



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:12 PM GMT

PDB ID : 4KT0  
Title : Crystal structure of a virus like photosystem I from the cyanobacterium Synechocystis PCC 6803  
Authors : Mazor, Y.; Nataf, D.; Toporik, H.; Nelson, N.  
Deposited on : 2013-05-19  
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

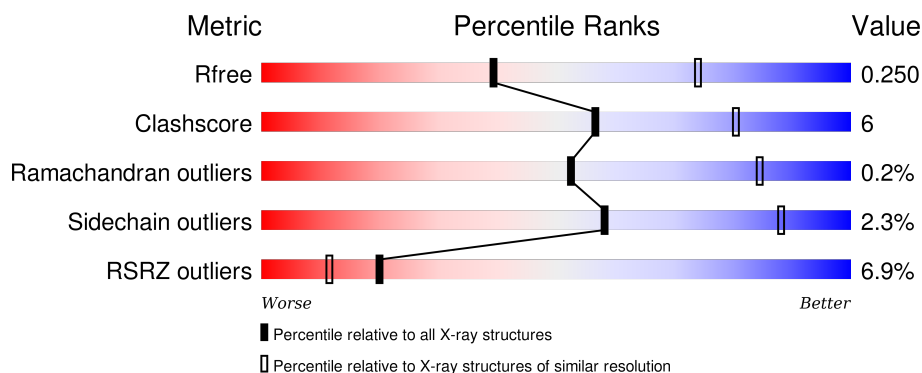
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 91344                       | 2393 (2.80-2.80)                                      |
| Clashscore            | 102246                      | 2827 (2.80-2.80)                                      |
| Ramachandran outliers | 100387                      | 2782 (2.80-2.80)                                      |
| Sidechain outliers    | 100360                      | 2784 (2.80-2.80)                                      |
| RSRZ outliers         | 91569                       | 2404 (2.80-2.80)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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 electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | A     | 751    | <div> <div>8%</div> <div>90%</div> <div>9%</div> </div>               |
| 2   | B     | 731    | <div> <div>3%</div> <div>91%</div> <div>8%</div> </div>               |
| 3   | C     | 81     | <div> <div>94%</div> <div>...</div> </div>                            |
| 4   | D     | 141    | <div> <div>17%</div> <div>89%</div> <div>8%</div> </div>              |
| 5   | E     | 74     | <div> <div>4%</div> <div>81%</div> <div>9%</div> <div>8%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 6   | F     | 165    |                  |
| 7   | J     | 40     |                  |
| 8   | K     | 128    |                  |
| 9   | M     | 31     |                  |

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

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 10  | PQN  | B     | 2002 | -         | -        | -       | X                |
| 11  | SF4  | A     | 3001 | -         | -        | -       | X                |
| 13  | CL0  | A     | 1011 | X         | -        | -       | -                |
| 13  | CL0  | A     | 1108 | X         | -        | -       | -                |
| 14  | BCR  | A     | 4003 | -         | -        | -       | X                |
| 14  | BCR  | A     | 4007 | -         | -        | -       | X                |
| 14  | BCR  | A     | 4012 | -         | -        | -       | X                |
| 14  | BCR  | B     | 4009 | -         | -        | -       | X                |
| 14  | BCR  | F     | 4015 | -         | -        | -       | X                |
| 14  | BCR  | J     | 4013 | -         | -        | -       | X                |
| 15  | CLA  | A     | 1012 | X         | -        | -       | -                |
| 15  | CLA  | A     | 1022 | X         | -        | -       | -                |
| 15  | CLA  | A     | 1101 | X         | -        | -       | -                |
| 15  | CLA  | A     | 1102 | X         | -        | -       | -                |
| 15  | CLA  | A     | 1103 | X         | -        | -       | -                |
| 15  | CLA  | A     | 1104 | X         | -        | -       | -                |
| 15  | CLA  | A     | 1105 | X         | -        | -       | -                |
| 15  | CLA  | A     | 1106 | X         | -        | -       | -                |
| 15  | CLA  | A     | 1107 | X         | -        | -       | -                |
| 15  | CLA  | A     | 1109 | X         | -        | -       | -                |
| 15  | CLA  | A     | 1110 | X         | -        | -       | -                |
| 15  | CLA  | A     | 1111 | X         | -        | -       | -                |
| 15  | CLA  | A     | 1112 | X         | -        | -       | -                |
| 15  | CLA  | A     | 1113 | X         | -        | -       | -                |
| 15  | CLA  | A     | 1114 | X         | -        | -       | -                |
| 15  | CLA  | A     | 1115 | X         | -        | -       | -                |
| 15  | CLA  | A     | 1116 | X         | -        | -       | -                |
| 15  | CLA  | A     | 1117 | X         | -        | -       | X                |
| 15  | CLA  | A     | 1118 | X         | -        | -       | -                |
| 15  | CLA  | A     | 1119 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 15  | CLA  | A     | 1120 | X         | -        | -       | -                |
| 15  | CLA  | A     | 1121 | X         | -        | -       | X                |
| 15  | CLA  | A     | 1122 | X         | -        | -       | -                |
| 15  | CLA  | A     | 1123 | X         | -        | -       | -                |
| 15  | CLA  | A     | 1124 | X         | -        | -       | -                |
| 15  | CLA  | A     | 1125 | X         | -        | -       | -                |
| 15  | CLA  | A     | 1126 | X         | -        | -       | -                |
| 15  | CLA  | A     | 1127 | X         | -        | -       | X                |
| 15  | CLA  | A     | 1128 | X         | -        | -       | -                |
| 15  | CLA  | A     | 1129 | X         | -        | -       | -                |
| 15  | CLA  | A     | 1130 | X         | -        | -       | -                |
| 15  | CLA  | A     | 1131 | X         | -        | -       | -                |
| 15  | CLA  | A     | 1132 | X         | -        | -       | -                |
| 15  | CLA  | A     | 1133 | X         | -        | -       | -                |
| 15  | CLA  | A     | 1134 | X         | -        | -       | -                |
| 15  | CLA  | A     | 1135 | X         | -        | -       | -                |
| 15  | CLA  | A     | 1136 | X         | -        | -       | -                |
| 15  | CLA  | A     | 1137 | X         | -        | -       | -                |
| 15  | CLA  | A     | 1138 | X         | -        | -       | -                |
| 15  | CLA  | A     | 1140 | X         | -        | -       | -                |
| 15  | CLA  | A     | 1801 | X         | -        | -       | X                |
| 15  | CLA  | B     | 1013 | X         | -        | -       | -                |
| 15  | CLA  | B     | 1021 | X         | -        | -       | -                |
| 15  | CLA  | B     | 1023 | X         | -        | -       | -                |
| 15  | CLA  | B     | 1201 | X         | -        | -       | -                |
| 15  | CLA  | B     | 1202 | X         | -        | -       | -                |
| 15  | CLA  | B     | 1203 | X         | -        | -       | -                |
| 15  | CLA  | B     | 1204 | X         | -        | -       | -                |
| 15  | CLA  | B     | 1205 | X         | -        | -       | -                |
| 15  | CLA  | B     | 1206 | X         | -        | -       | -                |
| 15  | CLA  | B     | 1207 | X         | -        | -       | -                |
| 15  | CLA  | B     | 1208 | X         | -        | -       | -                |
| 15  | CLA  | B     | 1209 | X         | -        | -       | -                |
| 15  | CLA  | B     | 1210 | X         | -        | -       | -                |
| 15  | CLA  | B     | 1211 | X         | -        | -       | -                |
| 15  | CLA  | B     | 1212 | X         | -        | -       | -                |
| 15  | CLA  | B     | 1213 | X         | -        | -       | -                |
| 15  | CLA  | B     | 1214 | X         | -        | -       | -                |
| 15  | CLA  | B     | 1215 | X         | -        | -       | -                |
| 15  | CLA  | B     | 1216 | X         | -        | -       | -                |
| 15  | CLA  | B     | 1217 | X         | -        | -       | -                |
| 15  | CLA  | B     | 1218 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 15  | CLA  | B     | 1219 | X         | -        | -       | -                |
| 15  | CLA  | B     | 1220 | X         | -        | -       | -                |
| 15  | CLA  | B     | 1221 | X         | -        | -       | -                |
| 15  | CLA  | B     | 1222 | X         | -        | -       | -                |
| 15  | CLA  | B     | 1223 | X         | -        | -       | -                |
| 15  | CLA  | B     | 1224 | X         | -        | -       | -                |
| 15  | CLA  | B     | 1225 | X         | -        | -       | -                |
| 15  | CLA  | B     | 1226 | X         | -        | -       | -                |
| 15  | CLA  | B     | 1227 | X         | -        | -       | -                |
| 15  | CLA  | B     | 1228 | X         | -        | -       | -                |
| 15  | CLA  | B     | 1229 | X         | -        | -       | -                |
| 15  | CLA  | B     | 1230 | X         | -        | -       | -                |
| 15  | CLA  | B     | 1231 | X         | -        | -       | -                |
| 15  | CLA  | B     | 1232 | X         | -        | -       | -                |
| 15  | CLA  | B     | 1234 | X         | -        | -       | -                |
| 15  | CLA  | B     | 1235 | X         | -        | -       | -                |
| 15  | CLA  | B     | 1236 | X         | -        | -       | -                |
| 15  | CLA  | B     | 1237 | X         | -        | -       | -                |
| 15  | CLA  | B     | 1238 | X         | -        | -       | -                |
| 15  | CLA  | B     | 1239 | X         | -        | -       | -                |
| 15  | CLA  | B     | 1240 | X         | -        | -       | -                |
| 15  | CLA  | F     | 1139 | X         | -        | -       | -                |
| 15  | CLA  | F     | 1301 | X         | -        | -       | -                |
| 15  | CLA  | F     | 1410 | X         | -        | -       | X                |
| 15  | CLA  | J     | 1302 | X         | -        | -       | X                |
| 15  | CLA  | J     | 1303 | X         | -        | -       | X                |
| 15  | CLA  | K     | 1401 | X         | -        | -       | -                |
| 15  | CLA  | K     | 1402 | X         | -        | -       | -                |

## 2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 22051 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 739      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 5787  | 3791 | 984 | 985 | 27 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | B     | 728      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 5765  | 3796 | 966 | 988 | 15 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 3   | C     | 80       | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 600   | 369 | 103 | 117 | 11 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4   | D     | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1075  | 681 | 187 | 204 | 3 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---------|---------|-------|
| 5   | E     | 68       | Total | C   | N  | O   | 0       | 0       | 0     |
|     |       |          | 533   | 335 | 94 | 104 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | F     | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1099  | 711 | 183 | 200 | 5 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 7   | J     | 40       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 319   | 215 | 47 | 54 | 3 |         |         |       |

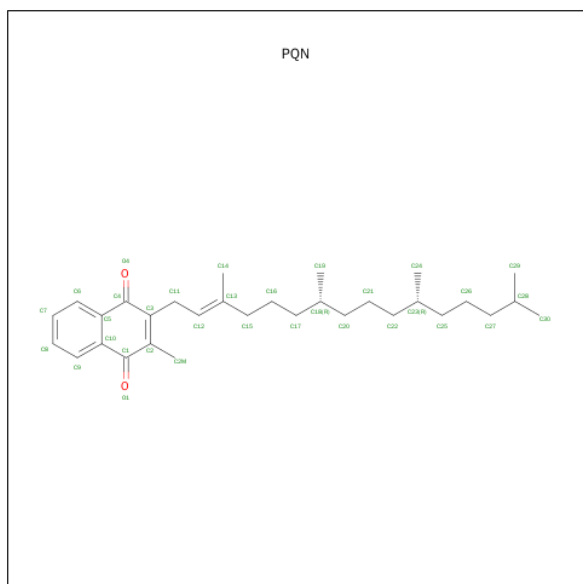
- Molecule 8 is a protein called Photosystem I reaction center subunit PsaK.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 8   | K     | 53       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 366   | 242 | 56 | 63 | 5 |         |         |       |

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

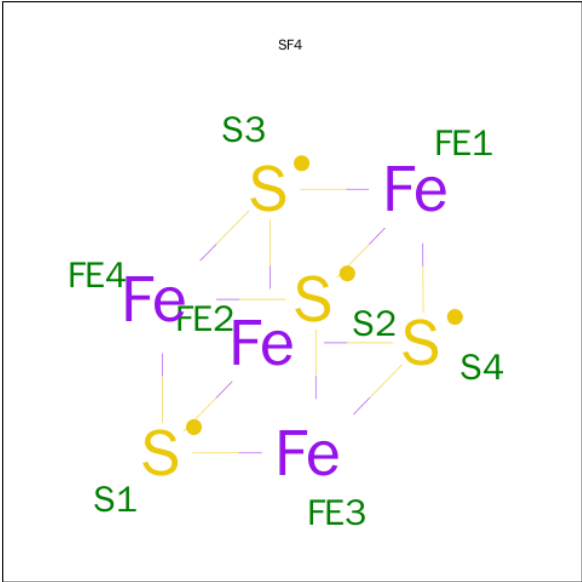
| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 9   | M     | 30       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 214   | 142 | 34 | 38 |         |         |       |

- Molecule 10 is PHYLLOQUINONE (three-letter code: PQN) (formula:  $C_{31}H_{46}O_2$ ).



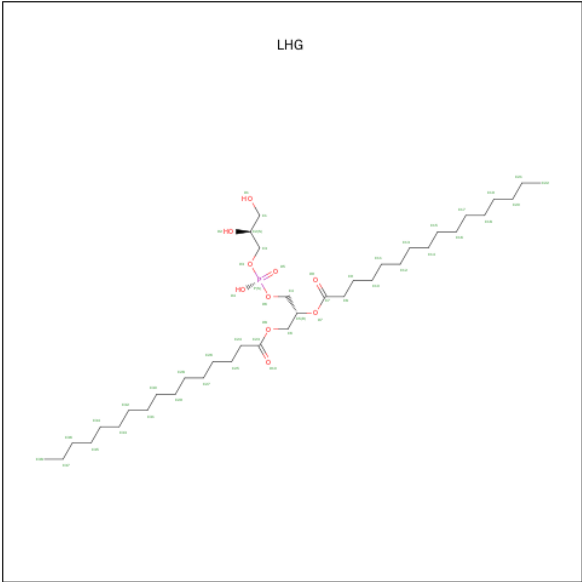
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 10  | A     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 33    | 31 | 2 |         |         |
| 10  | B     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 33    | 31 | 2 |         |         |

- Molecule 11 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $Fe_4S_4$ ).



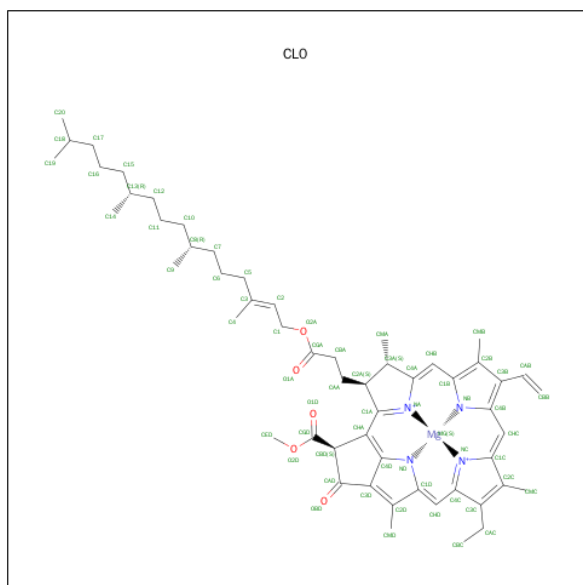
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 11  | A     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 11  | C     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 11  | C     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |

- Molecule 12 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



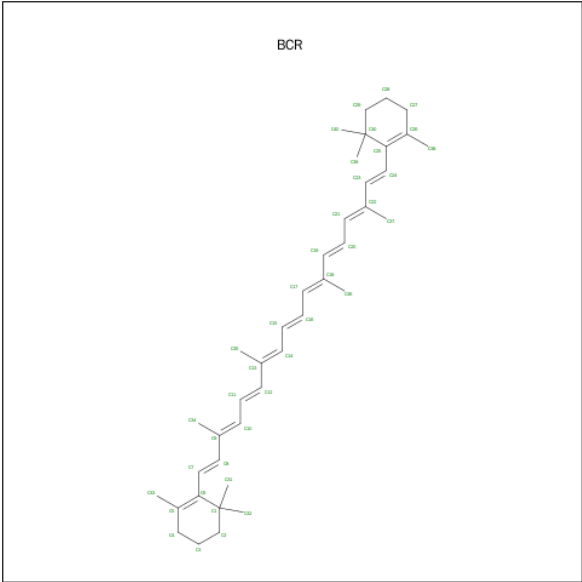
| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 12  | A     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |         |
| 12  | A     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |         |
| 12  | A     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 36    | 25 | 10 | 1 |         |         |
| 12  | B     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |         |

- Molecule 13 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula:  $C_{55}H_{72}MgN_4O_5$ ).



| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 13  | A     | 1        | Total | C  | Mg | N | O       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5       | 0       |
| 13  | A     | 1        | Total | C  | Mg | N | O       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5       | 0       |

- Molecule 14 is BETA-CAROTENE (three-letter code: BCR) (formula:  $C_{40}H_{56}$ ).



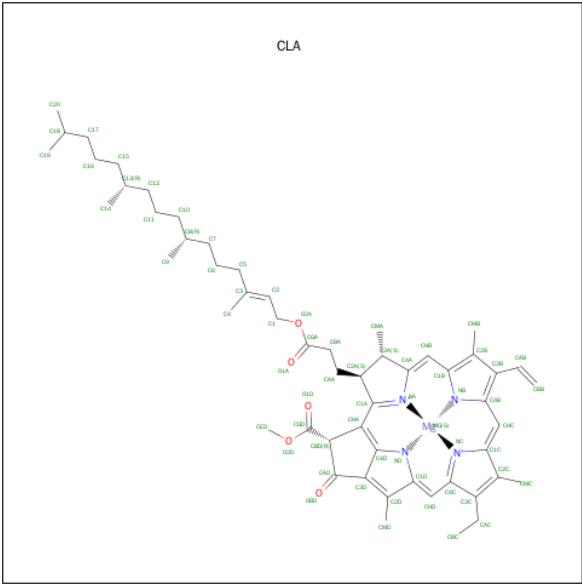
| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 14  | A     | 1        | Total C<br>40 40 | 0       | 0       |
| 14  | A     | 1        | Total C<br>40 40 | 0       | 0       |
| 14  | A     | 1        | Total C<br>40 40 | 0       | 0       |
| 14  | A     | 1        | Total C<br>40 40 | 0       | 0       |
| 14  | A     | 1        | Total C<br>40 40 | 0       | 0       |
| 14  | A     | 1        | Total C<br>40 40 | 0       | 0       |
| 14  | B     | 1        | Total C<br>40 40 | 0       | 0       |
| 14  | B     | 1        | Total C<br>40 40 | 0       | 0       |
| 14  | B     | 1        | Total C<br>40 40 | 0       | 0       |
| 14  | B     | 1        | Total C<br>40 40 | 0       | 0       |
| 14  | B     | 1        | Total C<br>40 40 | 0       | 0       |
| 14  | B     | 1        | Total C<br>40 40 | 0       | 0       |
| 14  | B     | 1        | Total C<br>40 40 | 0       | 0       |
| 14  | B     | 1        | Total C<br>40 40 | 0       | 0       |

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| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 14  | F     | 1        | Total C<br>40 40 | 0       | 0       |
| 14  | F     | 1        | Total C<br>40 40 | 0       | 0       |
| 14  | J     | 1        | Total C<br>40 40 | 0       | 0       |

- Molecule 15 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



| Mol | Chain | Residues | Atoms                         | ZeroOcc | AltConf |
|-----|-------|----------|-------------------------------|---------|---------|
| 15  | A     | 1        | Total C Mg N O<br>52 42 1 4 5 | 0       | 0       |
| 15  | A     | 1        | Total C Mg N O<br>65 55 1 4 5 | 0       | 0       |
| 15  | A     | 1        | Total C Mg N O<br>65 55 1 4 5 | 0       | 0       |
| 15  | A     | 1        | Total C Mg N O<br>65 55 1 4 5 | 0       | 0       |
| 15  | A     | 1        | Total C Mg N O<br>65 55 1 4 5 | 0       | 0       |
| 15  | A     | 1        | Total C Mg N O<br>65 55 1 4 5 | 0       | 0       |
| 15  | A     | 1        | Total C Mg N O<br>65 55 1 4 5 | 0       | 0       |

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| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 15  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |         |
| 15  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 15  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |         |
| 15  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |         |
| 15  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 15  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 15  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |         |
| 15  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 15  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |         |
| 15  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 64    | 54 | 1  | 4 | 5 |         |         |
| 15  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 15  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 15  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |         |
| 15  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 52    | 42 | 1  | 4 | 5 |         |         |
| 15  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 15  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 15  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 15  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 15  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |         |
| 15  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 15  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 15  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 15  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 49    | 39 | 1  | 4 | 5 |         |         |
| 15  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |         |
| 15  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 49    | 39 | 1  | 4 | 5 |         |         |
| 15  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |         |
| 15  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |         |
| 15  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |         |
| 15  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |         |
| 15  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 62    | 52 | 1  | 4 | 5 |         |         |
| 15  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |         |
| 15  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |         |
| 15  | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |         |
| 15  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 15  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 15  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 15  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 15  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 15  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |         |
| 15  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |         |
| 15  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |

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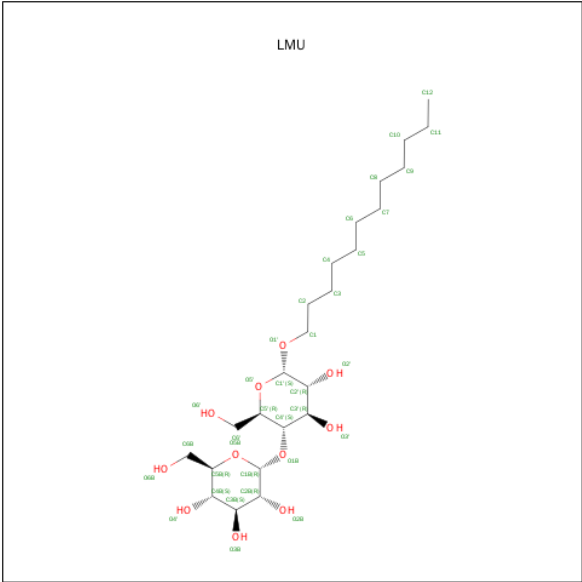
| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 15  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 15  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 15  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 15  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |         |
| 15  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 15  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 15  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 15  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 47    | 37 | 1  | 4 | 5 |         |         |
| 15  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |         |
| 15  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |         |
| 15  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 56    | 46 | 1  | 4 | 5 |         |         |
| 15  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 15  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 56    | 46 | 1  | 4 | 5 |         |         |
| 15  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 15  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 15  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 15  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 15  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 15  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 15  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |

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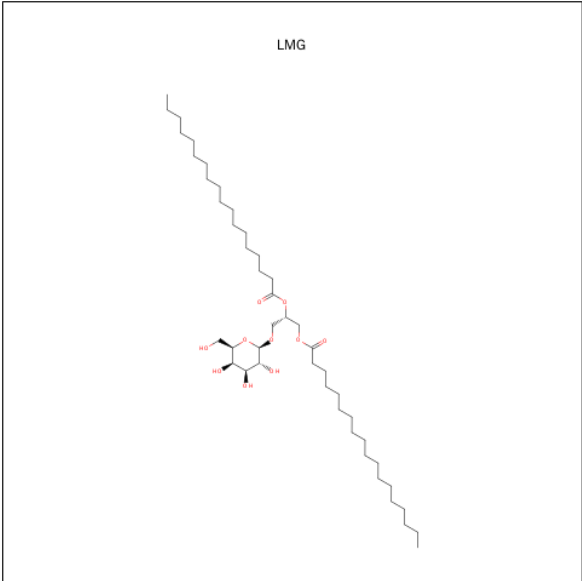
| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 15  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 15  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 15  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 15  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 15  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |         |
| 15  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |         |
| 15  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |         |
| 15  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |         |
| 15  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |         |
| 15  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |         |
| 15  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 44    | 35 | 1  | 4 | 4 |         |         |
| 15  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |         |
| 15  | F     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 15  | F     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 15  | F     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 15  | J     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |         |
| 15  | J     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 15  | K     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |         |
| 15  | K     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |         |

- Molecule 16 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula:  $C_{24}H_{46}O_{11}$ ).



| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 16  | B     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 16  | J     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |

- Molecule 17 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 17  | B     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 55    | 45 | 10 |         |         |

- Molecule 18 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 18  | B     | 1        | Total | Cl | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

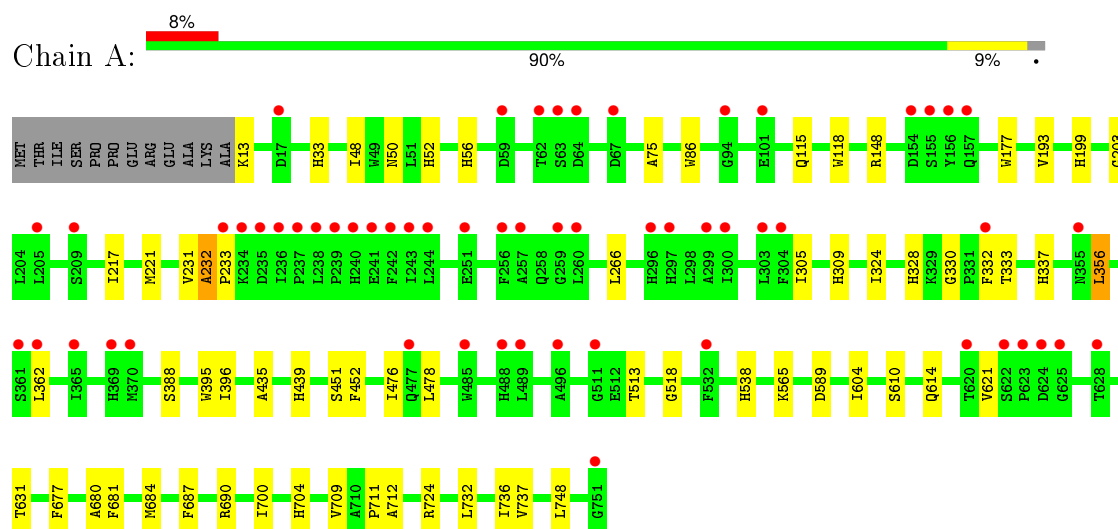
- Molecule 19 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 19  | A     | 10       | Total | O  | 0       | 0       |
|     |       |          | 10    | 10 |         |         |
| 19  | B     | 15       | Total | O  | 0       | 0       |
|     |       |          | 15    | 15 |         |         |
| 19  | C     | 3        | Total | O  | 0       | 0       |
|     |       |          | 3     | 3  |         |         |
| 19  | F     | 1        | Total | O  | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

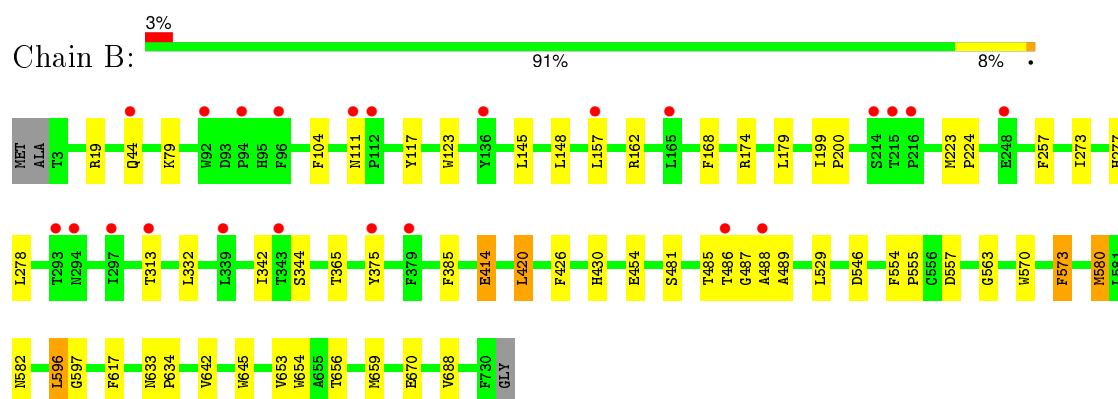
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

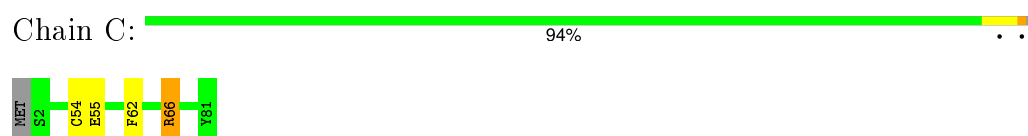
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



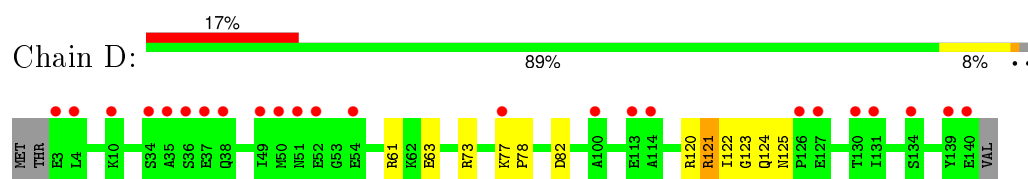
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



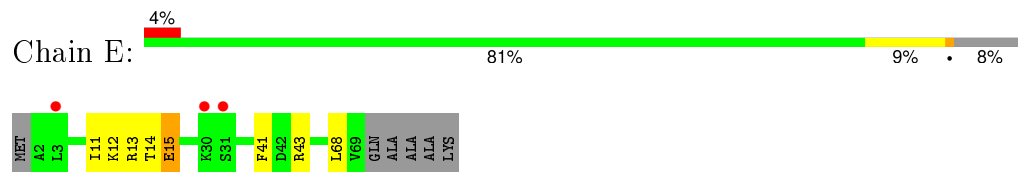
- Molecule 3: Photosystem I iron-sulfur center



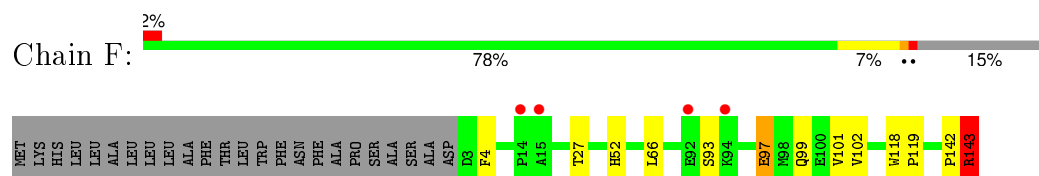
- Molecule 4: Photosystem I subunit II



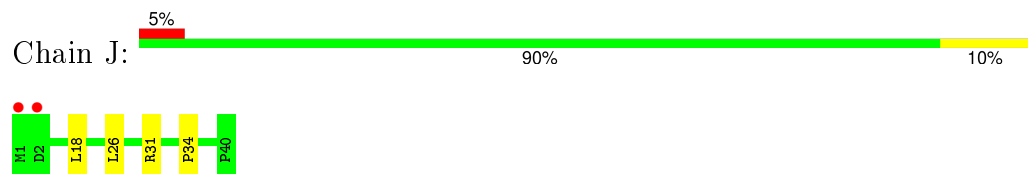
- Molecule 5: Photosystem I reaction center subunit IV



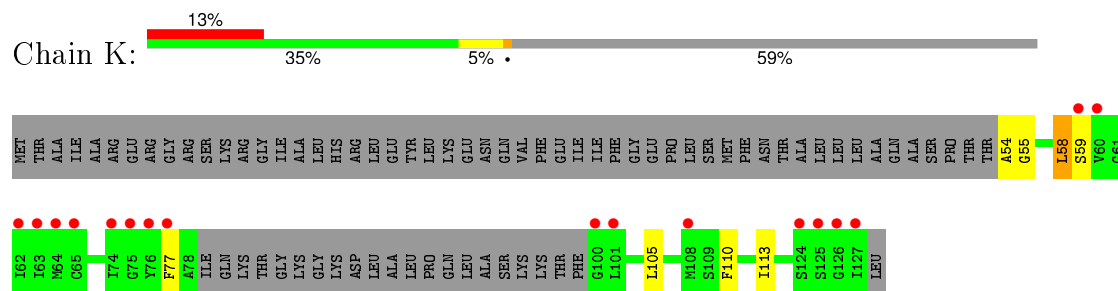
- Molecule 6: Photosystem I subunit III



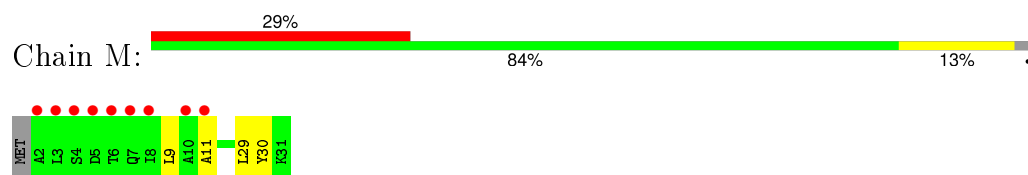
- Molecule 7: Photosystem I reaction center subunit IX



