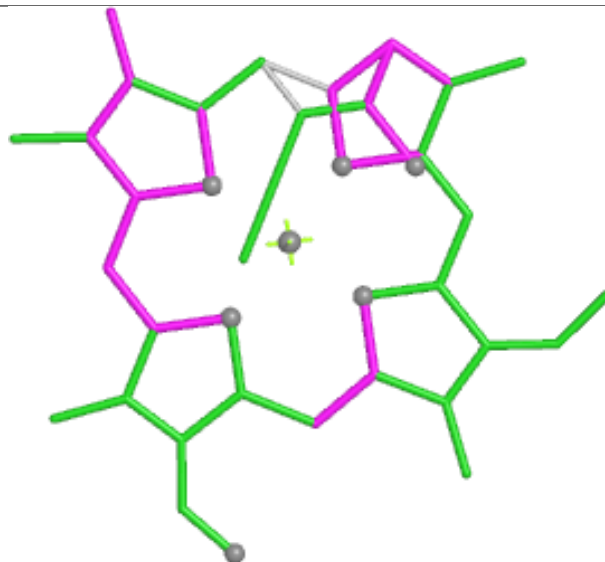
Rings



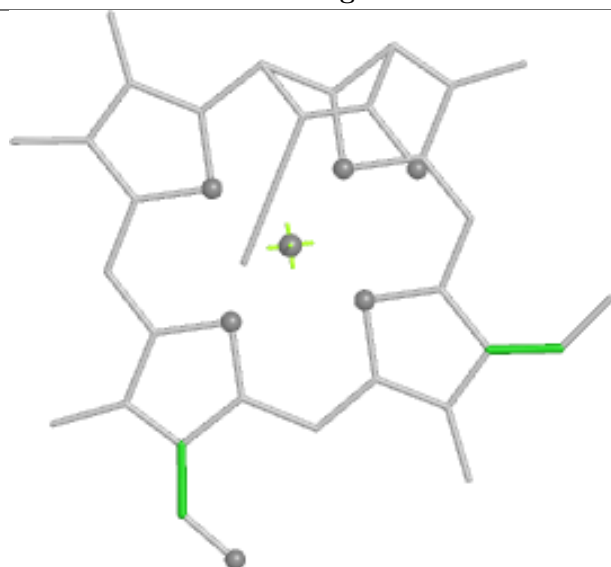
## Ligand CL7 aA 3119



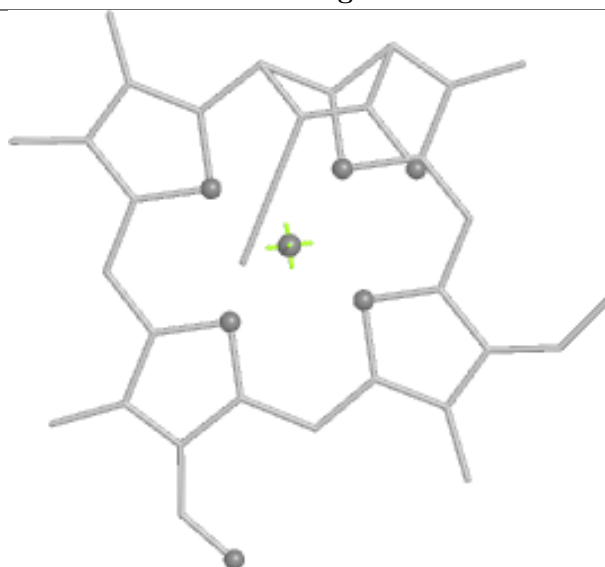
Bond lengths



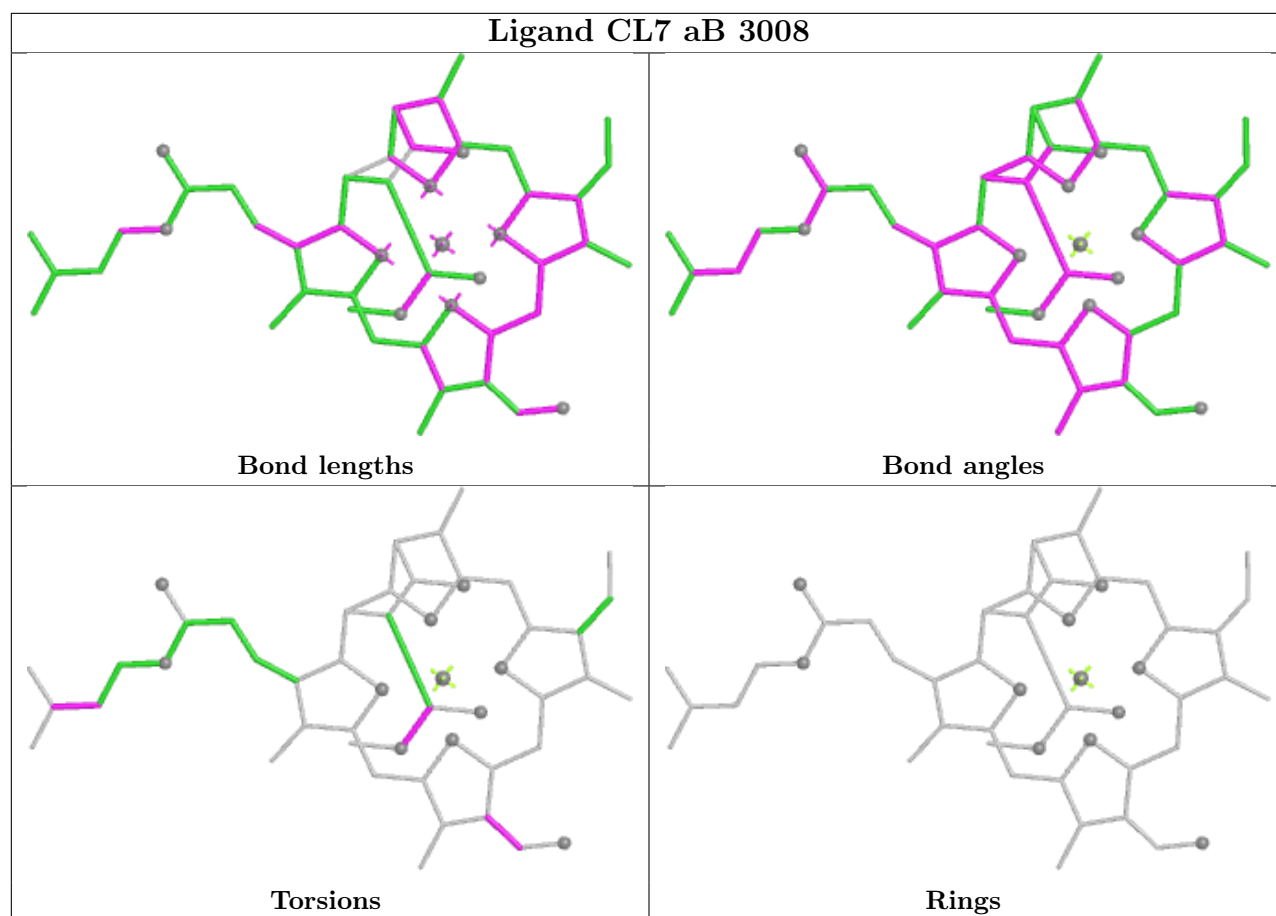
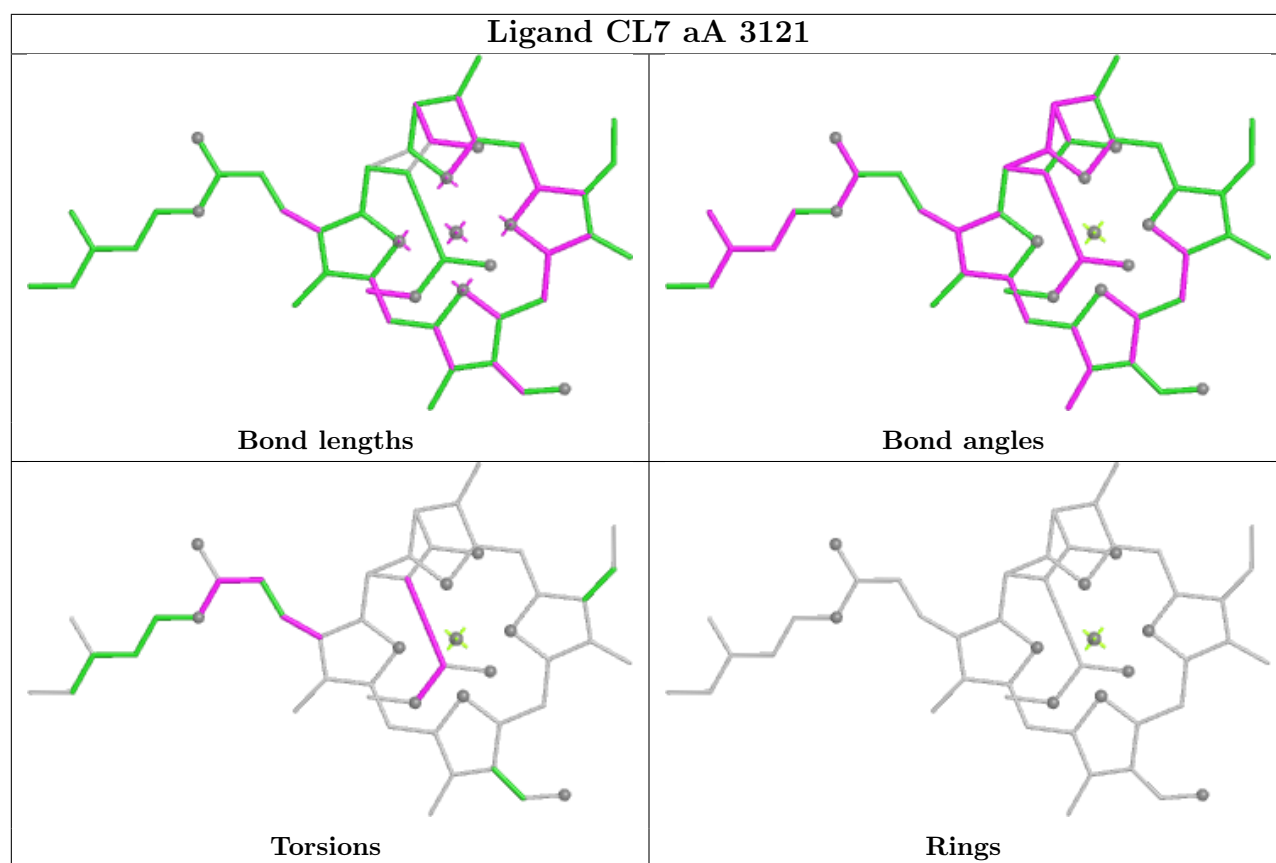
Bond angles



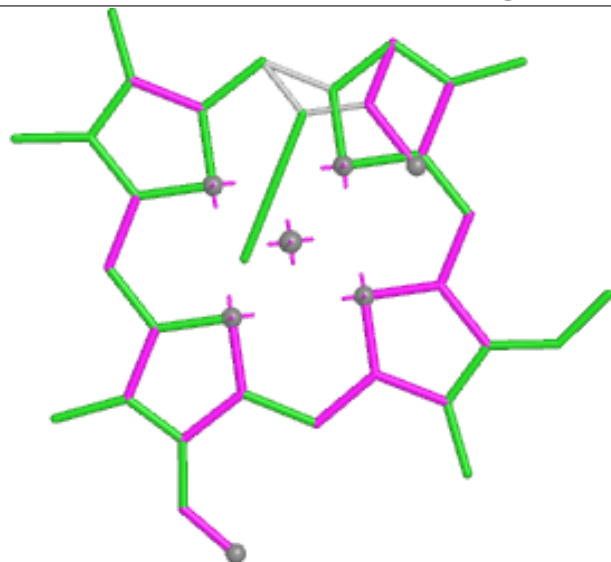
Torsions



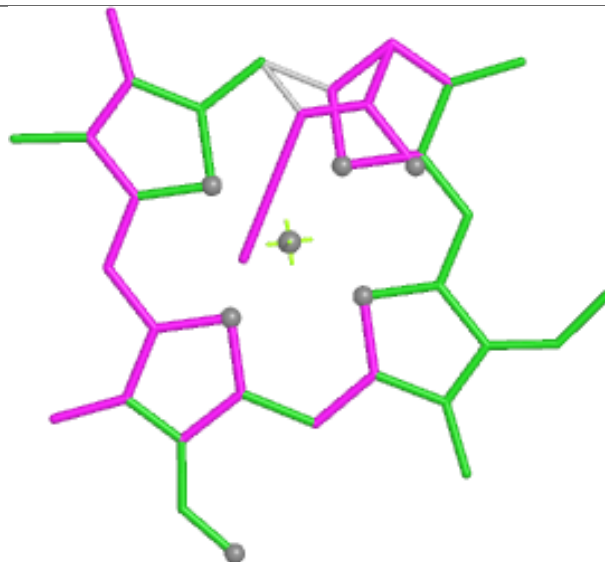
Rings



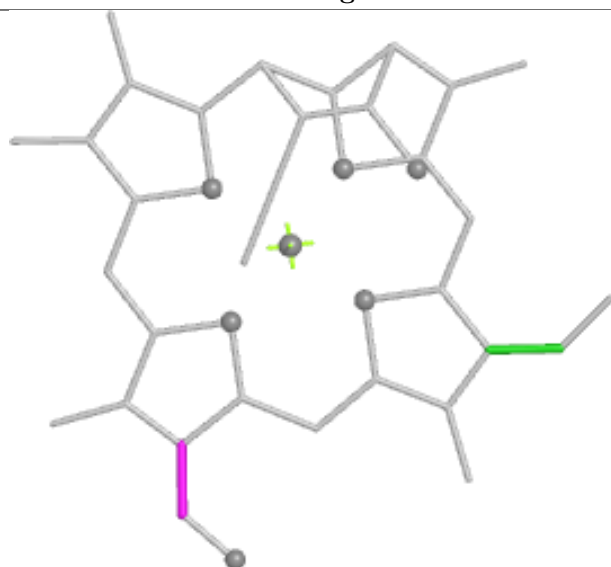
## Ligand CL7 bA 3117



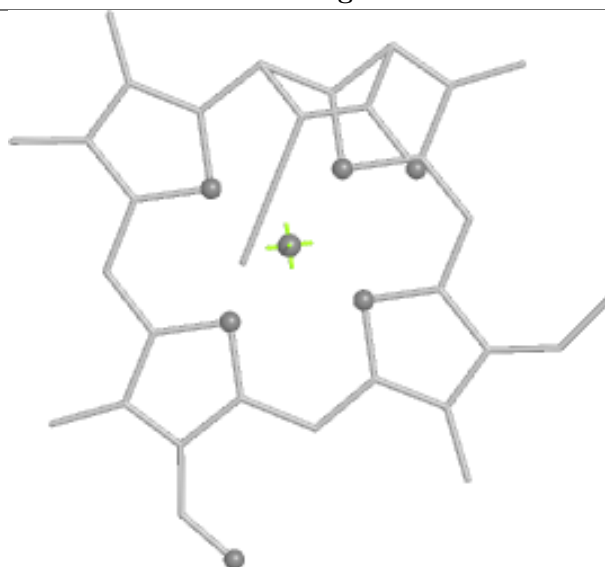
Bond lengths



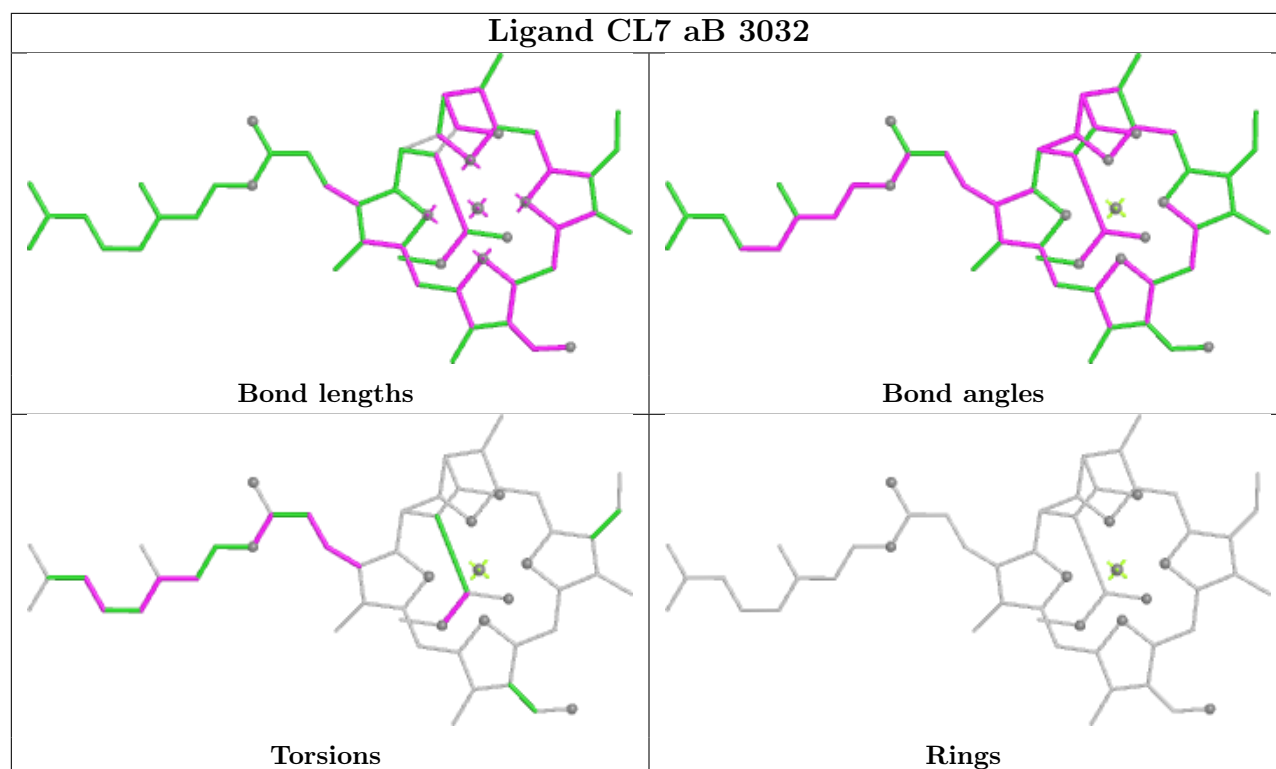
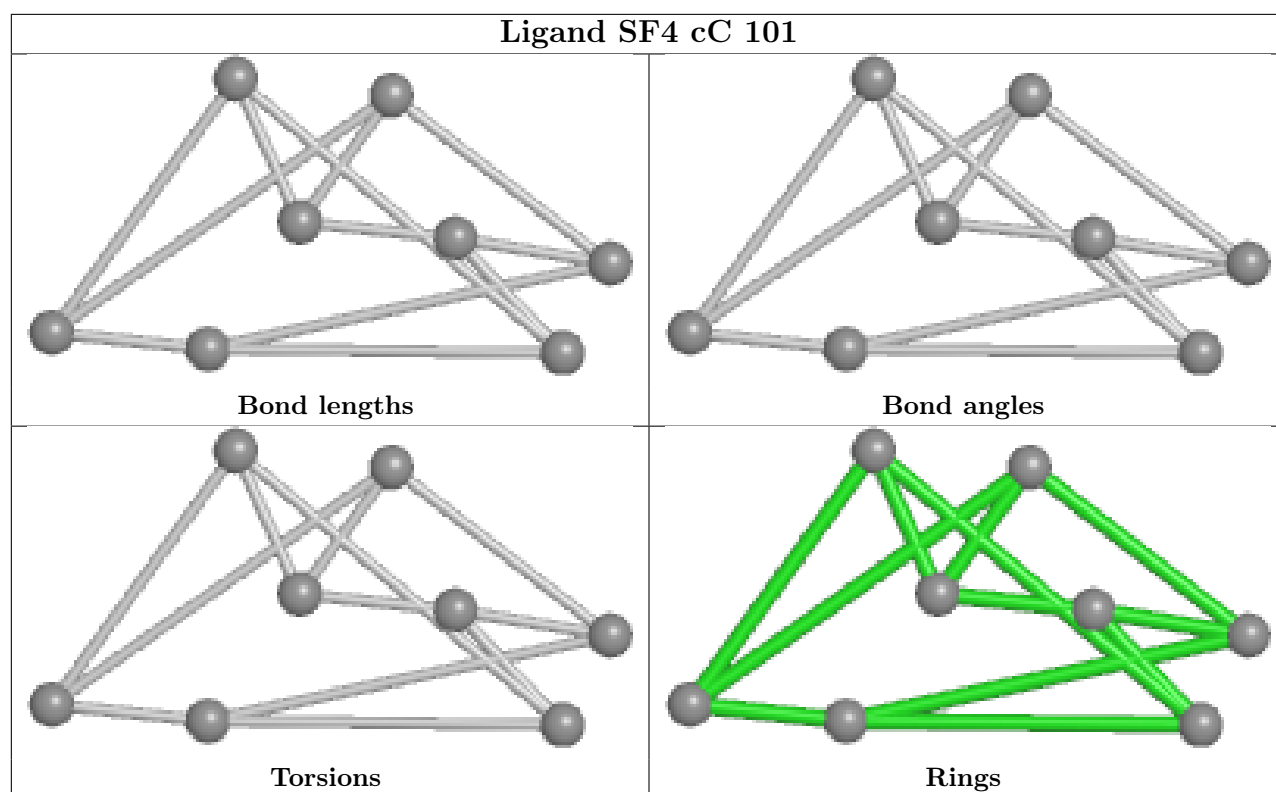
Bond angles



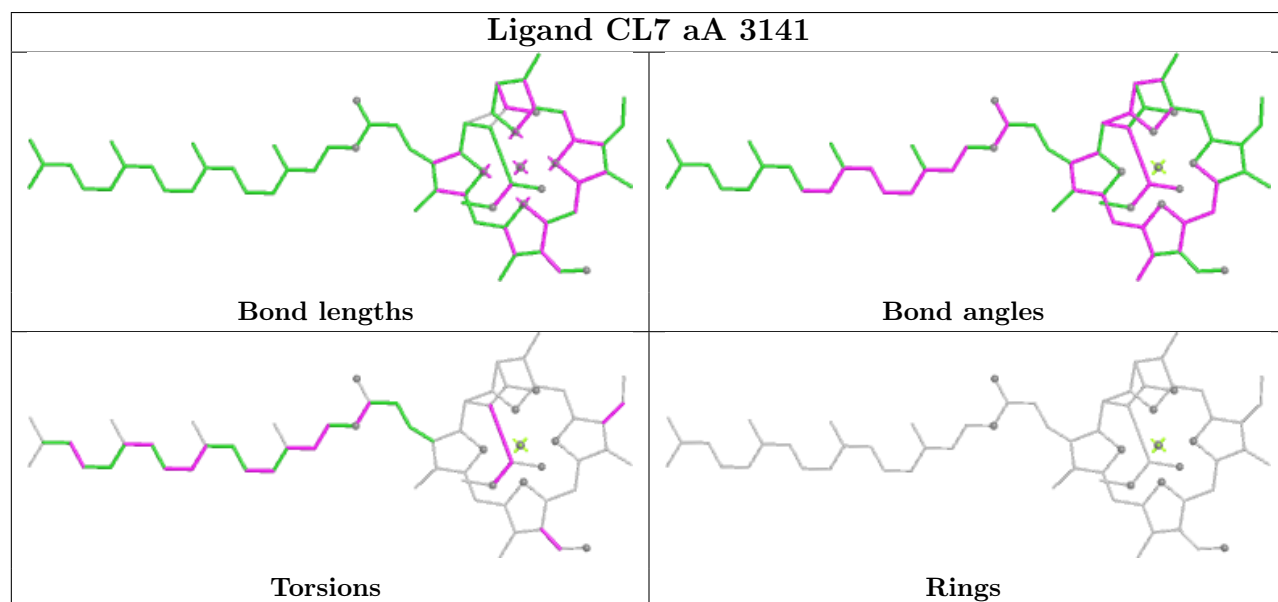
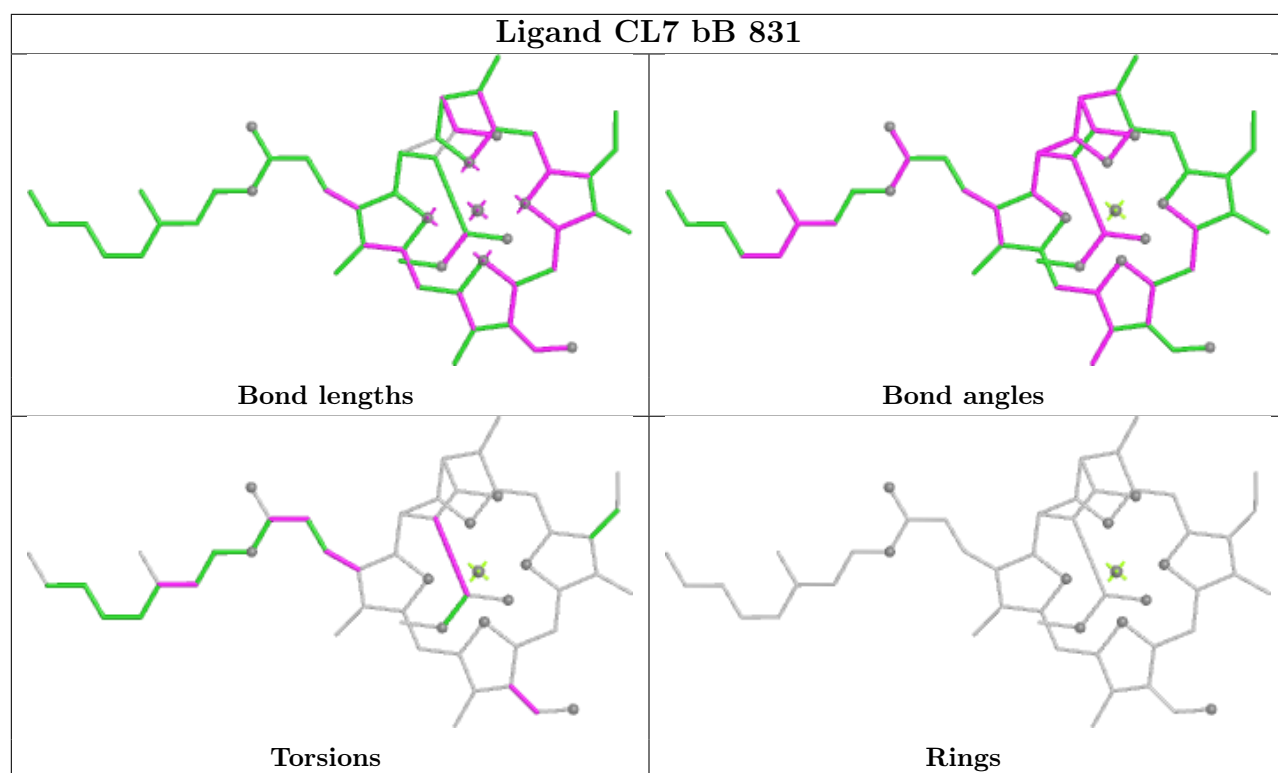
Torsions