- Molecule 8: Photosystem I reaction center subunit PsaK



- Molecule 9: Photosystem I reaction center subunit XII



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 120.18Å 173.31Å 179.14Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 29.98 – 2.80<br>48.55 – 2.60                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 98.6 (29.98-2.80)<br>79.2 (48.55-2.60)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.14  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.36 (at 2.61Å)   | Xtriage          |
| Refinement program  | PHENIX (phenix.refine: 1.8.4_1496)                          | Depositor        |
| R, $R_{free}$   | 0.198 , 0.245<br>0.206 , 0.250                              | Depositor<br>DCC |
| $R_{free}$ test set   | 4594 reflections (6.19%)                                    | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 57.4  | Xtriage          |
| Anisotropy  | 0.546   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.29 , 75.7   | EDS              |
| Estimated twinning fraction   | 0.001 for -h,l,k  | Xtriage          |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Outliers  | 1 of 114217 reflections (0.001%)                            | Xtriage          |
| $F_o, F_c$ correlation  | 0.92  | EDS              |
| Total number of atoms   | 22051   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 92.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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

| Mol | Chain | Bond lengths |             | Bond angles |             |
|-----|-------|--------------|-------------|-------------|-------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$ |
| 1   | A     | 0.22         | 0/5985      | 0.38        | 0/8158      |
| 2   | B     | 0.23         | 0/5976      | 0.40        | 0/8173      |
| 3   | C     | 0.24         | 0/610       | 0.45        | 0/826       |
| 4   | D     | 0.23         | 0/1099      | 0.40        | 0/1482      |
| 5   | E     | 0.24         | 0/542       | 0.45        | 0/733       |
| 6   | F     | 0.23         | 0/1129      | 0.40        | 0/1535      |
| 7   | J     | 0.26         | 0/328       | 0.38        | 0/443       |
| 8   | K     | 0.25         | 0/371       | 0.39        | 0/499       |
| 9   | M     | 0.22         | 0/217       | 0.35        | 0/295       |
| All | All   | 0.23         | 0/16257     | 0.39        | 0/22144     |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 4   | D     | 0                   | 1                   |
| 6   | F     | 0                   | 1                   |
| All | All   | 0                   | 2                   |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 4   | D     | 121 | ARG  | Sidechain |
| 6   | F     | 143 | ARG  | Sidechain |

## 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   | A     | 5787  | 0        | 5646     | 60      | 0            |
| 2   | B     | 5765  | 0        | 5544     | 56      | 0            |
| 3   | C     | 600   | 0        | 581      | 4       | 0            |
| 4   | D     | 1075  | 0        | 1069     | 7       | 0            |
| 5   | E     | 533   | 0        | 517      | 8       | 0            |
| 6   | F     | 1099  | 0        | 1096     | 7       | 0            |
| 7   | J     | 319   | 0        | 328      | 4       | 0            |
| 8   | K     | 366   | 0        | 376      | 7       | 0            |
| 9   | M     | 214   | 0        | 213      | 2       | 0            |
| 10  | A     | 33    | 0        | 46       | 1       | 0            |
| 10  | B     | 33    | 0        | 46       | 3       | 0            |
| 11  | A     | 8     | 0        | 0        | 0       | 0            |
| 11  | C     | 16    | 0        | 0        | 0       | 0            |
| 12  | A     | 134   | 0        | 190      | 18      | 0            |
| 12  | B     | 49    | 0        | 74       | 2       | 0            |
| 13  | A     | 110   | 0        | 105      | 12      | 0            |
| 14  | A     | 240   | 0        | 294      | 17      | 0            |
| 14  | B     | 320   | 0        | 390      | 26      | 0            |
| 14  | F     | 80    | 0        | 97       | 8       | 0            |
| 14  | J     | 40    | 0        | 49       | 3       | 0            |
| 15  | A     | 2352  | 0        | 2285     | 69      | 0            |
| 15  | B     | 2365  | 0        | 2272     | 58      | 0            |
| 15  | F     | 175   | 0        | 177      | 3       | 0            |
| 15  | J     | 91    | 0        | 66       | 2       | 0            |
| 15  | K     | 92    | 0        | 66       | 2       | 0            |
| 16  | B     | 35    | 0        | 46       | 0       | 0            |
| 16  | J     | 35    | 0        | 46       | 2       | 0            |
| 17  | B     | 55    | 0        | 86       | 2       | 0            |
| 18  | B     | 1     | 0        | 0        | 0       | 0            |
| 19  | A     | 10    | 0        | 0        | 5       | 0            |
| 19  | B     | 15    | 0        | 0        | 6       | 0            |
| 19  | C     | 3     | 0        | 0        | 0       | 0            |
| 19  | F     | 1     | 0        | 0        | 1       | 0            |
| All | All   | 22051 | 0        | 21705    | 267     | 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 6.

All (267) 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) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:A:1011:CL0:CMA  | 19:A:9109:HOH:O    | 1.91                     | 1.19              |
| 13:A:1011:CL0:H6   | 19:A:9109:HOH:O    | 1.48                     | 1.11              |
| 14:B:4004:BCR:H403 | 14:B:4004:BCR:H23C | 1.51                     | 0.92              |
| 13:A:1011:CL0:H71  | 19:A:9109:HOH:O    | 1.71                     | 0.88              |
| 15:A:1110:CLA:HBD  | 15:A:1110:CLA:HBA1 | 1.57                     | 0.86              |
| 12:A:5005:LHG:H251 | 12:A:5005:LHG:C8   | 2.11                     | 0.81              |
| 7:J:31:ARG:NH2     | 15:J:1302:CLA:O1D  | 2.15                     | 0.80              |
| 1:A:395:TRP:CD1    | 15:A:1126:CLA:HAB  | 2.16                     | 0.80              |
| 14:A:4008:BCR:HC8  | 15:A:1124:CLA:HAB  | 1.61                     | 0.80              |
| 1:A:604:ILE:HD11   | 13:A:1011:CL0:H35  | 1.66                     | 0.78              |
| 2:B:123:TRP:CZ2    | 15:B:1210:CLA:H201 | 2.18                     | 0.78              |
| 12:A:5005:LHG:HC81 | 12:A:5005:LHG:H251 | 1.66                     | 0.78              |
| 15:J:1302:CLA:HBB1 | 15:J:1302:CLA:HHC  | 1.66                     | 0.77              |
| 15:A:1113:CLA:HHC  | 15:A:1113:CLA:HBB1 | 1.67                     | 0.76              |
| 1:A:538:HIS:ND1    | 15:A:1135:CLA:HAB  | 2.01                     | 0.75              |
| 14:A:4003:BCR:H14C | 15:A:1103:CLA:H201 | 1.69                     | 0.74              |
| 1:A:13:LYS:HB2     | 15:A:1110:CLA:HAA1 | 1.69                     | 0.74              |
| 15:A:1128:CLA:HHC  | 15:A:1128:CLA:HBB1 | 1.70                     | 0.73              |
| 2:B:582:ASN:OD1    | 19:B:9102:HOH:O    | 2.05                     | 0.73              |
| 1:A:332:PHE:HB2    | 12:A:5003:LHG:HC41 | 1.71                     | 0.73              |
| 13:A:1011:CL0:C2A  | 19:A:9109:HOH:O    | 2.33                     | 0.72              |
| 15:A:1101:CLA:H203 | 15:A:1126:CLA:H202 | 1.73                     | 0.70              |
| 14:A:4008:BCR:C8   | 15:A:1124:CLA:HAB  | 2.21                     | 0.70              |
| 2:B:656:THR:HA     | 15:B:1023:CLA:HAB  | 1.72                     | 0.70              |
| 15:B:1203:CLA:HHB  | 15:B:1226:CLA:HAB  | 1.74                     | 0.70              |
| 15:B:1227:CLA:HAB  | 15:B:1236:CLA:HBB2 | 1.73                     | 0.69              |
| 1:A:330:GLY:HA3    | 12:A:5003:LHG:HC32 | 1.75                     | 0.69              |
| 15:A:1110:CLA:CBD  | 15:A:1110:CLA:HBA1 | 2.23                     | 0.69              |
| 15:A:1131:CLA:HBB1 | 15:A:1131:CLA:HHC  | 1.74                     | 0.69              |
| 15:A:1101:CLA:HBB1 | 15:A:1101:CLA:HHC  | 1.74                     | 0.69              |
| 19:B:9105:HOH:O    | 14:F:4015:BCR:HC32 | 1.94                     | 0.68              |
| 1:A:737:VAL:HG22   | 14:B:4011:BCR:HC21 | 1.76                     | 0.68              |
| 14:A:4001:BCR:H23C | 8:K:110:PHE:HB2    | 1.75                     | 0.68              |
| 5:E:13:ARG:O       | 5:E:14:THR:HB      | 1.93                     | 0.67              |
| 1:A:476:ILE:HD12   | 12:A:5005:LHG:HC81 | 1.75                     | 0.67              |
| 1:A:435:ALA:O      | 1:A:439:HIS:ND1    | 2.27                     | 0.66              |
| 15:A:1110:CLA:HMB3 | 15:A:1118:CLA:C3D  | 2.25                     | 0.66              |
| 15:A:1131:CLA:CBB  | 12:A:5005:LHG:H281 | 2.26                     | 0.65              |
| 15:B:1220:CLA:HMD2 | 15:B:1221:CLA:HAB  | 1.76                     | 0.65              |
| 14:A:4001:BCR:H24C | 15:A:1120:CLA:HMD2 | 1.78                     | 0.65              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:A:1012:CLA:H42  | 14:B:4011:BCR:H362 | 1.77                     | 0.65              |
| 2:B:332:LEU:HD11   | 15:B:1226:CLA:HBB1 | 1.79                     | 0.64              |
| 15:A:1107:CLA:HBB1 | 15:A:1107:CLA:HHC  | 1.79                     | 0.64              |
| 1:A:677:PHE:CG     | 14:B:4011:BCR:H363 | 2.33                     | 0.64              |
| 1:A:231:VAL:O      | 1:A:232:ALA:HB3    | 1.97                     | 0.64              |
| 15:A:1022:CLA:H202 | 14:B:4017:BCR:H343 | 1.80                     | 0.63              |
| 16:J:1304:LMU:H82  | 16:J:1304:LMU:H41  | 1.80                     | 0.63              |
| 13:A:1108:CL0:H2   | 13:A:1108:CL0:H15  | 1.81                     | 0.63              |
| 13:A:1011:CL0:H5   | 19:A:9109:HOH:O    | 1.79                     | 0.62              |
| 1:A:604:ILE:CD1    | 13:A:1011:CL0:H35  | 2.29                     | 0.62              |
| 12:A:5005:LHG:HC82 | 12:A:5005:LHG:H251 | 1.82                     | 0.62              |
| 12:B:5004:LHG:H202 | 14:B:4009:BCR:H353 | 1.82                     | 0.62              |
| 15:B:1229:CLA:H192 | 14:F:4016:BCR:H19C | 1.81                     | 0.61              |
| 1:A:680:ALA:C      | 15:B:1013:CLA:HAB  | 2.20                     | 0.61              |
| 2:B:430:HIS:HB2    | 14:F:4015:BCR:HC22 | 1.83                     | 0.61              |
| 12:A:5005:LHG:HC82 | 12:A:5005:LHG:O10  | 2.00                     | 0.61              |
| 15:B:1231:CLA:HHC  | 15:B:1231:CLA:HBB1 | 1.83                     | 0.60              |
| 4:D:120:ARG:NH1    | 4:D:125:ASN:OD1    | 2.33                     | 0.60              |
| 2:B:570:TRP:NE1    | 17:B:5002:LMG:O10  | 2.34                     | 0.60              |
| 1:A:118:TRP:HB3    | 14:J:4013:BCR:HC21 | 1.84                     | 0.60              |
| 1:A:589:ASP:OD1    | 1:A:724:ARG:NH1    | 2.34                     | 0.60              |
| 15:B:1235:CLA:HBC2 | 14:F:4015:BCR:HC7  | 1.82                     | 0.59              |
| 15:A:1110:CLA:HMB3 | 15:A:1118:CLA:CAD  | 2.32                     | 0.59              |
| 15:B:1227:CLA:HAB  | 15:B:1236:CLA:CBB  | 2.31                     | 0.59              |
| 15:F:1139:CLA:HHC  | 15:F:1139:CLA:HBB1 | 1.85                     | 0.59              |
| 15:B:1205:CLA:CGA  | 15:B:1205:CLA:C1A  | 2.81                     | 0.59              |
| 2:B:486:THR:N      | 2:B:487:GLY:CA     | 2.66                     | 0.58              |
| 15:A:1102:CLA:H202 | 15:A:1105:CLA:H92  | 1.85                     | 0.58              |
| 2:B:481:SER:O      | 2:B:485:THR:HG23   | 2.04                     | 0.58              |
| 2:B:375:TYR:CD1    | 15:B:1224:CLA:HAB  | 2.39                     | 0.58              |
| 15:A:1104:CLA:HHC  | 15:A:1104:CLA:HBB1 | 1.86                     | 0.57              |
| 15:A:1110:CLA:HHC  | 15:A:1110:CLA:HBB1 | 1.86                     | 0.57              |
| 14:J:4013:BCR:H392 | 14:J:4013:BCR:H23C | 1.86                     | 0.57              |
| 4:D:123:GLY:HA3    | 5:E:15:GLU:HG2     | 1.87                     | 0.57              |
| 4:D:121:ARG:NH1    | 4:D:124:GLN:HG3    | 2.20                     | 0.57              |
| 2:B:486:THR:N      | 2:B:487:GLY:HA2    | 2.19                     | 0.56              |
| 14:A:4002:BCR:H342 | 15:A:1112:CLA:CHB  | 2.36                     | 0.56              |
| 2:B:597:GLY:HA3    | 19:B:9112:HOH:O    | 2.05                     | 0.55              |
| 2:B:656:THR:CA     | 15:B:1023:CLA:HAB  | 2.36                     | 0.55              |
| 1:A:677:PHE:CD2    | 14:B:4011:BCR:H363 | 2.41                     | 0.55              |
| 15:B:1231:CLA:C4C  | 15:B:1232:CLA:HAB  | 2.37                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:B:1218:CLA:HHC  | 15:B:1218:CLA:HBB1 | 1.89                     | 0.55              |
| 1:A:736:ILE:HG22   | 14:B:4011:BCR:HC31 | 1.88                     | 0.55              |
| 15:A:1122:CLA:HHC  | 15:A:1122:CLA:HBB1 | 1.89                     | 0.54              |
| 5:E:14:THR:O       | 5:E:14:THR:HG22    | 2.07                     | 0.54              |
| 5:E:12:LYS:O       | 5:E:12:LYS:HD3     | 2.07                     | 0.54              |
| 2:B:385:PHE:CZ     | 14:B:4010:BCR:H373 | 2.42                     | 0.54              |
| 15:A:1106:CLA:HAB  | 15:A:1126:CLA:H142 | 1.90                     | 0.54              |
| 1:A:217:ILE:HA     | 1:A:221:MET:HE2    | 1.90                     | 0.53              |
| 9:M:9:LEU:O        | 9:M:11:ALA:N       | 2.37                     | 0.53              |
| 15:A:1110:CLA:CHA  | 15:A:1110:CLA:HBA1 | 2.39                     | 0.53              |
| 15:A:1101:CLA:H203 | 15:A:1126:CLA:C20  | 2.36                     | 0.53              |
| 15:B:1230:CLA:OBD  | 19:B:9106:HOH:O    | 2.18                     | 0.53              |
| 2:B:645:TRP:CZ3    | 14:B:4017:BCR:HC41 | 2.44                     | 0.53              |
| 14:A:4003:BCR:H14C | 15:A:1103:CLA:C20  | 2.38                     | 0.53              |
| 2:B:385:PHE:CE2    | 14:B:4010:BCR:H373 | 2.44                     | 0.53              |
| 2:B:19:ARG:HD2     | 19:B:9108:HOH:O    | 2.09                     | 0.53              |
| 2:B:168:PHE:O      | 2:B:174:ARG:NH2    | 2.42                     | 0.52              |
| 2:B:557:ASP:OD2    | 3:C:66:ARG:NH2     | 2.42                     | 0.52              |
| 14:B:4014:BCR:HC41 | 15:B:1229:CLA:HBB2 | 1.91                     | 0.52              |
| 15:A:1110:CLA:CBB  | 15:A:1110:CLA:HHC  | 2.40                     | 0.52              |
| 1:A:395:TRP:NE1    | 15:A:1126:CLA:HAB  | 2.23                     | 0.52              |
| 1:A:395:TRP:HD1    | 15:A:1126:CLA:HAB  | 1.73                     | 0.52              |
| 1:A:56:HIS:CG      | 15:A:1103:CLA:HAB  | 2.45                     | 0.52              |
| 10:B:2002:PQN:H302 | 17:B:5002:LMG:H192 | 1.92                     | 0.52              |
| 4:D:61:ARG:NH2     | 4:D:63:GLU:OE1     | 2.43                     | 0.52              |
| 2:B:385:PHE:HZ     | 15:B:1222:CLA:HAB  | 1.75                     | 0.52              |
| 10:B:2002:PQN:H303 | 15:B:1239:CLA:O1A  | 2.11                     | 0.51              |
| 2:B:554:PHE:HB2    | 2:B:555:PRO:HD2    | 1.92                     | 0.51              |
| 13:A:1108:CL0:H27  | 15:A:1110:CLA:HMD1 | 1.93                     | 0.51              |
| 1:A:711:PRO:HB2    | 19:F:9301:HOH:O    | 2.09                     | 0.51              |
| 15:B:1229:CLA:HAB  | 15:B:1230:CLA:C2B  | 2.40                     | 0.51              |
| 2:B:430:HIS:CG     | 14:F:4015:BCR:HC42 | 2.46                     | 0.51              |
| 1:A:362:LEU:CD2    | 15:A:1127:CLA:H202 | 2.41                     | 0.51              |
| 2:B:44:GLN:OE1     | 2:B:162:ARG:NH1    | 2.42                     | 0.51              |
| 1:A:305:ILE:HG21   | 14:A:4001:BCR:H14C | 1.93                     | 0.51              |
| 15:B:1212:CLA:HAB  | 15:B:1211:CLA:CMC  | 2.40                     | 0.51              |
| 8:K:58:LEU:N       | 8:K:58:LEU:CD1     | 2.73                     | 0.51              |
| 1:A:681:PHE:HA     | 15:B:1013:CLA:HAB  | 1.92                     | 0.50              |
| 1:A:324:ILE:O      | 1:A:328:HIS:ND1    | 2.36                     | 0.50              |
| 1:A:231:VAL:O      | 1:A:232:ALA:CB     | 2.58                     | 0.50              |
| 14:A:4002:BCR:HC41 | 15:A:1103:CLA:H122 | 1.94                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:426:PHE:CZ     | 14:F:4015:BCR:HC41 | 2.47                     | 0.50              |
| 2:B:123:TRP:CE2    | 15:B:1210:CLA:H201 | 2.46                     | 0.49              |
| 13:A:1108:CL0:OBD  | 15:A:1110:CLA:H71  | 2.13                     | 0.49              |
| 1:A:333:HIS:NE2    | 15:A:1109:CLA:O1A  | 2.32                     | 0.49              |
| 2:B:454:GLU:OE2    | 6:F:52:HIS:ND1     | 2.41                     | 0.49              |
| 2:B:642:VAL:HG22   | 15:B:1206:CLA:HHD  | 1.95                     | 0.49              |
| 8:K:58:LEU:HD13    | 8:K:58:LEU:H       | 1.78                     | 0.48              |
| 12:A:5005:LHG:HC82 | 12:A:5005:LHG:C23  | 2.43                     | 0.48              |
| 1:A:75:ALA:HB1     | 15:A:1103:CLA:HBB1 | 1.95                     | 0.48              |
| 1:A:333:THR:OG1    | 12:A:5003:LHG:HC2  | 2.13                     | 0.48              |
| 1:A:684:MET:HE2    | 10:A:2001:PQN:H2M3 | 1.95                     | 0.48              |
| 2:B:420:LEU:HD22   | 2:B:529:LEU:HB2    | 1.94                     | 0.48              |
| 14:A:4007:BCR:H15C | 14:A:4007:BCR:H351 | 1.70                     | 0.48              |
| 15:B:1235:CLA:H122 | 14:F:4016:BCR:H23C | 1.95                     | 0.48              |
| 15:A:1133:CLA:HHC  | 15:A:1133:CLA:HBB1 | 1.95                     | 0.48              |
| 1:A:396:ILE:HD12   | 15:A:1127:CLA:HAB  | 1.94                     | 0.48              |
| 14:A:4008:BCR:H371 | 14:A:4008:BCR:H24C | 1.73                     | 0.47              |
| 14:B:4006:BCR:H403 | 14:B:4006:BCR:C23  | 2.44                     | 0.47              |
| 5:E:11:ILE:HD12    | 5:E:11:ILE:N       | 2.30                     | 0.47              |
| 1:A:690:ARG:NH1    | 2:B:563:GLY:O      | 2.46                     | 0.47              |
| 12:A:5005:LHG:H112 | 12:A:5005:LHG:H262 | 1.95                     | 0.47              |
| 1:A:330:GLY:CA     | 12:A:5003:LHG:HC32 | 2.44                     | 0.47              |
| 2:B:179:LEU:CD2    | 15:B:1216:CLA:HAB  | 2.44                     | 0.47              |
| 15:B:1235:CLA:C1A  | 15:B:1235:CLA:CGA  | 2.93                     | 0.47              |
| 15:B:1215:CLA:H3A  | 15:B:1215:CLA:CGA  | 2.44                     | 0.47              |
| 15:A:1022:CLA:CAD  | 15:B:1021:CLA:HMB3 | 2.44                     | 0.47              |
| 1:A:610:SER:OG     | 1:A:614:GLN:NE2    | 2.47                     | 0.47              |
| 2:B:633:ASN:HB2    | 2:B:634:PRO:CD     | 2.44                     | 0.47              |
| 2:B:486:THR:OG1    | 2:B:487:GLY:HA2    | 2.13                     | 0.47              |
| 15:B:1224:CLA:H3A  | 15:B:1224:CLA:CGA  | 2.45                     | 0.47              |
| 15:A:1119:CLA:HMB2 | 15:A:1123:CLA:HMA3 | 1.97                     | 0.47              |
| 13:A:1011:CL0:H13  | 15:A:1012:CLA:HMD1 | 1.97                     | 0.47              |
| 1:A:687:PHE:HB2    | 15:B:1013:CLA:HBC2 | 1.97                     | 0.47              |
| 8:K:58:LEU:HD13    | 8:K:58:LEU:N       | 2.29                     | 0.47              |
| 15:B:1013:CLA:CGA  | 15:B:1013:CLA:H3A  | 2.46                     | 0.46              |
| 14:B:4010:BCR:H351 | 14:B:4010:BCR:H15C | 1.69                     | 0.46              |
| 14:A:4003:BCR:H24C | 15:A:1127:CLA:H2   | 1.97                     | 0.46              |
| 8:K:54:ALA:O       | 8:K:58:LEU:HD22    | 2.14                     | 0.46              |
| 1:A:712:ALA:HB1    | 6:F:97:GLU:OE1     | 2.15                     | 0.46              |
| 1:A:199:HIS:O      | 1:A:203:GLY:N      | 2.48                     | 0.46              |
| 2:B:111:ASN:N      | 2:B:111:ASN:OD1    | 2.49                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:A:1137:CLA:HAB  | 15:A:1129:CLA:CBB  | 2.45                     | 0.46              |
| 14:J:4013:BCR:H15C | 14:J:4013:BCR:H351 | 1.67                     | 0.46              |
| 1:A:86:TRP:HA      | 15:A:1105:CLA:HBB2 | 1.98                     | 0.46              |
| 2:B:273:ILE:O      | 2:B:277:HIS:ND1    | 2.43                     | 0.46              |
| 15:A:1022:CLA:H171 | 14:B:4017:BCR:H343 | 1.96                     | 0.46              |
| 15:B:1203:CLA:OBD  | 15:B:1201:CLA:HHC  | 2.16                     | 0.46              |
| 14:B:4017:BCR:H15C | 14:B:4017:BCR:H351 | 1.68                     | 0.46              |
| 15:B:1215:CLA:HBB2 | 15:B:1221:CLA:H201 | 1.99                     | 0.45              |
| 1:A:681:PHE:N      | 15:B:1013:CLA:HAB  | 2.30                     | 0.45              |
| 2:B:199:ILE:HB     | 2:B:200:PRO:HD3    | 1.99                     | 0.45              |
| 1:A:362:LEU:HD22   | 15:A:1127:CLA:H202 | 1.97                     | 0.45              |
| 2:B:546:ASP:OD2    | 3:C:66:ARG:NH1     | 2.48                     | 0.45              |
| 15:A:1114:CLA:HBB1 | 15:A:1114:CLA:HHC  | 1.97                     | 0.45              |
| 2:B:688:VAL:HG11   | 15:B:1237:CLA:HAB  | 1.99                     | 0.45              |
| 15:A:1110:CLA:C3C  | 15:A:1111:CLA:HBB2 | 2.47                     | 0.45              |
| 15:B:1236:CLA:HHC  | 15:B:1236:CLA:HBB1 | 1.99                     | 0.45              |
| 1:A:305:ILE:O      | 1:A:309:HIS:ND1    | 2.45                     | 0.45              |
| 14:B:4010:BCR:C23  | 14:B:4010:BCR:H403 | 2.46                     | 0.45              |
| 1:A:565:LYS:NZ     | 2:B:670:GLU:OE2    | 2.44                     | 0.45              |
| 1:A:476:ILE:CD1    | 12:A:5005:LHG:HC81 | 2.45                     | 0.45              |
| 5:E:13:ARG:O       | 5:E:14:THR:CB      | 2.59                     | 0.45              |
| 14:B:4010:BCR:H14C | 15:B:1222:CLA:HMA1 | 1.99                     | 0.45              |
| 2:B:573:PHE:CE2    | 15:B:1226:CLA:HMD2 | 2.52                     | 0.45              |
| 2:B:104:PHE:CZ     | 2:B:642:VAL:HG23   | 2.52                     | 0.44              |
| 14:B:4005:BCR:H15C | 14:B:4005:BCR:H351 | 1.74                     | 0.44              |
| 2:B:656:THR:N      | 15:B:1023:CLA:HAB  | 2.32                     | 0.44              |
| 15:B:1212:CLA:HAB  | 15:B:1211:CLA:HMC3 | 1.99                     | 0.44              |
| 15:A:1110:CLA:CGA  | 15:A:1110:CLA:C1A  | 2.95                     | 0.44              |
| 14:A:4008:BCR:H351 | 14:A:4008:BCR:H15C | 1.63                     | 0.44              |
| 14:A:4012:BCR:C8   | 14:A:4012:BCR:H331 | 2.45                     | 0.44              |
| 1:A:700:ILE:O      | 1:A:704:HIS:ND1    | 2.46                     | 0.44              |
| 1:A:193:VAL:CG1    | 15:A:1123:CLA:HHD  | 2.48                     | 0.44              |
| 8:K:54:ALA:HB3     | 15:K:1402:CLA:C1   | 2.48                     | 0.44              |
| 16:J:1304:LMU:H71  | 16:J:1304:LMU:H101 | 1.82                     | 0.44              |
| 1:A:680:ALA:O      | 15:B:1013:CLA:HAB  | 2.17                     | 0.44              |
| 14:B:4011:BCR:H392 | 14:B:4011:BCR:H23C | 2.00                     | 0.44              |
| 14:A:4002:BCR:H24C | 14:A:4002:BCR:H371 | 1.72                     | 0.44              |
| 15:A:1106:CLA:H43  | 15:A:1126:CLA:HMD2 | 2.00                     | 0.43              |
| 15:A:1801:CLA:HAB  | 15:A:1122:CLA:HHB  | 2.00                     | 0.43              |
| 1:A:337:HIS:CE1    | 12:A:5003:LHG:HC12 | 2.53                     | 0.43              |
| 15:B:1215:CLA:HBB1 | 15:B:1215:CLA:HHC  | 2.00                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:A:1122:CLA:HBB1 | 15:A:1129:CLA:HMD2 | 2.00                     | 0.43              |
| 2:B:426:PHE:CE1    | 14:F:4015:BCR:HC41 | 2.53                     | 0.43              |
| 2:B:117:TYR:HA     | 2:B:365:THR:HG22   | 2.01                     | 0.43              |
| 2:B:645:TRP:CE3    | 14:B:4017:BCR:HC41 | 2.54                     | 0.43              |
| 5:E:11:ILE:HD11    | 5:E:41:PHE:HE1     | 1.82                     | 0.43              |
| 14:A:4008:BCR:HC8  | 15:A:1124:CLA:CAB  | 2.42                     | 0.43              |
| 5:E:14:THR:O       | 6:F:142:PRO:HG3    | 2.19                     | 0.43              |
| 2:B:278:LEU:HG     | 15:B:1213:CLA:HAB  | 2.01                     | 0.43              |
| 14:B:4014:BCR:HC8  | 15:B:1229:CLA:HBB1 | 2.01                     | 0.43              |
| 15:A:1110:CLA:HMB3 | 15:A:1118:CLA:C4D  | 2.48                     | 0.42              |
| 15:A:1114:CLA:HHC  | 15:A:1114:CLA:CBB  | 2.49                     | 0.42              |
| 4:D:77:LYS:HB2     | 4:D:78:PRO:HD3     | 2.01                     | 0.42              |
| 15:B:1222:CLA:H3A  | 15:B:1222:CLA:HBA2 | 1.88                     | 0.42              |
| 15:B:1215:CLA:HHC  | 15:B:1215:CLA:CBB  | 2.49                     | 0.42              |
| 14:A:4012:BCR:HC7  | 7:J:26:LEU:HD13    | 2.01                     | 0.42              |
| 12:A:5003:LHG:H282 | 15:A:1122:CLA:H202 | 2.02                     | 0.42              |
| 2:B:654:TRP:CE3    | 15:B:1021:CLA:HMA1 | 2.55                     | 0.42              |
| 1:A:681:PHE:HA     | 15:B:1013:CLA:CAB  | 2.49                     | 0.42              |
| 2:B:596:LEU:HD12   | 2:B:596:LEU:HA     | 1.81                     | 0.42              |
| 1:A:356:LEU:HD11   | 15:A:1128:CLA:CBB  | 2.50                     | 0.42              |
| 1:A:177:TRP:HB2    | 15:A:1109:CLA:HMC3 | 2.01                     | 0.42              |
| 15:B:1235:CLA:HAB  | 19:B:9105:HOH:O    | 2.19                     | 0.42              |
| 1:A:48:ILE:O       | 1:A:52:HIS:ND1     | 2.51                     | 0.42              |
| 14:B:4004:BCR:H351 | 14:B:4004:BCR:H15C | 1.67                     | 0.42              |
| 6:F:93:SER:OG      | 6:F:99:GLN:NE2     | 2.53                     | 0.42              |
| 2:B:223:MET:N      | 2:B:224:PRO:CD     | 2.83                     | 0.42              |
| 1:A:737:VAL:HG22   | 14:B:4011:BCR:H323 | 2.01                     | 0.42              |
| 2:B:488:ALA:O      | 2:B:489:ALA:HB3    | 2.19                     | 0.42              |
| 1:A:518:GLY:O      | 1:A:621:VAL:N      | 2.52                     | 0.42              |
| 1:A:337:HIS:HE1    | 12:A:5003:LHG:HC12 | 1.83                     | 0.41              |
| 2:B:313:THR:OG1    | 12:B:5004:LHG:HC11 | 2.19                     | 0.41              |
| 15:A:1138:CLA:H203 | 15:F:1139:CLA:H62  | 2.02                     | 0.41              |
| 6:F:118:TRP:N      | 6:F:119:PRO:CD     | 2.83                     | 0.41              |
| 1:A:50:ASN:ND2     | 12:A:5001:LHG:HC12 | 2.35                     | 0.41              |
| 15:F:1139:CLA:H41  | 7:J:18:LEU:HD22    | 2.02                     | 0.41              |
| 3:C:62:PHE:HD2     | 4:D:122:ILE:HG21   | 1.85                     | 0.41              |
| 15:A:1121:CLA:HHC  | 15:A:1121:CLA:CBB  | 2.50                     | 0.41              |
| 1:A:604:ILE:HD11   | 13:A:1011:CL0:C4   | 2.45                     | 0.41              |
| 2:B:385:PHE:CZ     | 15:B:1222:CLA:HAB  | 2.53                     | 0.41              |
| 6:F:27:THR:HG21    | 7:J:34:PRO:HG3     | 2.03                     | 0.41              |
| 15:K:1401:CLA:HHC  | 15:K:1401:CLA:CBB  | 2.51                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:342:ILE:HG21   | 15:B:1221:CLA:H41  | 2.02                     | 0.41              |
| 15:B:1216:CLA:HMB2 | 15:B:1221:CLA:HMA3 | 2.03                     | 0.41              |
| 14:B:4017:BCR:H24C | 14:B:4017:BCR:H371 | 1.78                     | 0.41              |
| 2:B:414:GLU:OE2    | 6:F:143:ARG:NH2    | 2.54                     | 0.41              |
| 2:B:580:MET:HB3    | 2:B:580:MET:HE2    | 1.92                     | 0.41              |
| 15:A:1121:CLA:HBB1 | 15:A:1121:CLA:HHC  | 2.02                     | 0.41              |
| 2:B:157:LEU:HD11   | 9:M:29:LEU:HD12    | 2.03                     | 0.41              |
| 4:D:120:ARG:HG2    | 4:D:124:GLN:HB2    | 2.01                     | 0.41              |
| 2:B:653:VAL:HG22   | 15:B:1239:CLA:HMB3 | 2.03                     | 0.41              |
| 3:C:54:CYS:SG      | 3:C:55:GLU:N       | 2.94                     | 0.41              |
| 8:K:55:GLY:O       | 8:K:59:SER:OG      | 2.30                     | 0.41              |
| 1:A:451:SER:OG     | 1:A:452:PHE:N      | 2.54                     | 0.41              |
| 15:B:1231:CLA:CBB  | 15:B:1231:CLA:HHC  | 2.51                     | 0.40              |
| 15:A:1102:CLA:HMA2 | 15:A:1109:CLA:HMD2 | 2.02                     | 0.40              |
| 1:A:681:PHE:CA     | 15:B:1013:CLA:HAB  | 2.50                     | 0.40              |
| 2:B:659:MET:HE2    | 10:B:2002:PQN:H2M3 | 2.02                     | 0.40              |
| 15:A:1133:CLA:HHC  | 15:A:1133:CLA:CBB  | 2.51                     | 0.40              |
| 14:B:4004:BCR:H321 | 14:B:4004:BCR:HC8  | 2.03                     | 0.40              |
| 12:A:5005:LHG:HC2  | 12:A:5005:LHG:O4   | 2.22                     | 0.40              |
| 15:A:1102:CLA:HMB1 | 15:A:1102:CLA:HBB1 | 2.04                     | 0.40              |
| 1:A:388:SER:HB3    | 15:A:1126:CLA:HMA1 | 2.04                     | 0.40              |
| 15:B:1218:CLA:CBB  | 15:B:1218:CLA:HHC  | 2.50                     | 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 X-ray entries followed by that with respect to entries of similar resolution.

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   | A     | 737/751 (98%) | 694 (94%) | 40 (5%) | 3 (0%)   | 39          | 74  |
| 2   | B     | 726/731 (99%) | 695 (96%) | 31 (4%) | 0        | 100         | 100 |
| 3   | C     | 78/81 (96%)   | 74 (95%)  | 4 (5%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 4   | D     | 136/141 (96%)   | 123 (90%)  | 13 (10%) | 0        | 100         | 100 |
| 5   | E     | 66/74 (89%)     | 57 (86%)   | 9 (14%)  | 0        | 100         | 100 |
| 6   | F     | 139/165 (84%)   | 135 (97%)  | 4 (3%)   | 0        | 100         | 100 |
| 7   | J     | 38/40 (95%)     | 38 (100%)  | 0        | 0        | 100         | 100 |
| 8   | K     | 49/128 (38%)    | 46 (94%)   | 3 (6%)   | 0        | 100         | 100 |
| 9   | M     | 28/31 (90%)     | 25 (89%)   | 3 (11%)  | 0        | 100         | 100 |
| All | All   | 1997/2142 (93%) | 1887 (94%) | 107 (5%) | 3 (0%)   | 52          | 84  |

All (3) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 115 | GLN  |
| 1   | A     | 232 | ALA  |
| 1   | A     | 233 | PRO  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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   | A     | 593/603 (98%)   | 584 (98%)  | 9 (2%)   | 72          | 93  |
| 2   | B     | 582/583 (100%)  | 571 (98%)  | 11 (2%)  | 65          | 91  |
| 3   | C     | 68/69 (99%)     | 67 (98%)   | 1 (2%)   | 72          | 93  |
| 4   | D     | 112/116 (97%)   | 110 (98%)  | 2 (2%)   | 66          | 91  |
| 5   | E     | 57/60 (95%)     | 54 (95%)   | 3 (5%)   | 28          | 61  |
| 6   | F     | 118/137 (86%)   | 112 (95%)  | 6 (5%)   | 29          | 63  |
| 7   | J     | 35/35 (100%)    | 35 (100%)  | 0        | 100         | 100 |
| 8   | K     | 37/100 (37%)    | 33 (89%)   | 4 (11%)  | 8           | 23  |
| 9   | M     | 19/25 (76%)     | 18 (95%)   | 1 (5%)   | 28          | 61  |
| All | All   | 1621/1728 (94%) | 1584 (98%) | 37 (2%)  | 58          | 88  |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 148 | ARG  |
| 1   | A     | 266 | LEU  |
| 1   | A     | 356 | LEU  |
| 1   | A     | 478 | LEU  |
| 1   | A     | 513 | THR  |
| 1   | A     | 631 | THR  |
| 1   | A     | 709 | VAL  |
| 1   | A     | 732 | LEU  |
| 1   | A     | 748 | LEU  |
| 2   | B     | 79  | LYS  |
| 2   | B     | 145 | LEU  |
| 2   | B     | 148 | LEU  |
| 2   | B     | 257 | PHE  |
| 2   | B     | 344 | SER  |
| 2   | B     | 414 | GLU  |
| 2   | B     | 420 | LEU  |
| 2   | B     | 573 | PHE  |
| 2   | B     | 580 | MET  |
| 2   | B     | 596 | LEU  |
| 2   | B     | 617 | PHE  |
| 3   | C     | 66  | ARG  |
| 4   | D     | 73  | ARG  |
| 4   | D     | 82  | ASP  |
| 5   | E     | 15  | GLU  |
| 5   | E     | 43  | ARG  |
| 5   | E     | 68  | LEU  |
| 6   | F     | 4   | PHE  |
| 6   | F     | 66  | LEU  |
| 6   | F     | 97  | GLU  |
| 6   | F     | 101 | VAL  |
| 6   | F     | 102 | VAL  |
| 6   | F     | 143 | ARG  |
| 8   | K     | 58  | LEU  |
| 8   | K     | 77  | PHE  |
| 8   | K     | 105 | LEU  |
| 8   | K     | 113 | ILE  |
| 9   | M     | 30  | TYR  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 138 | GLN  |
| 1   | A     | 441 | ASN  |
| 1   | A     | 538 | HIS  |
| 1   | A     | 614 | GLN  |
| 2   | B     | 34  | HIS  |
| 2   | B     | 114 | ASN  |
| 4   | D     | 81  | GLN  |
| 4   | D     | 95  | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 122 ligands modelled in this entry, 1 is monoatomic - leaving 121 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 | $\# Z  > 2$ |
| 13  | CL0  | A     | 1011 | -    | 55,73,73     | 1.82 | 12 (21%)    | 61,113,113  | 2.14 | 11 (18%)    |
| 15  | CLA  | A     | 1012 | 19   | 55,73,73     | 1.87 | 12 (21%)    | 61,113,113  | 2.17 | 16 (26%)    |
| 15  | CLA  | A     | 1022 | 19   | 55,73,73     | 1.86 | 11 (20%)    | 61,113,113  | 2.18 | 13 (21%)    |
| 15  | CLA  | A     | 1101 | -    | 55,73,73     | 1.85 | 12 (21%)    | 61,113,113  | 2.18 | 14 (22%)    |
| 15  | CLA  | A     | 1102 | 15   | 55,73,73     | 1.89 | 12 (21%)    | 61,113,113  | 2.05 | 12 (19%)    |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 15  | CLA  | A     | 1103 | -    | 55,73,73     | 1.85 | 12 (21%) | 61,113,113  | 1.95 | 14 (22%) |
| 15  | CLA  | A     | 1104 | -    | 55,73,73     | 1.83 | 12 (21%) | 61,113,113  | 2.02 | 13 (21%) |
| 15  | CLA  | A     | 1105 | -    | 55,73,73     | 1.86 | 12 (21%) | 61,113,113  | 2.18 | 11 (18%) |
| 15  | CLA  | A     | 1106 | 1    | 55,73,73     | 1.88 | 12 (21%) | 61,113,113  | 2.15 | 12 (19%) |
| 15  | CLA  | A     | 1107 | 1    | 40,58,73     | 2.18 | 12 (30%) | 44,95,113   | 2.34 | 15 (34%) |
| 13  | CL0  | A     | 1108 | -    | 32,53,73     | 2.25 | 10 (31%) | 37,89,113   | 2.22 | 9 (24%)  |
| 15  | CLA  | A     | 1109 | 15   | 55,73,73     | 1.89 | 12 (21%) | 61,113,113  | 2.06 | 13 (21%) |
| 15  | CLA  | A     | 1110 | -    | 44,62,73     | 2.02 | 12 (27%) | 47,99,113   | 2.26 | 12 (25%) |
| 15  | CLA  | A     | 1111 | -    | 50,68,73     | 1.94 | 12 (24%) | 55,107,113  | 2.07 | 13 (23%) |
| 15  | CLA  | A     | 1112 | -    | 32,53,73     | 2.27 | 11 (34%) | 37,89,113   | 2.31 | 10 (27%) |
| 15  | CLA  | A     | 1113 | -    | 32,53,73     | 2.27 | 11 (34%) | 37,89,113   | 2.22 | 10 (27%) |
| 15  | CLA  | A     | 1114 | -    | 39,57,73     | 2.20 | 12 (30%) | 43,93,113   | 2.43 | 13 (30%) |
| 15  | CLA  | A     | 1115 | -    | 36,54,73     | 2.39 | 11 (30%) | 41,90,113   | 2.23 | 11 (26%) |
| 15  | CLA  | A     | 1116 | -    | 44,62,73     | 2.08 | 12 (27%) | 47,99,113   | 2.37 | 12 (25%) |
| 15  | CLA  | A     | 1117 | -    | 55,73,73     | 1.86 | 12 (21%) | 61,113,113  | 1.95 | 12 (19%) |
| 15  | CLA  | A     | 1118 | -    | 36,54,73     | 2.37 | 11 (30%) | 41,90,113   | 2.32 | 11 (26%) |
| 15  | CLA  | A     | 1119 | -    | 54,72,73     | 1.87 | 13 (24%) | 61,111,113  | 2.08 | 12 (19%) |
| 15  | CLA  | A     | 1120 | -    | 39,57,73     | 2.20 | 12 (30%) | 43,93,113   | 2.43 | 13 (30%) |
| 15  | CLA  | A     | 1121 | -    | 36,54,73     | 2.38 | 12 (33%) | 41,90,113   | 2.31 | 11 (26%) |
| 15  | CLA  | A     | 1122 | -    | 55,73,73     | 1.85 | 13 (23%) | 61,113,113  | 2.03 | 12 (19%) |
| 15  | CLA  | A     | 1123 | -    | 55,73,73     | 1.83 | 12 (21%) | 61,113,113  | 2.17 | 15 (24%) |
| 15  | CLA  | A     | 1124 | -    | 45,63,73     | 2.05 | 12 (26%) | 49,101,113  | 2.15 | 13 (26%) |
| 15  | CLA  | A     | 1125 | -    | 42,60,73     | 2.09 | 12 (28%) | 45,97,113   | 2.39 | 14 (31%) |
| 15  | CLA  | A     | 1126 | -    | 55,73,73     | 1.85 | 12 (21%) | 61,113,113  | 2.03 | 14 (22%) |
| 15  | CLA  | A     | 1127 | -    | 55,73,73     | 1.87 | 12 (21%) | 61,113,113  | 2.08 | 16 (26%) |
| 15  | CLA  | A     | 1128 | -    | 55,73,73     | 1.83 | 11 (20%) | 61,113,113  | 2.13 | 12 (19%) |
| 15  | CLA  | A     | 1129 | -    | 36,54,73     | 2.35 | 11 (30%) | 41,90,113   | 2.36 | 13 (31%) |
| 15  | CLA  | A     | 1130 | -    | 45,63,73     | 2.05 | 12 (26%) | 49,101,113  | 2.19 | 10 (20%) |
| 15  | CLA  | A     | 1131 | -    | 45,63,73     | 2.07 | 12 (26%) | 49,101,113  | 2.36 | 11 (22%) |
| 15  | CLA  | A     | 1132 | -    | 52,70,73     | 1.89 | 11 (21%) | 56,109,113  | 2.21 | 11 (19%) |
| 15  | CLA  | A     | 1133 | -    | 36,54,73     | 2.37 | 12 (33%) | 41,90,113   | 2.31 | 11 (26%) |
| 15  | CLA  | A     | 1134 | 1    | 36,54,73     | 2.38 | 12 (33%) | 41,90,113   | 2.15 | 10 (24%) |
| 15  | CLA  | A     | 1135 | -    | 45,63,73     | 2.05 | 12 (26%) | 49,101,113  | 2.32 | 14 (28%) |
| 15  | CLA  | A     | 1136 | -    | 55,73,73     | 1.86 | 12 (21%) | 61,113,113  | 2.14 | 13 (21%) |
| 15  | CLA  | A     | 1137 | -    | 40,58,73     | 2.18 | 12 (30%) | 44,95,113   | 2.41 | 11 (25%) |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 15  | CLA  | A     | 1138 | -    | 55,73,73     | 1.89 | 11 (20%) | 61,113,113  | 1.88 | 14 (22%) |
| 15  | CLA  | A     | 1140 | -    | 55,73,73     | 1.87 | 12 (21%) | 61,113,113  | 1.95 | 12 (19%) |
| 15  | CLA  | A     | 1801 | 12   | 42,60,73     | 2.15 | 13 (30%) | 45,97,113   | 2.41 | 15 (33%) |
| 10  | PQN  | A     | 2001 | -    | 34,34,34     | 1.39 | 2 (5%)   | 44,45,45    | 0.99 | 3 (6%)   |
| 11  | SF4  | A     | 3001 | 1,2  | 0,12,12      | 0.00 | -        | 0,24,24     | 0.00 | -        |
| 14  | BCR  | A     | 4001 | -    | 41,41,41     | 2.76 | 6 (14%)  | 56,56,56    | 6.17 | 25 (44%) |
| 14  | BCR  | A     | 4002 | -    | 41,41,41     | 2.75 | 6 (14%)  | 56,56,56    | 6.38 | 26 (46%) |
| 14  | BCR  | A     | 4003 | -    | 41,41,41     | 2.73 | 6 (14%)  | 56,56,56    | 6.41 | 25 (44%) |
| 14  | BCR  | A     | 4007 | -    | 41,41,41     | 2.71 | 6 (14%)  | 56,56,56    | 6.61 | 25 (44%) |
| 14  | BCR  | A     | 4008 | -    | 41,41,41     | 2.72 | 7 (17%)  | 56,56,56    | 6.68 | 23 (41%) |
| 14  | BCR  | A     | 4012 | -    | 41,41,41     | 2.80 | 6 (14%)  | 56,56,56    | 6.11 | 22 (39%) |
| 12  | LHG  | A     | 5001 | -    | 48,48,48     | 0.90 | 2 (4%)   | 49,54,54    | 1.09 | 3 (6%)   |
| 12  | LHG  | A     | 5003 | 15   | 48,48,48     | 0.91 | 2 (4%)   | 49,54,54    | 1.12 | 3 (6%)   |
| 12  | LHG  | A     | 5005 | -    | 35,35,48     | 1.04 | 2 (5%)   | 36,41,54    | 1.17 | 3 (8%)   |
| 15  | CLA  | B     | 1013 | -    | 55,73,73     | 1.86 | 12 (21%) | 61,113,113  | 2.09 | 13 (21%) |
| 15  | CLA  | B     | 1021 | -    | 55,73,73     | 1.84 | 13 (23%) | 61,113,113  | 2.06 | 15 (24%) |
| 15  | CLA  | B     | 1023 | -    | 55,73,73     | 1.83 | 12 (21%) | 61,113,113  | 2.01 | 13 (21%) |
| 15  | CLA  | B     | 1201 | -    | 36,54,73     | 2.38 | 12 (33%) | 41,90,113   | 2.42 | 11 (26%) |
| 15  | CLA  | B     | 1202 | -    | 55,73,73     | 1.87 | 12 (21%) | 61,113,113  | 2.07 | 13 (21%) |
| 15  | CLA  | B     | 1203 | -    | 55,73,73     | 1.83 | 12 (21%) | 61,113,113  | 1.99 | 11 (18%) |
| 15  | CLA  | B     | 1204 | -    | 36,54,73     | 2.36 | 12 (33%) | 41,90,113   | 2.38 | 12 (29%) |
| 15  | CLA  | B     | 1205 | -    | 45,63,73     | 2.04 | 11 (24%) | 49,101,113  | 2.47 | 11 (22%) |
| 15  | CLA  | B     | 1206 | 2    | 36,54,73     | 2.37 | 12 (33%) | 41,90,113   | 2.28 | 13 (31%) |
| 15  | CLA  | B     | 1207 | -    | 36,54,73     | 2.37 | 12 (33%) | 41,90,113   | 2.36 | 11 (26%) |
| 15  | CLA  | B     | 1208 | -    | 32,53,73     | 2.33 | 11 (34%) | 37,89,113   | 2.22 | 8 (21%)  |
| 15  | CLA  | B     | 1209 | -    | 32,53,73     | 2.26 | 11 (34%) | 37,89,113   | 2.40 | 11 (29%) |
| 15  | CLA  | B     | 1210 | -    | 55,73,73     | 1.84 | 12 (21%) | 61,113,113  | 1.98 | 12 (19%) |
| 15  | CLA  | B     | 1211 | -    | 36,54,73     | 2.38 | 12 (33%) | 41,90,113   | 2.33 | 11 (26%) |
| 15  | CLA  | B     | 1212 | -    | 32,53,73     | 2.30 | 12 (37%) | 37,89,113   | 2.34 | 9 (24%)  |
| 15  | CLA  | B     | 1213 | -    | 40,58,73     | 2.20 | 12 (30%) | 44,95,113   | 2.28 | 11 (25%) |
| 15  | CLA  | B     | 1214 | -    | 55,73,73     | 1.85 | 11 (20%) | 61,113,113  | 2.16 | 13 (21%) |
| 15  | CLA  | B     | 1215 | -    | 55,73,73     | 1.87 | 12 (21%) | 61,113,113  | 2.23 | 13 (21%) |
| 15  | CLA  | B     | 1216 | -    | 55,73,73     | 1.87 | 12 (21%) | 61,113,113  | 1.97 | 11 (18%) |
| 15  | CLA  | B     | 1217 | -    | 37,55,73     | 2.21 | 13 (35%) | 42,91,113   | 2.50 | 12 (28%) |
| 15  | CLA  | B     | 1218 | -    | 41,59,73     | 2.16 | 12 (29%) | 44,96,113   | 2.56 | 13 (29%) |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 15  | CLA  | B     | 1219 | -    | 45,63,73     | 2.11 | 12 (26%) | 49,101,113  | 2.30 | 12 (24%) |
| 15  | CLA  | B     | 1220 | -    | 46,64,73     | 2.09 | 12 (26%) | 50,102,113  | 2.12 | 12 (24%) |
| 15  | CLA  | B     | 1221 | -    | 55,73,73     | 1.85 | 13 (23%) | 61,113,113  | 2.19 | 12 (19%) |
| 15  | CLA  | B     | 1222 | -    | 46,64,73     | 2.03 | 11 (23%) | 50,102,113  | 2.41 | 13 (26%) |
| 15  | CLA  | B     | 1223 | -    | 55,73,73     | 1.83 | 11 (20%) | 61,113,113  | 2.04 | 13 (21%) |
| 15  | CLA  | B     | 1224 | -    | 55,73,73     | 1.86 | 11 (20%) | 61,113,113  | 2.09 | 11 (18%) |
| 15  | CLA  | B     | 1225 | -    | 55,73,73     | 1.84 | 12 (21%) | 61,113,113  | 2.16 | 14 (22%) |
| 15  | CLA  | B     | 1226 | -    | 55,73,73     | 1.84 | 10 (18%) | 61,113,113  | 2.16 | 12 (19%) |
| 15  | CLA  | B     | 1227 | -    | 32,53,73     | 2.23 | 12 (37%) | 37,89,113   | 2.41 | 9 (24%)  |
| 15  | CLA  | B     | 1228 | -    | 55,73,73     | 1.89 | 12 (21%) | 61,113,113  | 1.89 | 11 (18%) |
| 15  | CLA  | B     | 1229 | -    | 55,73,73     | 1.84 | 12 (21%) | 61,113,113  | 1.99 | 11 (18%) |
| 15  | CLA  | B     | 1230 | -    | 55,73,73     | 1.85 | 12 (21%) | 61,113,113  | 2.25 | 14 (22%) |
| 15  | CLA  | B     | 1231 | -    | 55,73,73     | 1.86 | 11 (20%) | 61,113,113  | 2.05 | 13 (21%) |
| 15  | CLA  | B     | 1232 | -    | 32,53,73     | 2.24 | 11 (34%) | 37,89,113   | 2.27 | 9 (24%)  |
| 15  | CLA  | B     | 1234 | -    | 55,73,73     | 1.86 | 12 (21%) | 61,113,113  | 2.07 | 14 (22%) |
| 15  | CLA  | B     | 1235 | -    | 55,73,73     | 1.87 | 11 (20%) | 61,113,113  | 2.03 | 13 (21%) |
| 15  | CLA  | B     | 1236 | -    | 40,58,73     | 2.15 | 11 (27%) | 44,95,113   | 2.33 | 12 (27%) |
| 15  | CLA  | B     | 1237 | 19   | 45,63,73     | 2.04 | 13 (28%) | 49,101,113  | 2.29 | 14 (28%) |
| 15  | CLA  | B     | 1238 | 19   | 34,52,73     | 2.21 | 11 (32%) | 36,87,113   | 2.26 | 9 (25%)  |
| 15  | CLA  | B     | 1239 | -    | 36,54,73     | 2.38 | 12 (33%) | 41,90,113   | 2.42 | 12 (29%) |
| 15  | CLA  | B     | 1240 | 12   | 32,53,73     | 2.29 | 11 (34%) | 37,89,113   | 2.21 | 9 (24%)  |
| 16  | LMU  | B     | 1301 | -    | 36,36,36     | 0.44 | 0        | 47,47,47    | 0.91 | 5 (10%)  |
| 10  | PQN  | B     | 2002 | -    | 34,34,34     | 1.39 | 2 (5%)   | 44,45,45    | 1.09 | 3 (6%)   |
| 14  | BCR  | B     | 4004 | -    | 41,41,41     | 2.75 | 6 (14%)  | 56,56,56    | 6.26 | 26 (46%) |
| 14  | BCR  | B     | 4005 | -    | 41,41,41     | 2.74 | 6 (14%)  | 56,56,56    | 6.33 | 22 (39%) |
| 14  | BCR  | B     | 4006 | -    | 41,41,41     | 2.83 | 6 (14%)  | 56,56,56    | 6.59 | 24 (42%) |
| 14  | BCR  | B     | 4009 | -    | 41,41,41     | 2.74 | 7 (17%)  | 56,56,56    | 6.66 | 24 (42%) |
| 14  | BCR  | B     | 4010 | -    | 41,41,41     | 2.72 | 6 (14%)  | 56,56,56    | 6.54 | 21 (37%) |
| 14  | BCR  | B     | 4011 | -    | 41,41,41     | 2.75 | 6 (14%)  | 56,56,56    | 6.62 | 24 (42%) |
| 14  | BCR  | B     | 4014 | -    | 41,41,41     | 2.74 | 6 (14%)  | 56,56,56    | 6.57 | 22 (39%) |
| 14  | BCR  | B     | 4017 | -    | 41,41,41     | 2.72 | 6 (14%)  | 56,56,56    | 6.48 | 24 (42%) |
| 17  | LMG  | B     | 5002 | -    | 55,55,55     | 0.88 | 2 (3%)   | 63,63,63    | 0.98 | 2 (3%)   |
| 12  | LHG  | B     | 5004 | 15   | 48,48,48     | 0.91 | 2 (4%)   | 49,54,54    | 1.16 | 3 (6%)   |
| 11  | SF4  | C     | 3002 | 3    | 0,12,12      | 0.00 | -        | 0,24,24     | 0.00 | -        |
| 11  | SF4  | C     | 3003 | 3    | 0,12,12      | 0.00 | -        | 0,24,24     | 0.00 | -        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 15  | CLA  | F     | 1139 | 19   | 55,73,73     | 1.84 | 13 (23%) | 61,113,113  | 1.95 | 10 (16%) |
| 15  | CLA  | F     | 1301 | -    | 32,53,73     | 2.27 | 10 (31%) | 37,89,113   | 2.24 | 10 (27%) |
| 15  | CLA  | F     | 1410 | 6    | 55,73,73     | 1.84 | 12 (21%) | 61,113,113  | 2.20 | 14 (22%) |
| 14  | BCR  | F     | 4015 | -    | 41,41,41     | 2.74 | 7 (17%)  | 56,56,56    | 6.54 | 26 (46%) |
| 14  | BCR  | F     | 4016 | -    | 41,41,41     | 2.72 | 6 (14%)  | 56,56,56    | 6.63 | 24 (42%) |
| 15  | CLA  | J     | 1302 | 7    | 32,53,73     | 2.27 | 11 (34%) | 37,89,113   | 2.24 | 7 (18%)  |
| 15  | CLA  | J     | 1303 | -    | 36,54,73     | 2.39 | 13 (36%) | 41,90,113   | 2.28 | 10 (24%) |
| 16  | LMU  | J     | 1304 | -    | 36,36,36     | 0.41 | 0        | 47,47,47    | 0.64 | 1 (2%)   |
| 14  | BCR  | J     | 4013 | -    | 41,41,41     | 2.72 | 6 (14%)  | 56,56,56    | 6.52 | 26 (46%) |
| 15  | CLA  | K     | 1401 | -    | 36,54,73     | 2.38 | 12 (33%) | 41,90,113   | 2.34 | 14 (34%) |
| 15  | CLA  | K     | 1402 | -    | 36,54,73     | 2.38 | 12 (33%) | 41,90,113   | 2.25 | 10 (24%) |