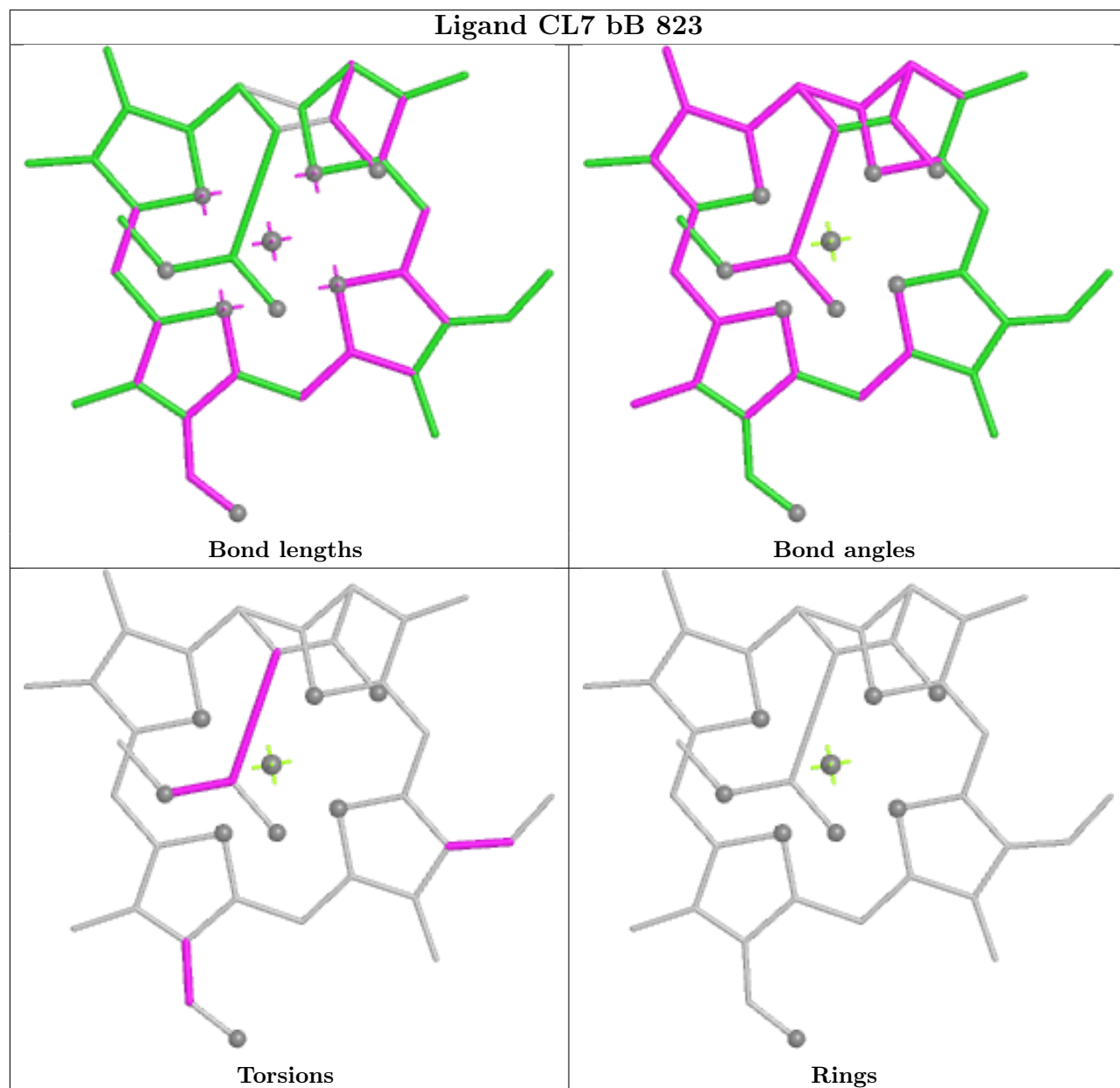


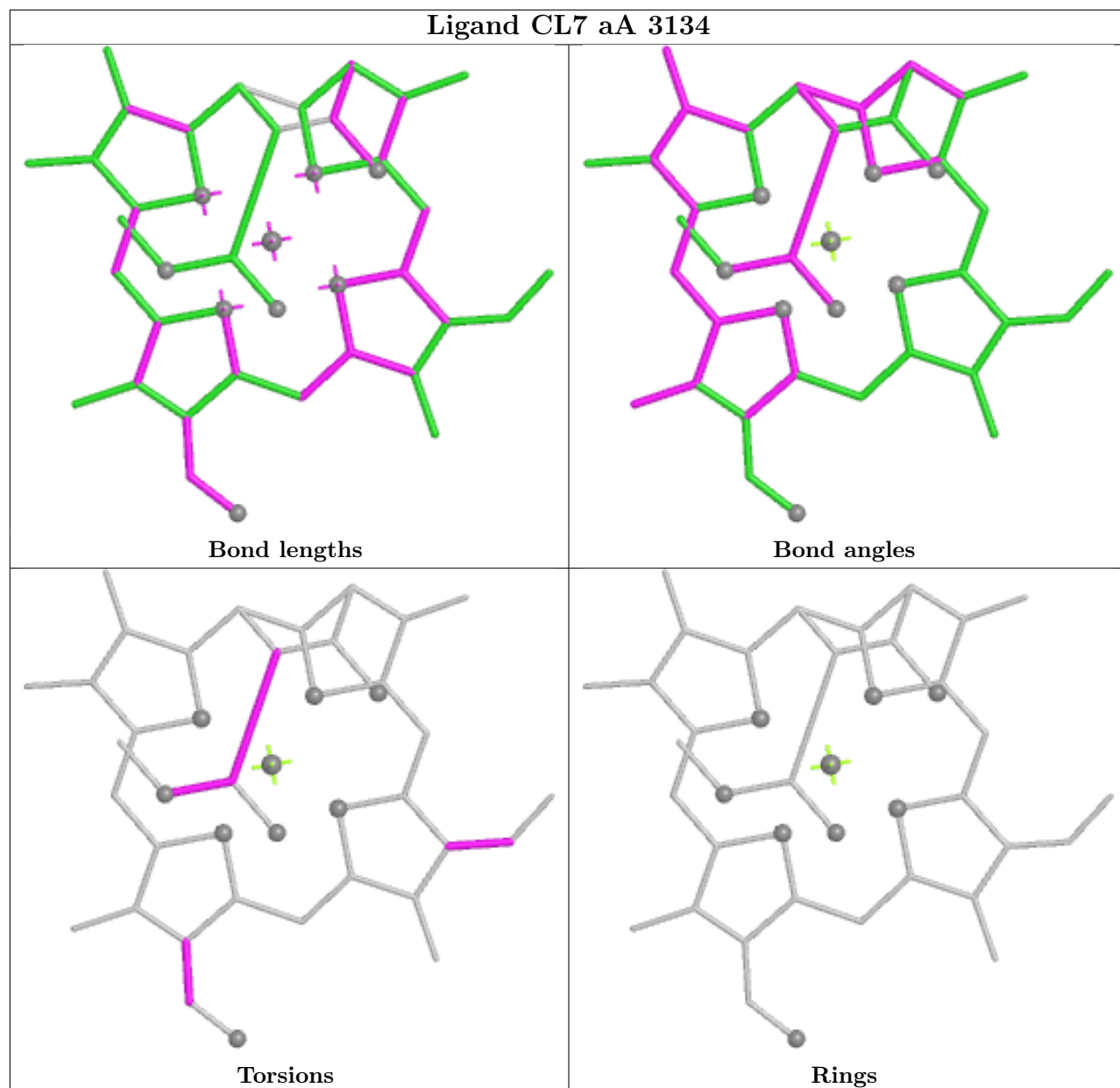
Rings

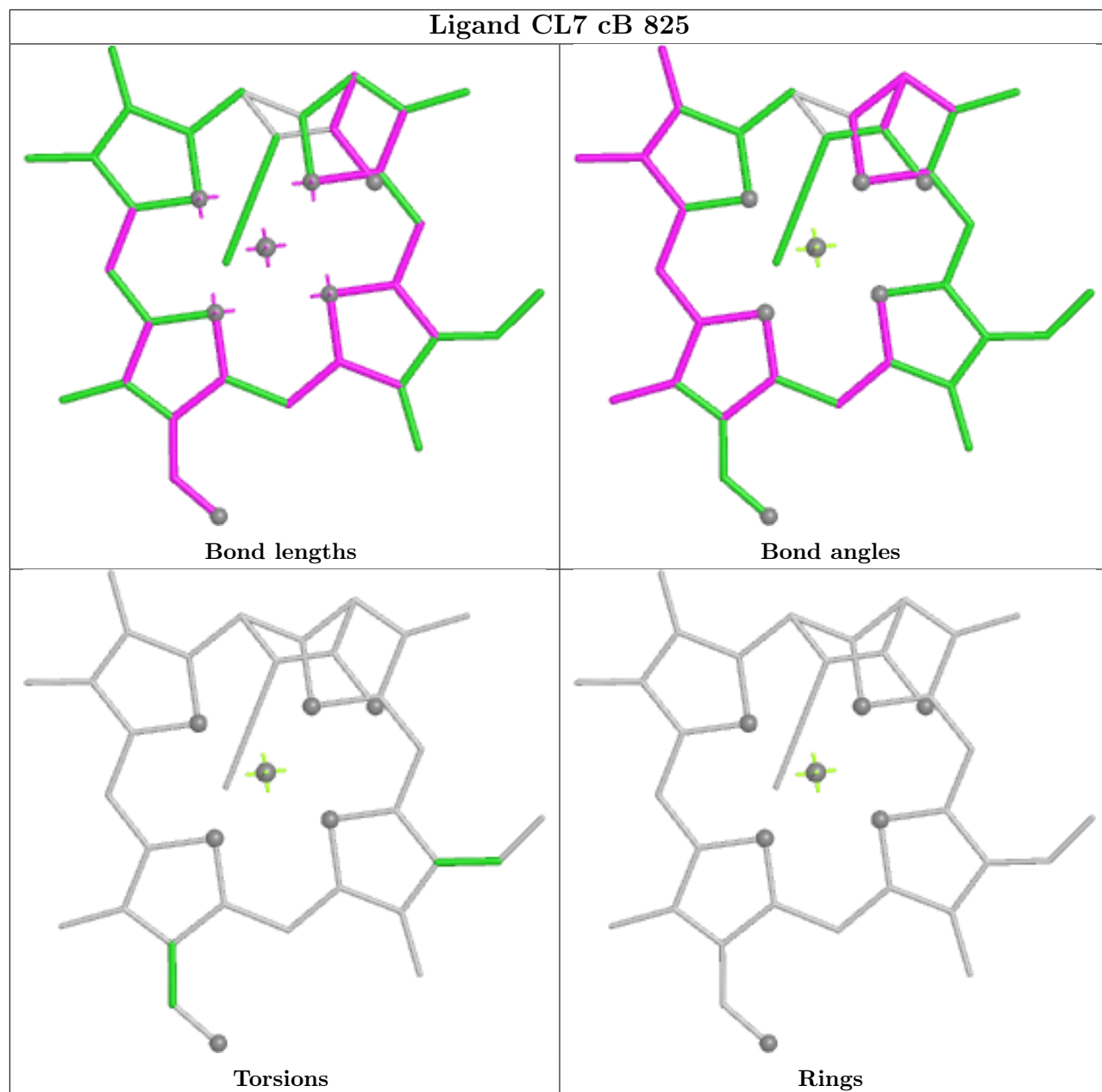


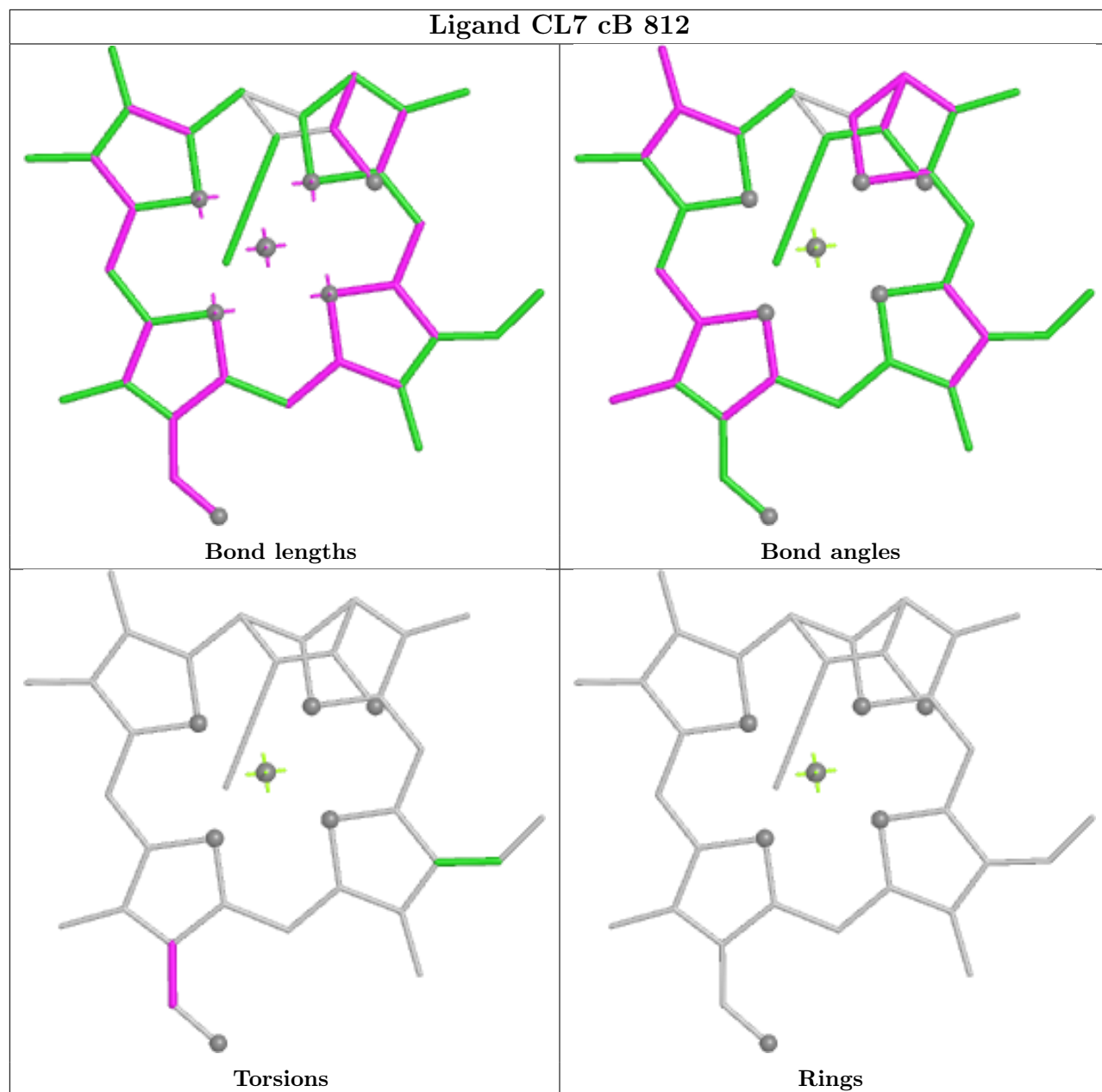


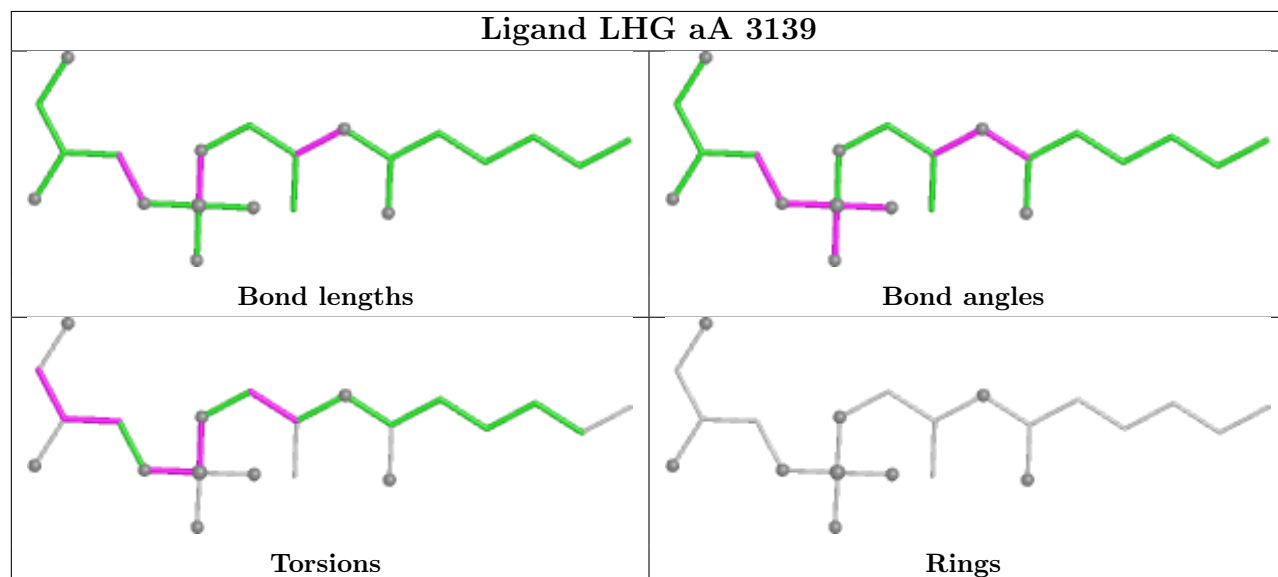
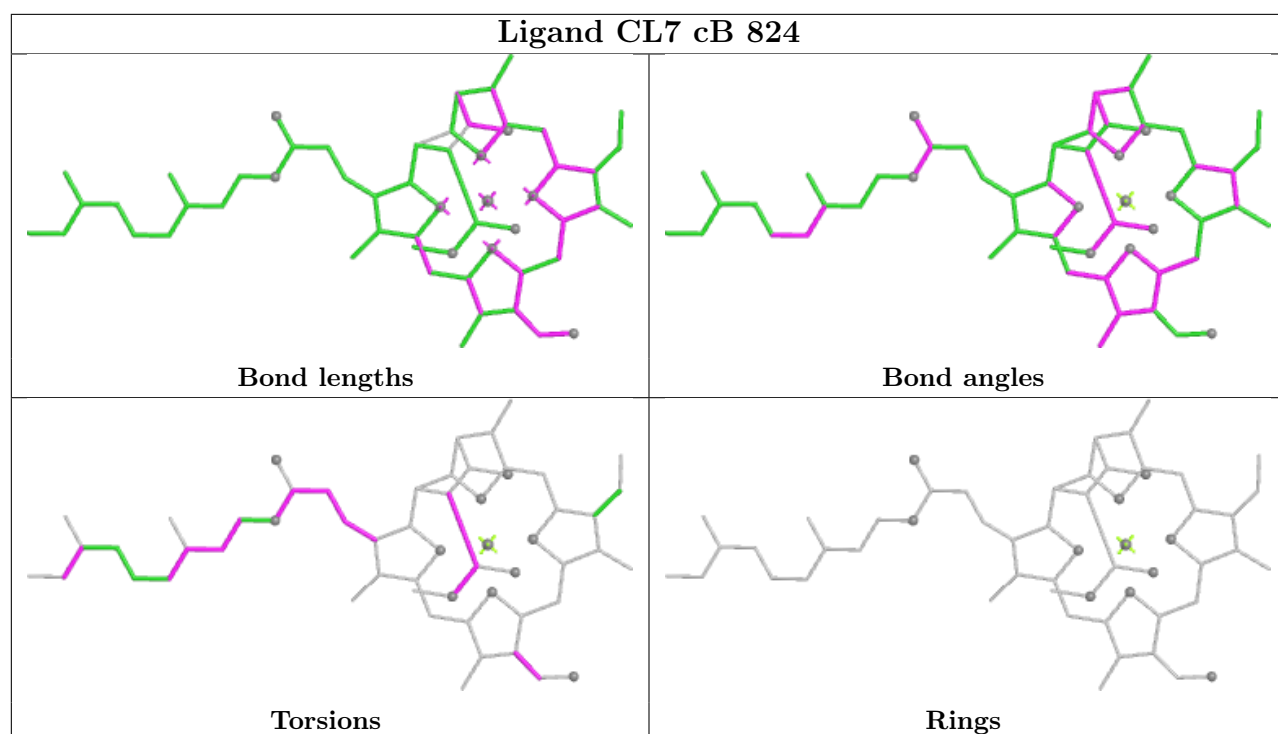