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   |
|-----|------|-------|------|------|-----------|--------------|---------|
| 13  | CL0  | A     | 1011 | -    | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 15  | CLA  | A     | 1012 | 19   | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 15  | CLA  | A     | 1022 | 19   | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 15  | CLA  | A     | 1101 | -    | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 15  | CLA  | A     | 1102 | 15   | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 15  | CLA  | A     | 1103 | -    | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 15  | CLA  | A     | 1104 | -    | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 15  | CLA  | A     | 1105 | -    | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 15  | CLA  | A     | 1106 | 1    | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 15  | CLA  | A     | 1107 | 1    | 2/2/17/25 | 0/19/117/135 | 0/0/9/9 |
| 13  | CL0  | A     | 1108 | -    | 3/3/16/25 | 0/11/111/135 | 0/0/9/9 |
| 15  | CLA  | A     | 1109 | 15   | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 15  | CLA  | A     | 1110 | -    | 3/3/17/25 | 0/24/122/135 | 0/0/9/9 |
| 15  | CLA  | A     | 1111 | -    | 3/3/19/25 | 0/31/129/135 | 0/0/9/9 |
| 15  | CLA  | A     | 1112 | -    | 3/3/16/25 | 0/11/111/135 | 0/0/9/9 |
| 15  | CLA  | A     | 1113 | -    | 3/3/16/25 | 0/11/111/135 | 0/0/9/9 |
| 15  | CLA  | A     | 1114 | -    | 3/3/16/25 | 0/18/116/135 | 0/0/9/9 |
| 15  | CLA  | A     | 1115 | -    | 3/3/16/25 | 0/15/113/135 | 0/0/9/9 |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions     | Rings   |
|-----|------|-------|------|------|-----------|--------------|---------|
| 15  | CLA  | A     | 1116 | -    | 3/3/17/25 | 0/24/122/135 | 0/0/9/9 |
| 15  | CLA  | A     | 1117 | -    | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 15  | CLA  | A     | 1118 | -    | 3/3/16/25 | 0/15/113/135 | 0/0/9/9 |
| 15  | CLA  | A     | 1119 | -    | 2/2/19/25 | 0/35/133/135 | 0/0/9/9 |
| 15  | CLA  | A     | 1120 | -    | 3/3/16/25 | 0/18/116/135 | 0/0/9/9 |
| 15  | CLA  | A     | 1121 | -    | 3/3/16/25 | 0/15/113/135 | 0/0/9/9 |
| 15  | CLA  | A     | 1122 | -    | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 15  | CLA  | A     | 1123 | -    | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 15  | CLA  | A     | 1124 | -    | 3/3/18/25 | 0/25/123/135 | 0/0/9/9 |
| 15  | CLA  | A     | 1125 | -    | 2/2/17/25 | 0/22/120/135 | 0/0/9/9 |
| 15  | CLA  | A     | 1126 | -    | 1/1/20/25 | 0/37/135/135 | 0/0/9/9 |
| 15  | CLA  | A     | 1127 | -    | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 15  | CLA  | A     | 1128 | -    | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 15  | CLA  | A     | 1129 | -    | 3/3/16/25 | 0/15/113/135 | 0/0/9/9 |
| 15  | CLA  | A     | 1130 | -    | 3/3/18/25 | 0/25/123/135 | 0/0/9/9 |
| 15  | CLA  | A     | 1131 | -    | 3/3/18/25 | 0/25/123/135 | 0/0/9/9 |
| 15  | CLA  | A     | 1132 | -    | 3/3/19/25 | 0/34/132/135 | 0/0/9/9 |
| 15  | CLA  | A     | 1133 | -    | 3/3/16/25 | 0/15/113/135 | 0/0/9/9 |
| 15  | CLA  | A     | 1134 | 1    | 3/3/16/25 | 0/15/113/135 | 0/0/9/9 |
| 15  | CLA  | A     | 1135 | -    | 3/3/18/25 | 0/25/123/135 | 0/0/9/9 |
| 15  | CLA  | A     | 1136 | -    | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 15  | CLA  | A     | 1137 | -    | 3/3/17/25 | 0/19/117/135 | 0/0/9/9 |
| 15  | CLA  | A     | 1138 | -    | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 15  | CLA  | A     | 1140 | -    | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 15  | CLA  | A     | 1801 | 12   | 3/3/17/25 | 0/22/120/135 | 0/0/9/9 |
| 10  | PQN  | A     | 2001 | -    | -         | 0/23/43/43   | 0/2/2/2 |
| 11  | SF4  | A     | 3001 | 1,2  | -         | 0/0/48/48    | 0/6/5/5 |
| 14  | BCR  | A     | 4001 | -    | -         | 0/29/63/63   | 0/2/2/2 |
| 14  | BCR  | A     | 4002 | -    | -         | 0/29/63/63   | 0/2/2/2 |
| 14  | BCR  | A     | 4003 | -    | -         | 0/29/63/63   | 0/2/2/2 |
| 14  | BCR  | A     | 4007 | -    | -         | 0/29/63/63   | 0/2/2/2 |
| 14  | BCR  | A     | 4008 | -    | -         | 0/29/63/63   | 0/2/2/2 |
| 14  | BCR  | A     | 4012 | -    | -         | 0/29/63/63   | 0/2/2/2 |
| 12  | LHG  | A     | 5001 | -    | -         | 0/53/53/53   | 0/0/0/0 |
| 12  | LHG  | A     | 5003 | 15   | -         | 0/53/53/53   | 0/0/0/0 |
| 12  | LHG  | A     | 5005 | -    | -         | 0/40/40/53   | 0/0/0/0 |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions     | Rings   |
|-----|------|-------|------|------|-----------|--------------|---------|
| 15  | CLA  | B     | 1013 | -    | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 15  | CLA  | B     | 1021 | -    | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 15  | CLA  | B     | 1023 | -    | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 15  | CLA  | B     | 1201 | -    | 3/3/16/25 | 0/15/113/135 | 0/0/9/9 |
| 15  | CLA  | B     | 1202 | -    | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 15  | CLA  | B     | 1203 | -    | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 15  | CLA  | B     | 1204 | -    | 3/3/16/25 | 0/15/113/135 | 0/0/9/9 |
| 15  | CLA  | B     | 1205 | -    | 3/3/18/25 | 0/25/123/135 | 0/0/9/9 |
| 15  | CLA  | B     | 1206 | 2    | 3/3/16/25 | 0/15/113/135 | 0/0/9/9 |
| 15  | CLA  | B     | 1207 | -    | 3/3/16/25 | 0/15/113/135 | 0/0/9/9 |
| 15  | CLA  | B     | 1208 | -    | 3/3/16/25 | 0/11/111/135 | 0/0/9/9 |
| 15  | CLA  | B     | 1209 | -    | 3/3/16/25 | 0/11/111/135 | 0/0/9/9 |
| 15  | CLA  | B     | 1210 | -    | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 15  | CLA  | B     | 1211 | -    | 3/3/16/25 | 0/15/113/135 | 0/0/9/9 |
| 15  | CLA  | B     | 1212 | -    | 3/3/16/25 | 0/11/111/135 | 0/0/9/9 |
| 15  | CLA  | B     | 1213 | -    | 2/2/17/25 | 0/19/117/135 | 0/0/9/9 |
| 15  | CLA  | B     | 1214 | -    | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 15  | CLA  | B     | 1215 | -    | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 15  | CLA  | B     | 1216 | -    | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 15  | CLA  | B     | 1217 | -    | 3/3/16/25 | 0/16/114/135 | 0/0/9/9 |
| 15  | CLA  | B     | 1218 | -    | 3/3/17/25 | 0/21/119/135 | 0/0/9/9 |
| 15  | CLA  | B     | 1219 | -    | 3/3/18/25 | 0/25/123/135 | 0/0/9/9 |
| 15  | CLA  | B     | 1220 | -    | 3/3/18/25 | 0/27/125/135 | 0/0/9/9 |
| 15  | CLA  | B     | 1221 | -    | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 15  | CLA  | B     | 1222 | -    | 2/2/18/25 | 0/27/125/135 | 0/0/9/9 |
| 15  | CLA  | B     | 1223 | -    | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 15  | CLA  | B     | 1224 | -    | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 15  | CLA  | B     | 1225 | -    | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 15  | CLA  | B     | 1226 | -    | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 15  | CLA  | B     | 1227 | -    | 2/2/16/25 | 0/11/111/135 | 0/0/9/9 |
| 15  | CLA  | B     | 1228 | -    | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 15  | CLA  | B     | 1229 | -    | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 15  | CLA  | B     | 1230 | -    | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 15  | CLA  | B     | 1231 | -    | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions     | Rings   |
|-----|------|-------|------|------|-----------|--------------|---------|
| 15  | CLA  | B     | 1232 | -    | 3/3/16/25 | 0/11/111/135 | 0/0/9/9 |
| 15  | CLA  | B     | 1234 | -    | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 15  | CLA  | B     | 1235 | -    | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 15  | CLA  | B     | 1236 | -    | 2/2/17/25 | 0/19/117/135 | 0/0/9/9 |
| 15  | CLA  | B     | 1237 | 19   | 3/3/18/25 | 0/25/123/135 | 0/0/9/9 |
| 15  | CLA  | B     | 1238 | 19   | 3/3/15/25 | 0/11/110/135 | 0/0/9/9 |
| 15  | CLA  | B     | 1239 | -    | 3/3/16/25 | 0/15/113/135 | 0/0/9/9 |
| 15  | CLA  | B     | 1240 | 12   | 3/3/16/25 | 0/11/111/135 | 0/0/9/9 |
| 16  | LMU  | B     | 1301 | -    | -         | 0/21/61/61   | 0/2/2/2 |
| 10  | PQN  | B     | 2002 | -    | -         | 0/23/43/43   | 0/2/2/2 |
| 14  | BCR  | B     | 4004 | -    | -         | 0/29/63/63   | 0/2/2/2 |
| 14  | BCR  | B     | 4005 | -    | -         | 0/29/63/63   | 0/2/2/2 |
| 14  | BCR  | B     | 4006 | -    | -         | 0/29/63/63   | 0/2/2/2 |
| 14  | BCR  | B     | 4009 | -    | -         | 2/29/63/63   | 0/2/2/2 |
| 14  | BCR  | B     | 4010 | -    | -         | 0/29/63/63   | 0/2/2/2 |
| 14  | BCR  | B     | 4011 | -    | -         | 0/29/63/63   | 0/2/2/2 |
| 14  | BCR  | B     | 4014 | -    | -         | 0/29/63/63   | 0/2/2/2 |
| 14  | BCR  | B     | 4017 | -    | -         | 0/29/63/63   | 0/2/2/2 |
| 17  | LMG  | B     | 5002 | -    | -         | 0/50/70/70   | 0/1/1/1 |
| 12  | LHG  | B     | 5004 | 15   | -         | 0/53/53/53   | 0/0/0/0 |
| 11  | SF4  | C     | 3002 | 3    | -         | 0/0/48/48    | 0/6/5/5 |
| 11  | SF4  | C     | 3003 | 3    | -         | 0/0/48/48    | 0/6/5/5 |
| 15  | CLA  | F     | 1139 | 19   | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 15  | CLA  | F     | 1301 | -    | 3/3/16/25 | 0/11/111/135 | 0/0/9/9 |
| 15  | CLA  | F     | 1410 | 6    | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 14  | BCR  | F     | 4015 | -    | -         | 0/29/63/63   | 0/2/2/2 |
| 14  | BCR  | F     | 4016 | -    | -         | 0/29/63/63   | 0/2/2/2 |
| 15  | CLA  | J     | 1302 | 7    | 3/3/16/25 | 0/11/111/135 | 0/0/9/9 |
| 15  | CLA  | J     | 1303 | -    | 3/3/16/25 | 0/15/113/135 | 0/0/9/9 |
| 16  | LMU  | J     | 1304 | -    | -         | 0/21/61/61   | 0/2/2/2 |
| 14  | BCR  | J     | 4013 | -    | -         | 0/29/63/63   | 0/2/2/2 |
| 15  | CLA  | K     | 1401 | -    | 3/3/16/25 | 0/15/113/135 | 0/0/9/9 |
| 15  | CLA  | K     | 1402 | -    | 3/3/16/25 | 0/15/113/135 | 0/0/9/9 |