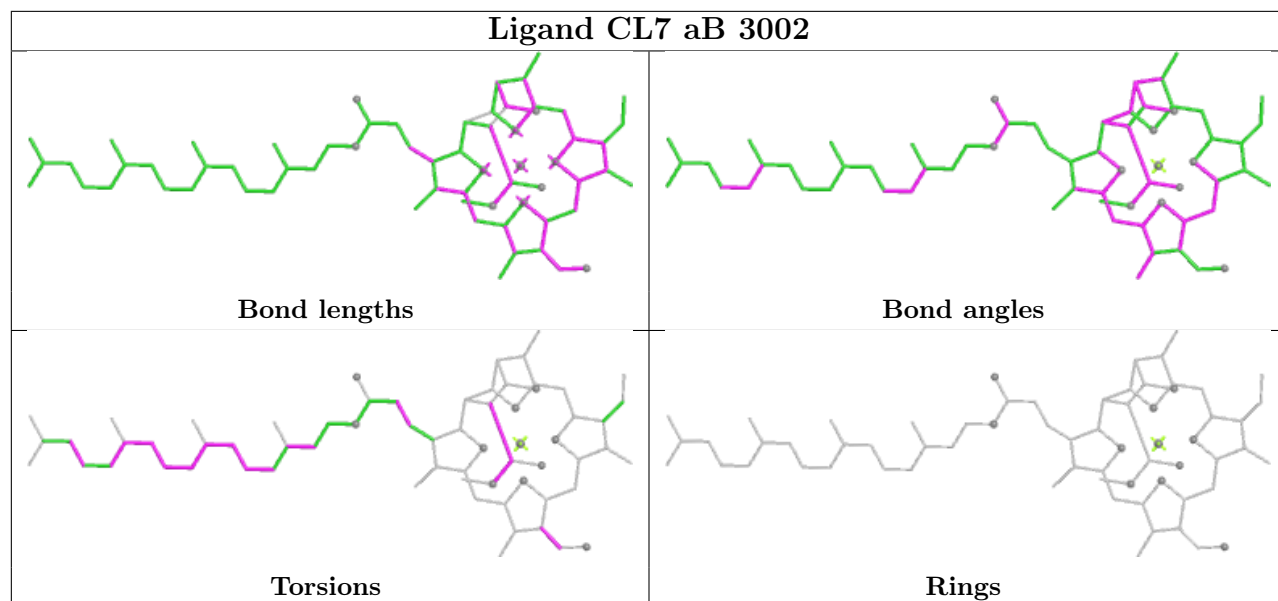


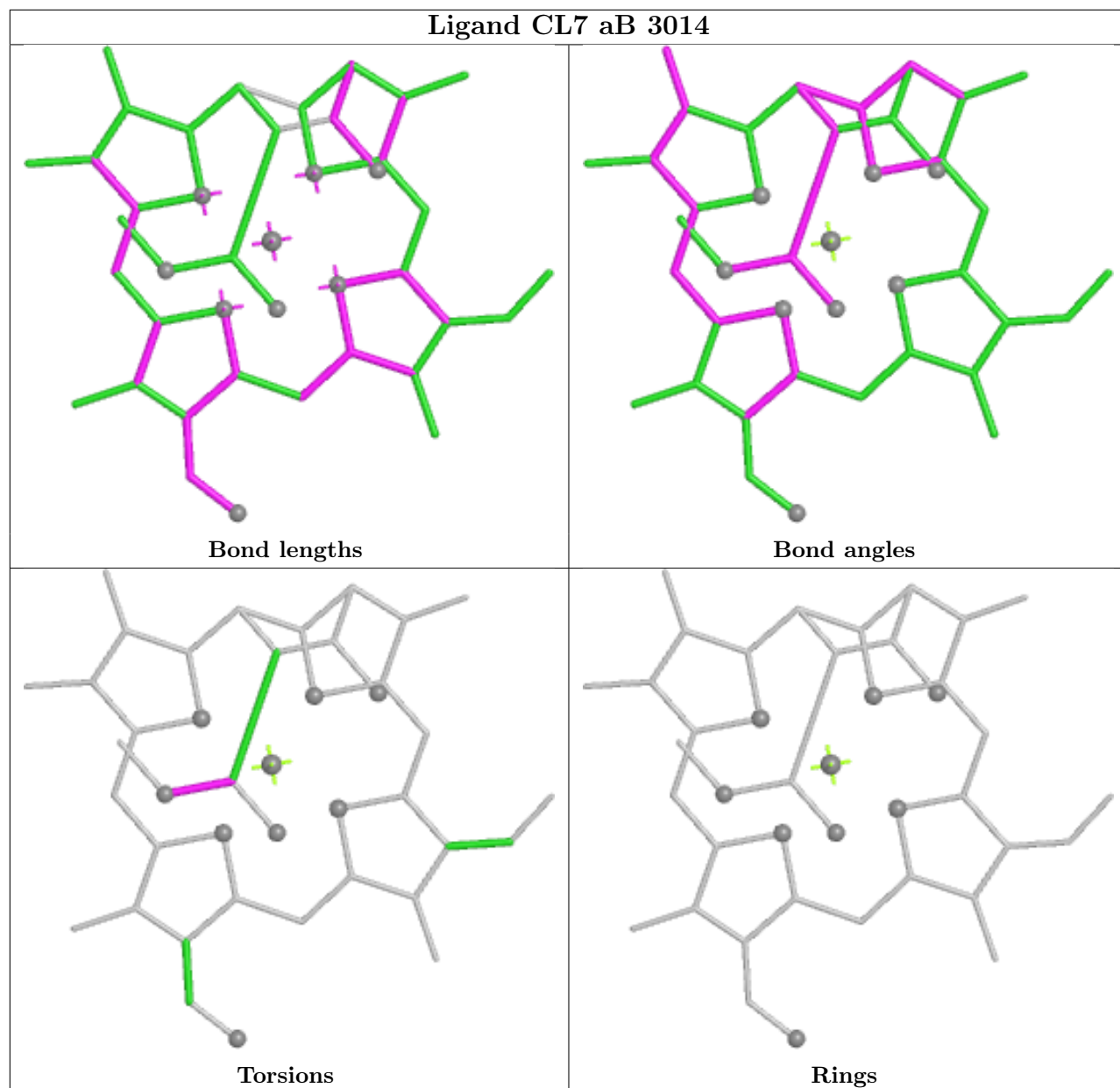




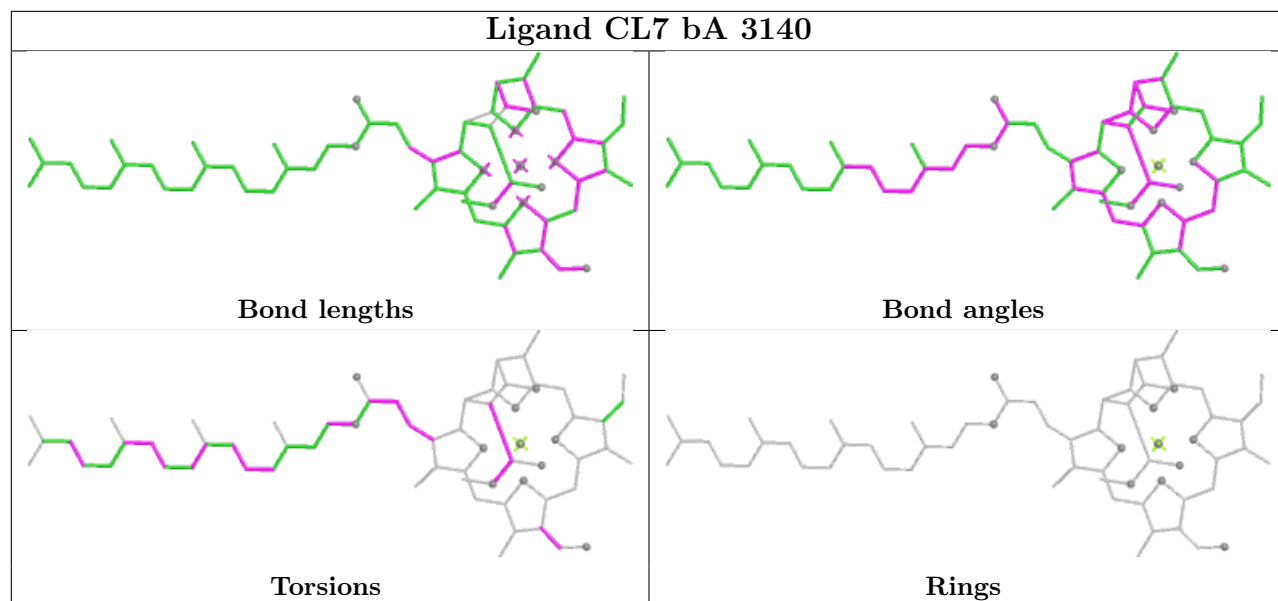


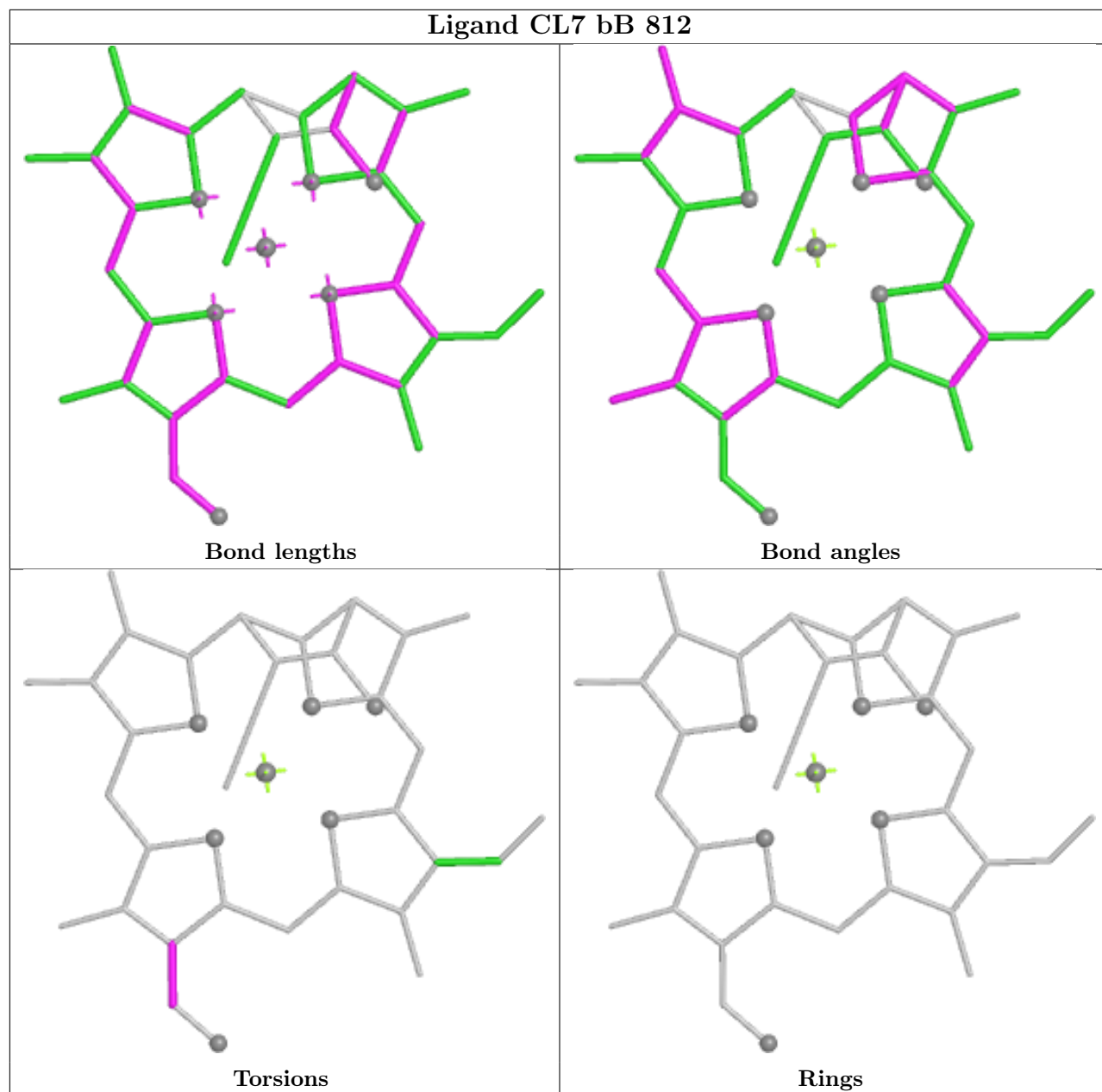


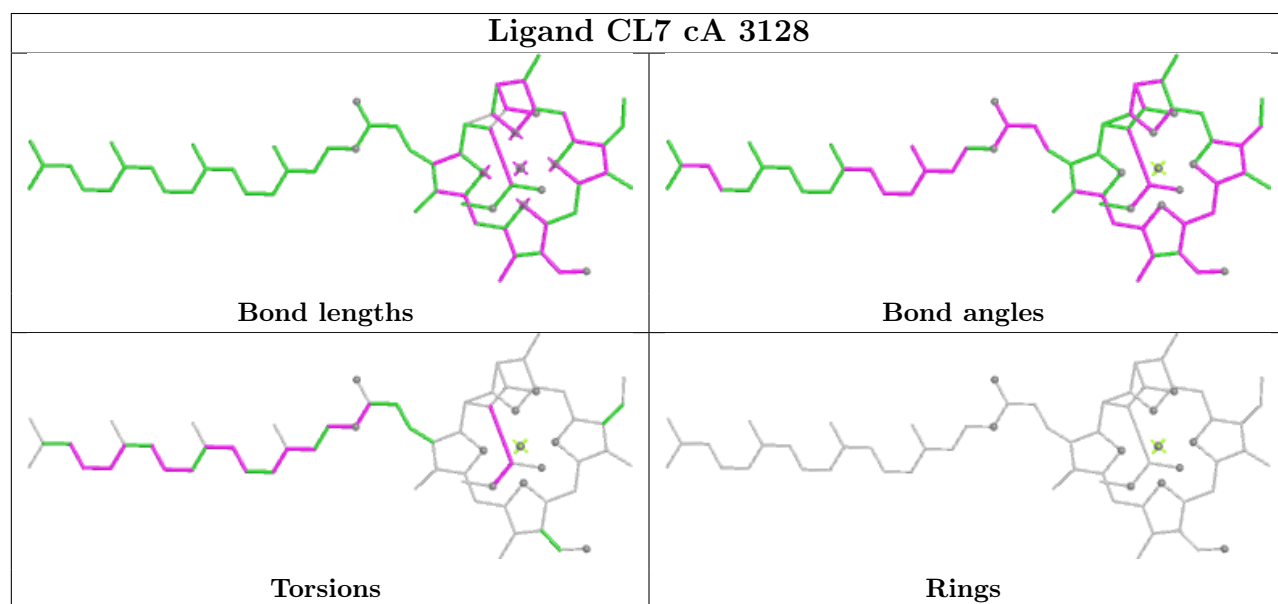
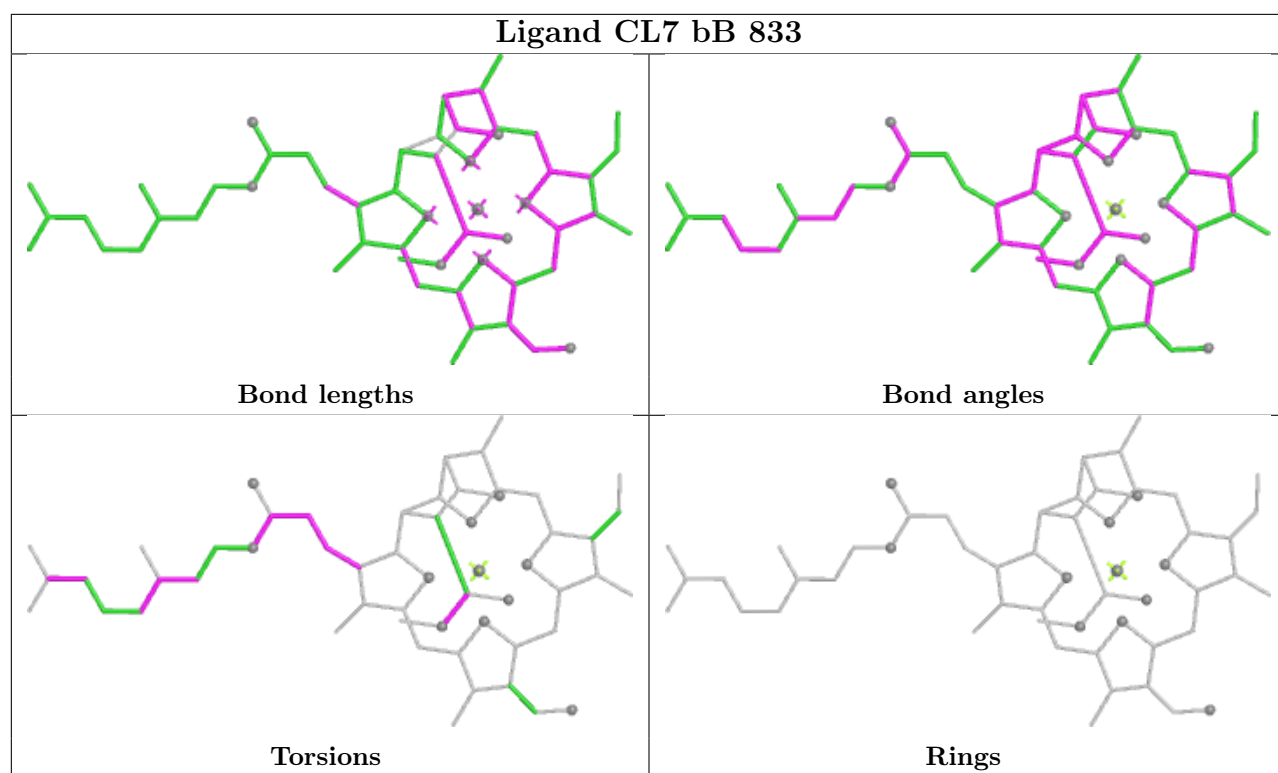


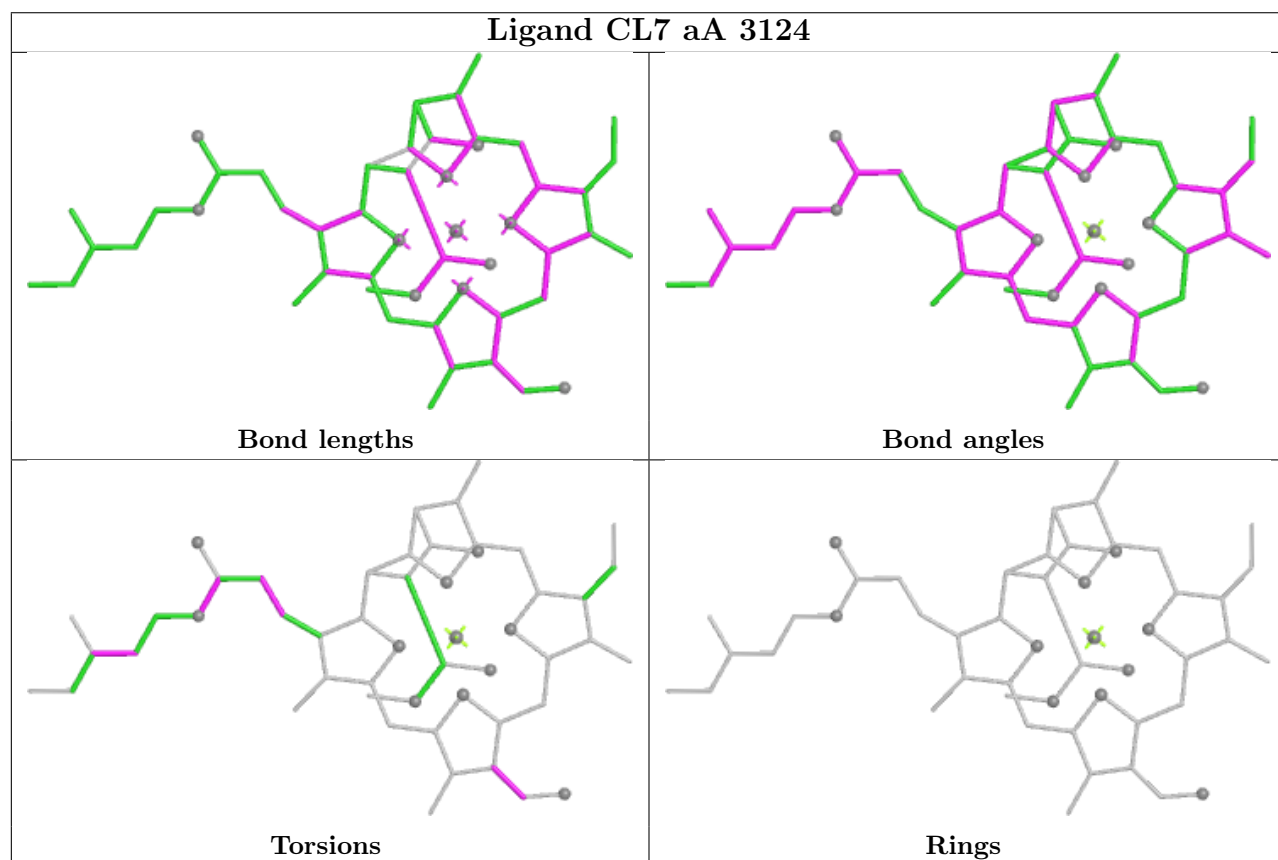
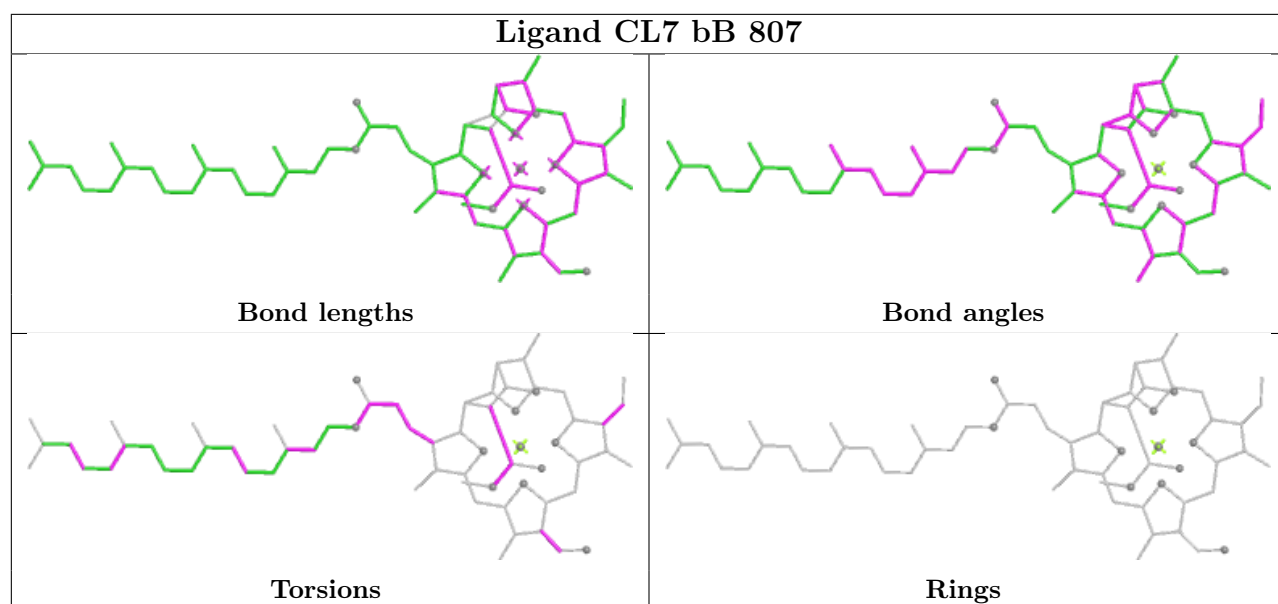