All (1203) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | A     | 4012 | BCR  | C11-C10 | -8.28 | 1.18        | 1.43     |
| 14  | B     | 4006 | BCR  | C11-C10 | -8.25 | 1.18        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | F     | 4016 | BCR  | C11-C10 | -8.15 | 1.18        | 1.43     |
| 14  | B     | 4004 | BCR  | C11-C10 | -8.12 | 1.18        | 1.43     |
| 14  | B     | 4010 | BCR  | C11-C10 | -8.09 | 1.18        | 1.43     |
| 14  | B     | 4011 | BCR  | C11-C10 | -8.06 | 1.18        | 1.43     |
| 14  | A     | 4002 | BCR  | C11-C10 | -8.03 | 1.18        | 1.43     |
| 14  | B     | 4014 | BCR  | C11-C10 | -8.01 | 1.18        | 1.43     |
| 14  | B     | 4009 | BCR  | C11-C10 | -8.01 | 1.18        | 1.43     |
| 14  | B     | 4005 | BCR  | C11-C10 | -8.00 | 1.18        | 1.43     |
| 14  | B     | 4006 | BCR  | C10-C9  | -7.98 | 1.25        | 1.35     |
| 14  | B     | 4009 | BCR  | C8-C9   | -7.98 | 1.28        | 1.45     |
| 14  | F     | 4015 | BCR  | C11-C10 | -7.98 | 1.19        | 1.43     |
| 14  | B     | 4017 | BCR  | C11-C10 | -7.97 | 1.19        | 1.43     |
| 14  | A     | 4003 | BCR  | C11-C10 | -7.96 | 1.19        | 1.43     |
| 14  | A     | 4007 | BCR  | C11-C10 | -7.95 | 1.19        | 1.43     |
| 14  | A     | 4001 | BCR  | C11-C10 | -7.94 | 1.19        | 1.43     |
| 14  | F     | 4015 | BCR  | C8-C9   | -7.93 | 1.28        | 1.45     |
| 14  | B     | 4014 | BCR  | C8-C9   | -7.92 | 1.28        | 1.45     |
| 14  | F     | 4016 | BCR  | C8-C9   | -7.92 | 1.28        | 1.45     |
| 14  | A     | 4008 | BCR  | C11-C10 | -7.91 | 1.19        | 1.43     |
| 14  | J     | 4013 | BCR  | C11-C10 | -7.89 | 1.19        | 1.43     |
| 14  | A     | 4012 | BCR  | C8-C9   | -7.88 | 1.28        | 1.45     |
| 14  | B     | 4005 | BCR  | C8-C9   | -7.88 | 1.28        | 1.45     |
| 14  | J     | 4013 | BCR  | C8-C9   | -7.86 | 1.28        | 1.45     |
| 14  | B     | 4006 | BCR  | C8-C9   | -7.82 | 1.28        | 1.45     |
| 14  | A     | 4003 | BCR  | C8-C9   | -7.81 | 1.28        | 1.45     |
| 14  | B     | 4011 | BCR  | C8-C9   | -7.77 | 1.28        | 1.45     |
| 14  | A     | 4008 | BCR  | C8-C9   | -7.76 | 1.28        | 1.45     |
| 14  | A     | 4001 | BCR  | C8-C9   | -7.76 | 1.28        | 1.45     |
| 14  | A     | 4001 | BCR  | C10-C9  | -7.71 | 1.25        | 1.35     |
| 14  | A     | 4002 | BCR  | C8-C9   | -7.70 | 1.28        | 1.45     |
| 14  | B     | 4004 | BCR  | C8-C9   | -7.68 | 1.28        | 1.45     |
| 14  | A     | 4007 | BCR  | C8-C9   | -7.66 | 1.28        | 1.45     |
| 14  | B     | 4017 | BCR  | C8-C9   | -7.66 | 1.28        | 1.45     |
| 14  | B     | 4010 | BCR  | C8-C9   | -7.62 | 1.29        | 1.45     |
| 14  | B     | 4017 | BCR  | C20-C21 | -7.44 | 1.20        | 1.43     |
| 14  | B     | 4011 | BCR  | C20-C21 | -7.43 | 1.20        | 1.43     |
| 14  | A     | 4002 | BCR  | C20-C21 | -7.40 | 1.20        | 1.43     |
| 14  | A     | 4012 | BCR  | C20-C21 | -7.40 | 1.20        | 1.43     |
| 14  | A     | 4008 | BCR  | C20-C21 | -7.39 | 1.20        | 1.43     |
| 14  | A     | 4012 | BCR  | C10-C9  | -7.39 | 1.26        | 1.35     |
| 14  | B     | 4006 | BCR  | C20-C21 | -7.39 | 1.20        | 1.43     |
| 14  | A     | 4012 | BCR  | C16-C17 | -7.37 | 1.20        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | B     | 4004 | BCR  | C10-C9  | -7.37 | 1.26        | 1.35     |
| 14  | F     | 4015 | BCR  | C20-C21 | -7.35 | 1.20        | 1.43     |
| 14  | B     | 4006 | BCR  | C16-C17 | -7.35 | 1.20        | 1.43     |
| 14  | B     | 4009 | BCR  | C20-C21 | -7.33 | 1.21        | 1.43     |
| 14  | B     | 4005 | BCR  | C20-C21 | -7.31 | 1.21        | 1.43     |
| 14  | A     | 4001 | BCR  | C20-C21 | -7.31 | 1.21        | 1.43     |
| 14  | A     | 4007 | BCR  | C20-C21 | -7.31 | 1.21        | 1.43     |
| 14  | J     | 4013 | BCR  | C20-C21 | -7.30 | 1.21        | 1.43     |
| 14  | F     | 4016 | BCR  | C20-C21 | -7.30 | 1.21        | 1.43     |
| 14  | A     | 4003 | BCR  | C20-C21 | -7.29 | 1.21        | 1.43     |
| 14  | A     | 4008 | BCR  | C16-C17 | -7.29 | 1.21        | 1.43     |
| 14  | A     | 4002 | BCR  | C16-C17 | -7.29 | 1.21        | 1.43     |
| 14  | B     | 4009 | BCR  | C16-C17 | -7.29 | 1.21        | 1.43     |
| 14  | A     | 4002 | BCR  | C10-C9  | -7.28 | 1.26        | 1.35     |
| 14  | A     | 4001 | BCR  | C16-C17 | -7.28 | 1.21        | 1.43     |
| 14  | B     | 4004 | BCR  | C20-C21 | -7.28 | 1.21        | 1.43     |
| 14  | B     | 4011 | BCR  | C16-C17 | -7.27 | 1.21        | 1.43     |
| 14  | A     | 4003 | BCR  | C16-C17 | -7.26 | 1.21        | 1.43     |
| 14  | B     | 4005 | BCR  | C16-C17 | -7.26 | 1.21        | 1.43     |
| 14  | B     | 4014 | BCR  | C20-C21 | -7.25 | 1.21        | 1.43     |
| 14  | B     | 4010 | BCR  | C20-C21 | -7.25 | 1.21        | 1.43     |
| 14  | B     | 4010 | BCR  | C10-C9  | -7.24 | 1.26        | 1.35     |
| 14  | F     | 4015 | BCR  | C16-C17 | -7.24 | 1.21        | 1.43     |
| 14  | B     | 4004 | BCR  | C16-C17 | -7.23 | 1.21        | 1.43     |
| 14  | B     | 4017 | BCR  | C16-C17 | -7.22 | 1.21        | 1.43     |
| 14  | J     | 4013 | BCR  | C16-C17 | -7.21 | 1.21        | 1.43     |
| 14  | B     | 4014 | BCR  | C16-C17 | -7.21 | 1.21        | 1.43     |
| 14  | B     | 4005 | BCR  | C10-C9  | -7.21 | 1.26        | 1.35     |
| 14  | B     | 4014 | BCR  | C10-C9  | -7.20 | 1.26        | 1.35     |
| 14  | B     | 4011 | BCR  | C10-C9  | -7.20 | 1.26        | 1.35     |
| 14  | F     | 4016 | BCR  | C16-C17 | -7.18 | 1.21        | 1.43     |
| 14  | A     | 4007 | BCR  | C16-C17 | -7.17 | 1.21        | 1.43     |
| 14  | A     | 4007 | BCR  | C10-C9  | -7.15 | 1.26        | 1.35     |
| 14  | A     | 4003 | BCR  | C10-C9  | -7.14 | 1.26        | 1.35     |
| 14  | F     | 4015 | BCR  | C10-C9  | -7.13 | 1.26        | 1.35     |
| 14  | B     | 4010 | BCR  | C16-C17 | -7.11 | 1.21        | 1.43     |
| 14  | J     | 4013 | BCR  | C10-C9  | -7.05 | 1.26        | 1.35     |
| 14  | B     | 4017 | BCR  | C10-C9  | -7.00 | 1.26        | 1.35     |
| 14  | B     | 4009 | BCR  | C10-C9  | -7.00 | 1.26        | 1.35     |
| 14  | A     | 4008 | BCR  | C10-C9  | -6.94 | 1.26        | 1.35     |
| 14  | F     | 4016 | BCR  | C10-C9  | -6.91 | 1.26        | 1.35     |
| 14  | A     | 4012 | BCR  | C11-C12 | -3.38 | 1.25        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | B     | 4006 | BCR  | C11-C12 | -3.31 | 1.25        | 1.34     |
| 14  | F     | 4016 | BCR  | C11-C12 | -3.26 | 1.25        | 1.34     |
| 14  | B     | 4004 | BCR  | C11-C12 | -3.23 | 1.26        | 1.34     |
| 14  | B     | 4010 | BCR  | C11-C12 | -3.18 | 1.26        | 1.34     |
| 14  | B     | 4014 | BCR  | C11-C12 | -3.11 | 1.26        | 1.34     |
| 14  | B     | 4011 | BCR  | C11-C12 | -3.11 | 1.26        | 1.34     |
| 14  | B     | 4005 | BCR  | C11-C12 | -3.10 | 1.26        | 1.34     |
| 14  | A     | 4002 | BCR  | C11-C12 | -3.06 | 1.26        | 1.34     |
| 14  | A     | 4003 | BCR  | C11-C12 | -3.02 | 1.26        | 1.34     |
| 14  | B     | 4017 | BCR  | C11-C12 | -3.00 | 1.26        | 1.34     |
| 14  | A     | 4007 | BCR  | C11-C12 | -2.99 | 1.26        | 1.34     |
| 14  | F     | 4015 | BCR  | C11-C12 | -2.98 | 1.26        | 1.34     |
| 14  | B     | 4009 | BCR  | C11-C12 | -2.97 | 1.26        | 1.34     |
| 14  | A     | 4008 | BCR  | C11-C12 | -2.96 | 1.26        | 1.34     |
| 14  | J     | 4013 | BCR  | C11-C12 | -2.95 | 1.26        | 1.34     |
| 14  | A     | 4001 | BCR  | C11-C12 | -2.77 | 1.27        | 1.34     |
| 15  | A     | 1128 | CLA  | C1C-NC  | -2.46 | 1.33        | 1.37     |
| 15  | B     | 1231 | CLA  | C1C-NC  | -2.39 | 1.33        | 1.37     |
| 15  | A     | 1107 | CLA  | C1C-NC  | -2.36 | 1.33        | 1.37     |
| 15  | A     | 1110 | CLA  | C1C-NC  | -2.23 | 1.34        | 1.37     |
| 15  | F     | 1139 | CLA  | C1C-NC  | -2.19 | 1.34        | 1.37     |
| 15  | B     | 1234 | CLA  | C1C-NC  | -2.19 | 1.34        | 1.37     |
| 15  | A     | 1115 | CLA  | C1C-NC  | -2.17 | 1.34        | 1.37     |
| 15  | B     | 1023 | CLA  | C1C-NC  | -2.17 | 1.34        | 1.37     |
| 15  | A     | 1131 | CLA  | C1C-NC  | -2.17 | 1.34        | 1.37     |
| 15  | B     | 1013 | CLA  | C1C-NC  | -2.16 | 1.34        | 1.37     |
| 15  | A     | 1801 | CLA  | C1C-NC  | -2.16 | 1.34        | 1.37     |
| 15  | B     | 1239 | CLA  | C1C-NC  | -2.15 | 1.34        | 1.37     |
| 15  | A     | 1106 | CLA  | C1C-NC  | -2.15 | 1.34        | 1.37     |
| 15  | B     | 1215 | CLA  | C1C-NC  | -2.15 | 1.34        | 1.37     |
| 15  | B     | 1222 | CLA  | C1C-NC  | -2.14 | 1.34        | 1.37     |
| 15  | B     | 1208 | CLA  | C1C-NC  | -2.13 | 1.34        | 1.37     |
| 15  | A     | 1140 | CLA  | C1C-NC  | -2.12 | 1.34        | 1.37     |
| 15  | B     | 1203 | CLA  | C1C-NC  | -2.12 | 1.34        | 1.37     |
| 15  | B     | 1211 | CLA  | C1C-NC  | -2.12 | 1.34        | 1.37     |
| 14  | A     | 4008 | BCR  | C30-C25 | -2.12 | 1.50        | 1.53     |
| 15  | A     | 1113 | CLA  | C1C-NC  | -2.12 | 1.34        | 1.37     |
| 15  | A     | 1102 | CLA  | C1C-NC  | -2.11 | 1.34        | 1.37     |
| 15  | K     | 1401 | CLA  | C1C-NC  | -2.11 | 1.34        | 1.37     |
| 15  | A     | 1103 | CLA  | C1C-NC  | -2.11 | 1.34        | 1.37     |
| 13  | A     | 1011 | CL0  | C1C-NC  | -2.11 | 1.34        | 1.37     |
| 15  | A     | 1105 | CLA  | C1C-NC  | -2.11 | 1.34        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 15  | B     | 1210 | CLA  | C1C-NC  | -2.11 | 1.34        | 1.37     |
| 15  | B     | 1229 | CLA  | C1C-NC  | -2.11 | 1.34        | 1.37     |
| 15  | A     | 1121 | CLA  | C1C-NC  | -2.11 | 1.34        | 1.37     |
| 15  | B     | 1218 | CLA  | C1C-NC  | -2.10 | 1.34        | 1.37     |
| 15  | B     | 1205 | CLA  | C1C-NC  | -2.10 | 1.34        | 1.37     |
| 15  | J     | 1302 | CLA  | C1C-NC  | -2.09 | 1.34        | 1.37     |
| 15  | A     | 1111 | CLA  | C1C-NC  | -2.09 | 1.34        | 1.37     |
| 15  | B     | 1238 | CLA  | C1C-NC  | -2.09 | 1.34        | 1.37     |
| 15  | A     | 1109 | CLA  | C1C-NC  | -2.09 | 1.34        | 1.37     |
| 15  | B     | 1212 | CLA  | C1C-NC  | -2.09 | 1.34        | 1.37     |
| 15  | A     | 1101 | CLA  | C1C-NC  | -2.08 | 1.34        | 1.37     |
| 15  | A     | 1135 | CLA  | C1C-NC  | -2.08 | 1.34        | 1.37     |
| 15  | B     | 1227 | CLA  | C1C-NC  | -2.08 | 1.34        | 1.37     |
| 15  | A     | 1116 | CLA  | C1C-NC  | -2.08 | 1.34        | 1.37     |
| 15  | B     | 1202 | CLA  | C1C-NC  | -2.08 | 1.34        | 1.37     |
| 15  | A     | 1122 | CLA  | C1C-NC  | -2.07 | 1.34        | 1.37     |
| 14  | F     | 4015 | BCR  | C30-C25 | -2.07 | 1.50        | 1.53     |
| 15  | A     | 1136 | CLA  | C1C-NC  | -2.07 | 1.34        | 1.37     |
| 13  | A     | 1011 | CL0  | C4C-NC  | -2.07 | 1.34        | 1.37     |
| 15  | J     | 1303 | CLA  | C1C-NC  | -2.06 | 1.34        | 1.37     |
| 15  | A     | 1120 | CLA  | C1C-NC  | -2.06 | 1.34        | 1.37     |
| 15  | B     | 1206 | CLA  | C1C-NC  | -2.06 | 1.34        | 1.37     |
| 15  | B     | 1216 | CLA  | C1C-NC  | -2.06 | 1.34        | 1.37     |
| 15  | K     | 1402 | CLA  | C1C-NC  | -2.06 | 1.34        | 1.37     |
| 15  | A     | 1133 | CLA  | C1C-NC  | -2.05 | 1.34        | 1.37     |
| 15  | B     | 1232 | CLA  | C1C-NC  | -2.05 | 1.34        | 1.37     |
| 15  | A     | 1127 | CLA  | C1C-NC  | -2.04 | 1.34        | 1.37     |
| 15  | B     | 1207 | CLA  | C1C-NC  | -2.04 | 1.34        | 1.37     |
| 15  | A     | 1137 | CLA  | C1C-NC  | -2.04 | 1.34        | 1.37     |
| 15  | A     | 1104 | CLA  | C1C-NC  | -2.04 | 1.34        | 1.37     |
| 15  | B     | 1230 | CLA  | C1C-NC  | -2.04 | 1.34        | 1.37     |
| 15  | B     | 1201 | CLA  | C1C-NC  | -2.04 | 1.34        | 1.37     |
| 15  | A     | 1125 | CLA  | C1C-NC  | -2.04 | 1.34        | 1.37     |
| 14  | B     | 4009 | BCR  | C30-C25 | -2.04 | 1.50        | 1.53     |
| 15  | A     | 1134 | CLA  | C1C-NC  | -2.03 | 1.34        | 1.37     |
| 15  | A     | 1114 | CLA  | C1C-NC  | -2.03 | 1.34        | 1.37     |
| 15  | B     | 1221 | CLA  | C1C-NC  | -2.03 | 1.34        | 1.37     |
| 15  | A     | 1123 | CLA  | C1C-NC  | -2.03 | 1.34        | 1.37     |
| 15  | A     | 1124 | CLA  | C1C-NC  | -2.03 | 1.34        | 1.37     |
| 15  | B     | 1204 | CLA  | C1C-NC  | -2.03 | 1.34        | 1.37     |
| 15  | A     | 1132 | CLA  | C1C-NC  | -2.03 | 1.34        | 1.37     |
| 15  | B     | 1237 | CLA  | C1C-NC  | -2.03 | 1.34        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 15  | A     | 1118 | CLA  | C1C-NC  | -2.02 | 1.34        | 1.37     |
| 15  | A     | 1119 | CLA  | C1C-NC  | -2.02 | 1.34        | 1.37     |
| 15  | B     | 1224 | CLA  | C1C-NC  | -2.02 | 1.34        | 1.37     |
| 15  | A     | 1117 | CLA  | C1C-NC  | -2.02 | 1.34        | 1.37     |
| 15  | B     | 1013 | CLA  | C4C-NC  | -2.01 | 1.34        | 1.37     |
| 15  | B     | 1209 | CLA  | C1C-NC  | -2.01 | 1.34        | 1.37     |
| 15  | B     | 1021 | CLA  | C1C-NC  | -2.00 | 1.34        | 1.37     |
| 15  | B     | 1217 | CLA  | C1C-NC  | -2.00 | 1.34        | 1.37     |
| 15  | B     | 1237 | CLA  | C1C-C2C | 2.00  | 1.48        | 1.44     |
| 15  | A     | 1122 | CLA  | C4C-C3C | 2.01  | 1.48        | 1.45     |
| 15  | J     | 1303 | CLA  | C1C-C2C | 2.01  | 1.48        | 1.44     |
| 15  | B     | 1234 | CLA  | C4C-C3C | 2.01  | 1.48        | 1.45     |
| 15  | F     | 1139 | CLA  | C4C-C3C | 2.01  | 1.48        | 1.45     |
| 15  | A     | 1127 | CLA  | C4C-C3C | 2.02  | 1.48        | 1.45     |
| 15  | B     | 1212 | CLA  | C4C-C3C | 2.02  | 1.48        | 1.45     |
| 15  | B     | 1225 | CLA  | C4C-C3C | 2.02  | 1.48        | 1.45     |
| 15  | A     | 1801 | CLA  | C1C-C2C | 2.02  | 1.48        | 1.44     |
| 15  | F     | 1410 | CLA  | C4C-C3C | 2.02  | 1.48        | 1.45     |
| 15  | B     | 1211 | CLA  | C1C-C2C | 2.02  | 1.48        | 1.44     |
| 15  | B     | 1221 | CLA  | C1C-C2C | 2.02  | 1.48        | 1.44     |
| 15  | A     | 1103 | CLA  | C4C-C3C | 2.03  | 1.48        | 1.45     |
| 15  | B     | 1212 | CLA  | C1C-C2C | 2.03  | 1.48        | 1.44     |
| 15  | A     | 1106 | CLA  | C4C-C3C | 2.03  | 1.48        | 1.45     |
| 15  | B     | 1219 | CLA  | C1C-C2C | 2.03  | 1.48        | 1.44     |
| 15  | A     | 1119 | CLA  | C1C-C2C | 2.03  | 1.48        | 1.44     |
| 15  | B     | 1225 | CLA  | C1C-C2C | 2.04  | 1.48        | 1.44     |
| 15  | B     | 1228 | CLA  | C4C-C3C | 2.04  | 1.48        | 1.45     |
| 15  | B     | 1229 | CLA  | C1C-C2C | 2.05  | 1.48        | 1.44     |
| 15  | A     | 1126 | CLA  | C1C-C2C | 2.05  | 1.48        | 1.44     |
| 15  | B     | 1227 | CLA  | C1C-C2C | 2.05  | 1.48        | 1.44     |
| 15  | A     | 1112 | CLA  | C4C-C3C | 2.06  | 1.48        | 1.45     |
| 15  | B     | 1217 | CLA  | C1C-C2C | 2.06  | 1.48        | 1.44     |
| 15  | A     | 1112 | CLA  | C1C-C2C | 2.06  | 1.48        | 1.44     |
| 15  | F     | 1410 | CLA  | C1C-C2C | 2.06  | 1.48        | 1.44     |
| 15  | B     | 1021 | CLA  | C4C-C3C | 2.06  | 1.48        | 1.45     |
| 15  | A     | 1117 | CLA  | C4C-C3C | 2.06  | 1.48        | 1.45     |
| 15  | A     | 1101 | CLA  | C1C-C2C | 2.07  | 1.48        | 1.44     |
| 15  | B     | 1213 | CLA  | C1C-C2C | 2.07  | 1.48        | 1.44     |
| 15  | B     | 1228 | CLA  | C1C-C2C | 2.07  | 1.48        | 1.44     |
| 15  | A     | 1801 | CLA  | C4C-C3C | 2.07  | 1.48        | 1.45     |
| 15  | B     | 1221 | CLA  | C4C-C3C | 2.07  | 1.48        | 1.45     |
| 15  | A     | 1102 | CLA  | C4C-C3C | 2.08  | 1.48        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 15  | A     | 1126 | CLA  | C4C-C3C | 2.08 | 1.48        | 1.45     |
| 15  | B     | 1021 | CLA  | C1C-C2C | 2.08 | 1.48        | 1.44     |
| 15  | A     | 1110 | CLA  | C4C-C3C | 2.08 | 1.48        | 1.45     |
| 15  | A     | 1130 | CLA  | C4C-C3C | 2.08 | 1.48        | 1.45     |
| 15  | B     | 1240 | CLA  | C1C-C2C | 2.08 | 1.48        | 1.44     |
| 15  | B     | 1201 | CLA  | C4C-C3C | 2.08 | 1.48        | 1.45     |
| 15  | B     | 1202 | CLA  | C4C-C3C | 2.09 | 1.48        | 1.45     |
| 15  | B     | 1218 | CLA  | C4C-C3C | 2.09 | 1.48        | 1.45     |
| 15  | B     | 1230 | CLA  | C1C-C2C | 2.09 | 1.48        | 1.44     |
| 15  | A     | 1107 | CLA  | C4C-C3C | 2.09 | 1.48        | 1.45     |
| 15  | B     | 1238 | CLA  | C4C-C3C | 2.09 | 1.48        | 1.45     |
| 13  | A     | 1108 | CL0  | C1C-C2C | 2.10 | 1.48        | 1.44     |
| 15  | B     | 1217 | CLA  | C4C-C3C | 2.11 | 1.48        | 1.45     |
| 15  | J     | 1302 | CLA  | C4C-C3C | 2.11 | 1.48        | 1.45     |
| 15  | A     | 1022 | CLA  | C1C-C2C | 2.11 | 1.48        | 1.44     |
| 15  | B     | 1213 | CLA  | C4C-C3C | 2.11 | 1.48        | 1.45     |
| 15  | A     | 1140 | CLA  | C1C-C2C | 2.12 | 1.48        | 1.44     |
| 15  | A     | 1012 | CLA  | C1C-C2C | 2.12 | 1.48        | 1.44     |
| 15  | K     | 1402 | CLA  | C4C-C3C | 2.12 | 1.48        | 1.45     |
| 15  | A     | 1122 | CLA  | C1C-C2C | 2.13 | 1.48        | 1.44     |
| 15  | B     | 1023 | CLA  | C4C-C3C | 2.13 | 1.48        | 1.45     |
| 15  | F     | 1301 | CLA  | C1C-C2C | 2.14 | 1.48        | 1.44     |
| 15  | A     | 1136 | CLA  | C4C-C3C | 2.14 | 1.48        | 1.45     |
| 15  | B     | 1219 | CLA  | C4C-C3C | 2.15 | 1.48        | 1.45     |
| 15  | B     | 1232 | CLA  | C4C-C3C | 2.15 | 1.48        | 1.45     |
| 15  | B     | 1220 | CLA  | C1C-C2C | 2.15 | 1.48        | 1.44     |
| 15  | B     | 1210 | CLA  | C4C-C3C | 2.15 | 1.48        | 1.45     |
| 15  | A     | 1129 | CLA  | C4C-C3C | 2.15 | 1.48        | 1.45     |
| 15  | A     | 1012 | CLA  | C4C-C3C | 2.15 | 1.48        | 1.45     |
| 15  | B     | 1220 | CLA  | C4C-C3C | 2.15 | 1.48        | 1.45     |
| 15  | A     | 1130 | CLA  | C1C-C2C | 2.15 | 1.48        | 1.44     |
| 15  | A     | 1124 | CLA  | C4C-C3C | 2.15 | 1.48        | 1.45     |
| 15  | A     | 1109 | CLA  | C1C-C2C | 2.16 | 1.48        | 1.44     |
| 15  | A     | 1134 | CLA  | C4C-C3C | 2.16 | 1.48        | 1.45     |
| 15  | A     | 1111 | CLA  | C4C-C3C | 2.16 | 1.48        | 1.45     |
| 15  | B     | 1203 | CLA  | C4C-C3C | 2.16 | 1.48        | 1.45     |
| 15  | A     | 1119 | CLA  | C4C-C3C | 2.16 | 1.48        | 1.45     |
| 15  | B     | 1208 | CLA  | C4C-C3C | 2.17 | 1.48        | 1.45     |
| 15  | B     | 1237 | CLA  | C4C-C3C | 2.18 | 1.49        | 1.45     |
| 15  | B     | 1207 | CLA  | C4C-C3C | 2.19 | 1.49        | 1.45     |
| 15  | A     | 1104 | CLA  | C1C-C2C | 2.19 | 1.49        | 1.44     |
| 15  | B     | 1214 | CLA  | C4C-C3C | 2.20 | 1.49        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 15  | A     | 1135 | CLA  | C4C-C3C | 2.20 | 1.49        | 1.45     |
| 15  | B     | 1227 | CLA  | C4C-C3C | 2.20 | 1.49        | 1.45     |
| 15  | K     | 1401 | CLA  | C4C-C3C | 2.20 | 1.49        | 1.45     |
| 15  | F     | 1139 | CLA  | C1C-C2C | 2.20 | 1.49        | 1.44     |
| 15  | B     | 1240 | CLA  | C4C-C3C | 2.21 | 1.49        | 1.45     |
| 15  | A     | 1121 | CLA  | C4C-C3C | 2.21 | 1.49        | 1.45     |
| 15  | A     | 1131 | CLA  | C4C-C3C | 2.21 | 1.49        | 1.45     |
| 15  | B     | 1215 | CLA  | C4C-C3C | 2.22 | 1.49        | 1.45     |
| 15  | J     | 1303 | CLA  | C4C-C3C | 2.22 | 1.49        | 1.45     |
| 15  | A     | 1120 | CLA  | C4C-C3C | 2.22 | 1.49        | 1.45     |
| 15  | A     | 1137 | CLA  | C4C-C3C | 2.22 | 1.49        | 1.45     |
| 15  | B     | 1204 | CLA  | C4C-C3C | 2.23 | 1.49        | 1.45     |
| 15  | A     | 1113 | CLA  | C4C-C3C | 2.23 | 1.49        | 1.45     |
| 15  | A     | 1125 | CLA  | C1C-C2C | 2.25 | 1.49        | 1.44     |
| 15  | B     | 1223 | CLA  | C1C-C2C | 2.26 | 1.49        | 1.44     |
| 15  | B     | 1235 | CLA  | C1C-C2C | 2.26 | 1.49        | 1.44     |
| 15  | A     | 1116 | CLA  | C4C-C3C | 2.26 | 1.49        | 1.45     |
| 15  | A     | 1105 | CLA  | C4C-C3C | 2.27 | 1.49        | 1.45     |
| 15  | A     | 1133 | CLA  | C4C-C3C | 2.28 | 1.49        | 1.45     |
| 15  | B     | 1216 | CLA  | C4C-C3C | 2.30 | 1.49        | 1.45     |
| 15  | B     | 1206 | CLA  | C4C-C3C | 2.32 | 1.49        | 1.45     |
| 15  | B     | 1239 | CLA  | C4C-C3C | 2.33 | 1.49        | 1.45     |
| 15  | A     | 1114 | CLA  | C4C-C3C | 2.34 | 1.49        | 1.45     |
| 15  | A     | 1138 | CLA  | C1C-C2C | 2.36 | 1.49        | 1.44     |
| 15  | B     | 1209 | CLA  | C4C-C3C | 2.36 | 1.49        | 1.45     |
| 15  | B     | 1236 | CLA  | C1C-C2C | 2.41 | 1.49        | 1.44     |
| 15  | A     | 1123 | CLA  | C4C-C3C | 2.46 | 1.49        | 1.45     |
| 15  | A     | 1125 | CLA  | CHD-C4C | 2.66 | 1.47        | 1.41     |
| 13  | A     | 1108 | CL0  | C3D-C2D | 2.67 | 1.46        | 1.40     |
| 15  | B     | 1221 | CLA  | CHD-C4C | 2.68 | 1.47        | 1.41     |
| 15  | F     | 1139 | CLA  | C3D-C2D | 2.68 | 1.46        | 1.40     |
| 15  | A     | 1125 | CLA  | C3D-C2D | 2.70 | 1.46        | 1.40     |
| 15  | A     | 1107 | CLA  | C3D-C2D | 2.73 | 1.46        | 1.40     |
| 15  | A     | 1115 | CLA  | CHD-C4C | 2.74 | 1.47        | 1.41     |
| 15  | B     | 1205 | CLA  | CHD-C4C | 2.75 | 1.47        | 1.41     |
| 13  | A     | 1108 | CL0  | CHD-C4C | 2.76 | 1.47        | 1.41     |
| 15  | B     | 1230 | CLA  | CHD-C4C | 2.77 | 1.47        | 1.41     |
| 15  | A     | 1126 | CLA  | C3D-C2D | 2.77 | 1.46        | 1.40     |
| 15  | B     | 1013 | CLA  | CHD-C4C | 2.77 | 1.47        | 1.41     |
| 15  | A     | 1124 | CLA  | C1B-CHB | 2.78 | 1.47        | 1.39     |
| 15  | B     | 1235 | CLA  | CHD-C4C | 2.79 | 1.47        | 1.41     |
| 15  | A     | 1130 | CLA  | C1B-CHB | 2.80 | 1.47        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 15  | A     | 1127 | CLA  | CHD-C4C | 2.80 | 1.47        | 1.41     |
| 15  | A     | 1128 | CLA  | CHD-C4C | 2.81 | 1.47        | 1.41     |
| 13  | A     | 1011 | CL0  | CHD-C4C | 2.81 | 1.47        | 1.41     |
| 15  | A     | 1122 | CLA  | C3D-C2D | 2.81 | 1.46        | 1.40     |
| 15  | A     | 1132 | CLA  | CHD-C4C | 2.82 | 1.47        | 1.41     |
| 15  | K     | 1401 | CLA  | C3D-C2D | 2.82 | 1.46        | 1.40     |
| 15  | B     | 1229 | CLA  | CHD-C4C | 2.83 | 1.47        | 1.41     |
| 15  | B     | 1223 | CLA  | CHD-C4C | 2.83 | 1.47        | 1.41     |
| 15  | B     | 1237 | CLA  | C3D-C2D | 2.83 | 1.46        | 1.40     |
| 15  | A     | 1103 | CLA  | C3D-C2D | 2.84 | 1.46        | 1.40     |
| 15  | B     | 1214 | CLA  | C1B-CHB | 2.84 | 1.47        | 1.39     |
| 15  | A     | 1107 | CLA  | C1B-CHB | 2.84 | 1.47        | 1.39     |
| 15  | B     | 1230 | CLA  | C3D-C2D | 2.84 | 1.46        | 1.40     |
| 15  | B     | 1013 | CLA  | C1B-CHB | 2.85 | 1.47        | 1.39     |
| 15  | A     | 1137 | CLA  | C3D-C2D | 2.85 | 1.47        | 1.40     |
| 15  | A     | 1101 | CLA  | CHD-C4C | 2.85 | 1.47        | 1.41     |
| 15  | A     | 1129 | CLA  | C3D-C2D | 2.85 | 1.47        | 1.40     |
| 15  | A     | 1118 | CLA  | CHD-C4C | 2.86 | 1.47        | 1.41     |
| 15  | A     | 1120 | CLA  | C3D-C2D | 2.86 | 1.47        | 1.40     |
| 15  | B     | 1226 | CLA  | C3D-C2D | 2.86 | 1.47        | 1.40     |
| 15  | A     | 1134 | CLA  | C3D-C2D | 2.87 | 1.47        | 1.40     |
| 15  | A     | 1140 | CLA  | C3D-C2D | 2.87 | 1.47        | 1.40     |
| 15  | A     | 1140 | CLA  | CHD-C4C | 2.87 | 1.47        | 1.41     |
| 15  | K     | 1402 | CLA  | C3D-C2D | 2.87 | 1.47        | 1.40     |
| 13  | A     | 1011 | CL0  | C1B-CHB | 2.87 | 1.47        | 1.39     |
| 15  | A     | 1136 | CLA  | C3D-C2D | 2.88 | 1.47        | 1.40     |
| 15  | A     | 1126 | CLA  | C1B-CHB | 2.88 | 1.47        | 1.39     |
| 15  | J     | 1303 | CLA  | C3D-C2D | 2.88 | 1.47        | 1.40     |
| 15  | A     | 1106 | CLA  | C1B-CHB | 2.88 | 1.47        | 1.39     |
| 15  | A     | 1101 | CLA  | C1B-CHB | 2.89 | 1.47        | 1.39     |
| 15  | B     | 1231 | CLA  | C3D-C2D | 2.89 | 1.47        | 1.40     |
| 15  | B     | 1225 | CLA  | CHD-C4C | 2.89 | 1.48        | 1.41     |
| 15  | J     | 1303 | CLA  | CHD-C4C | 2.89 | 1.48        | 1.41     |
| 15  | A     | 1012 | CLA  | CHD-C4C | 2.89 | 1.48        | 1.41     |
| 15  | F     | 1301 | CLA  | CHD-C4C | 2.89 | 1.48        | 1.41     |
| 15  | B     | 1226 | CLA  | CHD-C4C | 2.89 | 1.48        | 1.41     |
| 15  | J     | 1302 | CLA  | C3D-C2D | 2.90 | 1.47        | 1.40     |
| 15  | B     | 1203 | CLA  | C3D-C2D | 2.90 | 1.47        | 1.40     |
| 15  | B     | 1207 | CLA  | C3D-C2D | 2.90 | 1.47        | 1.40     |
| 15  | A     | 1138 | CLA  | C1B-CHB | 2.90 | 1.47        | 1.39     |
| 15  | B     | 1234 | CLA  | C3D-C2D | 2.90 | 1.47        | 1.40     |
| 15  | B     | 1201 | CLA  | CHD-C4C | 2.90 | 1.48        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 15  | A     | 1111 | CLA  | CHD-C4C | 2.91 | 1.48        | 1.41     |
| 15  | A     | 1112 | CLA  | CHD-C4C | 2.91 | 1.48        | 1.41     |
| 15  | B     | 1225 | CLA  | C3D-C2D | 2.91 | 1.47        | 1.40     |
| 15  | A     | 1123 | CLA  | C3D-C2D | 2.91 | 1.47        | 1.40     |
| 15  | F     | 1139 | CLA  | CHD-C4C | 2.91 | 1.48        | 1.41     |
| 15  | A     | 1117 | CLA  | C1B-CHB | 2.91 | 1.47        | 1.39     |
| 15  | B     | 1239 | CLA  | C3D-C2D | 2.91 | 1.47        | 1.40     |
| 15  | A     | 1137 | CLA  | CHD-C4C | 2.91 | 1.48        | 1.41     |
| 15  | B     | 1236 | CLA  | C3D-C2D | 2.91 | 1.47        | 1.40     |
| 15  | B     | 1228 | CLA  | C3D-C2D | 2.91 | 1.47        | 1.40     |
| 15  | K     | 1402 | CLA  | CHD-C4C | 2.92 | 1.48        | 1.41     |
| 15  | A     | 1104 | CLA  | C1B-CHB | 2.92 | 1.47        | 1.39     |
| 15  | B     | 1222 | CLA  | CHD-C4C | 2.92 | 1.48        | 1.41     |
| 15  | A     | 1134 | CLA  | CHD-C4C | 2.92 | 1.48        | 1.41     |
| 13  | A     | 1011 | CL0  | C3D-C2D | 2.92 | 1.47        | 1.40     |
| 15  | B     | 1212 | CLA  | CHD-C4C | 2.92 | 1.48        | 1.41     |
| 15  | F     | 1301 | CLA  | C1B-CHB | 2.93 | 1.47        | 1.39     |
| 15  | J     | 1302 | CLA  | CHD-C4C | 2.93 | 1.48        | 1.41     |
| 15  | A     | 1110 | CLA  | CHD-C4C | 2.93 | 1.48        | 1.41     |
| 15  | B     | 1023 | CLA  | CHD-C4C | 2.93 | 1.48        | 1.41     |
| 15  | A     | 1131 | CLA  | C3D-C2D | 2.93 | 1.47        | 1.40     |
| 15  | A     | 1113 | CLA  | C3D-C2D | 2.93 | 1.47        | 1.40     |
| 15  | A     | 1104 | CLA  | CHD-C4C | 2.93 | 1.48        | 1.41     |
| 15  | B     | 1021 | CLA  | CHD-C4C | 2.93 | 1.48        | 1.41     |
| 15  | B     | 1223 | CLA  | C3D-C2D | 2.93 | 1.47        | 1.40     |
| 15  | A     | 1801 | CLA  | CHD-C4C | 2.93 | 1.48        | 1.41     |
| 15  | A     | 1110 | CLA  | C3D-C2D | 2.93 | 1.47        | 1.40     |
| 15  | B     | 1236 | CLA  | C1B-CHB | 2.93 | 1.47        | 1.39     |
| 15  | B     | 1239 | CLA  | C4B-CHC | 2.93 | 1.47        | 1.39     |
| 15  | B     | 1202 | CLA  | C3D-C2D | 2.93 | 1.47        | 1.40     |
| 15  | B     | 1202 | CLA  | CHD-C4C | 2.93 | 1.48        | 1.41     |
| 15  | A     | 1118 | CLA  | C3D-C2D | 2.93 | 1.47        | 1.40     |
| 15  | B     | 1227 | CLA  | C3D-C2D | 2.93 | 1.47        | 1.40     |
| 15  | B     | 1232 | CLA  | CHD-C4C | 2.93 | 1.48        | 1.41     |
| 15  | B     | 1209 | CLA  | C3D-C2D | 2.93 | 1.47        | 1.40     |
| 15  | A     | 1801 | CLA  | C3D-C2D | 2.93 | 1.47        | 1.40     |
| 15  | B     | 1211 | CLA  | CHD-C4C | 2.94 | 1.48        | 1.41     |
| 15  | B     | 1234 | CLA  | CHD-C4C | 2.94 | 1.48        | 1.41     |
| 15  | A     | 1131 | CLA  | CHD-C4C | 2.94 | 1.48        | 1.41     |
| 15  | B     | 1224 | CLA  | C3D-C2D | 2.94 | 1.47        | 1.40     |
| 15  | B     | 1229 | CLA  | C3D-C2D | 2.94 | 1.47        | 1.40     |
| 15  | B     | 1224 | CLA  | C1B-CHB | 2.94 | 1.47        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 15  | A     | 1119 | CLA  | C1B-CHB | 2.94 | 1.47        | 1.39     |
| 15  | B     | 1210 | CLA  | C1B-CHB | 2.94 | 1.47        | 1.39     |
| 15  | A     | 1121 | CLA  | C3D-C2D | 2.94 | 1.47        | 1.40     |
| 15  | A     | 1111 | CLA  | C1B-CHB | 2.94 | 1.48        | 1.39     |
| 15  | B     | 1236 | CLA  | CHD-C4C | 2.94 | 1.48        | 1.41     |
| 15  | B     | 1205 | CLA  | C3D-C2D | 2.94 | 1.47        | 1.40     |
| 15  | A     | 1116 | CLA  | C3D-C2D | 2.95 | 1.47        | 1.40     |
| 15  | A     | 1115 | CLA  | C3D-C2D | 2.95 | 1.47        | 1.40     |
| 15  | A     | 1136 | CLA  | CHD-C4C | 2.95 | 1.48        | 1.41     |
| 15  | B     | 1207 | CLA  | CHD-C4C | 2.95 | 1.48        | 1.41     |
| 15  | A     | 1135 | CLA  | C3D-C2D | 2.95 | 1.47        | 1.40     |
| 15  | B     | 1023 | CLA  | C1B-CHB | 2.95 | 1.48        | 1.39     |
| 15  | A     | 1127 | CLA  | C3D-C2D | 2.95 | 1.47        | 1.40     |
| 15  | A     | 1128 | CLA  | C4B-CHC | 2.95 | 1.48        | 1.39     |
| 15  | B     | 1204 | CLA  | C3D-C2D | 2.95 | 1.47        | 1.40     |
| 15  | A     | 1114 | CLA  | C3D-C2D | 2.95 | 1.47        | 1.40     |
| 15  | B     | 1206 | CLA  | C3D-C2D | 2.95 | 1.47        | 1.40     |
| 15  | A     | 1022 | CLA  | C1B-CHB | 2.96 | 1.48        | 1.39     |
| 15  | K     | 1401 | CLA  | CHD-C4C | 2.96 | 1.48        | 1.41     |