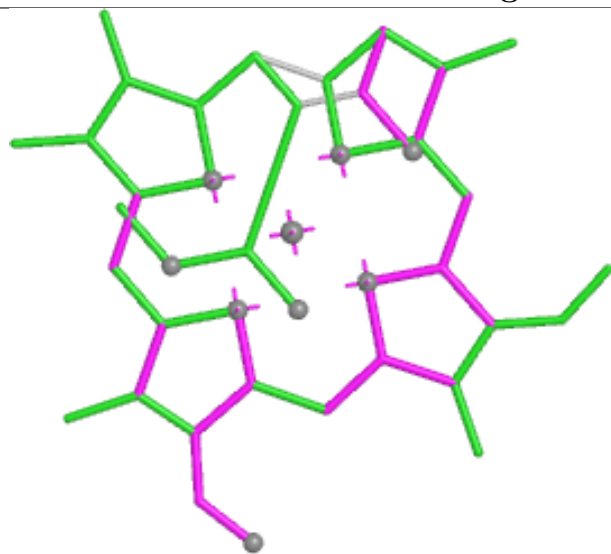




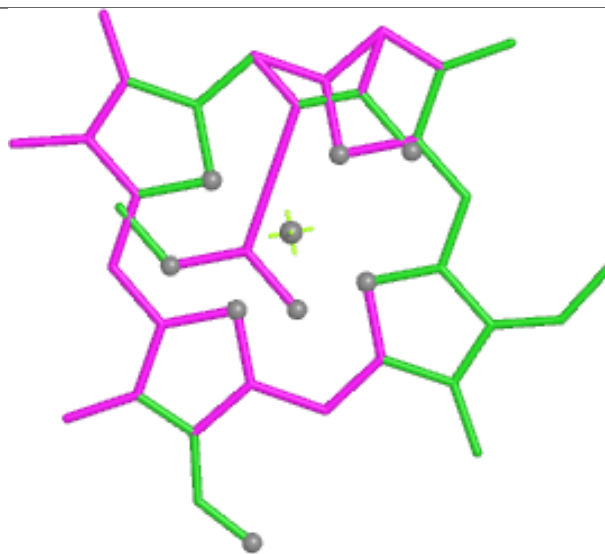




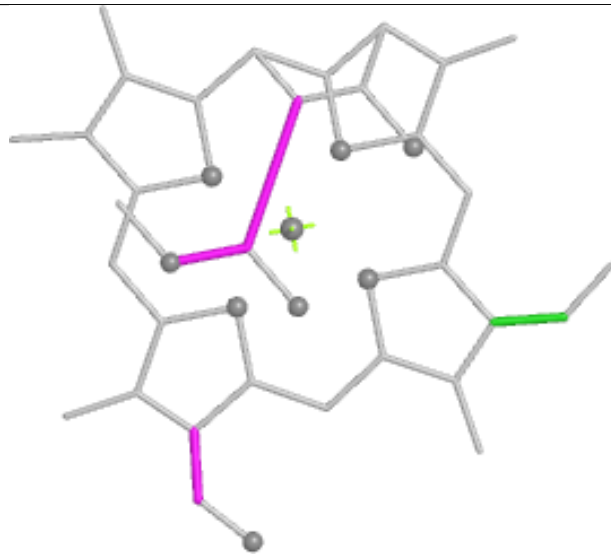
## Ligand CL7 aA 3132



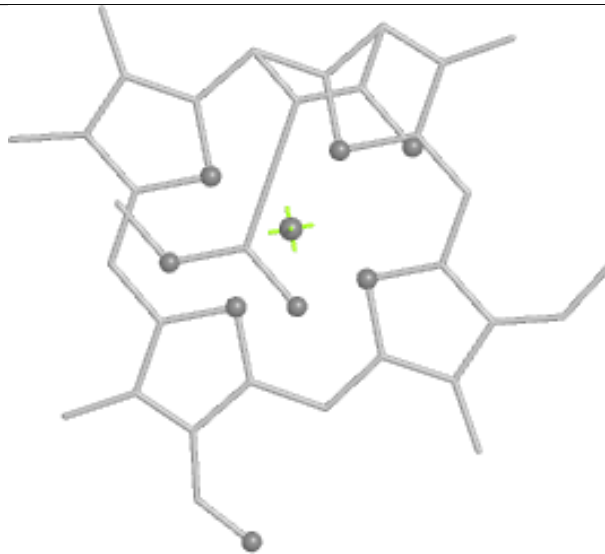
Bond lengths



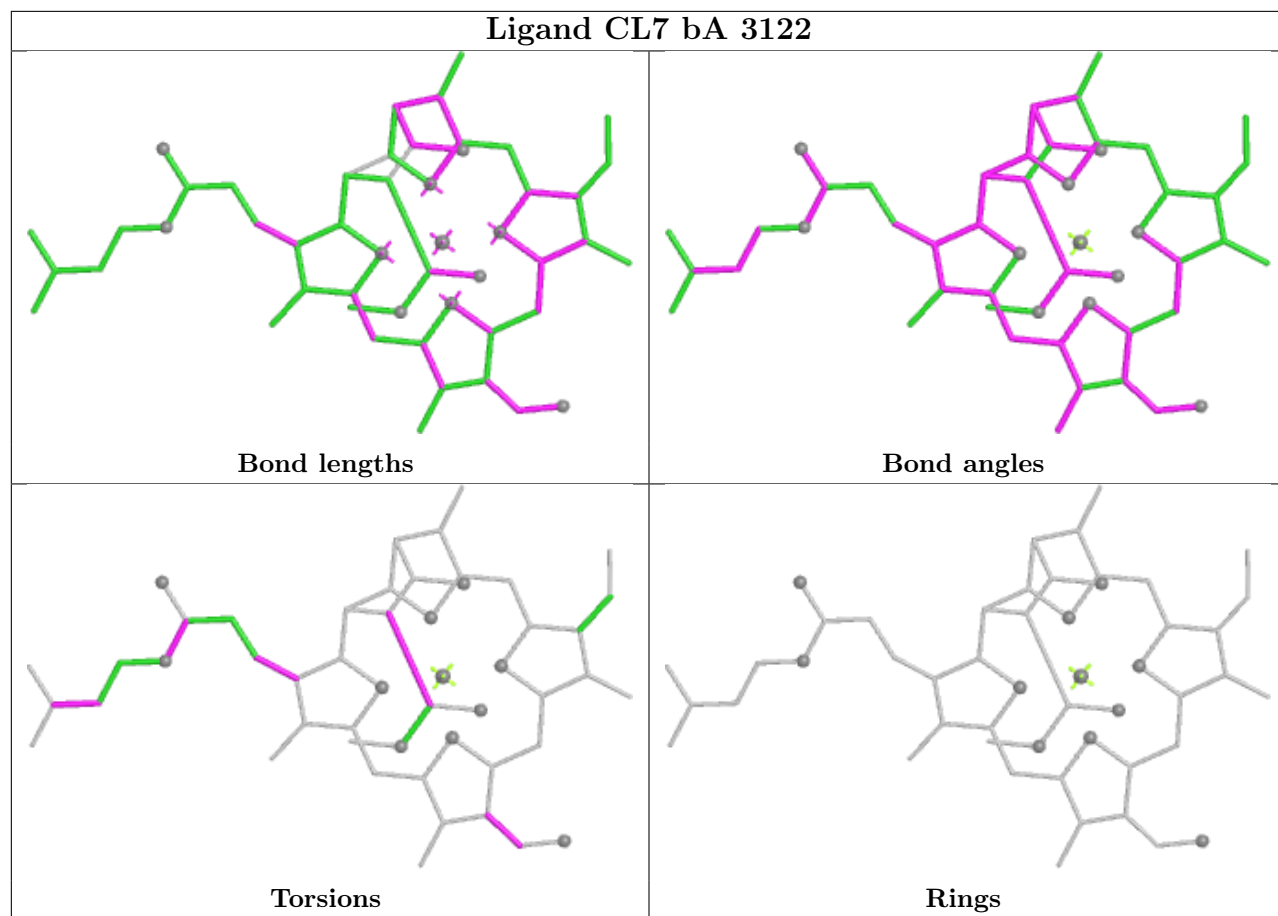
Bond angles

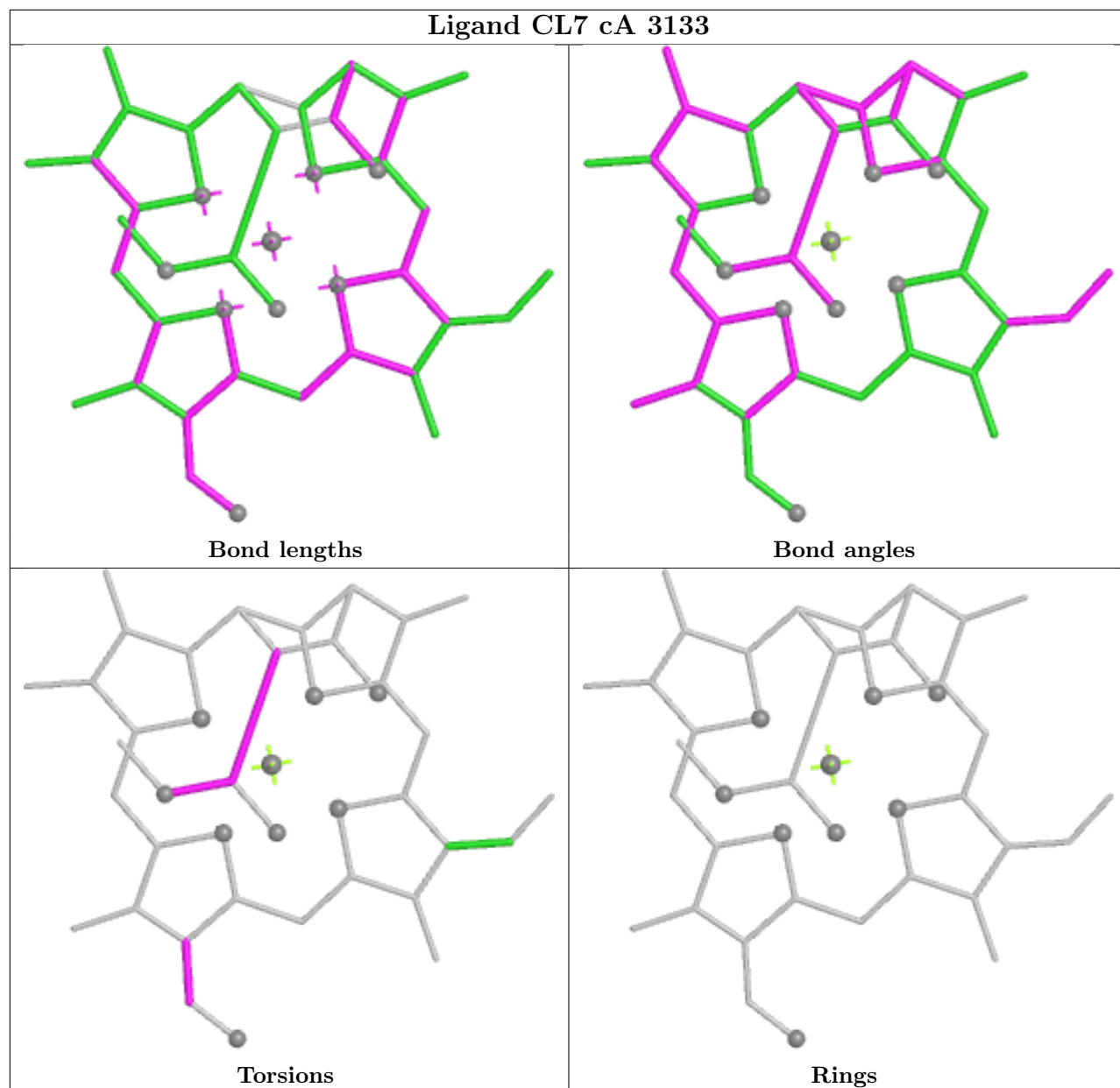


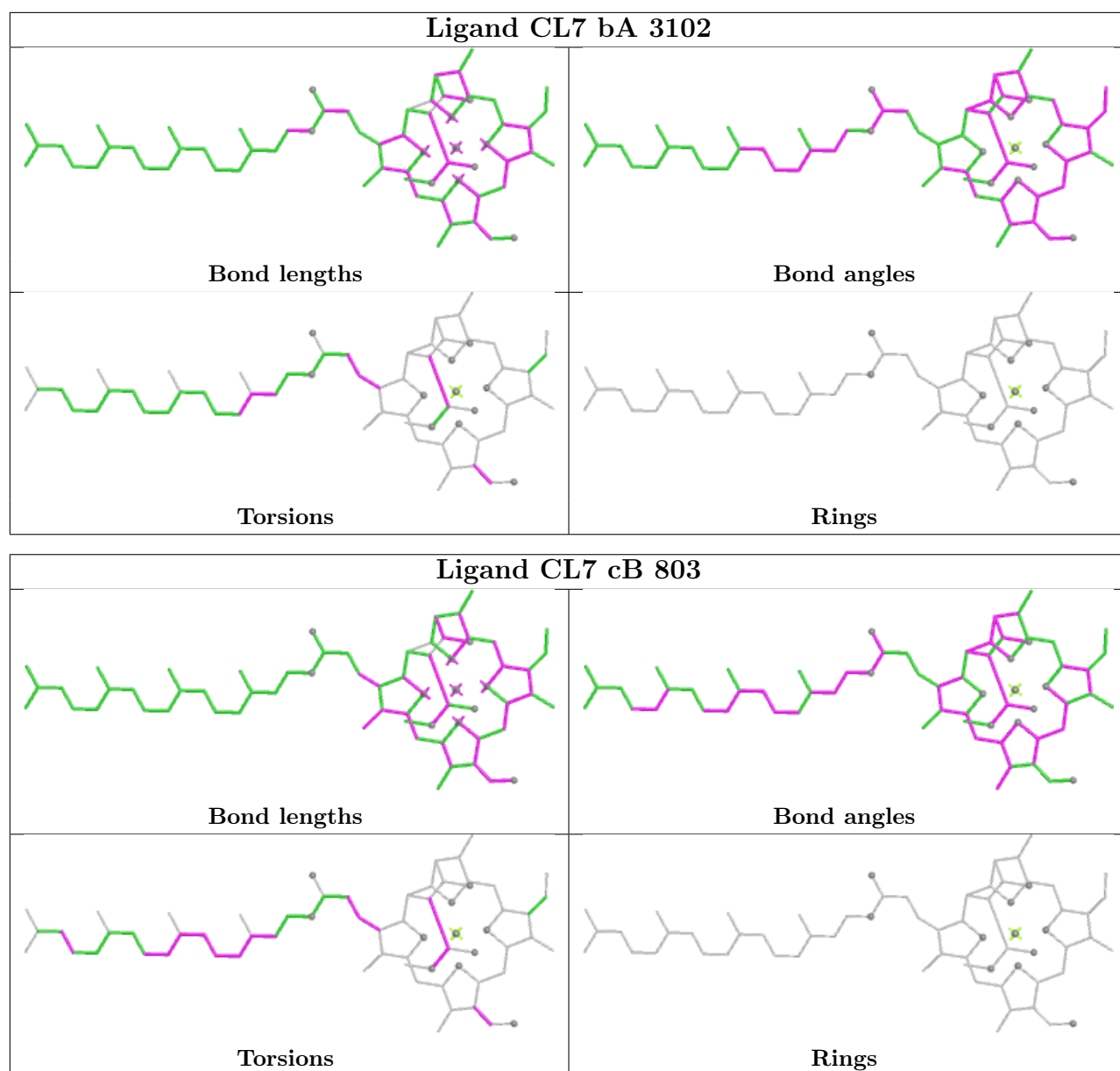
Torsions



Rings

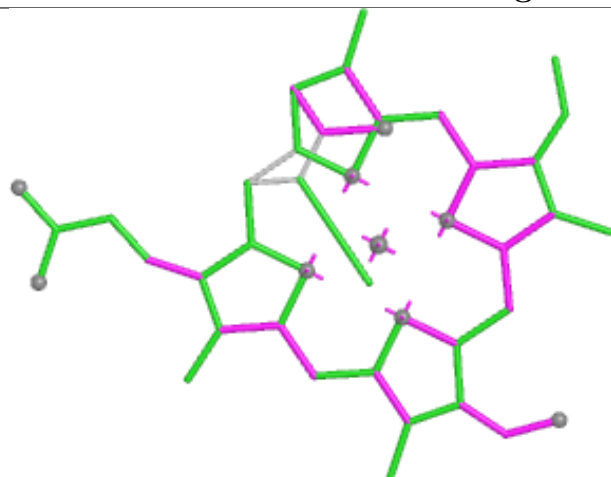




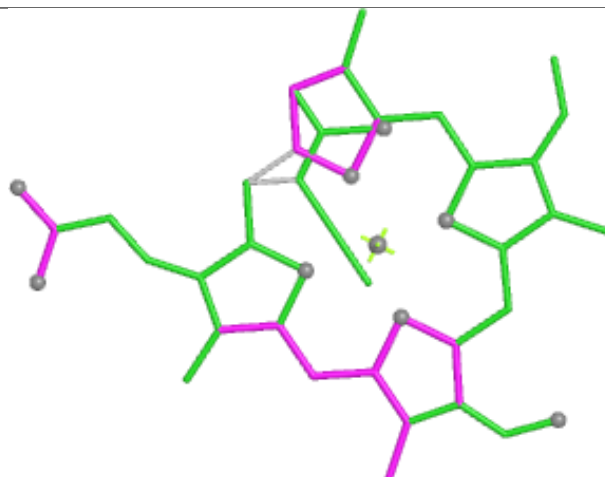




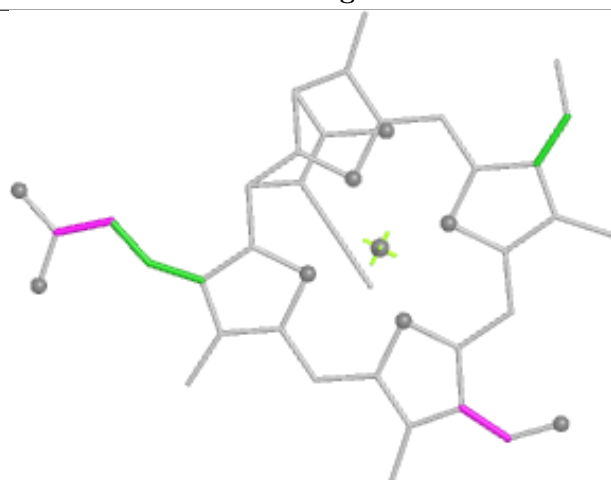
## Ligand CL7 cJ 101



Bond lengths



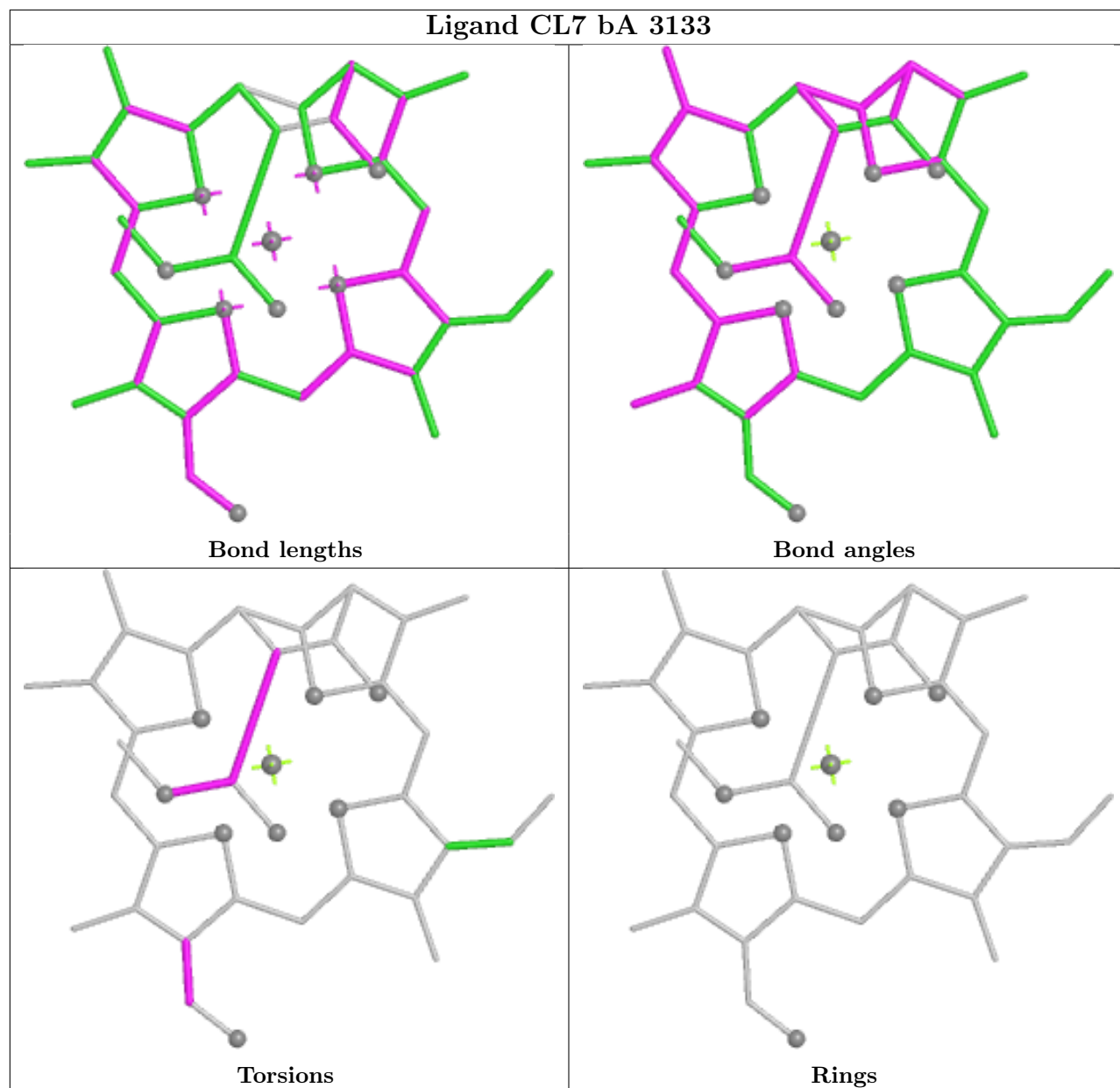
Bond angles

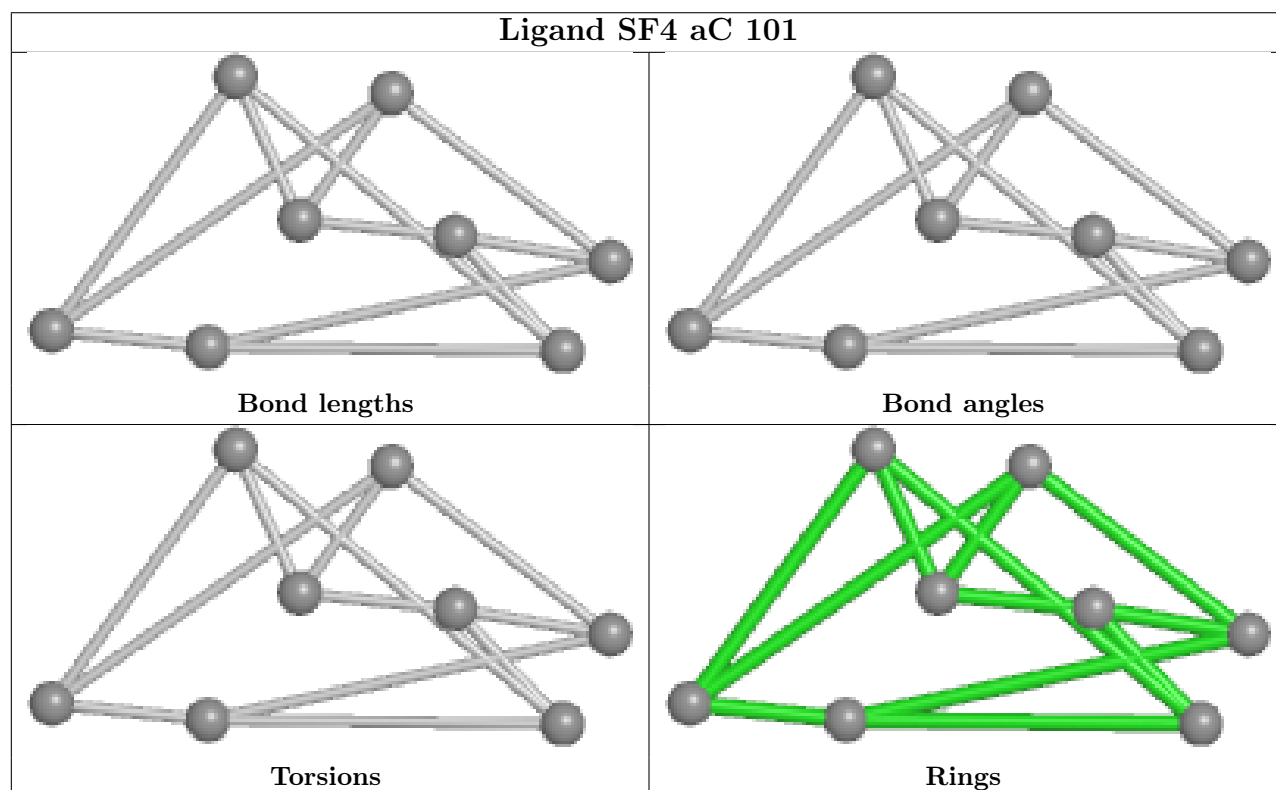
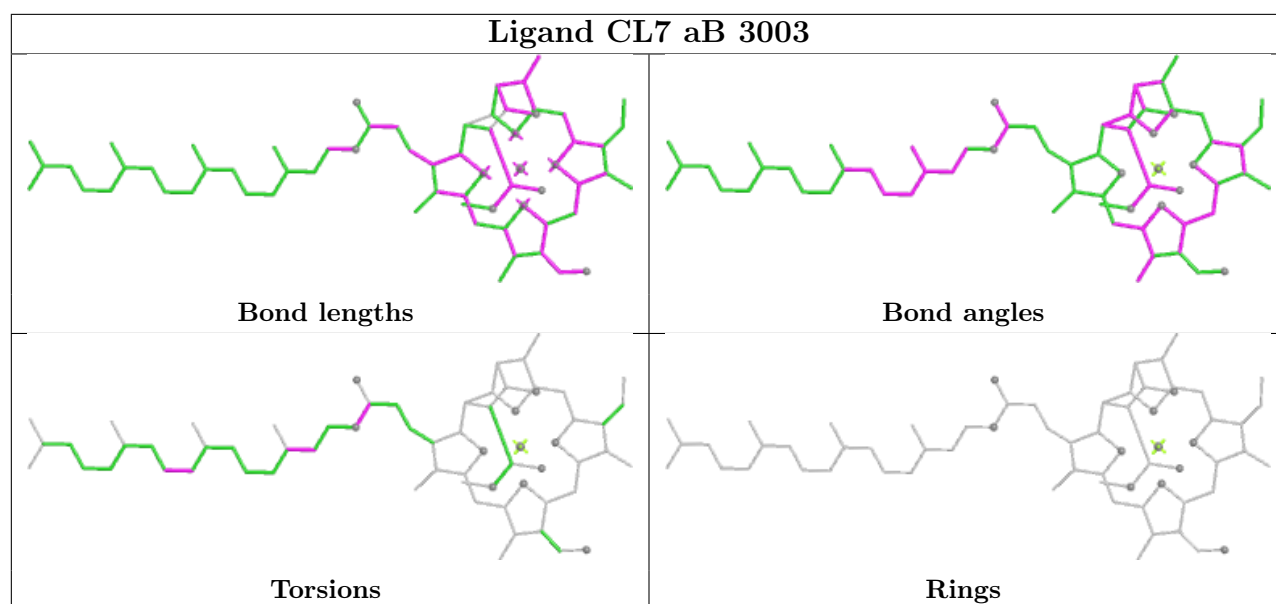