| 15  | B     | 1021 | CLA  | C3D-C2D | 2.96 | 1.47        | 1.40     |
| 15  | B     | 1228 | CLA  | CHD-C4C | 2.96 | 1.48        | 1.41     |
| 15  | A     | 1022 | CLA  | CHD-C4C | 2.96 | 1.48        | 1.41     |
| 15  | B     | 1238 | CLA  | CHD-C4C | 2.96 | 1.48        | 1.41     |
| 13  | A     | 1011 | CL0  | C4B-CHC | 2.96 | 1.48        | 1.39     |
| 15  | B     | 1219 | CLA  | C3D-C2D | 2.96 | 1.47        | 1.40     |
| 15  | A     | 1101 | CLA  | C3D-C2D | 2.97 | 1.47        | 1.40     |
| 15  | A     | 1132 | CLA  | C3D-C2D | 2.97 | 1.47        | 1.40     |
| 15  | A     | 1104 | CLA  | C3D-C2D | 2.97 | 1.47        | 1.40     |
| 15  | B     | 1240 | CLA  | C3D-C2D | 2.97 | 1.47        | 1.40     |
| 15  | A     | 1113 | CLA  | CHD-C4C | 2.97 | 1.48        | 1.41     |
| 15  | B     | 1221 | CLA  | C3D-C2D | 2.97 | 1.47        | 1.40     |
| 15  | B     | 1225 | CLA  | C1B-CHB | 2.97 | 1.48        | 1.39     |
| 15  | A     | 1129 | CLA  | CHD-C4C | 2.97 | 1.48        | 1.41     |
| 15  | A     | 1102 | CLA  | C1B-CHB | 2.97 | 1.48        | 1.39     |
| 15  | B     | 1209 | CLA  | CHD-C4C | 2.98 | 1.48        | 1.41     |
| 15  | B     | 1231 | CLA  | C4B-CHC | 2.98 | 1.48        | 1.39     |
| 15  | A     | 1112 | CLA  | C1B-CHB | 2.98 | 1.48        | 1.39     |
| 15  | B     | 1217 | CLA  | CHD-C4C | 2.98 | 1.48        | 1.41     |
| 15  | A     | 1111 | CLA  | C3D-C2D | 2.98 | 1.47        | 1.40     |
| 15  | B     | 1201 | CLA  | C3D-C2D | 2.98 | 1.47        | 1.40     |
| 15  | B     | 1227 | CLA  | C1B-CHB | 2.98 | 1.48        | 1.39     |
| 15  | A     | 1130 | CLA  | C3D-C2D | 2.98 | 1.47        | 1.40     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 15  | F     | 1410 | CLA  | C3D-C2D | 2.99 | 1.47        | 1.40     |
| 15  | B     | 1206 | CLA  | C1B-CHB | 2.99 | 1.48        | 1.39     |
| 15  | A     | 1138 | CLA  | CHD-C4C | 2.99 | 1.48        | 1.41     |
| 15  | B     | 1210 | CLA  | CHD-C4C | 2.99 | 1.48        | 1.41     |
| 15  | A     | 1103 | CLA  | CHD-C4C | 2.99 | 1.48        | 1.41     |
| 15  | A     | 1105 | CLA  | C3D-C2D | 2.99 | 1.47        | 1.40     |
| 15  | A     | 1133 | CLA  | CHD-C4C | 2.99 | 1.48        | 1.41     |
| 15  | A     | 1123 | CLA  | C4B-CHC | 2.99 | 1.48        | 1.39     |
| 15  | A     | 1133 | CLA  | C3D-C2D | 2.99 | 1.47        | 1.40     |
| 15  | B     | 1203 | CLA  | C4B-CHC | 2.99 | 1.48        | 1.39     |
| 15  | B     | 1021 | CLA  | C1B-CHB | 2.99 | 1.48        | 1.39     |
| 15  | B     | 1218 | CLA  | C3D-C2D | 2.99 | 1.47        | 1.40     |
| 15  | F     | 1410 | CLA  | CHD-C4C | 2.99 | 1.48        | 1.41     |
| 15  | B     | 1235 | CLA  | C3D-C2D | 2.99 | 1.47        | 1.40     |
| 15  | A     | 1110 | CLA  | C1B-CHB | 3.00 | 1.48        | 1.39     |
| 15  | B     | 1211 | CLA  | C3D-C2D | 3.00 | 1.47        | 1.40     |
| 15  | A     | 1112 | CLA  | C3D-C2D | 3.00 | 1.47        | 1.40     |
| 15  | B     | 1222 | CLA  | C1B-CHB | 3.00 | 1.48        | 1.39     |
| 15  | B     | 1210 | CLA  | C3D-C2D | 3.00 | 1.47        | 1.40     |
| 15  | A     | 1116 | CLA  | CHD-C4C | 3.00 | 1.48        | 1.41     |
| 15  | B     | 1208 | CLA  | C3D-C2D | 3.00 | 1.47        | 1.40     |
| 15  | A     | 1122 | CLA  | C1B-CHB | 3.00 | 1.48        | 1.39     |
| 15  | A     | 1128 | CLA  | C3D-C2D | 3.01 | 1.47        | 1.40     |
| 15  | B     | 1212 | CLA  | C3D-C2D | 3.01 | 1.47        | 1.40     |
| 15  | B     | 1240 | CLA  | CHD-C4C | 3.01 | 1.48        | 1.41     |
| 15  | B     | 1218 | CLA  | CHD-C4C | 3.01 | 1.48        | 1.41     |
| 15  | B     | 1203 | CLA  | CHD-C4C | 3.01 | 1.48        | 1.41     |
| 15  | B     | 1209 | CLA  | C1B-CHB | 3.01 | 1.48        | 1.39     |
| 15  | A     | 1121 | CLA  | CHD-C4C | 3.01 | 1.48        | 1.41     |
| 15  | A     | 1107 | CLA  | CHD-C4C | 3.01 | 1.48        | 1.41     |
| 15  | A     | 1105 | CLA  | CHD-C4C | 3.02 | 1.48        | 1.41     |
| 15  | A     | 1102 | CLA  | CHD-C4C | 3.02 | 1.48        | 1.41     |
| 15  | A     | 1125 | CLA  | C1B-CHB | 3.02 | 1.48        | 1.39     |
| 15  | A     | 1109 | CLA  | C3D-C2D | 3.02 | 1.47        | 1.40     |
| 15  | B     | 1220 | CLA  | C1B-CHB | 3.02 | 1.48        | 1.39     |
| 15  | B     | 1213 | CLA  | C3D-C2D | 3.02 | 1.47        | 1.40     |
| 15  | B     | 1223 | CLA  | C1B-CHB | 3.02 | 1.48        | 1.39     |
| 15  | B     | 1228 | CLA  | C1B-CHB | 3.02 | 1.48        | 1.39     |
| 15  | B     | 1224 | CLA  | CHD-C4C | 3.02 | 1.48        | 1.41     |
| 15  | A     | 1119 | CLA  | CHD-C4C | 3.02 | 1.48        | 1.41     |
| 15  | B     | 1237 | CLA  | CHD-C4C | 3.02 | 1.48        | 1.41     |
| 15  | B     | 1217 | CLA  | C3D-C2D | 3.02 | 1.47        | 1.40     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 15  | B     | 1234 | CLA  | C4B-CHC | 3.03 | 1.48        | 1.39     |
| 15  | A     | 1123 | CLA  | CHD-C4C | 3.03 | 1.48        | 1.41     |
| 15  | B     | 1216 | CLA  | C1B-CHB | 3.03 | 1.48        | 1.39     |
| 15  | A     | 1012 | CLA  | C1B-CHB | 3.03 | 1.48        | 1.39     |
| 15  | B     | 1222 | CLA  | C4B-CHC | 3.03 | 1.48        | 1.39     |
| 15  | B     | 1227 | CLA  | CHD-C4C | 3.03 | 1.48        | 1.41     |
| 15  | A     | 1124 | CLA  | C3D-C2D | 3.03 | 1.47        | 1.40     |
| 15  | A     | 1124 | CLA  | CHD-C4C | 3.03 | 1.48        | 1.41     |
| 15  | B     | 1218 | CLA  | C1B-CHB | 3.03 | 1.48        | 1.39     |
| 15  | B     | 1227 | CLA  | C4B-CHC | 3.03 | 1.48        | 1.39     |
| 15  | A     | 1119 | CLA  | C3D-C2D | 3.03 | 1.47        | 1.40     |
| 15  | F     | 1301 | CLA  | C3D-C2D | 3.03 | 1.47        | 1.40     |
| 15  | B     | 1231 | CLA  | CHD-C4C | 3.03 | 1.48        | 1.41     |
| 15  | A     | 1114 | CLA  | CHD-C4C | 3.04 | 1.48        | 1.41     |
| 15  | B     | 1232 | CLA  | C4B-CHC | 3.04 | 1.48        | 1.39     |
| 15  | B     | 1235 | CLA  | C1B-CHB | 3.04 | 1.48        | 1.39     |
| 15  | A     | 1128 | CLA  | C1B-CHB | 3.04 | 1.48        | 1.39     |
| 15  | B     | 1215 | CLA  | C4B-CHC | 3.04 | 1.48        | 1.39     |
| 15  | A     | 1135 | CLA  | CHD-C4C | 3.04 | 1.48        | 1.41     |
| 15  | B     | 1209 | CLA  | C4B-CHC | 3.04 | 1.48        | 1.39     |
| 15  | A     | 1110 | CLA  | C4B-CHC | 3.04 | 1.48        | 1.39     |
| 15  | A     | 1120 | CLA  | CHD-C4C | 3.04 | 1.48        | 1.41     |
| 15  | A     | 1136 | CLA  | C4B-CHC | 3.04 | 1.48        | 1.39     |
| 15  | A     | 1105 | CLA  | C1B-CHB | 3.04 | 1.48        | 1.39     |
| 15  | B     | 1023 | CLA  | C3D-C2D | 3.04 | 1.47        | 1.40     |
| 15  | B     | 1216 | CLA  | C3D-C2D | 3.05 | 1.47        | 1.40     |
| 15  | B     | 1216 | CLA  | CHD-C4C | 3.05 | 1.48        | 1.41     |
| 15  | B     | 1206 | CLA  | C4B-CHC | 3.05 | 1.48        | 1.39     |
| 15  | A     | 1120 | CLA  | C1B-CHB | 3.06 | 1.48        | 1.39     |
| 15  | K     | 1401 | CLA  | C1B-CHB | 3.06 | 1.48        | 1.39     |
| 15  | B     | 1204 | CLA  | CHD-C4C | 3.06 | 1.48        | 1.41     |
| 15  | A     | 1109 | CLA  | CHD-C4C | 3.06 | 1.48        | 1.41     |
| 15  | B     | 1215 | CLA  | CHD-C4C | 3.06 | 1.48        | 1.41     |
| 15  | B     | 1204 | CLA  | C4B-CHC | 3.06 | 1.48        | 1.39     |
| 15  | B     | 1202 | CLA  | C1B-CHB | 3.06 | 1.48        | 1.39     |
| 15  | F     | 1410 | CLA  | C1B-CHB | 3.06 | 1.48        | 1.39     |
| 15  | B     | 1238 | CLA  | C3D-C2D | 3.06 | 1.47        | 1.40     |
| 15  | A     | 1138 | CLA  | C3D-C2D | 3.06 | 1.47        | 1.40     |
| 15  | B     | 1215 | CLA  | C3D-C2D | 3.06 | 1.47        | 1.40     |
| 15  | B     | 1230 | CLA  | C1B-CHB | 3.06 | 1.48        | 1.39     |
| 15  | A     | 1113 | CLA  | C1B-CHB | 3.06 | 1.48        | 1.39     |
| 15  | A     | 1135 | CLA  | C4B-CHC | 3.06 | 1.48        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 15  | A     | 1116 | CLA  | C1B-CHB | 3.06 | 1.48        | 1.39     |
| 15  | B     | 1023 | CLA  | C4B-CHC | 3.07 | 1.48        | 1.39     |
| 15  | A     | 1134 | CLA  | C1B-CHB | 3.07 | 1.48        | 1.39     |
| 15  | A     | 1118 | CLA  | C4B-CHC | 3.07 | 1.48        | 1.39     |
| 15  | A     | 1117 | CLA  | CHD-C4C | 3.07 | 1.48        | 1.41     |
| 15  | A     | 1120 | CLA  | C4B-CHC | 3.07 | 1.48        | 1.39     |
| 15  | A     | 1106 | CLA  | C3D-C2D | 3.07 | 1.47        | 1.40     |
| 15  | B     | 1217 | CLA  | C1B-CHB | 3.07 | 1.48        | 1.39     |
| 15  | A     | 1131 | CLA  | C4B-CHC | 3.07 | 1.48        | 1.39     |
| 15  | B     | 1232 | CLA  | C3D-C2D | 3.07 | 1.47        | 1.40     |
| 15  | B     | 1207 | CLA  | C1B-CHB | 3.07 | 1.48        | 1.39     |
| 15  | B     | 1219 | CLA  | C4B-CHC | 3.07 | 1.48        | 1.39     |
| 15  | B     | 1210 | CLA  | C4B-CHC | 3.07 | 1.48        | 1.39     |
| 15  | A     | 1109 | CLA  | C1B-CHB | 3.07 | 1.48        | 1.39     |
| 15  | B     | 1204 | CLA  | C1B-CHB | 3.08 | 1.48        | 1.39     |
| 15  | B     | 1201 | CLA  | C1B-CHB | 3.08 | 1.48        | 1.39     |
| 15  | A     | 1106 | CLA  | C4B-CHC | 3.08 | 1.48        | 1.39     |
| 15  | B     | 1214 | CLA  | C3D-C2D | 3.08 | 1.47        | 1.40     |
| 15  | B     | 1213 | CLA  | CHD-C4C | 3.09 | 1.48        | 1.41     |
| 15  | A     | 1133 | CLA  | C1B-CHB | 3.09 | 1.48        | 1.39     |
| 15  | A     | 1105 | CLA  | C4B-CHC | 3.09 | 1.48        | 1.39     |
| 15  | A     | 1129 | CLA  | C4B-CHC | 3.09 | 1.48        | 1.39     |
| 15  | B     | 1231 | CLA  | C1B-CHB | 3.09 | 1.48        | 1.39     |
| 15  | B     | 1222 | CLA  | C3D-C2D | 3.09 | 1.47        | 1.40     |
| 15  | B     | 1206 | CLA  | CHD-C4C | 3.09 | 1.48        | 1.41     |
| 15  | B     | 1232 | CLA  | C1B-CHB | 3.10 | 1.48        | 1.39     |
| 15  | B     | 1013 | CLA  | C3D-C2D | 3.10 | 1.47        | 1.40     |
| 15  | B     | 1205 | CLA  | C4B-CHC | 3.10 | 1.48        | 1.39     |
| 15  | A     | 1106 | CLA  | CHD-C4C | 3.10 | 1.48        | 1.41     |
| 15  | B     | 1219 | CLA  | CHD-C4C | 3.10 | 1.48        | 1.41     |
| 15  | A     | 1122 | CLA  | CHD-C4C | 3.11 | 1.48        | 1.41     |
| 15  | B     | 1240 | CLA  | C1B-CHB | 3.11 | 1.48        | 1.39     |
| 15  | B     | 1238 | CLA  | C4B-CHC | 3.11 | 1.48        | 1.39     |
| 15  | A     | 1103 | CLA  | C1B-CHB | 3.11 | 1.48        | 1.39     |
| 15  | B     | 1220 | CLA  | CHD-C4C | 3.11 | 1.48        | 1.41     |
| 15  | B     | 1224 | CLA  | C4B-CHC | 3.11 | 1.48        | 1.39     |
| 15  | B     | 1208 | CLA  | C4B-CHC | 3.11 | 1.48        | 1.39     |
| 15  | B     | 1021 | CLA  | C4B-CHC | 3.11 | 1.48        | 1.39     |
| 15  | B     | 1216 | CLA  | C4B-CHC | 3.11 | 1.48        | 1.39     |
| 15  | K     | 1402 | CLA  | C4B-CHC | 3.11 | 1.48        | 1.39     |
| 15  | A     | 1133 | CLA  | C4B-CHC | 3.12 | 1.48        | 1.39     |
| 15  | B     | 1226 | CLA  | C4B-CHC | 3.12 | 1.48        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 15  | B     | 1221 | CLA  | C4B-CHC | 3.12 | 1.48        | 1.39     |
| 15  | A     | 1121 | CLA  | C4B-CHC | 3.12 | 1.48        | 1.39     |
| 15  | A     | 1102 | CLA  | C4B-CHC | 3.12 | 1.48        | 1.39     |
| 15  | A     | 1124 | CLA  | C4B-CHC | 3.12 | 1.48        | 1.39     |
| 15  | A     | 1137 | CLA  | C4B-CHC | 3.13 | 1.48        | 1.39     |
| 15  | B     | 1203 | CLA  | C1B-CHB | 3.13 | 1.48        | 1.39     |
| 15  | B     | 1239 | CLA  | CHD-C4C | 3.13 | 1.48        | 1.41     |
| 15  | B     | 1211 | CLA  | C1B-CHB | 3.13 | 1.48        | 1.39     |
| 15  | B     | 1219 | CLA  | C1B-CHB | 3.13 | 1.48        | 1.39     |
| 15  | J     | 1302 | CLA  | C1B-CHB | 3.13 | 1.48        | 1.39     |
| 15  | B     | 1217 | CLA  | C4B-CHC | 3.13 | 1.48        | 1.39     |
| 15  | B     | 1226 | CLA  | C1B-CHB | 3.14 | 1.48        | 1.39     |
| 15  | B     | 1207 | CLA  | C4B-CHC | 3.14 | 1.48        | 1.39     |
| 15  | A     | 1130 | CLA  | CHD-C4C | 3.14 | 1.48        | 1.41     |
| 15  | A     | 1129 | CLA  | C1B-CHB | 3.14 | 1.48        | 1.39     |
| 15  | A     | 1123 | CLA  | C1B-CHB | 3.14 | 1.48        | 1.39     |
| 15  | B     | 1201 | CLA  | C4B-CHC | 3.14 | 1.48        | 1.39     |
| 15  | A     | 1140 | CLA  | C1B-CHB | 3.14 | 1.48        | 1.39     |
| 15  | A     | 1116 | CLA  | C4B-CHC | 3.14 | 1.48        | 1.39     |
| 15  | B     | 1208 | CLA  | CHD-C4C | 3.14 | 1.48        | 1.41     |
| 15  | B     | 1215 | CLA  | C1B-CHB | 3.14 | 1.48        | 1.39     |
| 15  | B     | 1214 | CLA  | CHD-C4C | 3.14 | 1.48        | 1.41     |
| 15  | A     | 1117 | CLA  | C3D-C2D | 3.14 | 1.47        | 1.40     |
| 15  | B     | 1208 | CLA  | C1B-CHB | 3.14 | 1.48        | 1.39     |
| 15  | A     | 1118 | CLA  | C1B-CHB | 3.15 | 1.48        | 1.39     |
| 15  | B     | 1212 | CLA  | C4B-CHC | 3.15 | 1.48        | 1.39     |
| 15  | A     | 1114 | CLA  | C1B-CHB | 3.15 | 1.48        | 1.39     |
| 15  | A     | 1127 | CLA  | C1B-CHB | 3.15 | 1.48        | 1.39     |
| 15  | A     | 1801 | CLA  | C1B-CHB | 3.15 | 1.48        | 1.39     |
| 15  | B     | 1218 | CLA  | C4B-CHC | 3.15 | 1.48        | 1.39     |
| 15  | B     | 1237 | CLA  | C4B-CHC | 3.15 | 1.48        | 1.39     |
| 15  | F     | 1139 | CLA  | C1B-CHB | 3.15 | 1.48        | 1.39     |
| 15  | A     | 1012 | CLA  | C4B-CHC | 3.16 | 1.48        | 1.39     |
| 15  | B     | 1229 | CLA  | C4B-CHC | 3.16 | 1.48        | 1.39     |
| 15  | A     | 1114 | CLA  | C4B-CHC | 3.16 | 1.48        | 1.39     |
| 15  | B     | 1238 | CLA  | C1B-CHB | 3.16 | 1.48        | 1.39     |
| 15  | A     | 1113 | CLA  | C4B-CHC | 3.16 | 1.48        | 1.39     |
| 15  | A     | 1801 | CLA  | C4B-CHC | 3.16 | 1.48        | 1.39     |
| 15  | J     | 1302 | CLA  | C4B-CHC | 3.16 | 1.48        | 1.39     |
| 15  | B     | 1205 | CLA  | C1B-CHB | 3.16 | 1.48        | 1.39     |
| 15  | A     | 1115 | CLA  | C1B-CHB | 3.16 | 1.48        | 1.39     |
| 15  | A     | 1121 | CLA  | C1B-CHB | 3.16 | 1.48        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 15  | A     | 1135 | CLA  | C1B-CHB | 3.16 | 1.48        | 1.39     |
| 15  | K     | 1401 | CLA  | C4B-CHC | 3.16 | 1.48        | 1.39     |
| 15  | B     | 1214 | CLA  | C4B-CHC | 3.17 | 1.48        | 1.39     |
| 15  | B     | 1234 | CLA  | C1B-CHB | 3.17 | 1.48        | 1.39     |
| 15  | B     | 1213 | CLA  | C1B-CHB | 3.17 | 1.48        | 1.39     |
| 15  | A     | 1117 | CLA  | C4B-CHC | 3.17 | 1.48        | 1.39     |
| 15  | B     | 1212 | CLA  | C1B-CHB | 3.17 | 1.48        | 1.39     |
| 15  | A     | 1111 | CLA  | C4B-CHC | 3.17 | 1.48        | 1.39     |
| 15  | F     | 1139 | CLA  | C4B-CHC | 3.17 | 1.48        | 1.39     |
| 15  | B     | 1237 | CLA  | C1B-CHB | 3.17 | 1.48        | 1.39     |
| 15  | A     | 1119 | CLA  | C4B-CHC | 3.18 | 1.48        | 1.39     |
| 15  | B     | 1202 | CLA  | C4B-CHC | 3.18 | 1.48        | 1.39     |
| 15  | J     | 1303 | CLA  | C4B-CHC | 3.18 | 1.48        | 1.39     |
| 15  | A     | 1102 | CLA  | C3D-C2D | 3.18 | 1.47        | 1.40     |
| 15  | B     | 1013 | CLA  | C4B-CHC | 3.19 | 1.48        | 1.39     |
| 15  | B     | 1225 | CLA  | C4B-CHC | 3.19 | 1.48        | 1.39     |
| 15  | A     | 1137 | CLA  | C1B-CHB | 3.19 | 1.48        | 1.39     |
| 15  | A     | 1132 | CLA  | C1B-CHB | 3.19 | 1.48        | 1.39     |
| 15  | A     | 1109 | CLA  | C4B-CHC | 3.19 | 1.48        | 1.39     |
| 15  | J     | 1303 | CLA  | C1B-CHB | 3.19 | 1.48        | 1.39     |
| 15  | B     | 1220 | CLA  | C3D-C2D | 3.19 | 1.47        | 1.40     |
| 15  | A     | 1127 | CLA  | C4B-CHC | 3.19 | 1.48        | 1.39     |
| 15  | K     | 1402 | CLA  | C1B-CHB | 3.20 | 1.48        | 1.39     |
| 13  | A     | 1108 | CL0  | C4B-CHC | 3.20 | 1.48        | 1.39     |
| 15  | A     | 1132 | CLA  | C4B-CHC | 3.20 | 1.48        | 1.39     |
| 15  | B     | 1211 | CLA  | C4B-CHC | 3.20 | 1.48        | 1.39     |
| 15  | A     | 1103 | CLA  | C4B-CHC | 3.20 | 1.48        | 1.39     |
| 15  | A     | 1022 | CLA  | C4B-CHC | 3.20 | 1.48        | 1.39     |
| 15  | A     | 1126 | CLA  | CHD-C4C | 3.20 | 1.48        | 1.41     |
| 15  | F     | 1301 | CLA  | C4B-CHC | 3.21 | 1.48        | 1.39     |
| 15  | A     | 1115 | CLA  | C4B-CHC | 3.21 | 1.48        | 1.39     |
| 15  | A     | 1136 | CLA  | C1B-CHB | 3.21 | 1.48        | 1.39     |
| 15  | F     | 1410 | CLA  | C4B-CHC | 3.21 | 1.48        | 1.39     |
| 15  | A     | 1131 | CLA  | C1B-CHB | 3.21 | 1.48        | 1.39     |
| 15  | B     | 1240 | CLA  | C4B-CHC | 3.21 | 1.48        | 1.39     |
| 15  | A     | 1104 | CLA  | C4B-CHC | 3.22 | 1.48        | 1.39     |
| 15  | B     | 1221 | CLA  | C1B-CHB | 3.23 | 1.48        | 1.39     |
| 15  | A     | 1134 | CLA  | C4B-CHC | 3.23 | 1.48        | 1.39     |
| 15  | B     | 1229 | CLA  | C1B-CHB | 3.23 | 1.48        | 1.39     |
| 15  | B     | 1213 | CLA  | C4B-CHC | 3.24 | 1.48        | 1.39     |
| 15  | B     | 1239 | CLA  | C1B-CHB | 3.24 | 1.48        | 1.39     |
| 15  | A     | 1130 | CLA  | C4B-CHC | 3.26 | 1.48        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 15  | A     | 1140 | CLA  | C4B-CHC | 3.27 | 1.48        | 1.39     |
| 15  | B     | 1220 | CLA  | C4B-CHC | 3.28 | 1.48        | 1.39     |
| 13  | A     | 1108 | CL0  | C1B-CHB | 3.28 | 1.48        | 1.39     |
| 15  | B     | 1223 | CLA  | C4B-CHC | 3.28 | 1.48        | 1.39     |
| 15  | A     | 1112 | CLA  | C4B-CHC | 3.29 | 1.48        | 1.39     |
| 15  | A     | 1107 | CLA  | C4B-CHC | 3.30 | 1.48        | 1.39     |
| 15  | B     | 1235 | CLA  | C4B-CHC | 3.30 | 1.48        | 1.39     |
| 15  | A     | 1012 | CLA  | C3D-C2D | 3.30 | 1.48        | 1.40     |
| 15  | B     | 1230 | CLA  | C4B-CHC | 3.31 | 1.49        | 1.39     |
| 15  | A     | 1022 | CLA  | C3D-C2D | 3.32 | 1.48        | 1.40     |
| 15  | A     | 1122 | CLA  | C4B-CHC | 3.33 | 1.49        | 1.39     |
| 15  | A     | 1126 | CLA  | C4B-CHC | 3.34 | 1.49        | 1.39     |
| 15  | A     | 1101 | CLA  | C4B-CHC | 3.36 | 1.49        | 1.39     |
| 15  | B     | 1228 | CLA  | C4B-CHC | 3.37 | 1.49        | 1.39     |
| 15  | A     | 1125 | CLA  | C4B-CHC | 3.40 | 1.49        | 1.39     |
| 15  | B     | 1236 | CLA  | C4B-CHC | 3.40 | 1.49        | 1.39     |
| 15  | A     | 1138 | CLA  | C4B-CHC | 3.49 | 1.49        | 1.39     |
| 12  | A     | 5005 | LHG  | O7-C7   | 3.77 | 1.45        | 1.34     |
| 12  | A     | 5003 | LHG  | O7-C7   | 3.83 | 1.45        | 1.34     |
| 12  | A     | 5001 | LHG  | O7-C7   | 3.87 | 1.45        | 1.34     |
| 12  | B     | 5004 | LHG  | O7-C7   | 3.88 | 1.45        | 1.34     |
| 15  | B     | 1223 | CLA  | OBD-CAD | 3.90 | 1.28        | 1.22     |
| 17  | B     | 5002 | LMG  | O7-C10  | 3.92 | 1.46        | 1.34     |
| 15  | A     | 1129 | CLA  | OBD-CAD | 3.96 | 1.28        | 1.22     |
| 15  | A     | 1128 | CLA  | CHC-C1C | 3.99 | 1.47        | 1.35     |
| 15  | B     | 1203 | CLA  | CHC-C1C | 3.99 | 1.47        | 1.35     |
| 15  | B     | 1231 | CLA  | CHC-C1C | 4.03 | 1.47        | 1.35     |
| 15  | B     | 1239 | CLA  | CHC-C1C | 4.03 | 1.47        | 1.35     |
| 12  | A     | 5001 | LHG  | O8-C23  | 4.04 | 1.45        | 1.33     |
| 15  | B     | 1215 | CLA  | CHC-C1C | 4.05 | 1.48        | 1.35     |
| 15  | B     | 1232 | CLA  | CHC-C1C | 4.05 | 1.48        | 1.35     |
| 13  | A     | 1011 | CL0  | CHC-C1C | 4.06 | 1.48        | 1.35     |
| 15  | A     | 1127 | CLA  | OBD-CAD | 4.07 | 1.28        | 1.22     |
| 15  | A     | 1110 | CLA  | CHC-C1C | 4.07 | 1.48        | 1.35     |
| 15  | B     | 1217 | CLA  | O2A-C1  | 4.07 | 1.60        | 1.46     |
| 12  | B     | 5004 | LHG  | O8-C23  | 4.08 | 1.45        | 1.33     |
| 15  | B     | 1228 | CLA  | OBD-CAD | 4.08 | 1.28        | 1.22     |
| 15  | A     | 1125 | CLA  | OBD-CAD | 4.09 | 1.28        | 1.22     |
| 12  | A     | 5005 | LHG  | O8-C23  | 4.09 | 1.45        | 1.33     |
| 15  | B     | 1238 | CLA  | CHC-C1C | 4.10 | 1.48        | 1.35     |
| 15  | B     | 1222 | CLA  | CHC-C1C | 4.10 | 1.48        | 1.35     |
| 15  | B     | 1205 | CLA  | CHC-C1C | 4.11 | 1.48        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 15  | B     | 1227 | CLA  | OBD-CAD | 4.11 | 1.28        | 1.22     |
| 15  | A     | 1131 | CLA  | CHC-C1C | 4.12 | 1.48        | 1.35     |
| 15  | B     | 1221 | CLA  | CHC-C1C | 4.12 | 1.48        | 1.35     |
| 15  | A     | 1136 | CLA  | CHC-C1C | 4.12 | 1.48        | 1.35     |
| 15  | B     | 1206 | CLA  | CHC-C1C | 4.12 | 1.48        | 1.35     |
| 15  | A     | 1105 | CLA  | CHC-C1C | 4.12 | 1.48        | 1.35     |
| 15  | A     | 1135 | CLA  | CHC-C1C | 4.13 | 1.48        | 1.35     |
| 15  | A     | 1123 | CLA  | CHC-C1C | 4.14 | 1.48        | 1.35     |
| 15  | B     | 1227 | CLA  | CHC-C1C | 4.15 | 1.48        | 1.35     |
| 15  | A     | 1118 | CLA  | CHC-C1C | 4.15 | 1.48        | 1.35     |
| 15  | J     | 1302 | CLA  | CHC-C1C | 4.15 | 1.48        | 1.35     |
| 15  | F     | 1139 | CLA  | CHC-C1C | 4.15 | 1.48        | 1.35     |
| 15  | A     | 1121 | CLA  | CHC-C1C | 4.15 | 1.48        | 1.35     |
| 15  | B     | 1204 | CLA  | CHC-C1C | 4.15 | 1.48        | 1.35     |
| 15  | A     | 1120 | CLA  | CHC-C1C | 4.16 | 1.48        | 1.35     |
| 15  | B     | 1234 | CLA  | CHC-C1C | 4.16 | 1.48        | 1.35     |
| 15  | B     | 1224 | CLA  | CHC-C1C | 4.16 | 1.48        | 1.35     |
| 15  | B     | 1216 | CLA  | CHC-C1C | 4.17 | 1.48        | 1.35     |
| 15  | B     | 1237 | CLA  | CHC-C1C | 4.18 | 1.48        | 1.35     |
| 15  | A     | 1133 | CLA  | CHC-C1C | 4.18 | 1.48        | 1.35     |
| 15  | B     | 1235 | CLA  | OBD-CAD | 4.18 | 1.28        | 1.22     |
| 15  | B     | 1209 | CLA  | CHC-C1C | 4.18 | 1.48        | 1.35     |
| 15  | B     | 1218 | CLA  | CHC-C1C | 4.18 | 1.48        | 1.35     |
| 15  | A     | 1137 | CLA  | CHC-C1C | 4.18 | 1.48        | 1.35     |
| 15  | B     | 1201 | CLA  | CHC-C1C | 4.19 | 1.48        | 1.35     |
| 15  | B     | 1219 | CLA  | CHC-C1C | 4.19 | 1.48        | 1.35     |
| 15  | B     | 1021 | CLA  | CHC-C1C | 4.19 | 1.48        | 1.35     |
| 15  | A     | 1113 | CLA  | CHC-C1C | 4.19 | 1.48        | 1.35     |
| 17  | B     | 5002 | LMG  | O8-C28  | 4.19 | 1.45        | 1.33     |
| 15  | B     | 1208 | CLA  | CHC-C1C | 4.19 | 1.48        | 1.35     |
| 15  | B     | 1221 | CLA  | OBD-CAD | 4.19 | 1.28        | 1.22     |
| 15  | B     | 1023 | CLA  | CHC-C1C | 4.19 | 1.48        | 1.35     |
| 15  | B     | 1229 | CLA  | CHC-C1C | 4.19 | 1.48        | 1.35     |
| 15  | A     | 1124 | CLA  | CHC-C1C | 4.20 | 1.48        | 1.35     |
| 15  | A     | 1129 | CLA  | CHC-C1C | 4.20 | 1.48        | 1.35     |
| 15  | B     | 1207 | CLA  | CHC-C1C | 4.20 | 1.48        | 1.35     |
| 15  | A     | 1116 | CLA  | CHC-C1C | 4.20 | 1.48        | 1.35     |
| 15  | A     | 1114 | CLA  | CHC-C1C | 4.20 | 1.48        | 1.35     |
| 15  | A     | 1110 | CLA  | OBD-CAD | 4.21 | 1.28        | 1.22     |
| 15  | A     | 1104 | CLA  | CHC-C1C | 4.21 | 1.48        | 1.35     |
| 15  | B     | 1212 | CLA  | CHC-C1C | 4.21 | 1.48        | 1.35     |
| 15  | A     | 1012 | CLA  | CHC-C1C | 4.21 | 1.48        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 15  | F     | 1410 | CLA  | CHC-C1C | 4.21 | 1.48        | 1.35     |
| 15  | K     | 1402 | CLA  | CHC-C1C | 4.21 | 1.48        | 1.35     |
| 15  | B     | 1225 | CLA  | CHC-C1C | 4.21 | 1.48        | 1.35     |
| 15  | K     | 1401 | CLA  | CHC-C1C | 4.21 | 1.48        | 1.35     |
| 13  | A     | 1108 | CL0  | OBD-CAD | 4.22 | 1.28        | 1.22     |
| 15  | A     | 1801 | CLA  | CHC-C1C | 4.22 | 1.48        | 1.35     |
| 12  | A     | 5003 | LHG  | O8-C23  | 4.22 | 1.46        | 1.33     |
| 15  | A     | 1102 | CLA  | CHC-C1C | 4.22 | 1.48        | 1.35     |
| 15  | B     | 1226 | CLA  | CHC-C1C | 4.22 | 1.48        | 1.35     |
| 15  | A     | 1119 | CLA  | CHC-C1C | 4.22 | 1.48        | 1.35     |
| 15  | B     | 1211 | CLA  | CHC-C1C | 4.22 | 1.48        | 1.35     |
| 15  | B     | 1237 | CLA  | OBD-CAD | 4.23 | 1.28        | 1.22     |
| 15  | B     | 1213 | CLA  | CHC-C1C | 4.23 | 1.48        | 1.35     |
| 15  | B     | 1202 | CLA  | CHC-C1C | 4.23 | 1.48        | 1.35     |
| 15  | B     | 1210 | CLA  | CHC-C1C | 4.23 | 1.48        | 1.35     |
| 15  | B     | 1217 | CLA  | CHC-C1C | 4.24 | 1.48        | 1.35     |
| 15  | A     | 1132 | CLA  | CHC-C1C | 4.24 | 1.48        | 1.35     |
| 15  | B     | 1236 | CLA  | OBD-CAD | 4.24 | 1.28        | 1.22     |
| 15  | A     | 1121 | CLA  | OBD-CAD | 4.24 | 1.28        | 1.22     |
| 15  | F     | 1139 | CLA  | OBD-CAD | 4.24 | 1.28        | 1.22     |
| 15  | A     | 1127 | CLA  | CHC-C1C | 4.24 | 1.48        | 1.35     |
| 13  | A     | 1108 | CL0  | CHC-C1C | 4.24 | 1.48        | 1.35     |
| 15  | B     | 1013 | CLA  | CHC-C1C | 4.25 | 1.48        | 1.35     |
| 15  | A     | 1130 | CLA  | OBD-CAD | 4.25 | 1.28        | 1.22     |
| 15  | F     | 1301 | CLA  | CHC-C1C | 4.25 | 1.48        | 1.35     |
| 15  | J     | 1303 | CLA  | CHC-C1C | 4.25 | 1.48        | 1.35     |
| 15  | A     | 1022 | CLA  | CHC-C1C | 4.25 | 1.48        | 1.35     |
| 15  | B     | 1211 | CLA  | OBD-CAD | 4.25 | 1.28        | 1.22     |
| 15  | A     | 1136 | CLA  | OBD-CAD | 4.25 | 1.28        | 1.22     |
| 13  | A     | 1011 | CL0  | OBD-CAD | 4.25 | 1.28        | 1.22     |
| 15  | B     | 1214 | CLA  | CHC-C1C | 4.26 | 1.48        | 1.35     |
| 15  | A     | 1109 | CLA  | OBD-CAD | 4.26 | 1.28        | 1.22     |
| 15  | A     | 1109 | CLA  | CHC-C1C | 4.26 | 1.48        | 1.35     |
| 15  | A     | 1106 | CLA  | CHC-C1C | 4.26 | 1.48        | 1.35     |
| 15  | B     | 1240 | CLA  | CHC-C1C | 4.27 | 1.48        | 1.35     |
| 15  | A     | 1117 | CLA  | CHC-C1C | 4.28 | 1.48        | 1.35     |
| 15  | A     | 1113 | CLA  | OBD-CAD | 4.28 | 1.28        | 1.22     |
| 15  | A     | 1119 | CLA  | OBD-CAD | 4.28 | 1.28        | 1.22     |
| 15  | A     | 1132 | CLA  | OBD-CAD | 4.28 | 1.28        | 1.22     |
| 15  | A     | 1107 | CLA  | OBD-CAD | 4.28 | 1.28        | 1.22     |
| 15  | A     | 1134 | CLA  | CHC-C1C | 4.28 | 1.48        | 1.35     |
| 15  | B     | 1013 | CLA  | OBD-CAD | 4.29 | 1.28        | 1.22     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 15  | B     | 1223 | CLA  | CHC-C1C | 4.29 | 1.48        | 1.35     |
| 15  | A     | 1103 | CLA  | CHC-C1C | 4.29 | 1.48        | 1.35     |
| 15  | B     | 1234 | CLA  | OBD-CAD | 4.29 | 1.28        | 1.22     |
| 15  | B     | 1210 | CLA  | OBD-CAD | 4.29 | 1.28        | 1.22     |
| 15  | B     | 1230 | CLA  | CHC-C1C | 4.29 | 1.48        | 1.35     |
| 15  | A     | 1137 | CLA  | OBD-CAD | 4.29 | 1.28        | 1.22     |
| 15  | A     | 1104 | CLA  | OBD-CAD | 4.30 | 1.28        | 1.22     |
| 15  | B     | 1238 | CLA  | OBD-CAD | 4.30 | 1.28        | 1.22     |
| 15  | A     | 1123 | CLA  | OBD-CAD | 4.30 | 1.28        | 1.22     |
| 15  | B     | 1220 | CLA  | CHC-C1C | 4.30 | 1.48        | 1.35     |
| 15  | A     | 1105 | CLA  | OBD-CAD | 4.30 | 1.28        | 1.22     |
| 15  | B     | 1203 | CLA  | OBD-CAD | 4.31 | 1.28        | 1.22     |
| 15  | A     | 1128 | CLA  | OBD-CAD | 4.31 | 1.28        | 1.22     |
| 15  | A     | 1140 | CLA  | CHC-C1C | 4.31 | 1.48        | 1.35     |
| 15  | A     | 1135 | CLA  | OBD-CAD | 4.31 | 1.28        | 1.22     |
| 15  | B     | 1227 | CLA  | C3B-C2B | 4.31 | 1.46        | 1.40     |
| 15  | B     | 1023 | CLA  | OBD-CAD | 4.31 | 1.28        | 1.22     |
| 15  | A     | 1115 | CLA  | CHC-C1C | 4.31 | 1.48        | 1.35     |
| 15  | A     | 1111 | CLA  | CHC-C1C | 4.31 | 1.48        | 1.35     |
| 15  | A     | 1126 | CLA  | OBD-CAD | 4.32 | 1.28        | 1.22     |
| 15  | B     | 1208 | CLA  | OBD-CAD | 4.32 | 1.28        | 1.22     |
| 15  | B     | 1206 | CLA  | OBD-CAD | 4.32 | 1.28        | 1.22     |
| 15  | A     | 1103 | CLA  | OBD-CAD | 4.32 | 1.28        | 1.22     |
| 15  | B     | 1231 | CLA  | OBD-CAD | 4.32 | 1.28        | 1.22     |
| 15  | A     | 1115 | CLA  | OBD-CAD | 4.32 | 1.28        | 1.22     |
| 15  | J     | 1303 | CLA  | OBD-CAD | 4.32 | 1.29        | 1.22     |
| 15  | A     | 1122 | CLA  | OBD-CAD | 4.32 | 1.29        | 1.22     |
| 15  | A     | 1801 | CLA  | OBD-CAD | 4.32 | 1.29        | 1.22     |
| 15  | A     | 1133 | CLA  | OBD-CAD | 4.33 | 1.29        | 1.22     |
| 15  | A     | 1012 | CLA  | OBD-CAD | 4.33 | 1.29        | 1.22     |
| 15  | B     | 1232 | CLA  | OBD-CAD | 4.33 | 1.29        | 1.22     |
| 15  | B     | 1230 | CLA  | OBD-CAD | 4.33 | 1.29        | 1.22     |
| 13  | A     | 1108 | CL0  | C3C-C2C | 4.33 | 1.46        | 1.36     |
| 15  | K     | 1402 | CLA  | OBD-CAD | 4.34 | 1.29        | 1.22     |
| 15  | A     | 1107 | CLA  | CHC-C1C | 4.34 | 1.48        | 1.35     |
| 15  | F     | 1301 | CLA  | OBD-CAD | 4.34 | 1.29        | 1.22     |
| 15  | A     | 1130 | CLA  | CHC-C1C | 4.34 | 1.48        | 1.35     |
| 15  | A     | 1118 | CLA  | OBD-CAD | 4.34 | 1.29        | 1.22     |
| 15  | F     | 1410 | CLA  | OBD-CAD | 4.35 | 1.29        | 1.22     |
| 15  | J     | 1302 | CLA  | OBD-CAD | 4.35 | 1.29        | 1.22     |
| 15  | A     | 1131 | CLA  | OBD-CAD | 4.35 | 1.29        | 1.22     |
| 15  | A     | 1111 | CLA  | OBD-CAD | 4.35 | 1.29        | 1.22     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 15  | A     | 1112 | CLA  | OBD-CAD | 4.35 | 1.29        | 1.22     |
| 15  | A     | 1122 | CLA  | CHC-C1C | 4.35 | 1.49        | 1.35     |
| 15  | A     | 1114 | CLA  | OBD-CAD | 4.35 | 1.29        | 1.22     |
| 15  | B     | 1240 | CLA  | OBD-CAD | 4.35 | 1.29        | 1.22     |
| 15  | A     | 1134 | CLA  | OBD-CAD | 4.36 | 1.29        | 1.22     |
| 15  | A     | 1112 | CLA  | CHC-C1C | 4.36 | 1.49        | 1.35     |
| 15  | B     | 1217 | CLA  | OBD-CAD | 4.36 | 1.29        | 1.22     |
| 15  | B     | 1226 | CLA  | OBD-CAD | 4.36 | 1.29        | 1.22     |
| 15  | A     | 1101 | CLA  | CHC-C1C | 4.36 | 1.49        | 1.35     |
| 15  | B     | 1232 | CLA  | C3B-C2B | 4.36 | 1.46        | 1.40     |
| 15  | B     | 1201 | CLA  | OBD-CAD | 4.36 | 1.29        | 1.22     |
| 15  | A     | 1106 | CLA  | OBD-CAD | 4.37 | 1.29        | 1.22     |
| 15  | B     | 1212 | CLA  | OBD-CAD | 4.37 | 1.29        | 1.22     |
| 15  | B     | 1205 | CLA  | OBD-CAD | 4.37 | 1.29        | 1.22     |
| 15  | B     | 1220 | CLA  | OBD-CAD | 4.37 | 1.29        | 1.22     |
| 15  | A     | 1117 | CLA  | OBD-CAD | 4.37 | 1.29        | 1.22     |
| 15  | B     | 1204 | CLA  | OBD-CAD | 4.37 | 1.29        | 1.22     |
| 15  | A     | 1116 | CLA  | OBD-CAD | 4.37 | 1.29        | 1.22     |
| 15  | B     | 1214 | CLA  | OBD-CAD | 4.38 | 1.29        | 1.22     |
| 15  | A     | 1125 | CLA  | CHC-C1C | 4.38 | 1.49        | 1.35     |
| 15  | B     | 1209 | CLA  | OBD-CAD | 4.38 | 1.29        | 1.22     |
| 15  | A     | 1140 | CLA  | OBD-CAD | 4.38 | 1.29        | 1.22     |
| 15  | B     | 1219 | CLA  | OBD-CAD | 4.38 | 1.29        | 1.22     |
| 15  | B     | 1216 | CLA  | OBD-CAD | 4.39 | 1.29        | 1.22     |
| 15  | B     | 1224 | CLA  | OBD-CAD | 4.39 | 1.29        | 1.22     |
| 15  | B     | 1213 | CLA  | OBD-CAD | 4.39 | 1.29        | 1.22     |
| 15  | B     | 1239 | CLA  | OBD-CAD | 4.39 | 1.29        | 1.22     |
| 15  | B     | 1215 | CLA  | OBD-CAD | 4.39 | 1.29        | 1.22     |
| 15  | B     | 1235 | CLA  | CHC-C1C | 4.39 | 1.49        | 1.35     |
| 15  | F     | 1139 | CLA  | O2A-C1  | 4.40 | 1.59        | 1.46     |
| 15  | A     | 1103 | CLA  | C3C-C2C | 4.40 | 1.46        | 1.36     |
| 15  | A     | 1111 | CLA  | C3C-C2C | 4.40 | 1.46        | 1.36     |
| 15  | B     | 1021 | CLA  | OBD-CAD | 4.40 | 1.29        | 1.22     |
| 15  | B     | 1207 | CLA  | OBD-CAD | 4.40 | 1.29        | 1.22     |
| 15  | K     | 1401 | CLA  | OBD-CAD | 4.40 | 1.29        | 1.22     |
| 15  | B     | 1236 | CLA  | CHC-C1C | 4.41 | 1.49        | 1.35     |
| 15  | A     | 1120 | CLA  | OBD-CAD | 4.42 | 1.29        | 1.22     |
| 15  | A     | 1126 | CLA  | CHC-C1C | 4.42 | 1.49        | 1.35     |
| 15  | A     | 1123 | CLA  | C3C-C2C | 4.42 | 1.46        | 1.36     |
| 15  | A     | 1110 | CLA  | C3C-C2C | 4.42 | 1.46        | 1.36     |
| 15  | B     | 1236 | CLA  | C3C-C2C | 4.43 | 1.46        | 1.36     |
| 15  | A     | 1101 | CLA  | OBD-CAD | 4.43 | 1.29        | 1.22     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 15  | B     | 1210 | CLA  | C3C-C2C | 4.43 | 1.46        | 1.36     |
| 15  | B     | 1225 | CLA  | OBD-CAD | 4.44 | 1.29        | 1.22     |
| 15  | B     | 1228 | CLA  | CHC-C1C | 4.45 | 1.49        | 1.35     |
| 15  | B     | 1218 | CLA  | OBD-CAD | 4.45 | 1.29        | 1.22     |
| 15  | A     | 1022 | CLA  | OBD-CAD | 4.45 | 1.29        | 1.22     |
| 15  | A     | 1118 | CLA  | C3C-C2C | 4.46 | 1.46        | 1.36     |
| 15  | A     | 1102 | CLA  | OBD-CAD | 4.46 | 1.29        | 1.22     |
| 15  | A     | 1128 | CLA  | C3B-C2B | 4.46 | 1.46        | 1.40     |
| 15  | B     | 1202 | CLA  | OBD-CAD | 4.46 | 1.29        | 1.22     |
| 15  | B     | 1230 | CLA  | O2A-C1  | 4.46 | 1.60        | 1.46     |
| 15  | A     | 1138 | CLA  | OBD-CAD | 4.46 | 1.29        | 1.22     |
| 15  | A     | 1115 | CLA  | C3C-C2C | 4.47 | 1.46        | 1.36     |
| 15  | A     | 1133 | CLA  | C3C-C2C | 4.47 | 1.46        | 1.36     |
| 15  | B     | 1230 | CLA  | C3C-C2C | 4.47 | 1.46        | 1.36     |
| 15  | B     | 1225 | CLA  | C3C-C2C | 4.48 | 1.46        | 1.36     |
| 15  | B     | 1237 | CLA  | C3C-C2C | 4.48 | 1.46        | 1.36     |
| 15  | A     | 1103 | CLA  | O2A-C1  | 4.48 | 1.60        | 1.46     |
| 15  | B     | 1021 | CLA  | C3B-C2B | 4.48 | 1.46        | 1.40     |
| 15  | A     | 1125 | CLA  | C3C-C2C | 4.48 | 1.46        | 1.36     |
| 15  | B     | 1023 | CLA  | C3C-C2C | 4.49 | 1.46        | 1.36     |
| 15  | A     | 1136 | CLA  | C3C-C2C | 4.49 | 1.46        | 1.36     |
| 15  | B     | 1222 | CLA  | OBD-CAD | 4.49 | 1.29        | 1.22     |
| 15  | B     | 1211 | CLA  | C3C-C2C | 4.49 | 1.46        | 1.36     |
| 15  | B     | 1221 | CLA  | C3C-C2C | 4.49 | 1.46        | 1.36     |
| 15  | B     | 1224 | CLA  | C3C-C2C | 4.50 | 1.46        | 1.36     |
| 15  | B     | 1203 | CLA  | O2A-C1  | 4.50 | 1.60        | 1.46     |
| 15  | J     | 1302 | CLA  | C3C-C2C | 4.50 | 1.46        | 1.36     |
| 15  | A     | 1124 | CLA  | OBD-CAD | 4.50 | 1.29        | 1.22     |
| 15  | B     | 1201 | CLA  | C3C-C2C | 4.50 | 1.46        | 1.36     |
| 15  | A     | 1101 | CLA  | C3C-C2C | 4.50 | 1.46        | 1.36     |
| 15  | B     | 1206 | CLA  | C3C-C2C | 4.50 | 1.46        | 1.36     |
| 15  | A     | 1106 | CLA  | C3C-C2C | 4.50 | 1.46        | 1.36     |
| 15  | A     | 1131 | CLA  | C3C-C2C | 4.51 | 1.46        | 1.36     |
| 15  | B     | 1225 | CLA  | O2A-C1  | 4.51 | 1.60        | 1.46     |
| 15  | A     | 1113 | CLA  | C3C-C2C | 4.51 | 1.46        | 1.36     |
| 15  | A     | 1128 | CLA  | C3C-C2C | 4.52 | 1.46        | 1.36     |
| 15  | A     | 1101 | CLA  | O2A-C1  | 4.52 | 1.60        | 1.46     |
| 15  | B     | 1205 | CLA  | C3C-C2C | 4.52 | 1.46        | 1.36     |
| 13  | A     | 1011 | CL0  | C3C-C2C | 4.52 | 1.46        | 1.36     |
| 15  | K     | 1401 | CLA  | C3C-C2C | 4.52 | 1.46        | 1.36     |
| 15  | B     | 1204 | CLA  | C3C-C2C | 4.52 | 1.46        | 1.36     |
| 13  | A     | 1011 | CL0  | C3B-C2B | 4.52 | 1.46        | 1.40     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 15  | B     | 1215 | CLA  | C3C-C2C | 4.53 | 1.46        | 1.36     |
| 15  | B     | 1238 | CLA  | C3C-C2C | 4.53 | 1.46        | 1.36     |
| 15  | B     | 1229 | CLA  | OBD-CAD | 4.53 | 1.29        | 1.22     |
| 15  | B     | 1209 | CLA  | C3C-C2C | 4.53 | 1.46        | 1.36     |
| 15  | B     | 1213 | CLA  | C3C-C2C | 4.53 | 1.46        | 1.36     |
| 15  | B     | 1207 | CLA  | C3C-C2C | 4.54 | 1.46        | 1.36     |
| 15  | F     | 1410 | CLA  | C3C-C2C | 4.54 | 1.46        | 1.36     |
| 15  | B     | 1210 | CLA  | O2A-C1  | 4.54 | 1.60        | 1.46     |
| 15  | A     | 1104 | CLA  | O2A-C1  | 4.55 | 1.60        | 1.46     |
| 15  | A     | 1135 | CLA  | C3C-C2C | 4.55 | 1.46        | 1.36     |
| 15  | A     | 1110 | CLA  | O2A-C1  | 4.55 | 1.60        | 1.46     |
| 15  | B     | 1203 | CLA  | C3C-C2C | 4.55 | 1.46        | 1.36     |
| 15  | A     | 1123 | CLA  | O2A-C1  | 4.55 | 1.60        | 1.46     |
| 15  | A     | 1126 | CLA  | C3C-C2C | 4.55 | 1.46        | 1.36     |
| 15  | A     | 1122 | CLA  | O2A-C1  | 4.55 | 1.60        | 1.46     |
| 15  | A     | 1120 | CLA  | C3C-C2C | 4.56 | 1.46        | 1.36     |
| 15  | B     | 1023 | CLA  | O2A-C1  | 4.56 | 1.60        | 1.46     |
| 15  | B     | 1218 | CLA  | C3C-C2C | 4.56 | 1.46        | 1.36     |
| 15  | A     | 1121 | CLA  | C3C-C2C | 4.56 | 1.46        | 1.36     |
| 15  | B     | 1219 | CLA  | C3C-C2C | 4.56 | 1.46        | 1.36     |
| 15  | A     | 1104 | CLA  | C3C-C2C | 4.57 | 1.46        | 1.36     |
| 15  | K     | 1402 | CLA  | C3C-C2C | 4.57 | 1.46        | 1.36     |
| 15  | A     | 1138 | CLA  | CHC-C1C | 4.57 | 1.49        | 1.35     |
| 15  | F     | 1301 | CLA  | C3C-C2C | 4.57 | 1.46        | 1.36     |
| 15  | B     | 1214 | CLA  | O2A-C1  | 4.58 | 1.60        | 1.46     |
| 15  | A     | 1117 | CLA  | C3C-C2C | 4.58 | 1.46        | 1.36     |
| 15  | A     | 1129 | CLA  | C3C-C2C | 4.58 | 1.46        | 1.36     |
| 15  | A     | 1132 | CLA  | O2A-C1  | 4.58 | 1.60        | 1.46     |
| 15  | A     | 1022 | CLA  | C3B-C2B | 4.58 | 1.46        | 1.40     |
| 15  | A     | 1112 | CLA  | C3C-C2C | 4.58 | 1.46        | 1.36     |
| 15  | A     | 1102 | CLA  | C3C-C2C | 4.58 | 1.46        | 1.36     |
| 15  | A     | 1134 | CLA  | C3C-C2C | 4.58 | 1.46        | 1.36     |
| 15  | A     | 1114 | CLA  | C3C-C2C | 4.58 | 1.46        | 1.36     |
| 15  | F     | 1139 | CLA  | C3C-C2C | 4.58 | 1.46        | 1.36     |
| 15  | A     | 1140 | CLA  | O2A-C1  | 4.58 | 1.60        | 1.46     |
| 15  | B     | 1214 | CLA  | C3C-C2C | 4.58 | 1.46        | 1.36     |
| 15  | B     | 1231 | CLA  | C3C-C2C | 4.58 | 1.46        | 1.36     |
| 15  | A     | 1022 | CLA  | O2A-C1  | 4.59 | 1.60        | 1.46     |
| 15  | A     | 1126 | CLA  | O2A-C1  | 4.59 | 1.60        | 1.46     |
| 15  | A     | 1105 | CLA  | C3C-C2C | 4.59 | 1.46        | 1.36     |
| 15  | A     | 1119 | CLA  | C3C-C2C | 4.59 | 1.46        | 1.36     |
| 15  | A     | 1105 | CLA  | C3B-C2B | 4.59 | 1.46        | 1.40     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 15  | B     | 1217 | CLA  | C3C-C2C | 4.59 | 1.46        | 1.36     |
| 15  | B     | 1222 | CLA  | O2A-C1  | 4.59 | 1.60        | 1.46     |
| 15  | B     | 1229 | CLA  | O2A-C1  | 4.59 | 1.60        | 1.46     |
| 15  | A     | 1122 | CLA  | C3B-C2B | 4.59 | 1.46        | 1.40     |
| 15  | A     | 1012 | CLA  | C3C-C2C | 4.60 | 1.46        | 1.36     |
| 15  | B     | 1202 | CLA  | O2A-C1  | 4.60 | 1.60        | 1.46     |
| 15  | B     | 1236 | CLA  | C3B-C2B | 4.60 | 1.46        | 1.40     |
| 15  | A     | 1107 | CLA  | O2A-C1  | 4.60 | 1.60        | 1.46     |
| 15  | B     | 1021 | CLA  | O2A-C1  | 4.60 | 1.60        | 1.46     |
| 15  | B     | 1234 | CLA  | C3C-C2C | 4.60 | 1.46        | 1.36     |
| 15  | B     | 1229 | CLA  | C3C-C2C | 4.60 | 1.46        | 1.36     |
| 15  | B     | 1216 | CLA  | C3C-C2C | 4.61 | 1.46        | 1.36     |
| 15  | A     | 1132 | CLA  | C3C-C2C | 4.61 | 1.46        | 1.36     |
| 15  | A     | 1012 | CLA  | C3B-C2B | 4.61 | 1.46        | 1.40     |
| 15  | A     | 1124 | CLA  | C3C-C2C | 4.61 | 1.46        | 1.36     |
| 15  | A     | 1140 | CLA  | C3C-C2C | 4.61 | 1.46        | 1.36     |
| 15  | B     | 1239 | CLA  | C3C-C2C | 4.61 | 1.46        | 1.36     |
| 15  | B     | 1226 | CLA  | C3C-C2C | 4.61 | 1.46        | 1.36     |
| 15  | B     | 1021 | CLA  | C3C-C2C | 4.61 | 1.46        | 1.36     |
| 15  | A     | 1127 | CLA  | C3C-C2C | 4.61 | 1.46        | 1.36     |
| 15  | B     | 1023 | CLA  | C3B-C2B | 4.62 | 1.46        | 1.40     |
| 15  | B     | 1232 | CLA  | C3C-C2C | 4.62 | 1.46        | 1.36     |
| 15  | B     | 1212 | CLA  | C3C-C2C | 4.62 | 1.46        | 1.36     |
| 15  | B     | 1235 | CLA  | C3C-C2C | 4.62 | 1.46        | 1.36     |
| 15  | A     | 1137 | CLA  | C3C-C2C | 4.62 | 1.46        | 1.36     |
| 15  | A     | 1104 | CLA  | C3B-C2B | 4.62 | 1.46        | 1.40     |
| 15  | B     | 1234 | CLA  | O2D-CGD | 4.62 | 1.45        | 1.33     |
| 15  | B     | 1228 | CLA  | O2A-C1  | 4.63 | 1.60        | 1.46     |
| 15  | A     | 1138 | CLA  | C3C-C2C | 4.63 | 1.46        | 1.36     |
| 15  | B     | 1216 | CLA  | O2A-C1  | 4.63 | 1.60        | 1.46     |
| 15  | A     | 1119 | CLA  | C3B-C2B | 4.63 | 1.46        | 1.40     |
| 15  | J     | 1303 | CLA  | C3C-C2C | 4.63 | 1.46        | 1.36     |
| 15  | A     | 1122 | CLA  | C3C-C2C | 4.64 | 1.46        | 1.36     |
| 15  | A     | 1107 | CLA  | C3C-C2C | 4.64 | 1.46        | 1.36     |
| 15  | B     | 1229 | CLA  | C3B-C2B | 4.64 | 1.46        | 1.40     |
| 15  | B     | 1237 | CLA  | O2A-C1  | 4.64 | 1.60        | 1.46     |
| 15  | B     | 1013 | CLA  | C3C-C2C | 4.64 | 1.46        | 1.36     |
| 15  | A     | 1022 | CLA  | C3C-C2C | 4.64 | 1.46        | 1.36     |
| 15  | A     | 1116 | CLA  | C3C-C2C | 4.64 | 1.46        | 1.36     |
| 15  | A     | 1117 | CLA  | C3B-C2B | 4.65 | 1.46        | 1.40     |
| 15  | A     | 1127 | CLA  | O2A-C1  | 4.65 | 1.60        | 1.46     |
| 15  | A     | 1137 | CLA  | O2A-C1  | 4.65 | 1.60        | 1.46     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 15  | B     | 1223 | CLA  | O2A-C1  | 4.65 | 1.60        | 1.46     |
| 15  | F     | 1410 | CLA  | O2A-C1  | 4.65 | 1.60        | 1.46     |
| 15  | B     | 1202 | CLA  | C3C-C2C | 4.65 | 1.46        | 1.36     |
| 15  | A     | 1109 | CLA  | C3C-C2C | 4.65 | 1.46        | 1.36     |
| 15  | A     | 1111 | CLA  | O2A-C1  | 4.66 | 1.60        | 1.46     |
| 15  | A     | 1114 | CLA  | O2A-C1  | 4.66 | 1.60        | 1.46     |
| 15  | A     | 1801 | CLA  | O2A-C1  | 4.67 | 1.60        | 1.46     |
| 15  | B     | 1240 | CLA  | C3C-C2C | 4.67 | 1.46        | 1.36     |
| 15  | B     | 1223 | CLA  | C3C-C2C | 4.67 | 1.46        | 1.36     |
| 15  | A     | 1126 | CLA  | C3B-C2B | 4.67 | 1.46        | 1.40     |
| 15  | B     | 1221 | CLA  | O2A-C1  | 4.67 | 1.60        | 1.46     |
| 15  | A     | 1120 | CLA  | O2A-C1  | 4.68 | 1.60        | 1.46     |
| 15  | B     | 1219 | CLA  | O2A-C1  | 4.68 | 1.60        | 1.46     |
| 15  | B     | 1227 | CLA  | C3C-C2C | 4.68 | 1.46        | 1.36     |
| 15  | A     | 1124 | CLA  | O2A-C1  | 4.68 | 1.60        | 1.46     |
| 15  | A     | 1128 | CLA  | O2A-C1  | 4.68 | 1.60        | 1.46     |
| 15  | A     | 1124 | CLA  | C3B-C2B | 4.68 | 1.46        | 1.40     |
| 15  | B     | 1236 | CLA  | O2A-C1  | 4.68 | 1.60        | 1.46     |
| 15  | A     | 1130 | CLA  | O2A-C1  | 4.69 | 1.60        | 1.46     |
| 15  | B     | 1222 | CLA  | C3C-C2C | 4.69 | 1.46        | 1.36     |
| 15  | B     | 1226 | CLA  | O2A-C1  | 4.69 | 1.60        | 1.46     |
| 15  | B     | 1203 | CLA  | C3B-C2B | 4.69 | 1.46        | 1.40     |
| 15  | B     | 1220 | CLA  | C3C-C2C | 4.70 | 1.46        | 1.36     |
| 15  | A     | 1133 | CLA  | C3B-C2B | 4.70 | 1.46        | 1.40     |
| 15  | B     | 1205 | CLA  | C3B-C2B | 4.71 | 1.46        | 1.40     |
| 15  | A     | 1116 | CLA  | C3B-C2B | 4.71 | 1.46        | 1.40     |
| 13  | A     | 1011 | CL0  | O2A-C1  | 4.71 | 1.60        | 1.46     |
| 15  | A     | 1105 | CLA  | O2A-C1  | 4.71 | 1.60        | 1.46     |
| 15  | B     | 1226 | CLA  | C3B-C2B | 4.71 | 1.46        | 1.40     |
| 15  | B     | 1208 | CLA  | C3C-C2C | 4.72 | 1.46        | 1.36     |
| 15  | A     | 1130 | CLA  | C3C-C2C | 4.72 | 1.46        | 1.36     |
| 15  | B     | 1228 | CLA  | C3C-C2C | 4.72 | 1.46        | 1.36     |
| 15  | B     | 1218 | CLA  | O2A-C1  | 4.72 | 1.60        | 1.46     |
| 15  | F     | 1410 | CLA  | C3B-C2B | 4.73 | 1.46        | 1.40     |
| 15  | A     | 1125 | CLA  | C3B-C2B | 4.73 | 1.46        | 1.40     |
| 15  | A     | 1130 | CLA  | C3B-C2B | 4.73 | 1.46        | 1.40     |
| 15  | A     | 1110 | CLA  | C3B-C2B | 4.73 | 1.46        | 1.40     |
| 15  | B     | 1214 | CLA  | C3B-C2B | 4.73 | 1.46        | 1.40     |
| 15  | A     | 1138 | CLA  | C3B-C2B | 4.73 | 1.46        | 1.40     |
| 15  | B     | 1235 | CLA  | O2A-C1  | 4.74 | 1.60        | 1.46     |
| 15  | A     | 1102 | CLA  | O2A-C1  | 4.75 | 1.60        | 1.46     |
| 15  | A     | 1112 | CLA  | C3B-C2B | 4.75 | 1.46        | 1.40     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 15  | A     | 1136 | CLA  | O2A-C1  | 4.75 | 1.60        | 1.46     |
| 15  | B     | 1213 | CLA  | O2A-C1  | 4.75 | 1.60        | 1.46     |
| 15  | A     | 1106 | CLA  | C3B-C2B | 4.76 | 1.46        | 1.40     |
| 15  | B     | 1205 | CLA  | O2A-C1  | 4.76 | 1.61        | 1.46     |
| 15  | B     | 1204 | CLA  | C3B-C2B | 4.76 | 1.46        | 1.40     |
| 15  | B     | 1235 | CLA  | C3B-C2B | 4.76 | 1.46        | 1.40     |
| 15  | A     | 1129 | CLA  | C3B-C2B | 4.77 | 1.46        | 1.40     |
| 15  | A     | 1138 | CLA  | O2A-C1  | 4.77 | 1.61        | 1.46     |
| 15  | B     | 1013 | CLA  | O2A-C1  | 4.77 | 1.61        | 1.46     |
| 15  | A     | 1116 | CLA  | O2A-C1  | 4.77 | 1.61        | 1.46     |
| 15  | A     | 1125 | CLA  | O2A-C1  | 4.77 | 1.61        | 1.46     |
| 15  | A     | 1119 | CLA  | O2A-C1  | 4.77 | 1.61        | 1.46     |
| 15  | A     | 1135 | CLA  | O2A-C1  | 4.77 | 1.61        | 1.46     |
| 15  | B     | 1013 | CLA  | C3B-C2B | 4.78 | 1.46        | 1.40     |
| 15  | B     | 1217 | CLA  | C3B-C2B | 4.78 | 1.46        | 1.40     |
| 15  | A     | 1104 | CLA  | O2D-CGD | 4.78 | 1.45        | 1.33     |
| 15  | A     | 1134 | CLA  | O2D-CGD | 4.78 | 1.45        | 1.33     |
| 15  | B     | 1231 | CLA  | O2A-C1  | 4.79 | 1.61        | 1.46     |
| 15  | A     | 1131 | CLA  | O2A-C1  | 4.79 | 1.61        | 1.46     |
| 15  | A     | 1101 | CLA  | C3B-C2B | 4.79 | 1.46        | 1.40     |
| 15  | A     | 1121 | CLA  | C3B-C2B | 4.80 | 1.46        | 1.40     |
| 15  | A     | 1132 | CLA  | C3B-C2B | 4.80 | 1.46        | 1.40     |
| 15  | B     | 1226 | CLA  | O2D-CGD | 4.80 | 1.45        | 1.33     |
| 15  | B     | 1220 | CLA  | O2A-C1  | 4.81 | 1.61        | 1.46     |
| 15  | A     | 1107 | CLA  | C3B-C2B | 4.81 | 1.46        | 1.40     |
| 15  | B     | 1231 | CLA  | O2D-CGD | 4.82 | 1.45        | 1.33     |
| 15  | B     | 1234 | CLA  | O2A-C1  | 4.82 | 1.61        | 1.46     |
| 15  | B     | 1229 | CLA  | O2D-CGD | 4.82 | 1.45        | 1.33     |
| 15  | A     | 1135 | CLA  | O2D-CGD | 4.83 | 1.45        | 1.33     |
| 15  | B     | 1240 | CLA  | C3B-C2B | 4.83 | 1.46        | 1.40     |
| 15  | B     | 1210 | CLA  | O2D-CGD | 4.83 | 1.45        | 1.33     |
| 15  | A     | 1801 | CLA  | C3B-C2B | 4.84 | 1.46        | 1.40     |
| 15  | A     | 1110 | CLA  | O2D-CGD | 4.84 | 1.45        | 1.33     |
| 15  | A     | 1125 | CLA  | O2D-CGD | 4.84 | 1.45        | 1.33     |
| 15  | B     | 1223 | CLA  | C3B-C2B | 4.84 | 1.46        | 1.40     |
| 15  | B     | 1239 | CLA  | C3B-C2B | 4.84 | 1.46        | 1.40     |
| 15  | A     | 1101 | CLA  | O2D-CGD | 4.84 | 1.45        | 1.33     |
| 15  | A     | 1117 | CLA  | O2A-C1  | 4.84 | 1.61        | 1.46     |
| 15  | A     | 1109 | CLA  | C3B-C2B | 4.85 | 1.46        | 1.40     |
| 15  | B     | 1216 | CLA  | C3B-C2B | 4.85 | 1.46        | 1.40     |
| 15  | B     | 1215 | CLA  | C3B-C2B | 4.85 | 1.46        | 1.40     |
| 15  | B     | 1209 | CLA  | C3B-C2B | 4.85 | 1.46        | 1.40     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 15  | B     | 1218 | CLA  | C3B-C2B | 4.85 | 1.46        | 1.40     |
| 15  | B     | 1236 | CLA  | O2D-CGD | 4.85 | 1.45        | 1.33     |
| 15  | F     | 1301 | CLA  | C3B-C2B | 4.86 | 1.46        | 1.40     |
| 15  | K     | 1401 | CLA  | C3B-C2B | 4.86 | 1.46        | 1.40     |
| 15  | B     | 1206 | CLA  | C3B-C2B | 4.86 | 1.46        | 1.40     |
| 15  | A     | 1118 | CLA  | C3B-C2B | 4.86 | 1.46        | 1.40     |
| 15  | B     | 1222 | CLA  | C3B-C2B | 4.86 | 1.46        | 1.40     |
| 15  | B     | 1225 | CLA  | O2D-CGD | 4.86 | 1.45        | 1.33     |
| 15  | B     | 1207 | CLA  | C3B-C2B | 4.87 | 1.46        | 1.40     |
| 15  | A     | 1123 | CLA  | O2D-CGD | 4.87 | 1.45        | 1.33     |
| 15  | K     | 1402 | CLA  | C3B-C2B | 4.87 | 1.46        | 1.40     |
| 15  | A     | 1102 | CLA  | O2D-CGD | 4.87 | 1.45        | 1.33     |
| 15  | A     | 1120 | CLA  | C3B-C2B | 4.87 | 1.46        | 1.40     |
| 15  | J     | 1303 | CLA  | C3B-C2B | 4.87 | 1.46        | 1.40     |
| 15  | B     | 1222 | CLA  | O2D-CGD | 4.87 | 1.45        | 1.33     |
| 15  | A     | 1137 | CLA  | O2D-CGD | 4.88 | 1.45        | 1.33     |
| 15  | B     | 1217 | CLA  | O2D-CGD | 4.88 | 1.45        | 1.33     |
| 15  | B     | 1215 | CLA  | O2A-C1  | 4.88 | 1.61        | 1.46     |
| 15  | B     | 1223 | CLA  | O2D-CGD | 4.89 | 1.45        | 1.33     |
| 15  | A     | 1111 | CLA  | O2D-CGD | 4.89 | 1.45        | 1.33     |
| 15  | A     | 1130 | CLA  | O2D-CGD | 4.89 | 1.45        | 1.33     |
| 15  | F     | 1139 | CLA  | C3B-C2B | 4.90 | 1.46        | 1.40     |
| 15  | B     | 1238 | CLA  | O2D-CGD | 4.90 | 1.45        | 1.33     |
| 15  | J     | 1302 | CLA  | O2D-CGD | 4.90 | 1.45        | 1.33     |
| 15  | A     | 1109 | CLA  | O2A-C1  | 4.90 | 1.61        | 1.46     |
| 15  | A     | 1801 | CLA  | C3C-C2C | 4.90 | 1.47        | 1.36     |
| 15  | B     | 1023 | CLA  | O2D-CGD | 4.90 | 1.45        | 1.33     |
| 15  | A     | 1114 | CLA  | C3B-C2B | 4.90 | 1.46        | 1.40     |
| 15  | B     | 1213 | CLA  | O2D-CGD | 4.90 | 1.45        | 1.33     |
| 15  | B     | 1224 | CLA  | C3B-C2B | 4.90 | 1.46        | 1.40     |
| 15  | F     | 1410 | CLA  | O2D-CGD | 4.91 | 1.45        | 1.33     |
| 15  | A     | 1140 | CLA  | O2D-CGD | 4.91 | 1.45        | 1.33     |
| 15  | A     | 1111 | CLA  | C3B-C2B | 4.91 | 1.46        | 1.40     |
| 15  | B     | 1221 | CLA  | O2D-CGD | 4.91 | 1.45        | 1.33     |
| 15  | A     | 1128 | CLA  | O2D-CGD | 4.91 | 1.45        | 1.33     |
| 15  | B     | 1204 | CLA  | O2D-CGD | 4.92 | 1.45        | 1.33     |
| 15  | B     | 1239 | CLA  | O2D-CGD | 4.92 | 1.45        | 1.33     |
| 15  | A     | 1132 | CLA  | O2D-CGD | 4.92 | 1.45        | 1.33     |
| 15  | B     | 1201 | CLA  | O2D-CGD | 4.92 | 1.45        | 1.33     |
| 15  | B     | 1224 | CLA  | O2D-CGD | 4.92 | 1.45        | 1.33     |
| 15  | B     | 1224 | CLA  | O2A-C1  | 4.92 | 1.61        | 1.46     |
| 15  | A     | 1113 | CLA  | O2D-CGD | 4.92 | 1.45        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 15  | A     | 1123 | CLA  | C3B-C2B | 4.92 | 1.46        | 1.40     |
| 15  | B     | 1211 | CLA  | O2D-CGD | 4.93 | 1.45        | 1.33     |
| 15  | B     | 1225 | CLA  | C3B-C2B | 4.93 | 1.46        | 1.40     |
| 15  | A     | 1126 | CLA  | O2D-CGD | 4.93 | 1.45        | 1.33     |
| 15  | A     | 1129 | CLA  | O2D-CGD | 4.93 | 1.45        | 1.33     |
| 15  | A     | 1103 | CLA  | C3B-C2B | 4.93 | 1.46        | 1.40     |
| 15  | A     | 1106 | CLA  | O2D-CGD | 4.93 | 1.45        | 1.33     |
| 15  | A     | 1105 | CLA  | O2D-CGD | 4.94 | 1.45        | 1.33     |
| 15  | A     | 1135 | CLA  | C3B-C2B | 4.94 | 1.46        | 1.40     |
| 15  | A     | 1115 | CLA  | O2D-CGD | 4.94 | 1.45        | 1.33     |
| 15  | B     | 1209 | CLA  | O2D-CGD | 4.94 | 1.45        | 1.33     |
| 15  | B     | 1237 | CLA  | C3B-C2B | 4.94 | 1.46        | 1.40     |
| 15  | A     | 1114 | CLA  | O2D-CGD | 4.94 | 1.45        | 1.33     |
| 15  | A     | 1118 | CLA  | O2D-CGD | 4.94 | 1.45        | 1.33     |
| 15  | A     | 1107 | CLA  | O2D-CGD | 4.95 | 1.45        | 1.33     |
| 15  | B     | 1228 | CLA  | O2D-CGD | 4.95 | 1.45        | 1.33     |
| 15  | B     | 1206 | CLA  | O2D-CGD | 4.95 | 1.45        | 1.33     |
| 15  | B     | 1230 | CLA  | O2D-CGD | 4.95 | 1.45        | 1.33     |
| 15  | A     | 1122 | CLA  | O2D-CGD | 4.95 | 1.45        | 1.33     |
| 15  | B     | 1214 | CLA  | O2D-CGD | 4.95 | 1.45        | 1.33     |
| 15  | B     | 1212 | CLA  | O2D-CGD | 4.95 | 1.45        | 1.33     |
| 15  | A     | 1116 | CLA  | O2D-CGD | 4.95 | 1.45        | 1.33     |
| 15  | A     | 1134 | CLA  | C3B-C2B | 4.95 | 1.46        | 1.40     |
| 13  | A     | 1011 | CL0  | O2D-CGD | 4.95 | 1.45        | 1.33     |
| 15  | B     | 1220 | CLA  | O2D-CGD | 4.95 | 1.45        | 1.33     |
| 15  | A     | 1012 | CLA  | O2A-C1  | 4.95 | 1.61        | 1.46     |
| 15  | B     | 1207 | CLA  | O2D-CGD | 4.96 | 1.45        | 1.33     |
| 15  | A     | 1133 | CLA  | O2D-CGD | 4.96 | 1.45        | 1.33     |
| 15  | B     | 1231 | CLA  | C3B-C2B | 4.96 | 1.46        | 1.40     |
| 15  | B     | 1238 | CLA  | C3B-C2B | 4.96 | 1.46        | 1.40     |
| 15  | B     | 1205 | CLA  | O2D-CGD | 4.96 | 1.45        | 1.33     |
| 15  | A     | 1801 | CLA  | O2D-CGD | 4.96 | 1.45        | 1.33     |
| 15  | A     | 1106 | CLA  | O2A-C1  | 4.96 | 1.61        | 1.46     |
| 15  | A     | 1124 | CLA  | O2D-CGD | 4.96 | 1.45        | 1.33     |
| 15  | B     | 1211 | CLA  | C3B-C2B | 4.97 | 1.46        | 1.40     |
| 15  | A     | 1112 | CLA  | O2D-CGD | 4.97 | 1.45        | 1.33     |
| 15  | A     | 1113 | CLA  | C3B-C2B | 4.97 | 1.46        | 1.40     |
| 15  | B     | 1215 | CLA  | O2D-CGD | 4.98 | 1.45        | 1.33     |
| 15  | B     | 1218 | CLA  | O2D-CGD | 4.98 | 1.45        | 1.33     |
| 15  | B     | 1216 | CLA  | O2D-CGD | 4.98 | 1.45        | 1.33     |
| 15  | B     | 1201 | CLA  | C3B-C2B | 4.98 | 1.46        | 1.40     |
| 15  | A     | 1022 | CLA  | O2D-CGD | 4.98 | 1.45        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 15  | J     | 1302 | CLA  | C3B-C2B | 4.99 | 1.46        | 1.40     |
| 15  | B     | 1237 | CLA  | O2D-CGD | 4.99 | 1.45        | 1.33     |
| 15  | A     | 1140 | CLA  | C3B-C2B | 4.99 | 1.46        | 1.40     |
| 15  | B     | 1240 | CLA  | O2D-CGD | 4.99 | 1.45        | 1.33     |
| 15  | B     | 1202 | CLA  | C3B-C2B | 4.99 | 1.46        | 1.40     |
| 15  | A     | 1131 | CLA  | O2D-CGD | 4.99 | 1.45        | 1.33     |
| 15  | K     | 1402 | CLA  | O2D-CGD | 4.99 | 1.45        | 1.33     |
| 13  | A     | 1108 | CL0  | O2D-CGD | 5.00 | 1.46        | 1.33     |
| 15  | A     | 1117 | CLA  | O2D-CGD | 5.00 | 1.46        | 1.33     |
| 15  | J     | 1303 | CLA  | O2D-CGD | 5.00 | 1.46        | 1.33     |
| 15  | B     | 1208 | CLA  | O2D-CGD | 5.00 | 1.46        | 1.33     |
| 15  | B     | 1219 | CLA  | O2D-CGD | 5.00 | 1.46        | 1.33     |
| 15  | B     | 1021 | CLA  | O2D-CGD | 5.01 | 1.46        | 1.33     |
| 15  | B     | 1232 | CLA  | O2D-CGD | 5.01 | 1.46        | 1.33     |
| 15  | B     | 1230 | CLA  | C3B-C2B | 5.01 | 1.46        | 1.40     |
| 15  | B     | 1227 | CLA  | O2D-CGD | 5.01 | 1.46        | 1.33     |
| 15  | B     | 1202 | CLA  | O2D-CGD | 5.01 | 1.46        | 1.33     |
| 15  | A     | 1127 | CLA  | O2D-CGD | 5.01 | 1.46        | 1.33     |
| 15  | F     | 1301 | CLA  | O2D-CGD | 5.02 | 1.46        | 1.33     |
| 15  | A     | 1120 | CLA  | O2D-CGD | 5.02 | 1.46        | 1.33     |
| 15  | B     | 1213 | CLA  | C3B-C2B | 5.02 | 1.46        | 1.40     |
| 15  | B     | 1203 | CLA  | O2D-CGD | 5.03 | 1.46        | 1.33     |
| 15  | B     | 1234 | CLA  | C3B-C2B | 5.03 | 1.46        | 1.40     |
| 15  | A     | 1109 | CLA  | O2D-CGD | 5.03 | 1.46        | 1.33     |
| 15  | A     | 1136 | CLA  | C3B-C2B | 5.03 | 1.46        | 1.40     |
| 15  | A     | 1121 | CLA  | O2D-CGD | 5.03 | 1.46        | 1.33     |
| 15  | A     | 1136 | CLA  | O2D-CGD | 5.03 | 1.46        | 1.33     |
| 15  | B     | 1235 | CLA  | O2D-CGD | 5.04 | 1.46        | 1.33     |
| 15  | B     | 1221 | CLA  | C3B-C2B | 5.04 | 1.47        | 1.40     |
| 15  | B     | 1212 | CLA  | C3B-C2B | 5.04 | 1.47        | 1.40     |
| 15  | A     | 1103 | CLA  | O2D-CGD | 5.05 | 1.46        | 1.33     |
| 15  | K     | 1401 | CLA  | O2D-CGD | 5.05 | 1.46        | 1.33     |
| 10  | A     | 2001 | PQN  | C10-C5  | 5.05 | 1.48        | 1.40     |
| 13  | A     | 1108 | CL0  | C3B-C2B | 5.05 | 1.47        | 1.40     |
| 15  | A     | 1119 | CLA  | O2D-CGD | 5.05 | 1.46        | 1.33     |
| 15  | A     | 1012 | CLA  | O2D-CGD | 5.05 | 1.46        | 1.33     |
| 15  | F     | 1139 | CLA  | O2D-CGD | 5.05 | 1.46        | 1.33     |
| 10  | B     | 2002 | PQN  | C10-C5  | 5.06 | 1.48        | 1.40     |
| 15  | A     | 1138 | CLA  | O2D-CGD | 5.07 | 1.46        | 1.33     |
| 15  | B     | 1013 | CLA  | O2D-CGD | 5.09 | 1.46        | 1.33     |
| 15  | A     | 1131 | CLA  | C3B-C2B | 5.09 | 1.47        | 1.40     |
| 15  | A     | 1127 | CLA  | C3B-C2B | 5.10 | 1.47        | 1.40     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 15  | A     | 1137 | CLA  | C3B-C2B | 5.13 | 1.47        | 1.40     |
| 15  | B     | 1210 | CLA  | C3B-C2B | 5.15 | 1.47        | 1.40     |
| 15  | A     | 1115 | CLA  | C3B-C2B | 5.20 | 1.47        | 1.40     |
| 15  | A     | 1102 | CLA  | C3B-C2B | 5.21 | 1.47        | 1.40     |
| 15  | B     | 1220 | CLA  | C3B-C2B | 5.30 | 1.47        | 1.40     |
| 15  | B     | 1208 | CLA  | C3B-C2B | 5.36 | 1.47        | 1.40     |
| 15  | B     | 1228 | CLA  | C3B-C2B | 5.41 | 1.47        | 1.40     |
| 15  | B     | 1219 | CLA  | C3B-C2B | 5.75 | 1.47        | 1.40     |
| 10  | B     | 2002 | PQN  | C3-C2   | 5.86 | 1.49        | 1.35     |
| 10  | A     | 2001 | PQN  | C3-C2   | 5.91 | 1.49        | 1.35     |
| 15  | B     | 1204 | CLA  | O2A-C1  | 6.15 | 1.60        | 1.45     |
| 15  | B     | 1207 | CLA  | O2A-C1  | 6.15 | 1.60        | 1.45     |
| 15  | A     | 1133 | CLA  | O2A-C1  | 6.17 | 1.60        | 1.45     |
| 15  | A     | 1121 | CLA  | O2A-C1  | 6.20 | 1.60        | 1.45     |
| 15  | A     | 1115 | CLA  | O2A-C1  | 6.20 | 1.60        | 1.45     |
| 15  | B     | 1211 | CLA  | O2A-C1  | 6.20 | 1.60        | 1.45     |
| 15  | J     | 1303 | CLA  | O2A-C1  | 6.20 | 1.60        | 1.45     |
| 15  | K     | 1402 | CLA  | O2A-C1  | 6.21 | 1.60        | 1.45     |
| 15  | B     | 1206 | CLA  | O2A-C1  | 6.22 | 1.60        | 1.45     |
| 15  | B     | 1201 | CLA  | O2A-C1  | 6.22 | 1.60        | 1.45     |
| 15  | B     | 1239 | CLA  | O2A-C1  | 6.23 | 1.60        | 1.45     |
| 15  | K     | 1401 | CLA  | O2A-C1  | 6.24 | 1.60        | 1.45     |
| 15  | A     | 1134 | CLA  | O2A-C1  | 6.25 | 1.60        | 1.45     |
| 15  | A     | 1129 | CLA  | O2A-C1  | 6.27 | 1.60        | 1.45     |
| 15  | A     | 1118 | CLA  | O2A-C1  | 6.31 | 1.60        | 1.45     |