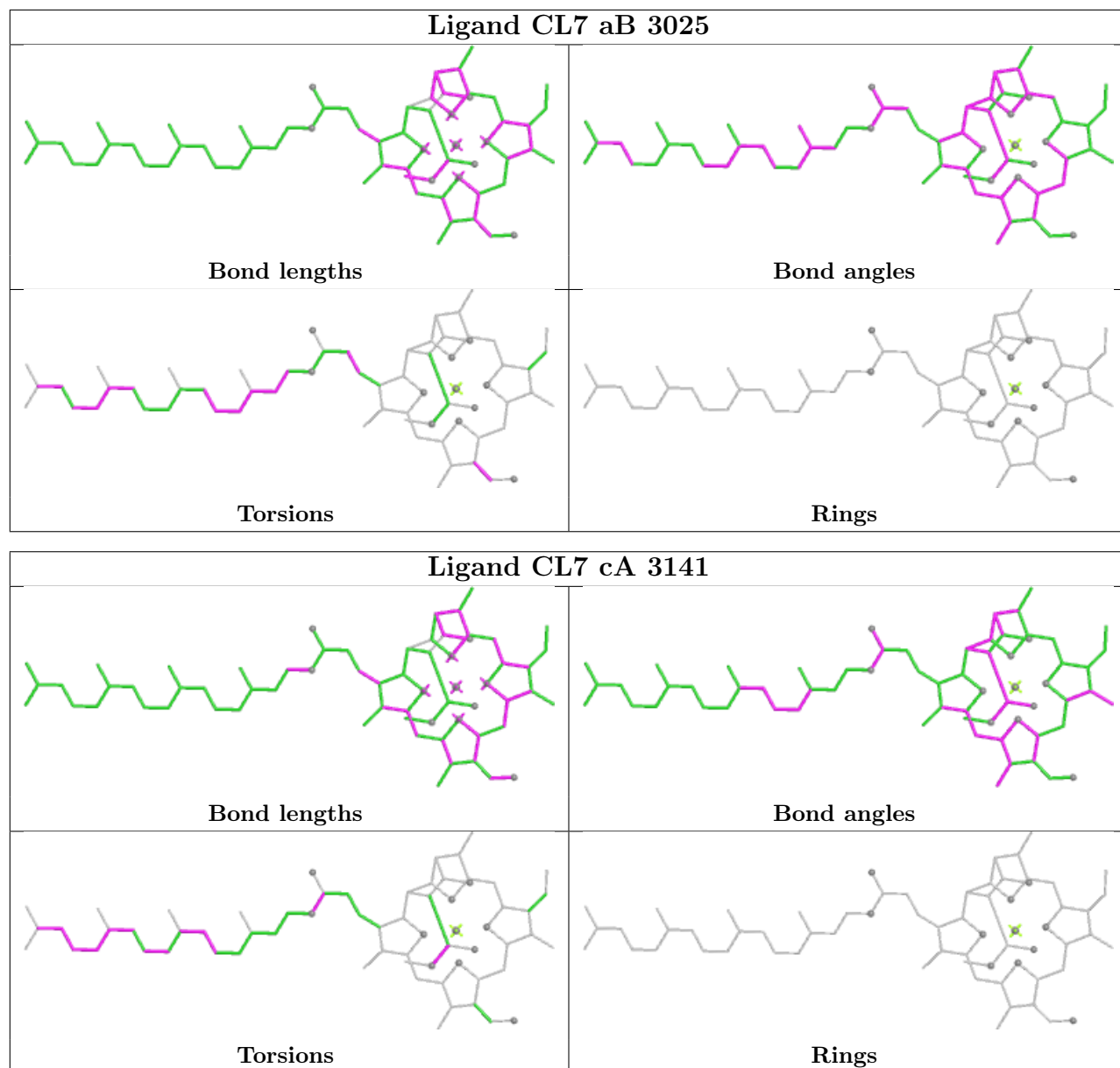
Torsions

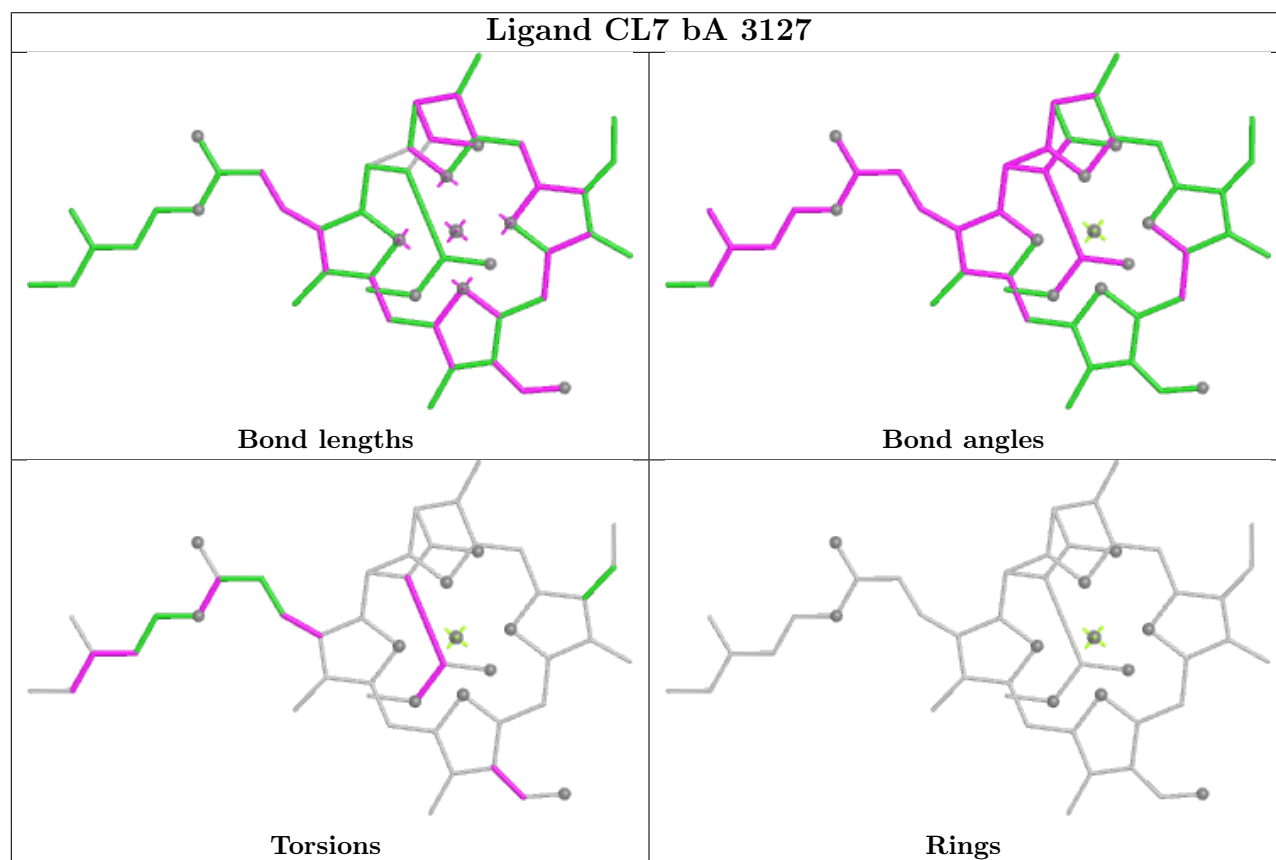
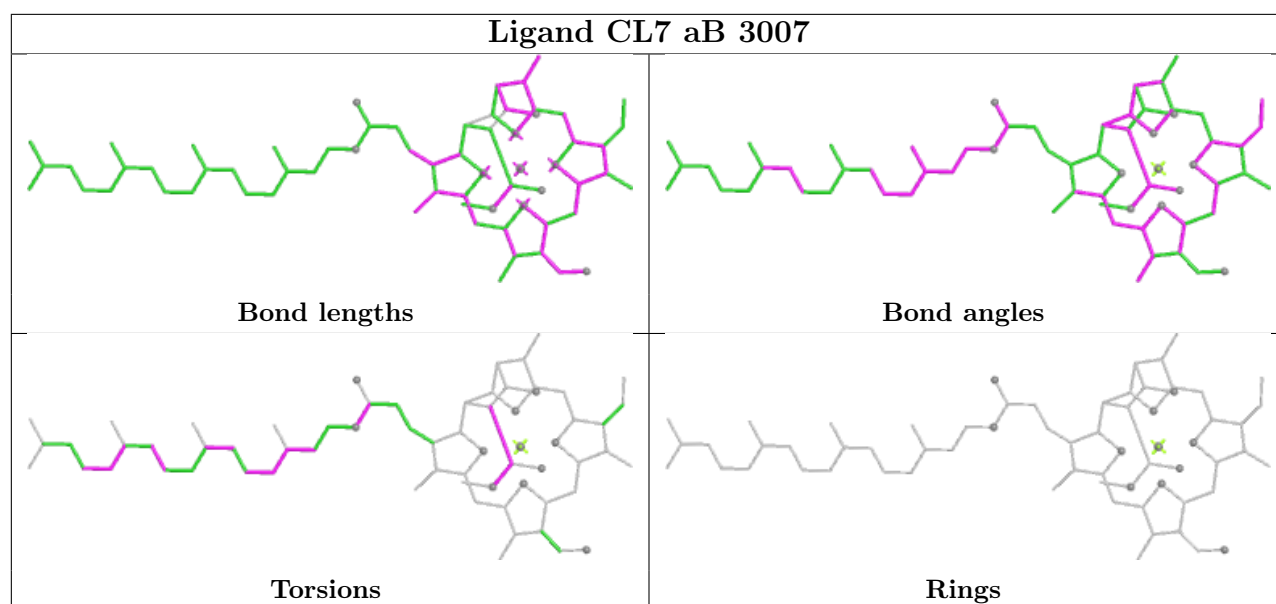


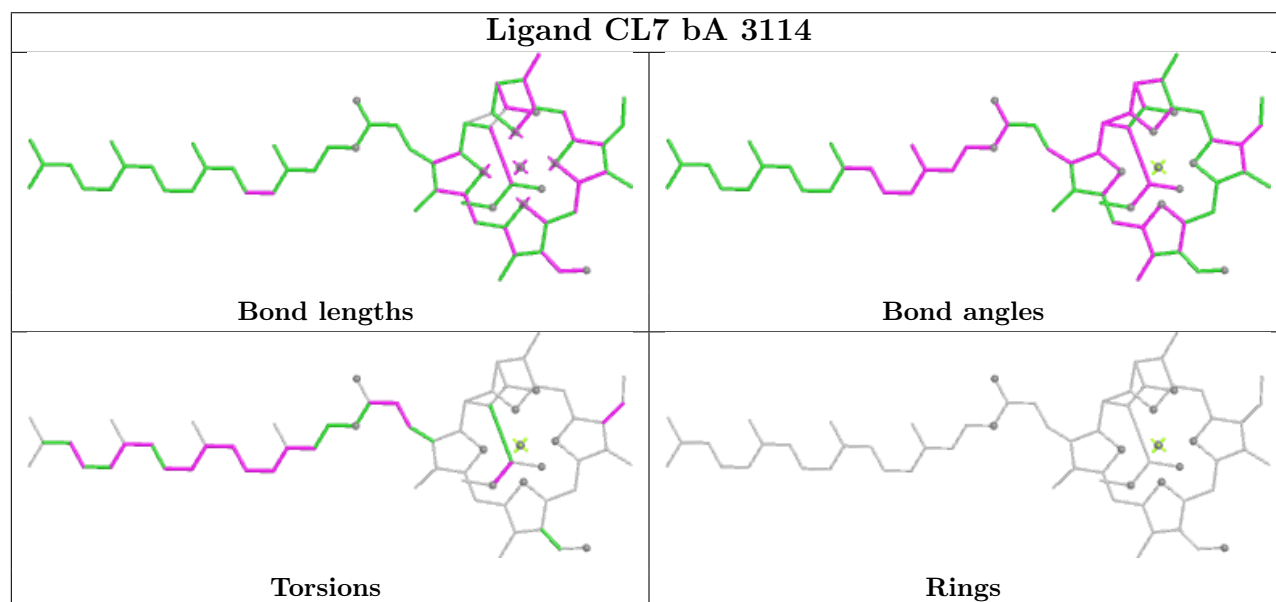
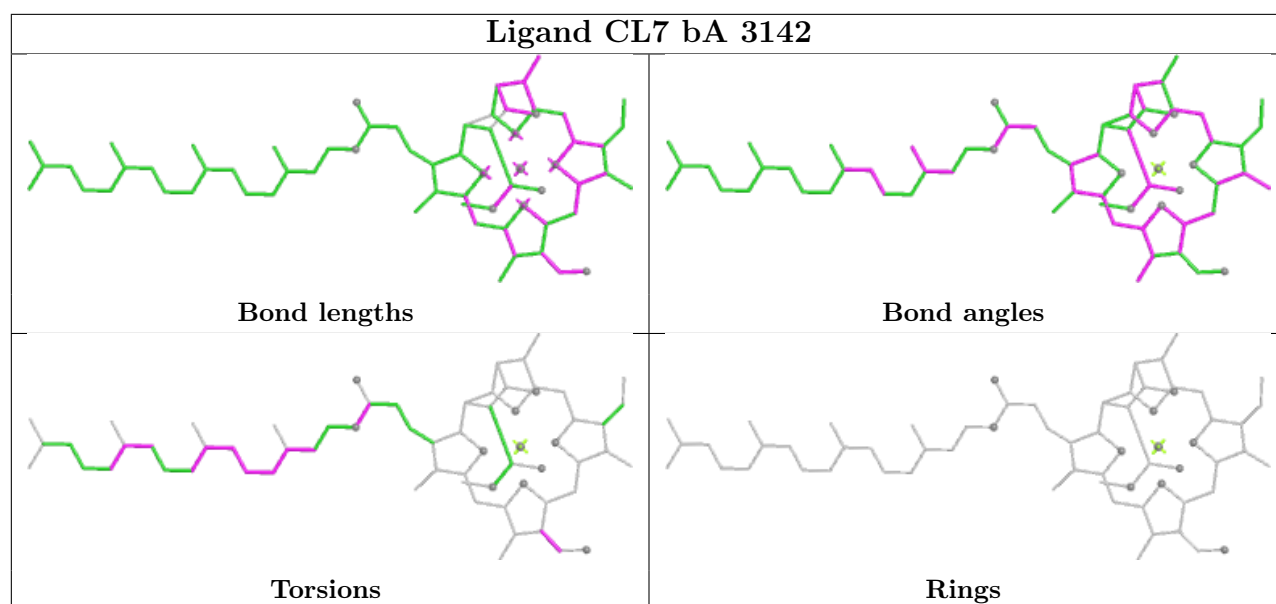
Rings

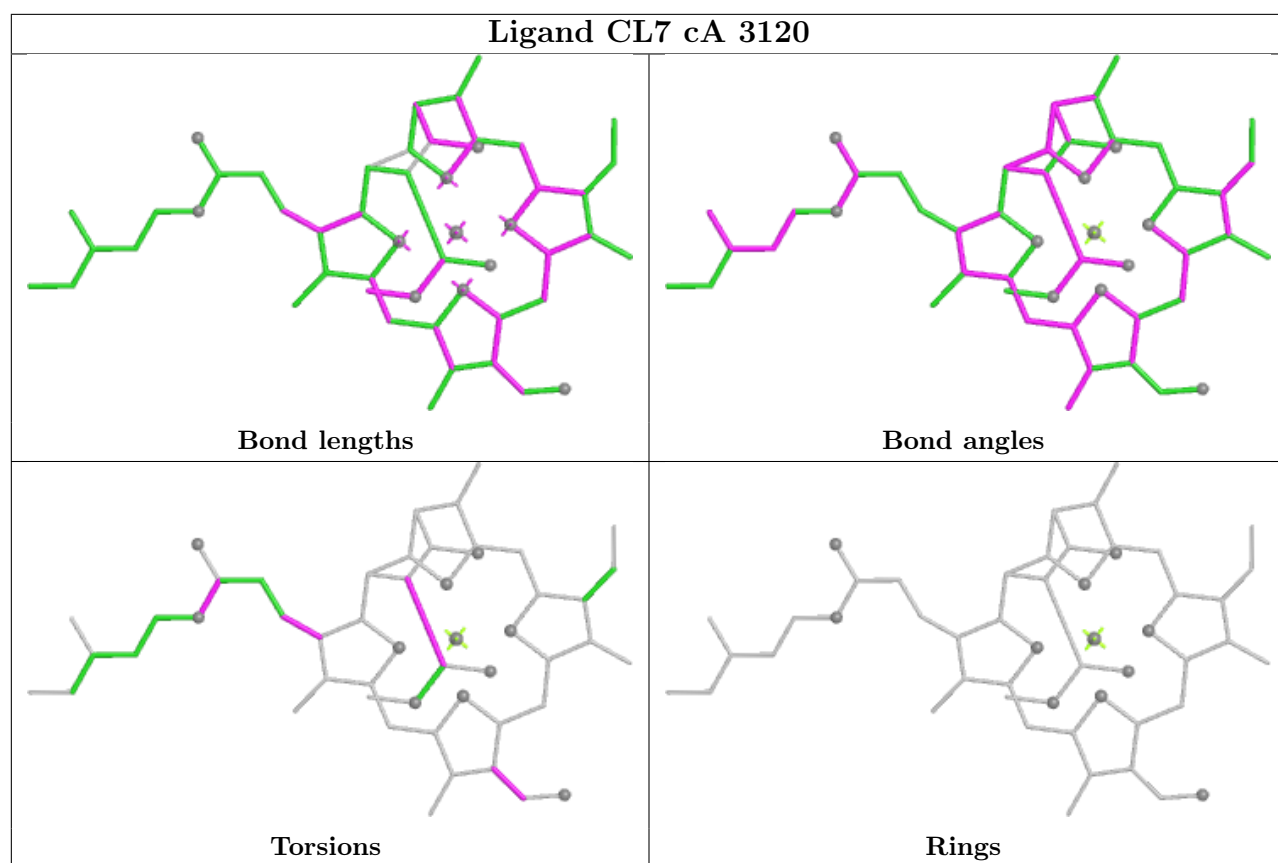




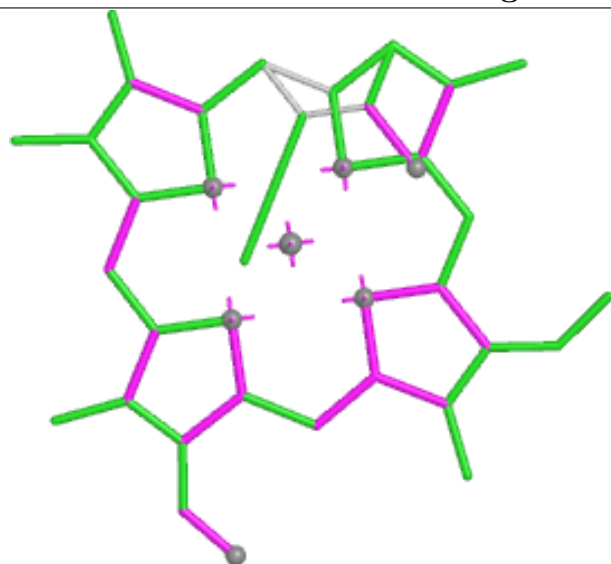




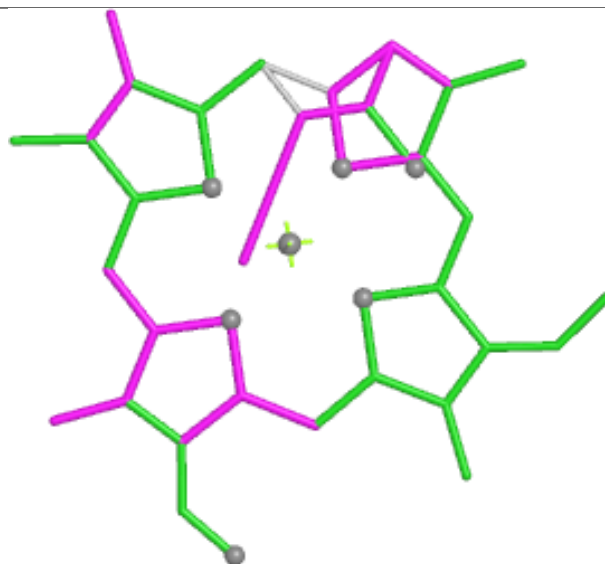




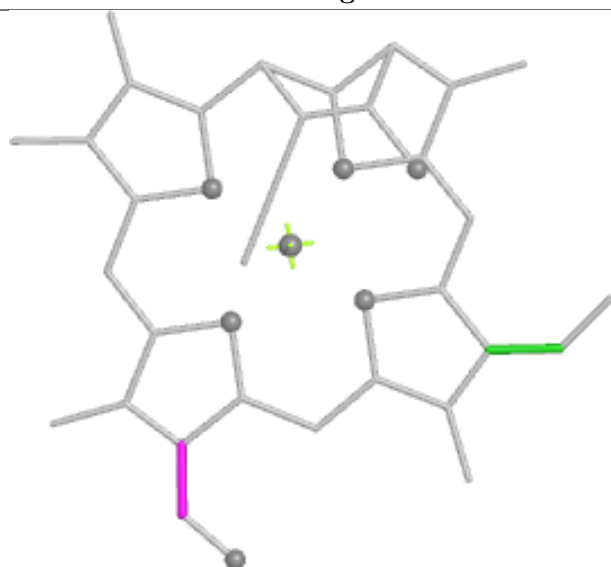
## Ligand CL7 aA 3112



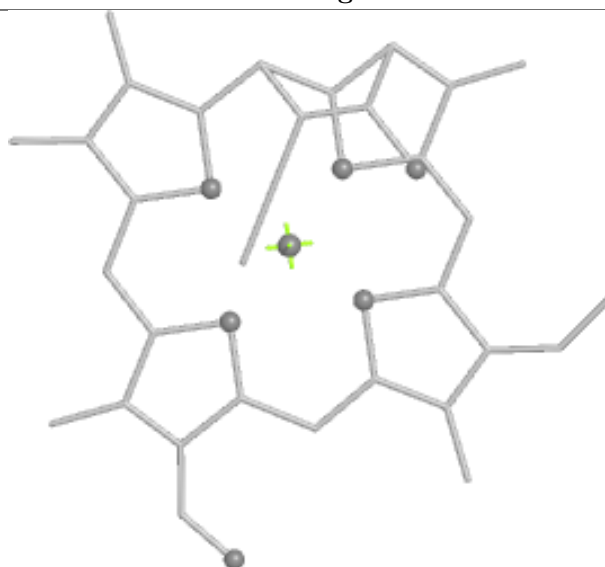
Bond lengths



Bond angles

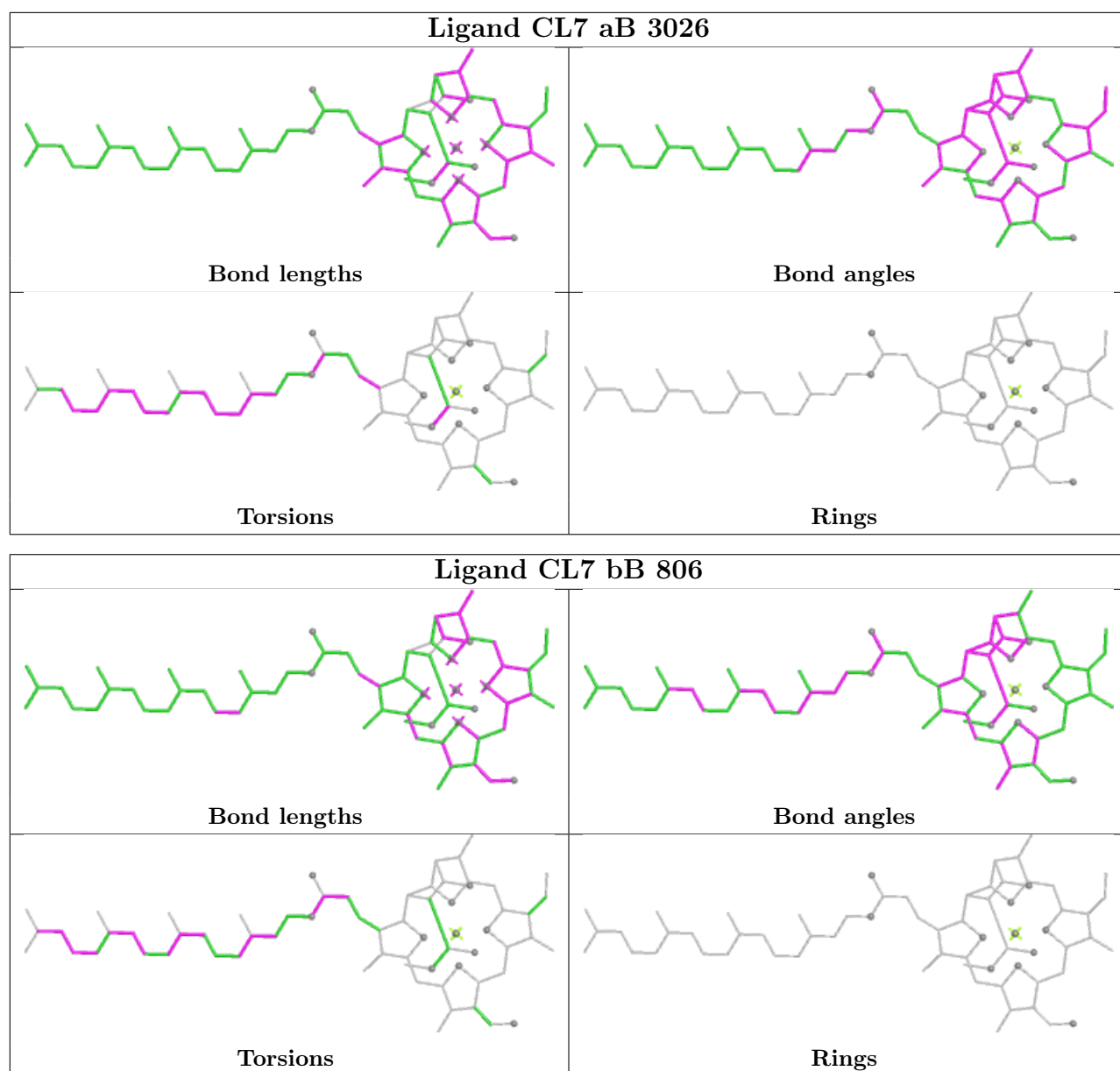


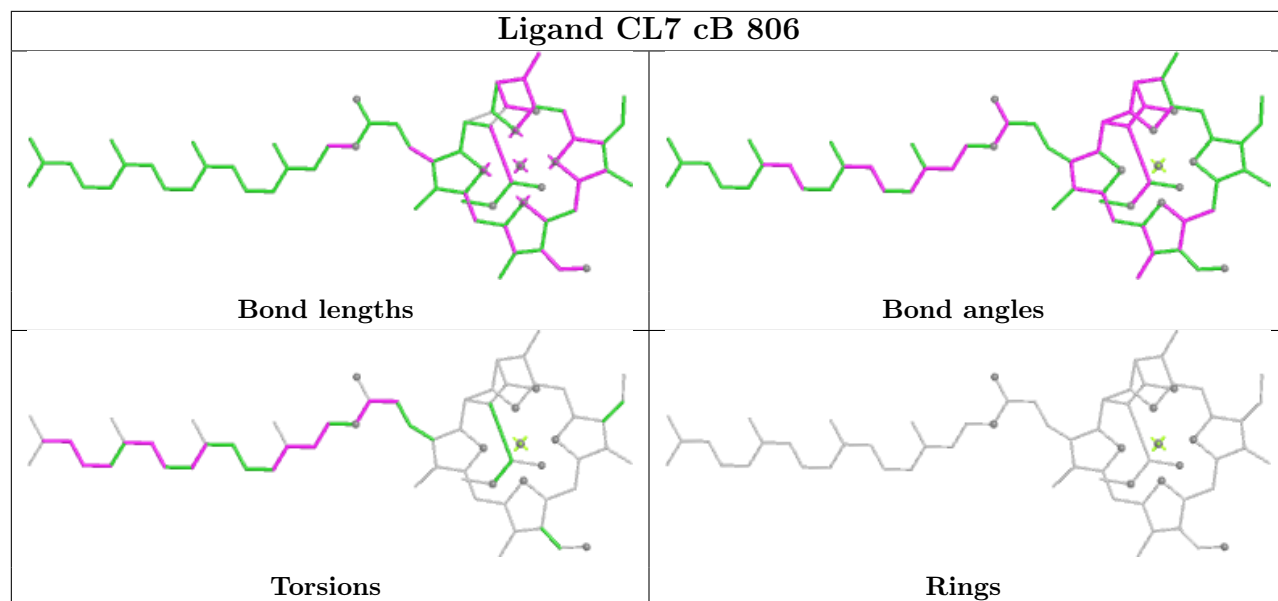
Torsions

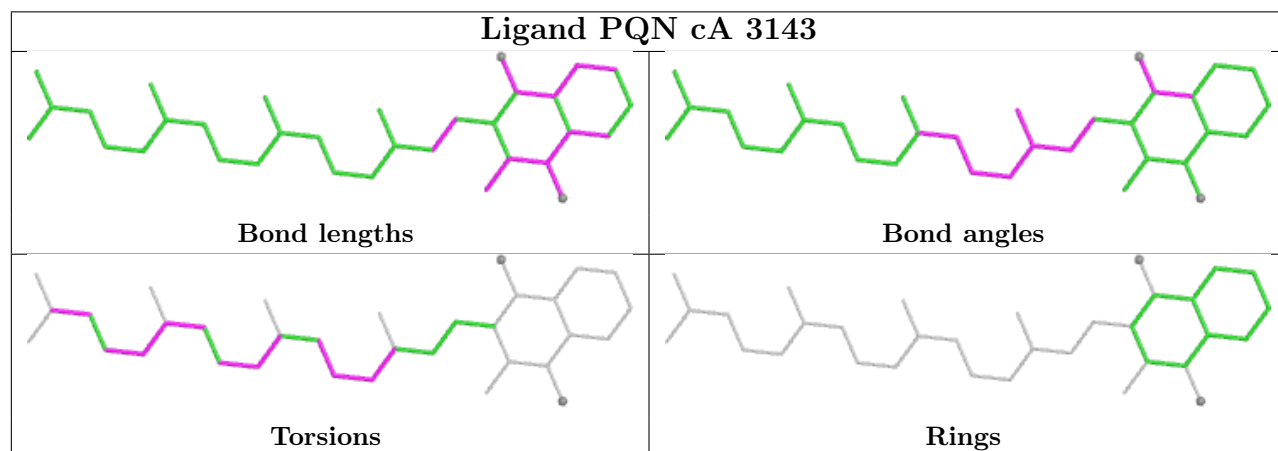
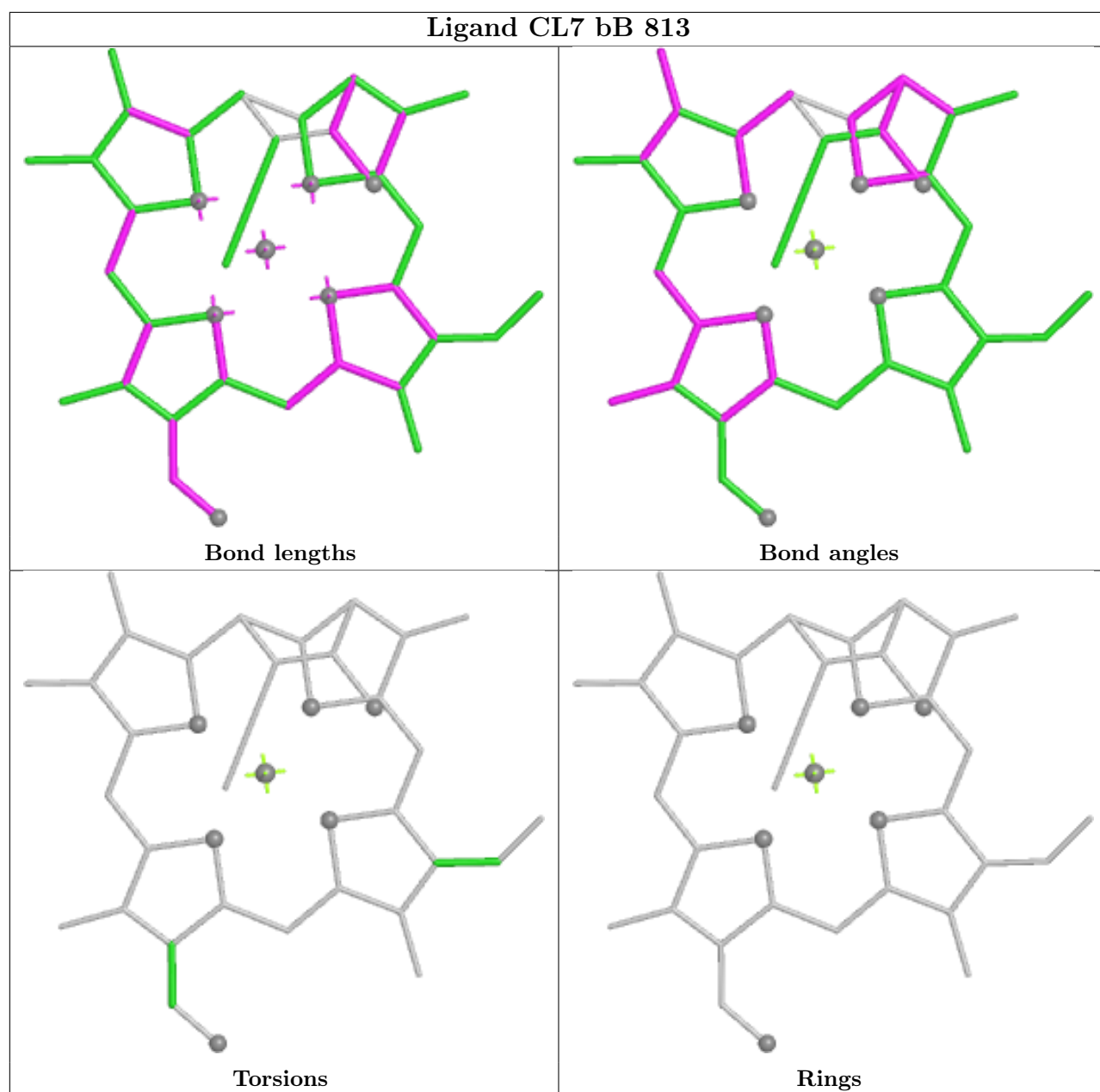


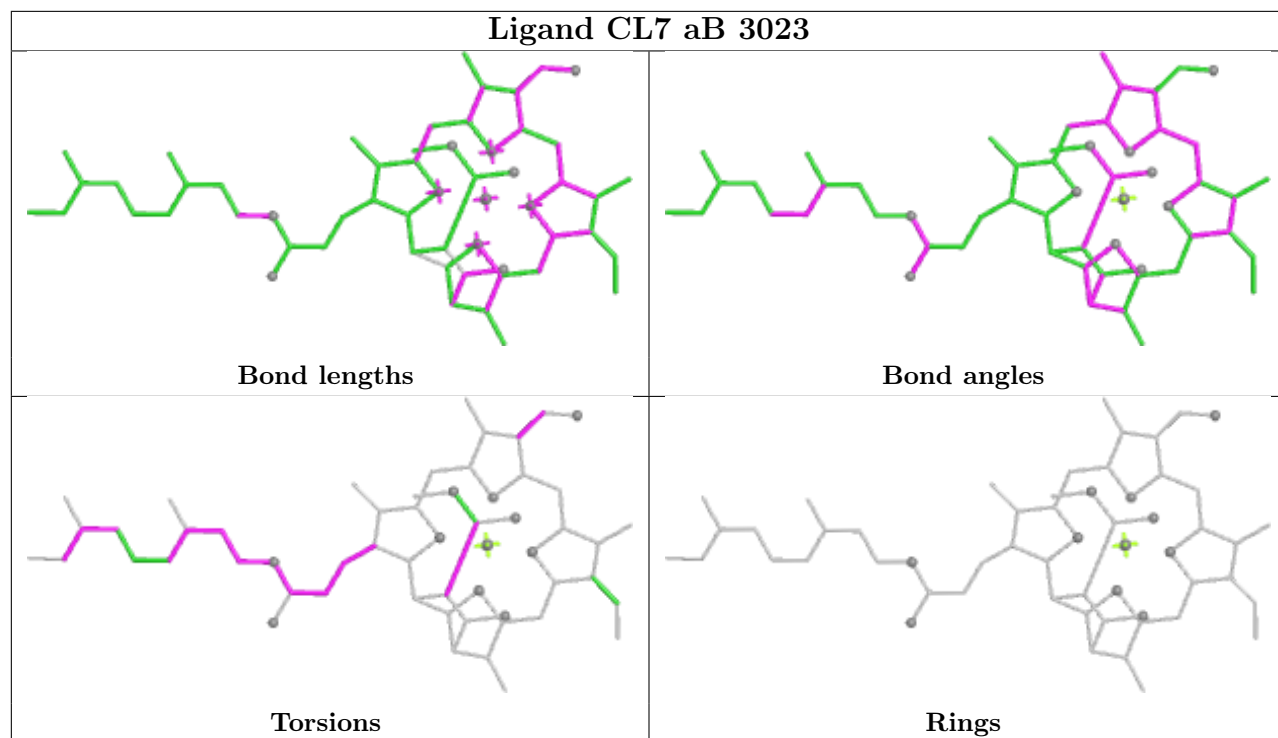
Rings



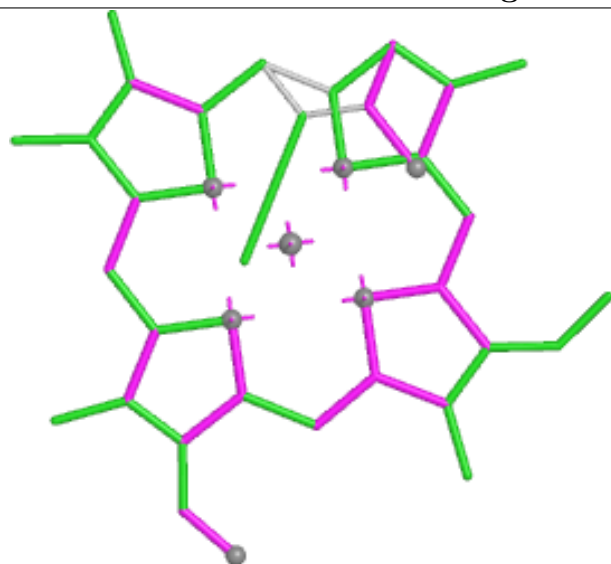




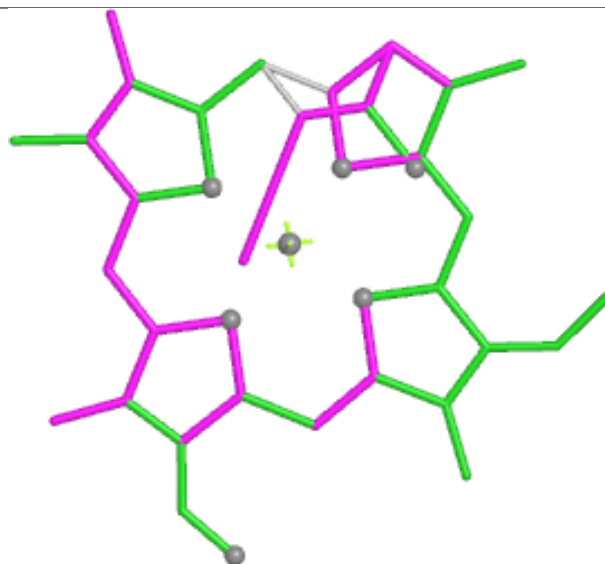




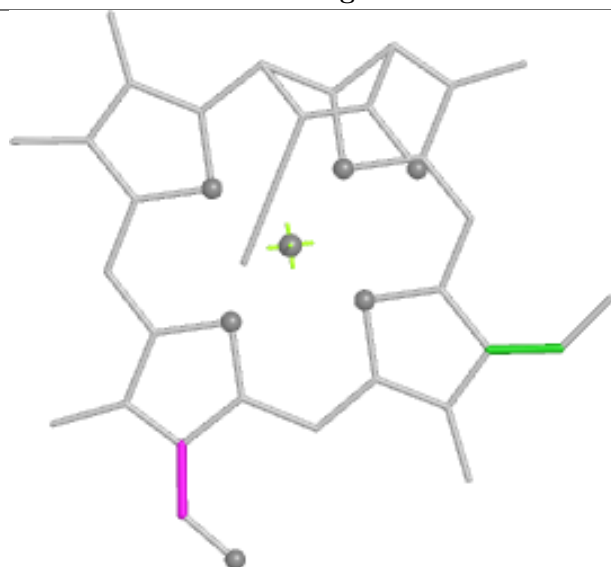
## Ligand CL7 aA 3118



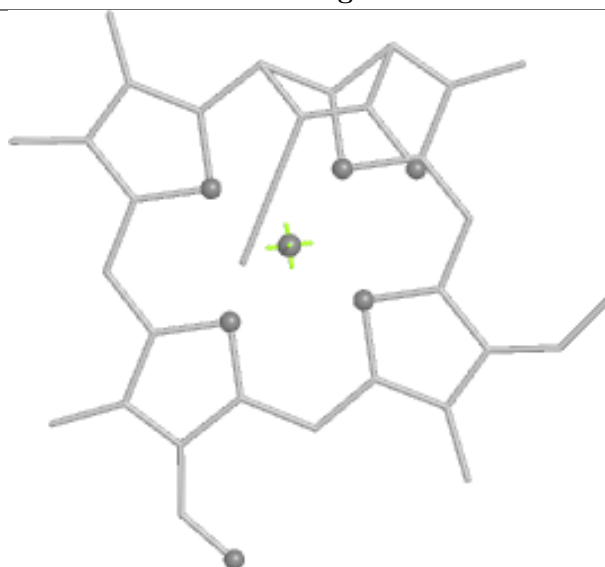
Bond lengths



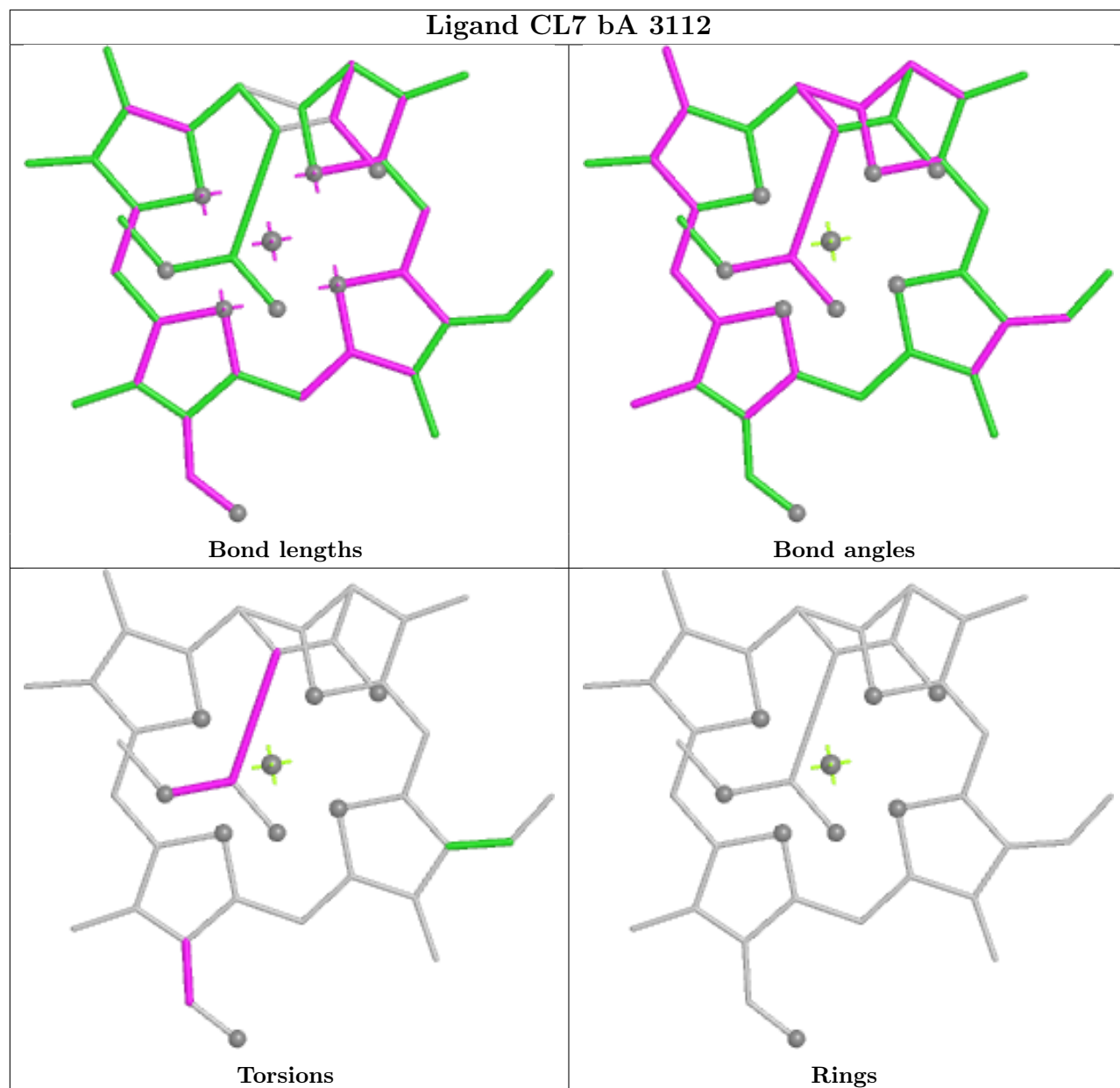
Bond angles



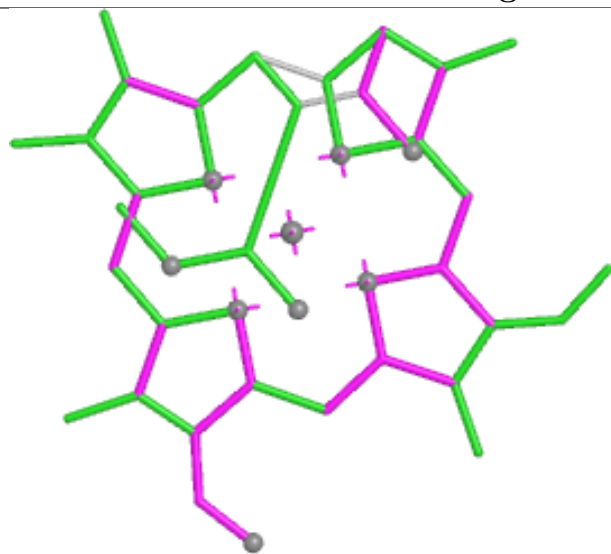
Torsions



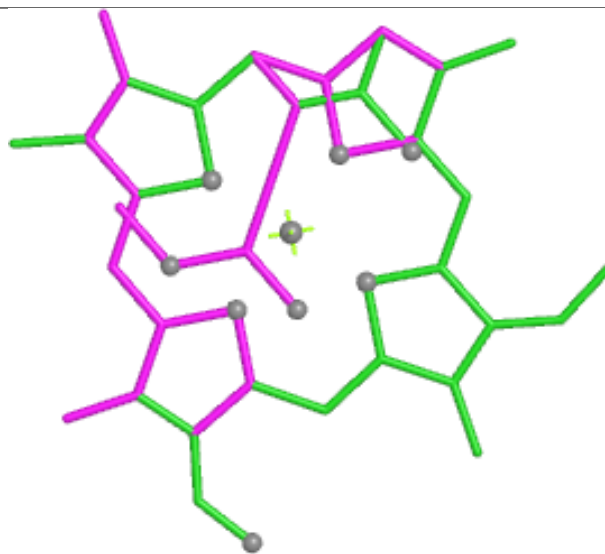
Rings



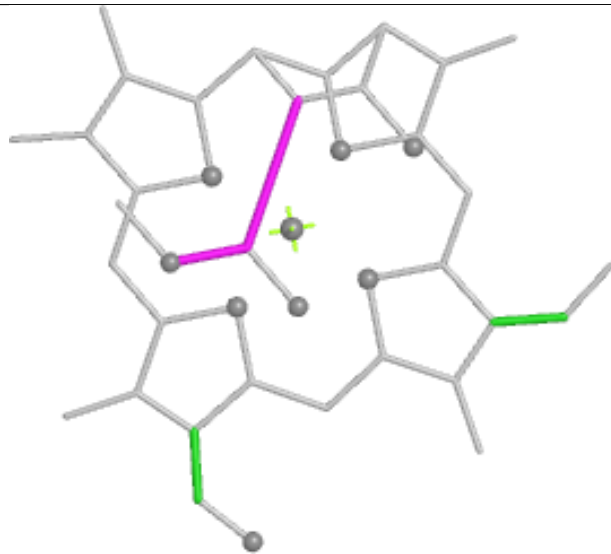
## Ligand CL7 bA 3110



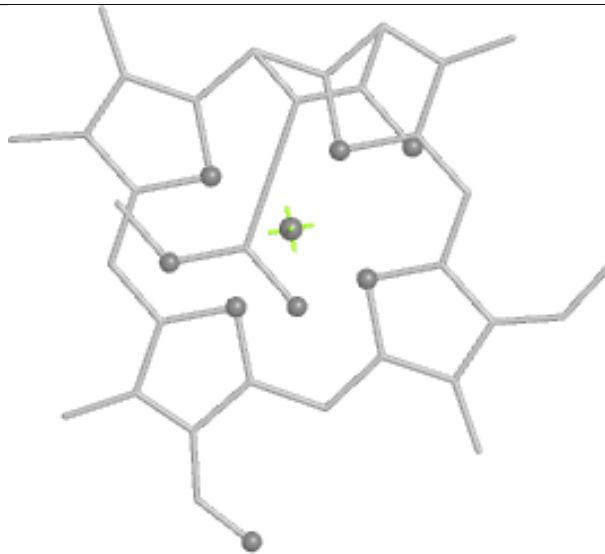
Bond lengths



Bond angles

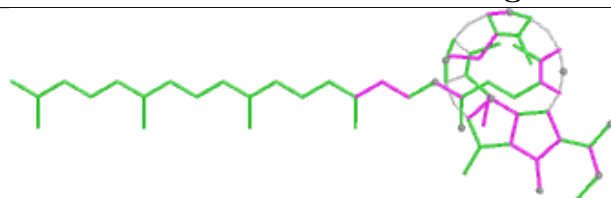


Torsions

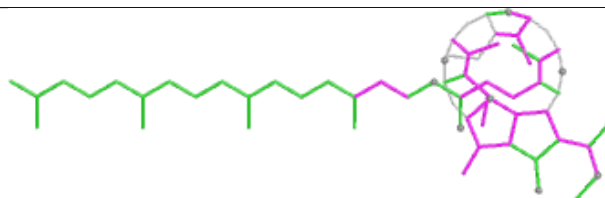


Rings

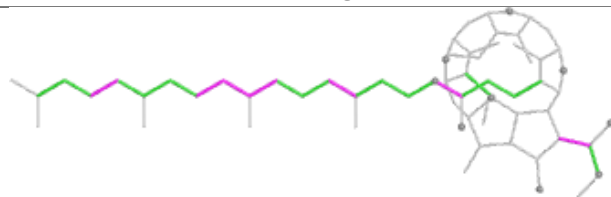
## Ligand PHO cB 801



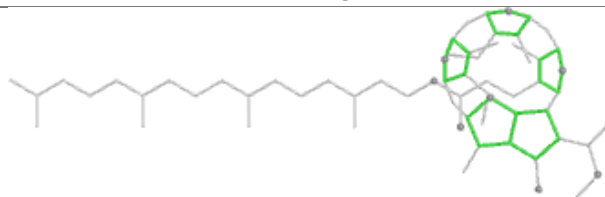
Bond lengths



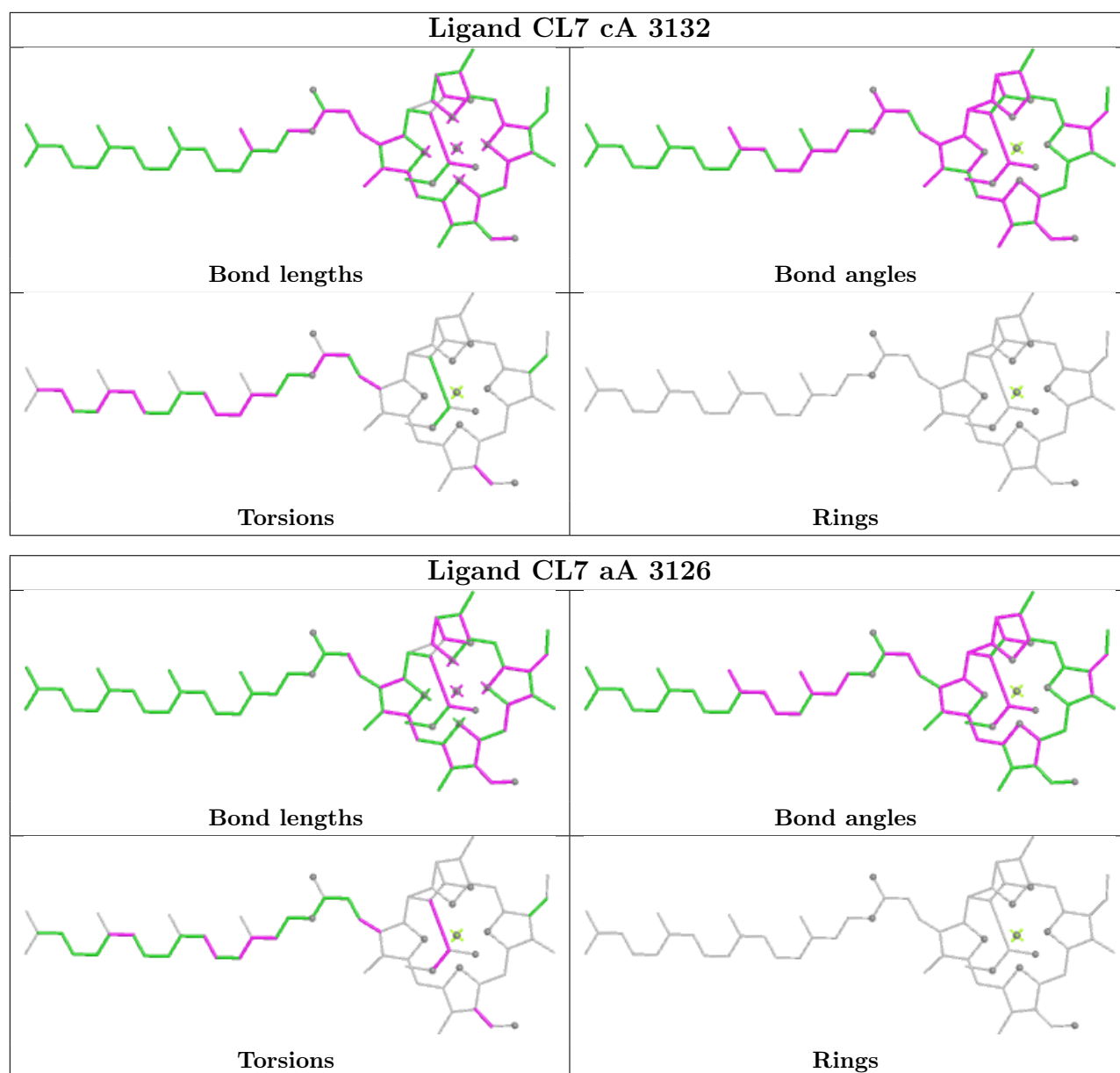
Bond angles



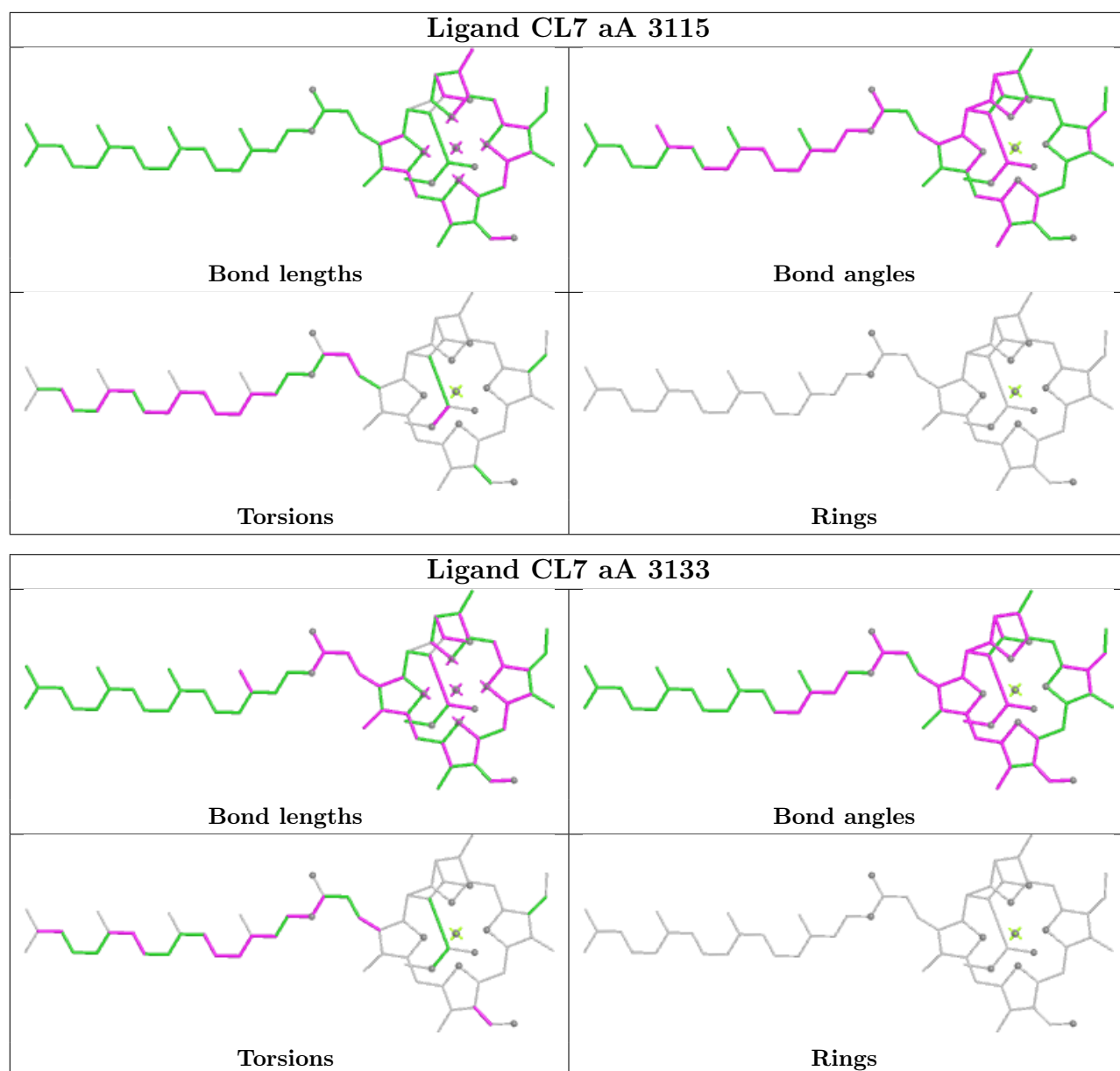
Torsions

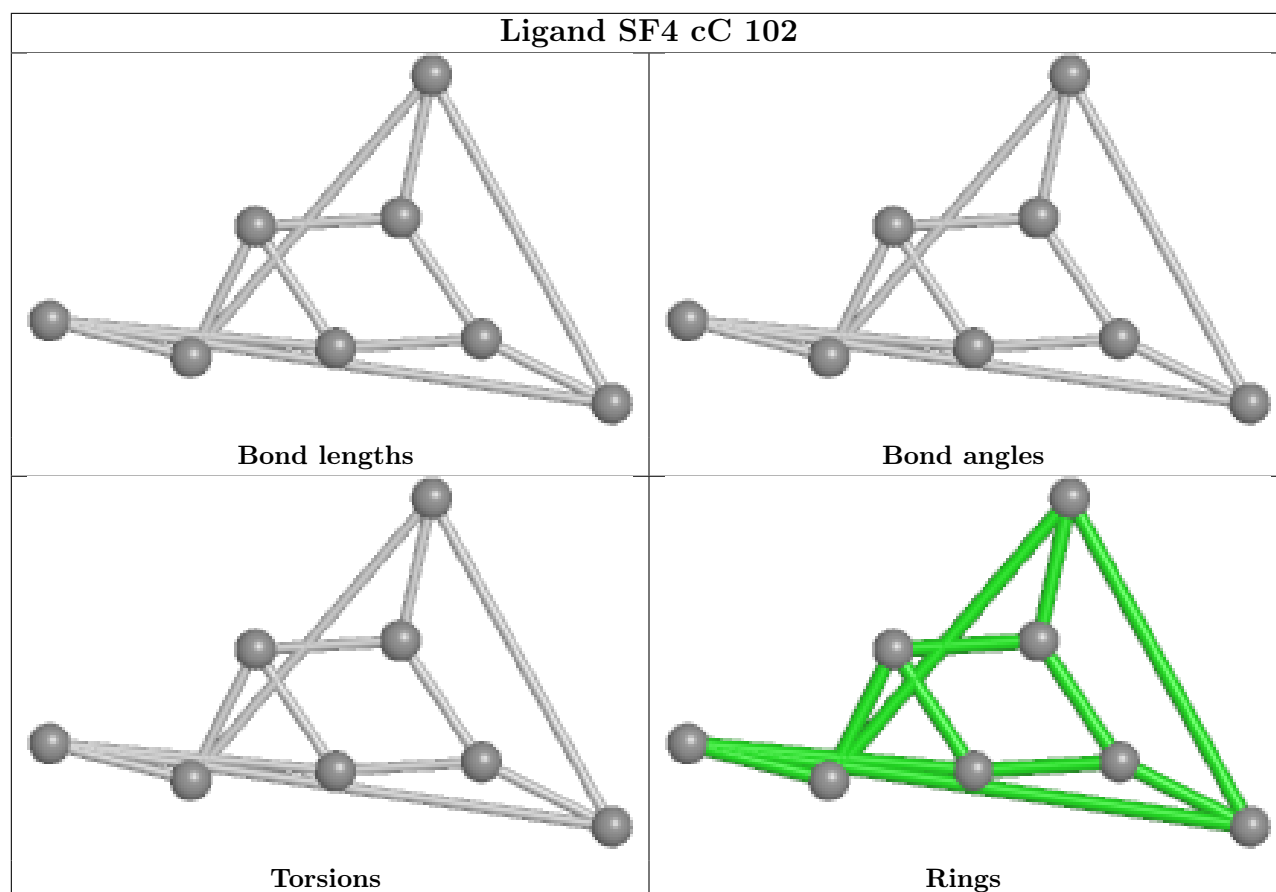
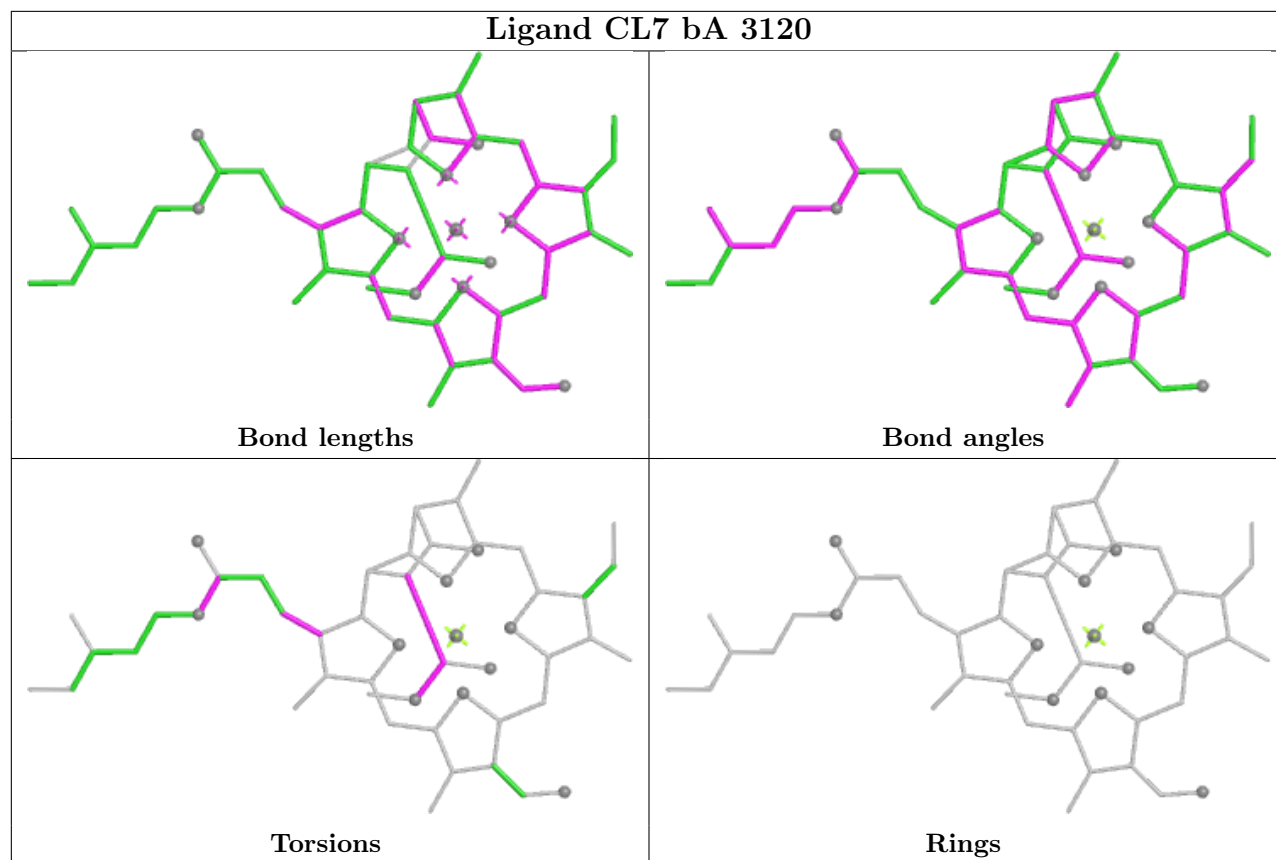


Rings









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

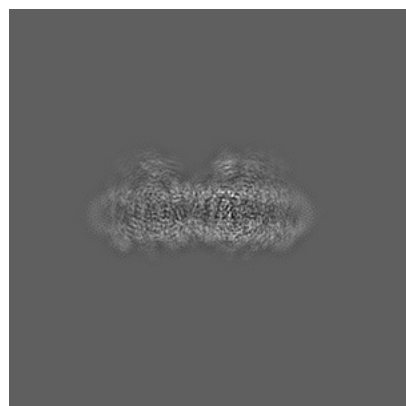
## 6 Map visualisation [i](#)

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

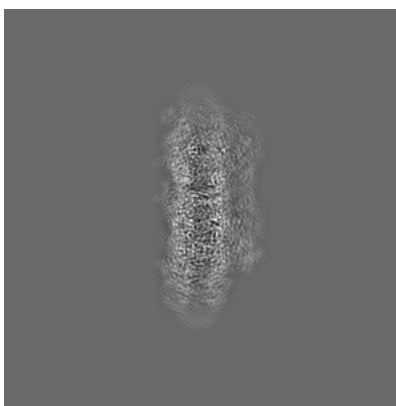
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

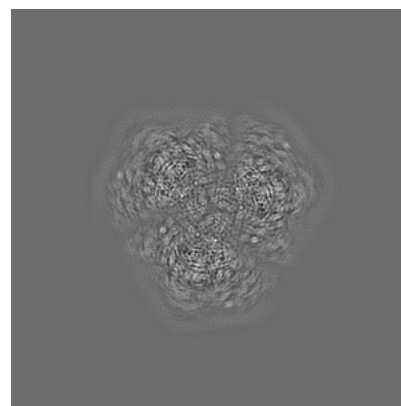
#### 6.1.1 Primary map



X

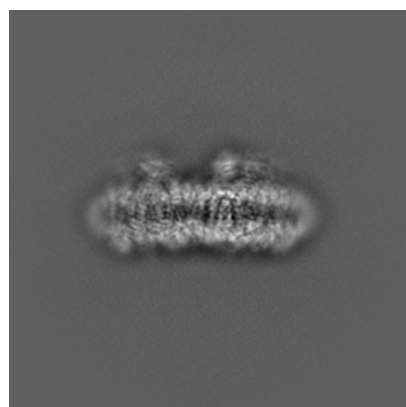


Y

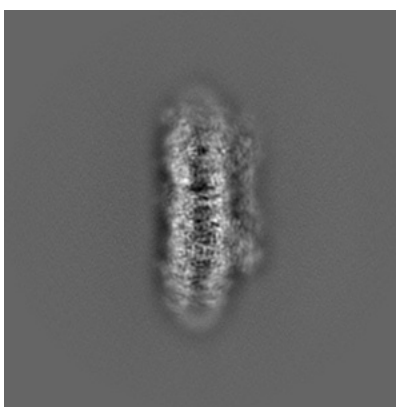


Z

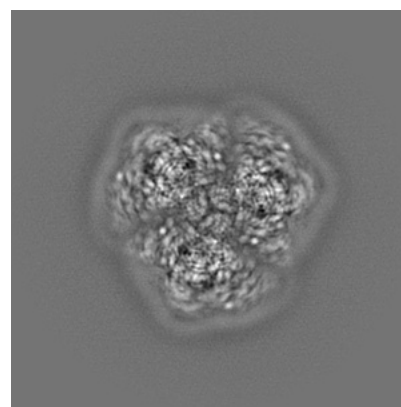
#### 6.1.2 Raw map



X



Y

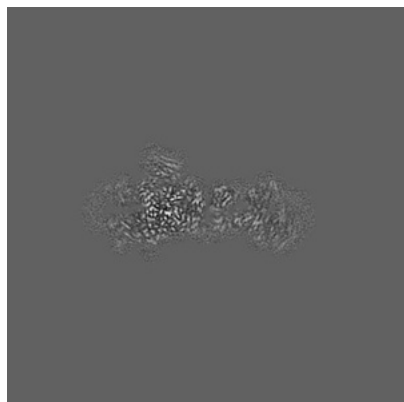


Z

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

## 6.2 Central slices [i](#)

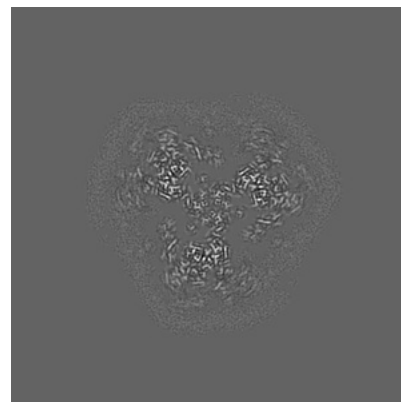
### 6.2.1 Primary map



X Index: 165

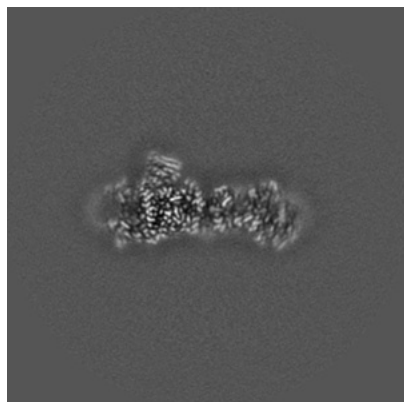


Y Index: 165

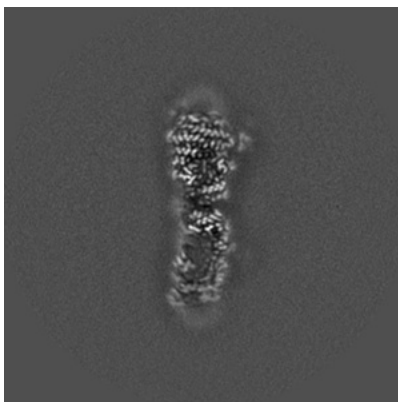


Z Index: 165

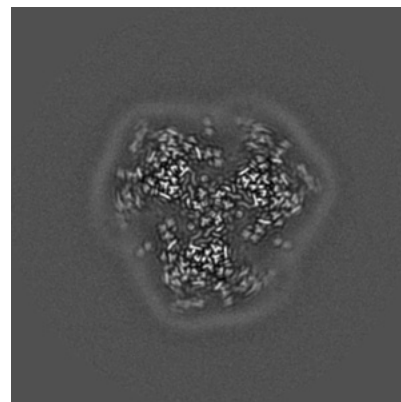
### 6.2.2 Raw map



X Index: 165



Y Index: 165

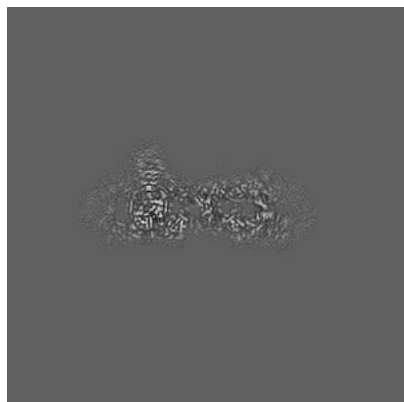


Z Index: 165

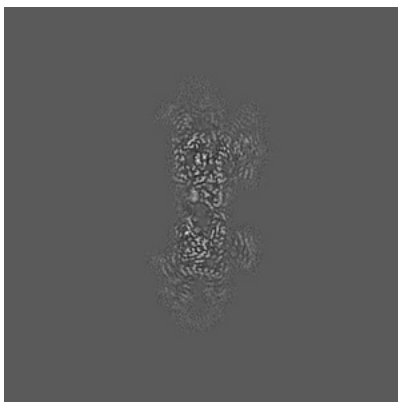
The images above show central slices of the map in three orthogonal directions.

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

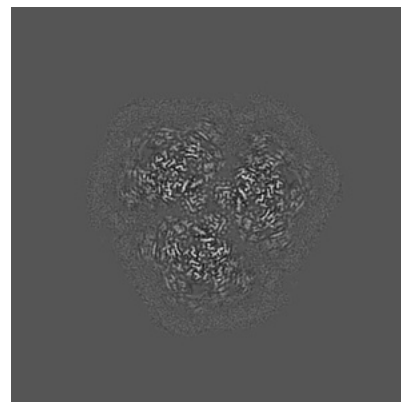
### 6.3.1 Primary map



X Index: 153

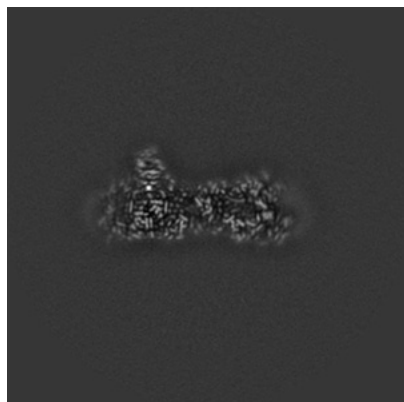


Y Index: 181

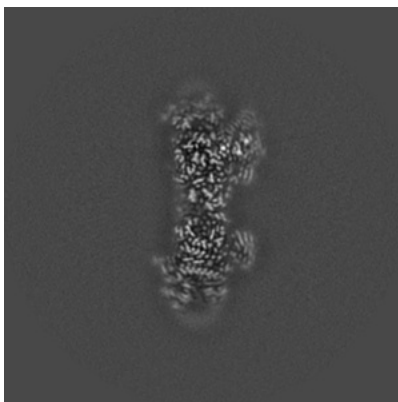


Z Index: 155

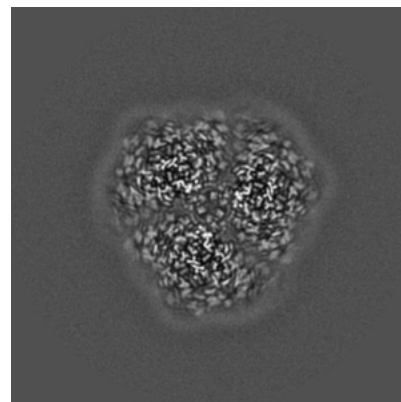
### 6.3.2 Raw map



X Index: 153



Y Index: 180

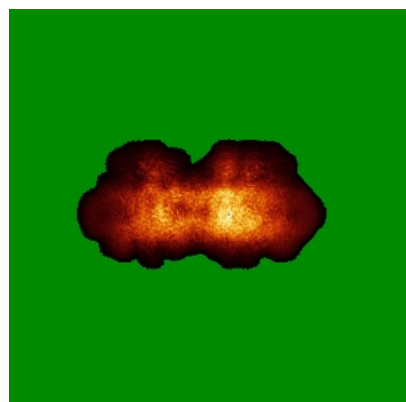


Z Index: 152

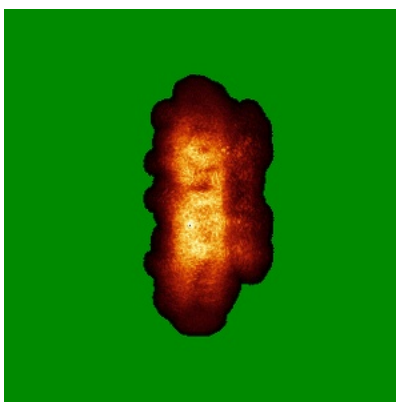
The images above show the largest variance slices of the map in three orthogonal directions.

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

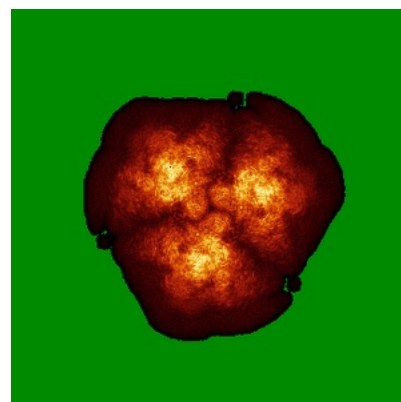
### 6.4.1 Primary map



X

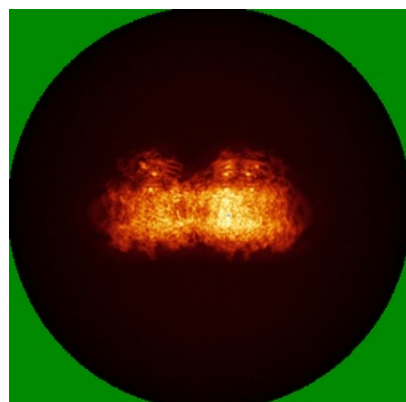


Y

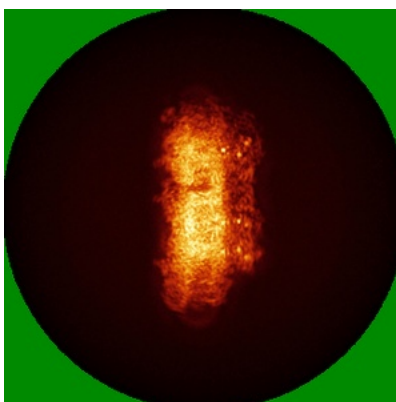


Z

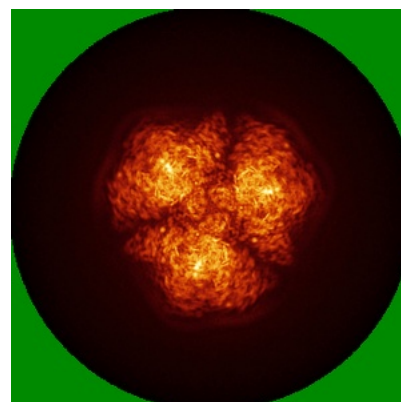
### 6.4.2 Raw map



X



Y

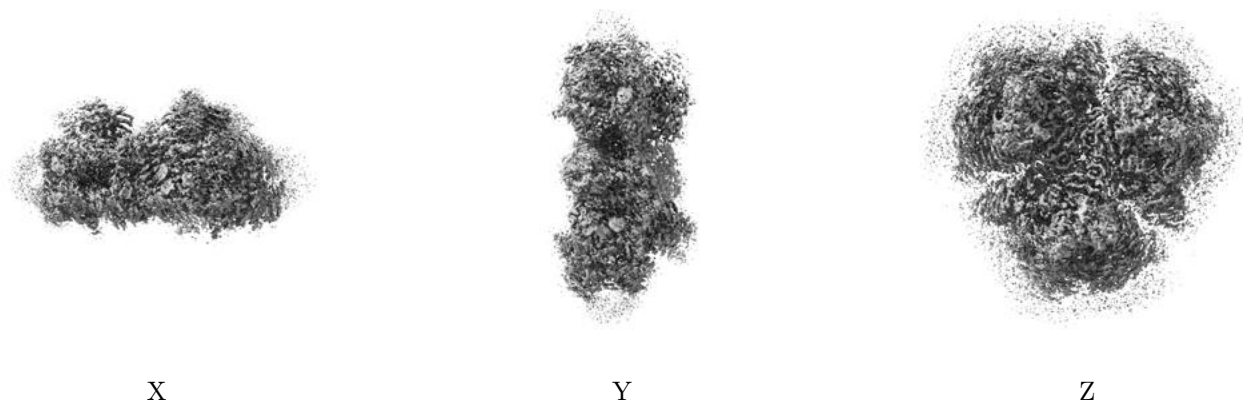


Z

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

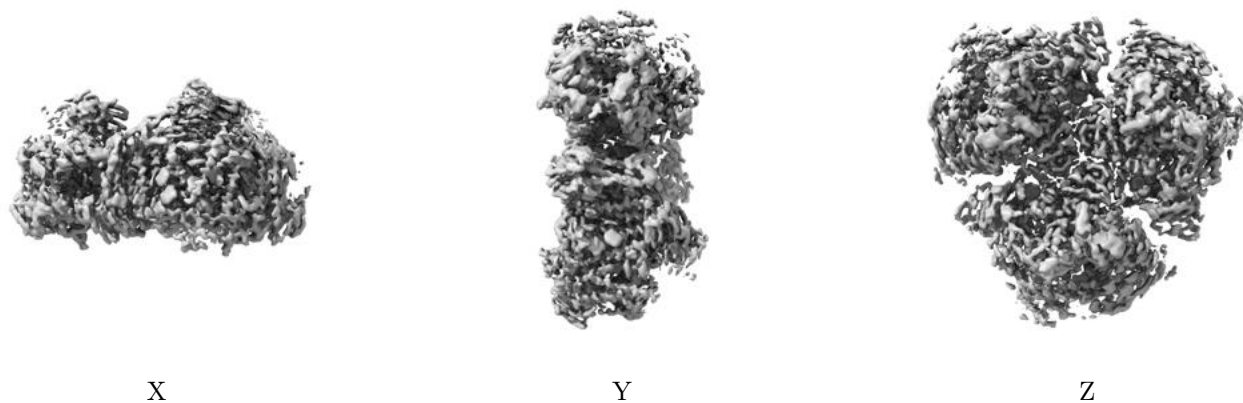
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00637. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

## 6.6 Mask visualisation [i](#)

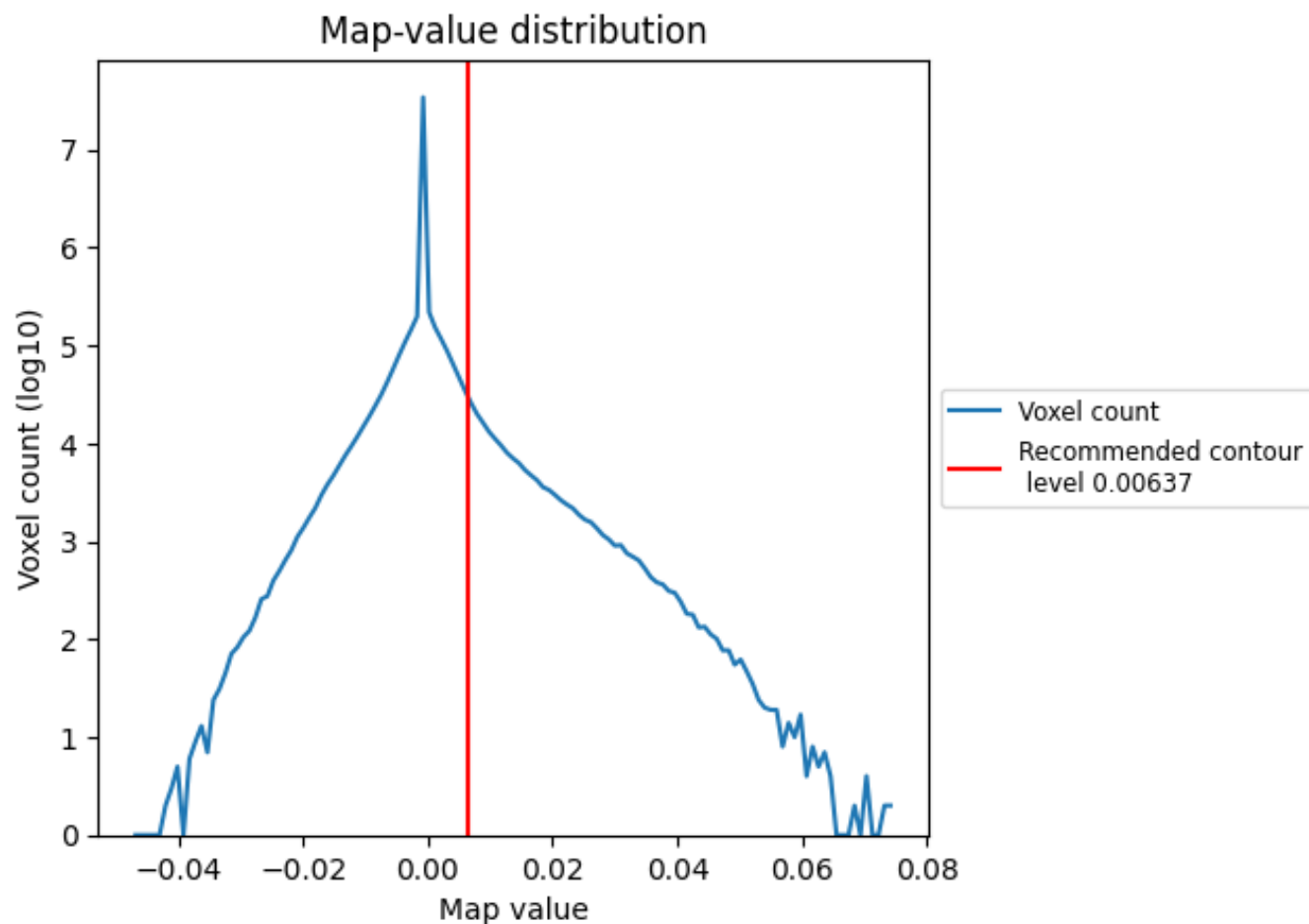
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

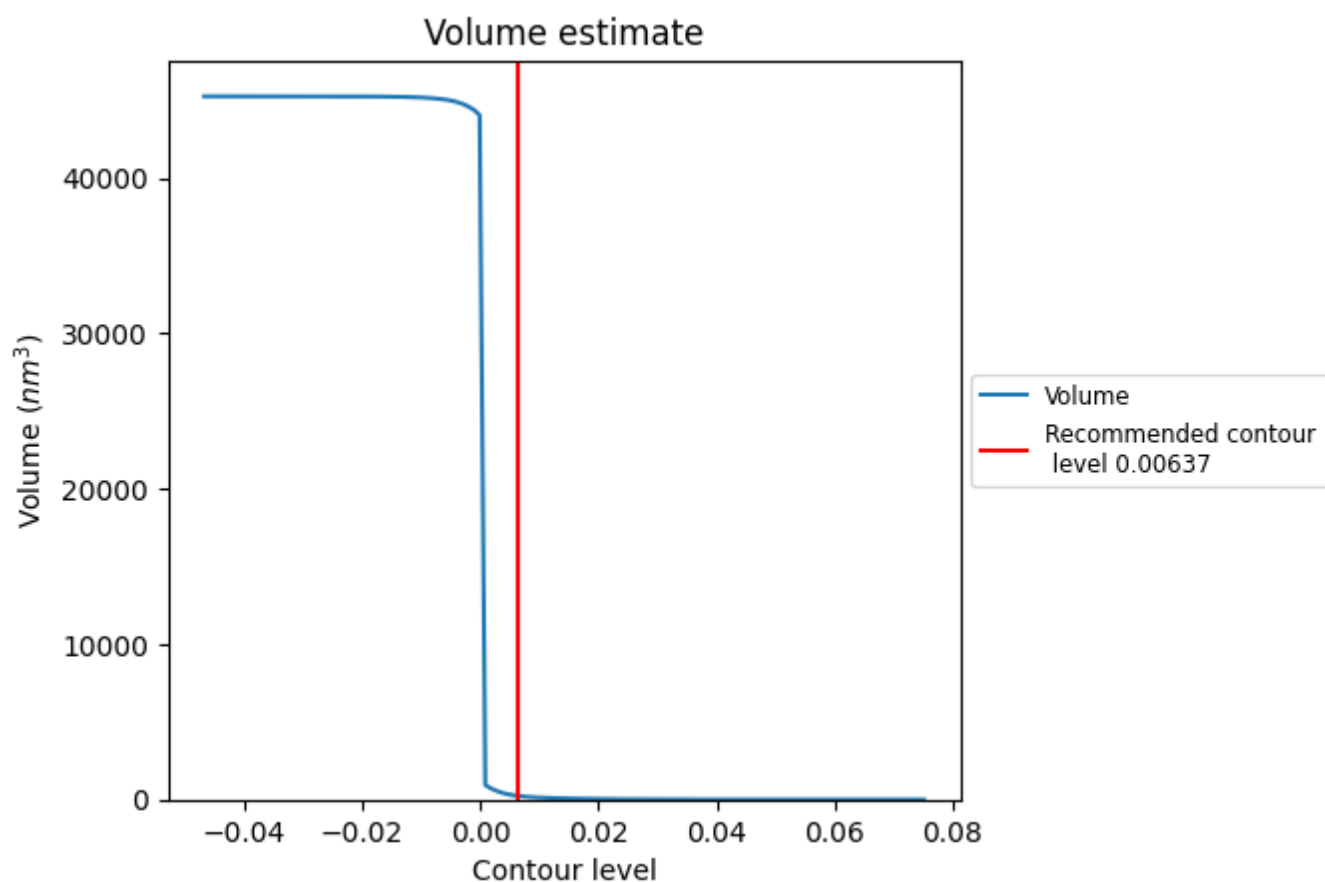
This section contains the results of statistical analysis of the map.

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



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

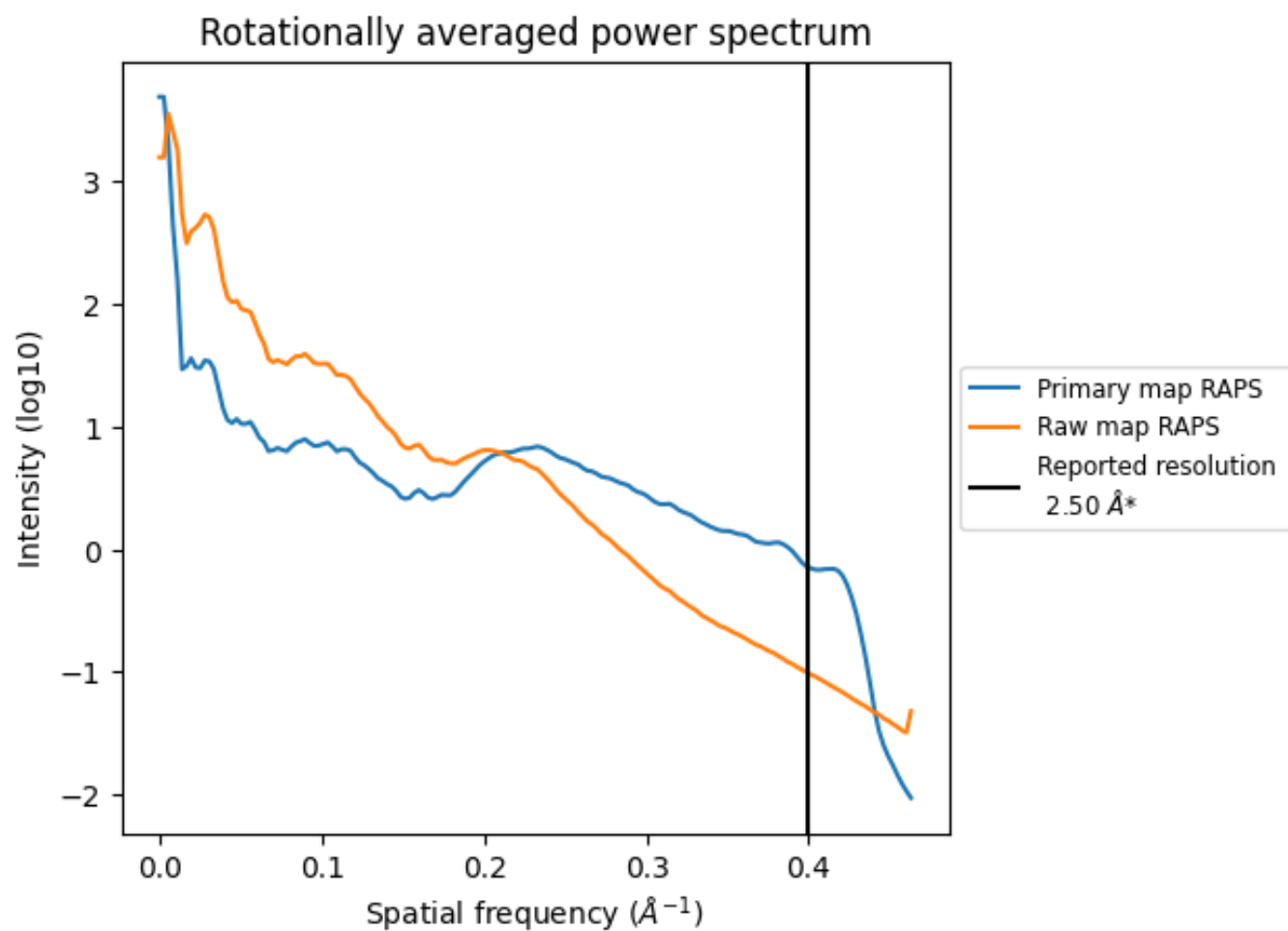
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 234 nm<sup>3</sup>; this corresponds to an approximate mass of 211 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

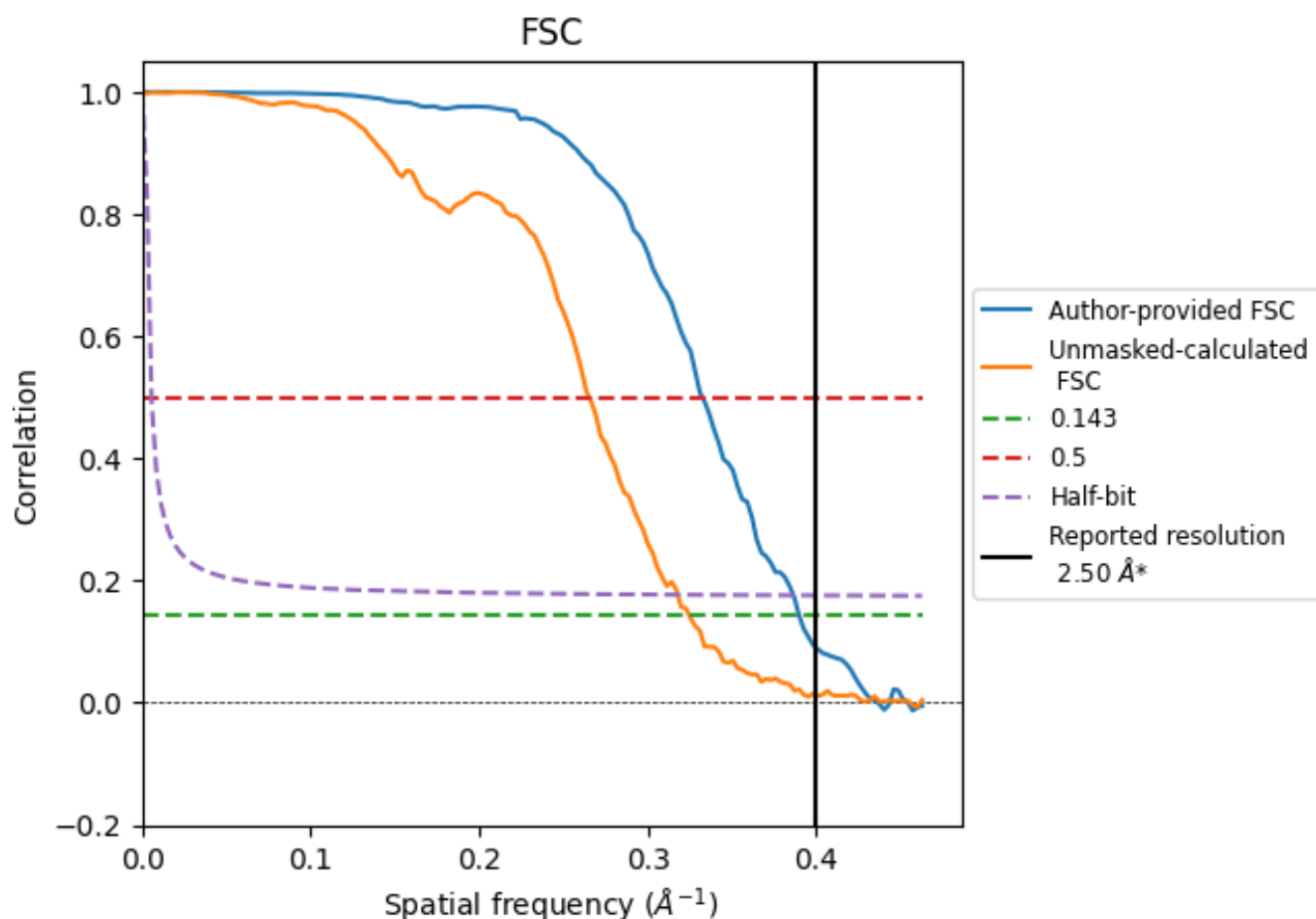


\*Reported resolution corresponds to spatial frequency of 0.400 Å<sup>-1</sup>

## 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 0.400 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

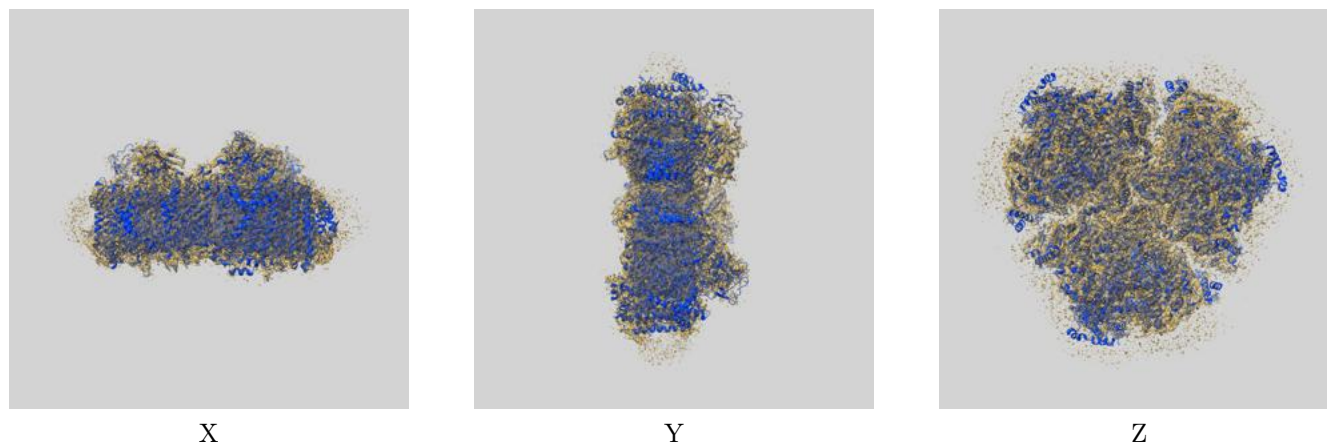
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.50           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

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

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

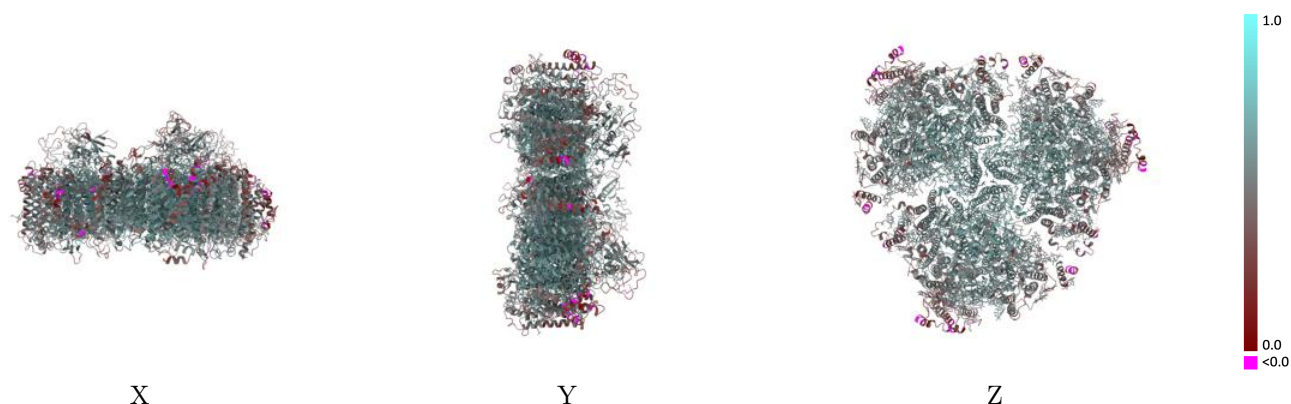
This section contains information regarding the fit between EMDB map EMD-30420 and PDB model 7COY. Per-residue inclusion information can be found in section [3](#) on page [30](#).

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



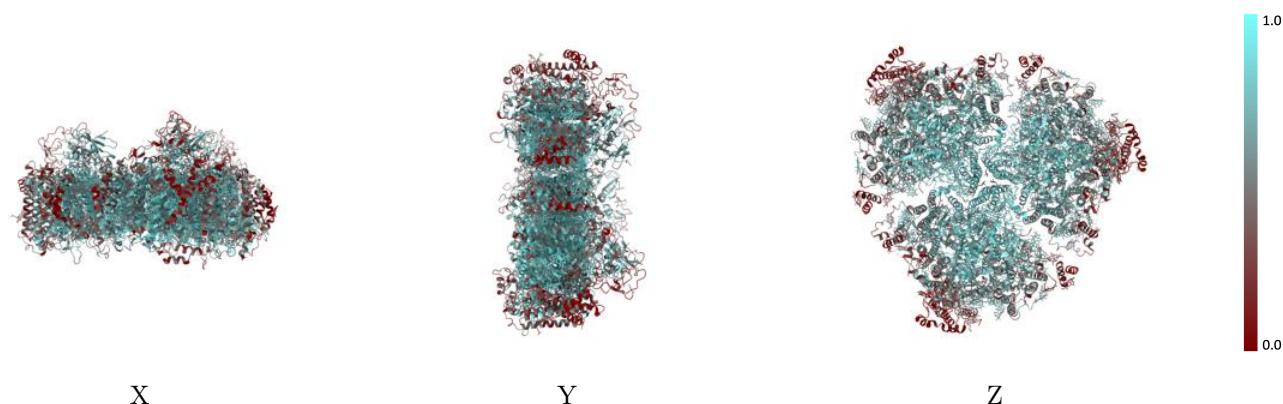
The images above show the 3D surface view of the map at the recommended contour level 0.00637 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



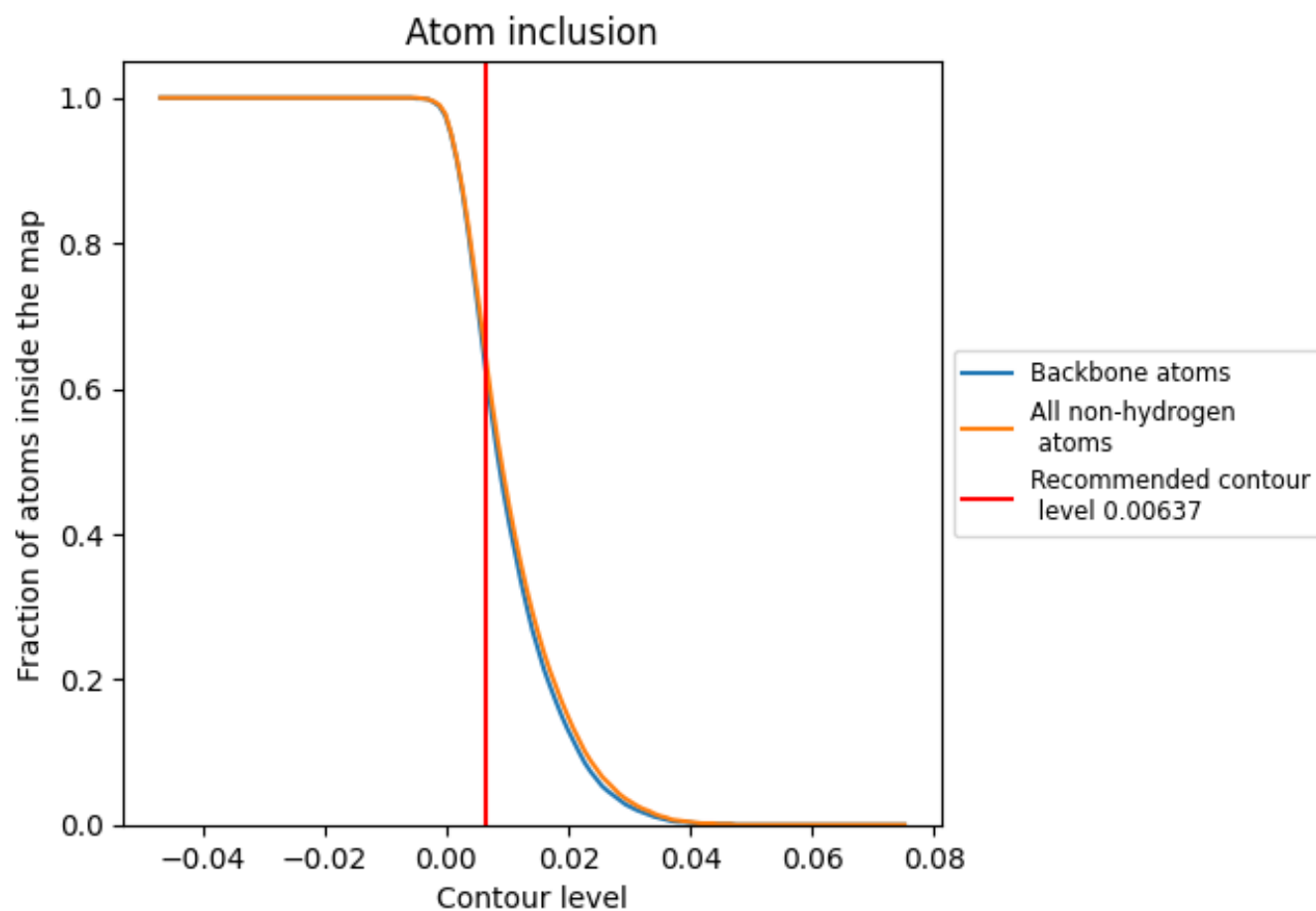
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 65% of all non-hydrogen atoms, are inside the map.



## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.00637) and Q-score for the entire model and for each chain.

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