All (1540) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15  | A     | 1105 | CLA  | C3B-CAB-CBB | -6.45 | 113.12      | 126.32   |
| 14  | F     | 4016 | BCR  | C38-C26-C25 | -6.01 | 118.70      | 124.61   |
| 14  | B     | 4009 | BCR  | C15-C14-C13 | -6.00 | 118.53      | 127.20   |
| 14  | A     | 4012 | BCR  | C38-C26-C25 | -5.85 | 118.86      | 124.61   |
| 14  | B     | 4006 | BCR  | C38-C26-C25 | -5.79 | 118.92      | 124.61   |
| 15  | B     | 1013 | CLA  | C3B-CAB-CBB | -5.69 | 114.67      | 126.32   |
| 14  | A     | 4003 | BCR  | C38-C26-C25 | -5.55 | 119.16      | 124.61   |
| 14  | A     | 4008 | BCR  | C33-C5-C6   | -5.55 | 119.16      | 124.61   |
| 14  | J     | 4013 | BCR  | C7-C8-C9    | -5.49 | 117.84      | 126.22   |
| 15  | A     | 1101 | CLA  | CAA-C2A-C3A | -5.44 | 97.58       | 113.22   |
| 14  | B     | 4011 | BCR  | C34-C9-C10  | -5.36 | 114.98      | 122.90   |
| 14  | B     | 4009 | BCR  | C33-C5-C6   | -5.30 | 119.40      | 124.61   |
| 15  | B     | 1013 | CLA  | O2A-CGA-O1A | -5.29 | 109.84      | 123.49   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | B     | 4004 | BCR  | C33-C5-C6   | -5.27 | 119.43      | 124.61   |
| 14  | B     | 4014 | BCR  | C33-C5-C6   | -5.26 | 119.44      | 124.61   |
| 15  | A     | 1119 | CLA  | O2A-CGA-O1A | -5.23 | 109.98      | 123.49   |
| 15  | B     | 1221 | CLA  | O2A-CGA-O1A | -5.23 | 110.00      | 123.49   |
| 15  | B     | 1205 | CLA  | O2A-CGA-O1A | -5.22 | 110.02      | 123.49   |
| 14  | B     | 4014 | BCR  | C38-C26-C25 | -5.21 | 119.49      | 124.61   |
| 15  | B     | 1235 | CLA  | O2A-CGA-O1A | -5.19 | 110.11      | 123.49   |
| 14  | F     | 4015 | BCR  | C33-C5-C6   | -5.18 | 119.52      | 124.61   |
| 14  | J     | 4013 | BCR  | C3-C4-C5    | -5.17 | 105.66      | 113.87   |
| 14  | B     | 4017 | BCR  | C24-C23-C22 | -5.13 | 118.39      | 126.22   |
| 15  | A     | 1136 | CLA  | O2A-CGA-O1A | -5.12 | 110.28      | 123.49   |
| 15  | A     | 1132 | CLA  | O2A-CGA-O1A | -5.11 | 110.31      | 123.49   |
| 14  | B     | 4017 | BCR  | C33-C5-C6   | -5.11 | 119.59      | 124.61   |
| 15  | A     | 1801 | CLA  | O2A-CGA-O1A | -5.07 | 110.41      | 123.49   |
| 15  | B     | 1202 | CLA  | O2A-CGA-O1A | -5.04 | 110.48      | 123.49   |
| 15  | B     | 1210 | CLA  | O2A-CGA-O1A | -5.04 | 110.49      | 123.49   |
| 15  | B     | 1231 | CLA  | O2A-CGA-O1A | -5.01 | 110.55      | 123.49   |
| 13  | A     | 1011 | CL0  | C1C-C2C-C3C | -4.99 | 100.94      | 106.91   |
| 14  | A     | 4001 | BCR  | C7-C8-C9    | -4.98 | 118.63      | 126.22   |
| 15  | A     | 1102 | CLA  | O2A-CGA-O1A | -4.97 | 110.67      | 123.49   |
| 15  | A     | 1104 | CLA  | C1C-C2C-C3C | -4.95 | 100.99      | 106.91   |
| 15  | A     | 1131 | CLA  | O2A-CGA-O1A | -4.94 | 110.75      | 123.49   |
| 15  | A     | 1111 | CLA  | O2A-CGA-O1A | -4.93 | 110.76      | 123.49   |
| 15  | B     | 1230 | CLA  | O2A-CGA-O1A | -4.93 | 110.77      | 123.49   |
| 15  | A     | 1135 | CLA  | O2A-CGA-O1A | -4.92 | 110.81      | 123.49   |
| 15  | B     | 1021 | CLA  | O2A-CGA-O1A | -4.91 | 110.83      | 123.49   |
| 15  | A     | 1118 | CLA  | C1C-C2C-C3C | -4.89 | 101.06      | 106.91   |
| 15  | A     | 1105 | CLA  | O2A-CGA-O1A | -4.88 | 110.89      | 123.49   |
| 14  | B     | 4010 | BCR  | C33-C5-C6   | -4.88 | 119.81      | 124.61   |
| 14  | A     | 4001 | BCR  | C33-C5-C6   | -4.88 | 119.81      | 124.61   |
| 15  | A     | 1104 | CLA  | O2A-CGA-O1A | -4.88 | 110.91      | 123.49   |
| 15  | A     | 1107 | CLA  | O2A-CGA-O1A | -4.87 | 110.92      | 123.49   |
| 15  | A     | 1109 | CLA  | O2A-CGA-O1A | -4.86 | 110.95      | 123.49   |
| 15  | B     | 1231 | CLA  | C1C-C2C-C3C | -4.86 | 101.10      | 106.91   |
| 15  | B     | 1218 | CLA  | O2A-CGA-O1A | -4.86 | 110.96      | 123.49   |
| 14  | B     | 4004 | BCR  | C38-C26-C25 | -4.85 | 119.84      | 124.61   |
| 14  | B     | 4011 | BCR  | C33-C5-C6   | -4.85 | 119.84      | 124.61   |
| 14  | A     | 4003 | BCR  | C7-C8-C9    | -4.85 | 118.83      | 126.22   |
| 15  | B     | 1226 | CLA  | O2A-CGA-O1A | -4.84 | 111.00      | 123.49   |
| 15  | B     | 1214 | CLA  | O2A-CGA-O1A | -4.84 | 111.01      | 123.49   |
| 15  | B     | 1203 | CLA  | C1C-C2C-C3C | -4.82 | 101.15      | 106.91   |
| 15  | B     | 1215 | CLA  | C1C-C2C-C3C | -4.81 | 101.16      | 106.91   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15  | A     | 1123 | CLA  | O2A-CGA-O1A | -4.80 | 111.09      | 123.49   |
| 15  | B     | 1232 | CLA  | C1C-C2C-C3C | -4.79 | 101.17      | 106.91   |
| 14  | A     | 4012 | BCR  | C33-C5-C6   | -4.79 | 119.90      | 124.61   |
| 15  | A     | 1135 | CLA  | C1C-C2C-C3C | -4.78 | 101.19      | 106.91   |
| 15  | B     | 1229 | CLA  | C1C-C2C-C3C | -4.78 | 101.19      | 106.91   |
| 15  | A     | 1022 | CLA  | O2A-CGA-O1A | -4.77 | 111.17      | 123.49   |
| 15  | B     | 1239 | CLA  | C1C-C2C-C3C | -4.76 | 101.21      | 106.91   |
| 15  | A     | 1130 | CLA  | O2A-CGA-O1A | -4.76 | 111.20      | 123.49   |
| 14  | B     | 4011 | BCR  | C38-C26-C25 | -4.75 | 119.94      | 124.61   |
| 15  | A     | 1131 | CLA  | C1C-C2C-C3C | -4.74 | 101.23      | 106.91   |
| 15  | B     | 1226 | CLA  | C1C-C2C-C3C | -4.74 | 101.23      | 106.91   |
| 15  | B     | 1219 | CLA  | C1C-C2C-C3C | -4.74 | 101.24      | 106.91   |
| 15  | A     | 1801 | CLA  | C1C-C2C-C3C | -4.74 | 101.24      | 106.91   |
| 15  | B     | 1219 | CLA  | O2A-CGA-O1A | -4.74 | 111.26      | 123.49   |
| 13  | A     | 1011 | CL0  | O2A-CGA-O1A | -4.74 | 111.27      | 123.49   |
| 15  | B     | 1217 | CLA  | O2A-CGA-O1A | -4.73 | 111.28      | 123.49   |
| 15  | B     | 1207 | CLA  | C1C-C2C-C3C | -4.73 | 101.25      | 106.91   |
| 13  | A     | 1108 | CL0  | C1C-C2C-C3C | -4.73 | 101.25      | 106.91   |
| 15  | B     | 1227 | CLA  | C1C-C2C-C3C | -4.73 | 101.25      | 106.91   |
| 15  | B     | 1224 | CLA  | C1C-C2C-C3C | -4.72 | 101.26      | 106.91   |
| 15  | J     | 1302 | CLA  | C1C-C2C-C3C | -4.72 | 101.26      | 106.91   |
| 14  | A     | 4003 | BCR  | C33-C5-C6   | -4.72 | 119.97      | 124.61   |
| 15  | A     | 1110 | CLA  | O2A-CGA-O1A | -4.72 | 111.32      | 123.49   |
| 15  | A     | 1140 | CLA  | O2A-CGA-O1A | -4.71 | 111.33      | 123.49   |
| 15  | A     | 1133 | CLA  | C1C-C2C-C3C | -4.71 | 101.27      | 106.91   |
| 15  | A     | 1128 | CLA  | C1C-C2C-C3C | -4.71 | 101.27      | 106.91   |
| 15  | B     | 1204 | CLA  | C1C-C2C-C3C | -4.71 | 101.28      | 106.91   |
| 15  | B     | 1236 | CLA  | O2A-CGA-O1A | -4.71 | 111.34      | 123.49   |
| 15  | A     | 1137 | CLA  | O2A-CGA-O1A | -4.70 | 111.35      | 123.49   |
| 14  | A     | 4002 | BCR  | C33-C5-C6   | -4.70 | 119.99      | 124.61   |
| 15  | B     | 1222 | CLA  | C1C-C2C-C3C | -4.70 | 101.29      | 106.91   |
| 15  | A     | 1022 | CLA  | C1C-C2C-C3C | -4.69 | 101.30      | 106.91   |
| 15  | A     | 1105 | CLA  | C1C-C2C-C3C | -4.69 | 101.30      | 106.91   |
| 15  | A     | 1120 | CLA  | C1C-C2C-C3C | -4.69 | 101.30      | 106.91   |
| 15  | B     | 1238 | CLA  | C1C-C2C-C3C | -4.69 | 101.30      | 106.91   |
| 15  | B     | 1205 | CLA  | C1C-C2C-C3C | -4.69 | 101.30      | 106.91   |
| 15  | B     | 1213 | CLA  | C1C-C2C-C3C | -4.69 | 101.30      | 106.91   |
| 14  | A     | 4002 | BCR  | C24-C23-C22 | -4.68 | 119.08      | 126.22   |
| 15  | A     | 1106 | CLA  | C1C-C2C-C3C | -4.68 | 101.31      | 106.91   |
| 15  | B     | 1220 | CLA  | O2A-CGA-O1A | -4.68 | 111.42      | 123.49   |
| 15  | B     | 1228 | CLA  | O2A-CGA-O1A | -4.68 | 111.42      | 123.49   |
| 15  | A     | 1136 | CLA  | C1C-C2C-C3C | -4.67 | 101.32      | 106.91   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15  | A     | 1137 | CLA  | C1C-C2C-C3C | -4.67 | 101.32      | 106.91   |
| 14  | F     | 4016 | BCR  | C33-C5-C6   | -4.67 | 120.02      | 124.61   |
| 15  | B     | 1221 | CLA  | C1C-C2C-C3C | -4.66 | 101.33      | 106.91   |
| 15  | A     | 1129 | CLA  | C1C-C2C-C3C | -4.66 | 101.33      | 106.91   |
| 15  | B     | 1023 | CLA  | C3B-CAB-CBB | -4.66 | 116.79      | 126.32   |
| 15  | F     | 1139 | CLA  | C1C-C2C-C3C | -4.65 | 101.34      | 106.91   |
| 15  | A     | 1128 | CLA  | O2A-CGA-O1A | -4.64 | 111.51      | 123.49   |
| 15  | B     | 1208 | CLA  | C1C-C2C-C3C | -4.64 | 101.36      | 106.91   |
| 15  | A     | 1127 | CLA  | C1C-C2C-C3C | -4.64 | 101.36      | 106.91   |
| 15  | A     | 1124 | CLA  | C1C-C2C-C3C | -4.64 | 101.36      | 106.91   |
| 15  | B     | 1218 | CLA  | C1C-C2C-C3C | -4.64 | 101.36      | 106.91   |
| 15  | B     | 1212 | CLA  | C1C-C2C-C3C | -4.64 | 101.36      | 106.91   |
| 15  | B     | 1225 | CLA  | C1C-C2C-C3C | -4.63 | 101.36      | 106.91   |
| 14  | B     | 4010 | BCR  | C38-C26-C25 | -4.63 | 120.06      | 124.61   |
| 15  | B     | 1202 | CLA  | C1C-C2C-C3C | -4.63 | 101.37      | 106.91   |
| 15  | A     | 1120 | CLA  | O2A-CGA-O1A | -4.63 | 111.55      | 123.49   |
| 15  | K     | 1402 | CLA  | C1C-C2C-C3C | -4.62 | 101.38      | 106.91   |
| 15  | A     | 1012 | CLA  | O2A-CGA-O1A | -4.62 | 111.57      | 123.49   |
| 14  | B     | 4005 | BCR  | C33-C5-C6   | -4.61 | 120.08      | 124.61   |
| 14  | B     | 4014 | BCR  | C7-C8-C9    | -4.61 | 119.19      | 126.22   |
| 15  | A     | 1110 | CLA  | C1C-C2C-C3C | -4.60 | 101.40      | 106.91   |
| 15  | B     | 1236 | CLA  | C1C-C2C-C3C | -4.60 | 101.41      | 106.91   |
| 15  | A     | 1122 | CLA  | O2A-CGA-O1A | -4.60 | 111.63      | 123.49   |
| 15  | B     | 1201 | CLA  | C1C-C2C-C3C | -4.60 | 101.41      | 106.91   |
| 15  | B     | 1214 | CLA  | C4-C3-C2    | -4.59 | 114.48      | 123.50   |
| 15  | A     | 1114 | CLA  | O2A-CGA-O1A | -4.59 | 111.64      | 123.49   |
| 15  | F     | 1410 | CLA  | C1C-C2C-C3C | -4.59 | 101.42      | 106.91   |
| 15  | B     | 1234 | CLA  | O2A-CGA-O1A | -4.59 | 111.64      | 123.49   |
| 15  | F     | 1410 | CLA  | O2A-CGA-O1A | -4.59 | 111.65      | 123.49   |
| 15  | A     | 1109 | CLA  | C1C-C2C-C3C | -4.59 | 101.42      | 106.91   |
| 15  | B     | 1206 | CLA  | C1C-C2C-C3C | -4.59 | 101.42      | 106.91   |
| 15  | A     | 1113 | CLA  | C1C-C2C-C3C | -4.59 | 101.42      | 106.91   |
| 15  | B     | 1217 | CLA  | C1C-C2C-C3C | -4.58 | 101.43      | 106.91   |
| 15  | A     | 1121 | CLA  | C1C-C2C-C3C | -4.58 | 101.43      | 106.91   |
| 15  | B     | 1209 | CLA  | C1C-C2C-C3C | -4.58 | 101.43      | 106.91   |
| 15  | B     | 1021 | CLA  | C1C-C2C-C3C | -4.58 | 101.43      | 106.91   |
| 15  | B     | 1023 | CLA  | O2A-CGA-O1A | -4.58 | 111.68      | 123.49   |
| 15  | A     | 1114 | CLA  | C1C-C2C-C3C | -4.58 | 101.44      | 106.91   |
| 15  | B     | 1216 | CLA  | C1C-C2C-C3C | -4.57 | 101.44      | 106.91   |
| 15  | A     | 1116 | CLA  | O2A-CGA-O1A | -4.57 | 111.71      | 123.49   |
| 15  | B     | 1013 | CLA  | C1C-C2C-C3C | -4.56 | 101.45      | 106.91   |
| 15  | B     | 1235 | CLA  | C1C-C2C-C3C | -4.56 | 101.46      | 106.91   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15  | B     | 1237 | CLA  | C1C-C2C-C3C | -4.56 | 101.46      | 106.91   |
| 15  | A     | 1116 | CLA  | C1C-C2C-C3C | -4.55 | 101.46      | 106.91   |
| 15  | B     | 1215 | CLA  | O2A-CGA-O1A | -4.54 | 111.77      | 123.49   |
| 15  | F     | 1301 | CLA  | C1C-C2C-C3C | -4.54 | 101.48      | 106.91   |
| 15  | B     | 1234 | CLA  | C1C-C2C-C3C | -4.54 | 101.48      | 106.91   |
| 14  | B     | 4009 | BCR  | C24-C23-C22 | -4.54 | 119.30      | 126.22   |
| 15  | B     | 1230 | CLA  | C1C-C2C-C3C | -4.54 | 101.48      | 106.91   |
| 14  | B     | 4009 | BCR  | C7-C8-C9    | -4.54 | 119.30      | 126.22   |
| 15  | A     | 1119 | CLA  | C1C-C2C-C3C | -4.53 | 101.49      | 106.91   |
| 15  | B     | 1214 | CLA  | C1C-C2C-C3C | -4.53 | 101.49      | 106.91   |
| 15  | A     | 1102 | CLA  | C1C-C2C-C3C | -4.52 | 101.50      | 106.91   |
| 15  | B     | 1223 | CLA  | C1C-C2C-C3C | -4.52 | 101.50      | 106.91   |
| 15  | A     | 1112 | CLA  | C1C-C2C-C3C | -4.51 | 101.51      | 106.91   |
| 15  | K     | 1401 | CLA  | C1C-C2C-C3C | -4.50 | 101.52      | 106.91   |
| 15  | A     | 1127 | CLA  | O2A-CGA-O1A | -4.50 | 111.88      | 123.49   |
| 15  | A     | 1134 | CLA  | C1C-C2C-C3C | -4.50 | 101.53      | 106.91   |
| 15  | B     | 1224 | CLA  | O2A-CGA-O1A | -4.49 | 111.89      | 123.49   |
| 15  | J     | 1303 | CLA  | C1C-C2C-C3C | -4.49 | 101.53      | 106.91   |
| 15  | B     | 1237 | CLA  | O2A-CGA-O1A | -4.49 | 111.89      | 123.49   |
| 15  | A     | 1123 | CLA  | C1C-C2C-C3C | -4.49 | 101.53      | 106.91   |
| 15  | A     | 1117 | CLA  | O2A-CGA-O1A | -4.48 | 111.92      | 123.49   |
| 15  | A     | 1012 | CLA  | C1C-C2C-C3C | -4.47 | 101.56      | 106.91   |
| 15  | B     | 1223 | CLA  | O2A-CGA-O1A | -4.46 | 111.98      | 123.49   |
| 15  | B     | 1240 | CLA  | C1C-C2C-C3C | -4.46 | 101.58      | 106.91   |
| 15  | A     | 1125 | CLA  | O2A-CGA-O1A | -4.46 | 111.99      | 123.49   |
| 14  | F     | 4015 | BCR  | C24-C23-C22 | -4.46 | 119.42      | 126.22   |
| 15  | A     | 1130 | CLA  | C1C-C2C-C3C | -4.46 | 101.58      | 106.91   |
| 14  | A     | 4008 | BCR  | C24-C23-C22 | -4.45 | 119.43      | 126.22   |
| 14  | A     | 4001 | BCR  | C38-C26-C25 | -4.45 | 120.24      | 124.61   |
| 15  | B     | 1023 | CLA  | C1C-C2C-C3C | -4.44 | 101.60      | 106.91   |
| 15  | B     | 1211 | CLA  | C1C-C2C-C3C | -4.44 | 101.60      | 106.91   |
| 14  | B     | 4014 | BCR  | C24-C23-C22 | -4.43 | 119.46      | 126.22   |
| 15  | A     | 1122 | CLA  | C1C-C2C-C3C | -4.43 | 101.61      | 106.91   |
| 15  | B     | 1220 | CLA  | C1C-C2C-C3C | -4.42 | 101.62      | 106.91   |
| 14  | B     | 4011 | BCR  | C24-C23-C22 | -4.41 | 119.49      | 126.22   |
| 14  | A     | 4007 | BCR  | C38-C26-C25 | -4.41 | 120.28      | 124.61   |
| 15  | A     | 1132 | CLA  | C1C-C2C-C3C | -4.40 | 101.64      | 106.91   |
| 15  | A     | 1140 | CLA  | C1C-C2C-C3C | -4.40 | 101.64      | 106.91   |
| 15  | A     | 1103 | CLA  | C1C-C2C-C3C | -4.40 | 101.65      | 106.91   |
| 15  | A     | 1117 | CLA  | C1C-C2C-C3C | -4.39 | 101.65      | 106.91   |
| 15  | B     | 1225 | CLA  | O2A-CGA-O1A | -4.39 | 112.16      | 123.49   |
| 14  | A     | 4012 | BCR  | C24-C23-C22 | -4.39 | 119.53      | 126.22   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | B     | 4006 | BCR  | C33-C5-C6   | -4.37 | 120.32      | 124.61   |
| 15  | A     | 1126 | CLA  | O2A-CGA-O1A | -4.37 | 112.22      | 123.49   |
| 15  | B     | 1229 | CLA  | O2A-CGA-O1A | -4.36 | 112.25      | 123.49   |
| 15  | A     | 1106 | CLA  | O2A-CGA-O1A | -4.35 | 112.27      | 123.49   |
| 15  | B     | 1203 | CLA  | O2A-CGA-O1A | -4.32 | 112.33      | 123.49   |
| 15  | A     | 1101 | CLA  | C1C-C2C-C3C | -4.31 | 101.76      | 106.91   |
| 15  | B     | 1213 | CLA  | O2A-CGA-O1A | -4.30 | 112.39      | 123.49   |
| 15  | B     | 1228 | CLA  | C1C-C2C-C3C | -4.29 | 101.77      | 106.91   |
| 15  | A     | 1022 | CLA  | C3B-CAB-CBB | -4.29 | 117.54      | 126.32   |
| 15  | B     | 1222 | CLA  | O2A-CGA-O1A | -4.28 | 112.44      | 123.49   |
| 15  | A     | 1022 | CLA  | OBD-CAD-CBD | -4.28 | 119.48      | 125.94   |
| 15  | B     | 1216 | CLA  | O2A-CGA-O1A | -4.27 | 112.48      | 123.49   |
| 15  | A     | 1122 | CLA  | C4-C3-C2    | -4.26 | 115.15      | 123.50   |
| 15  | A     | 1138 | CLA  | O2A-CGA-O1A | -4.25 | 112.52      | 123.49   |
| 15  | A     | 1126 | CLA  | C1C-C2C-C3C | -4.24 | 101.83      | 106.91   |
| 15  | A     | 1111 | CLA  | C1C-C2C-C3C | -4.23 | 101.85      | 106.91   |
| 15  | A     | 1115 | CLA  | C1C-C2C-C3C | -4.21 | 101.88      | 106.91   |
| 15  | F     | 1139 | CLA  | O2A-CGA-O1A | -4.20 | 112.64      | 123.49   |
| 15  | B     | 1204 | CLA  | C3B-CAB-CBB | -4.20 | 117.72      | 126.32   |
| 15  | A     | 1132 | CLA  | C3B-CAB-CBB | -4.18 | 117.76      | 126.32   |
| 15  | A     | 1107 | CLA  | C1C-C2C-C3C | -4.18 | 101.91      | 106.91   |
| 15  | A     | 1101 | CLA  | O2A-CGA-O1A | -4.18 | 112.72      | 123.49   |
| 14  | A     | 4003 | BCR  | C24-C23-C22 | -4.13 | 119.92      | 126.22   |
| 15  | B     | 1210 | CLA  | C1C-C2C-C3C | -4.12 | 101.98      | 106.91   |
| 14  | F     | 4015 | BCR  | C7-C8-C9    | -4.09 | 119.97      | 126.22   |
| 14  | B     | 4017 | BCR  | C7-C8-C9    | -4.08 | 119.99      | 126.22   |
| 15  | A     | 1103 | CLA  | O2A-CGA-O1A | -4.07 | 112.98      | 123.49   |
| 15  | A     | 1125 | CLA  | C1C-C2C-C3C | -4.04 | 102.07      | 106.91   |
| 15  | A     | 1125 | CLA  | OBD-CAD-C3D | -4.02 | 120.16      | 128.35   |
| 15  | A     | 1012 | CLA  | OBD-CAD-CBD | -3.98 | 119.93      | 125.94   |
| 14  | F     | 4015 | BCR  | C15-C14-C13 | -3.98 | 121.45      | 127.20   |
| 14  | B     | 4011 | BCR  | C7-C8-C9    | -3.98 | 120.15      | 126.22   |
| 15  | A     | 1138 | CLA  | C1C-C2C-C3C | -3.97 | 102.16      | 106.91   |
| 15  | F     | 1410 | CLA  | C4-C3-C2    | -3.97 | 115.71      | 123.50   |
| 15  | A     | 1124 | CLA  | O2A-CGA-O1A | -3.96 | 113.26      | 123.49   |
| 15  | B     | 1222 | CLA  | O1D-CGD-CBD | -3.90 | 119.04      | 124.62   |
| 15  | B     | 1239 | CLA  | O2A-CGA-O1A | -3.88 | 110.21      | 123.02   |
| 14  | F     | 4015 | BCR  | C38-C26-C25 | -3.88 | 120.80      | 124.61   |
| 14  | B     | 4005 | BCR  | C38-C26-C25 | -3.88 | 120.80      | 124.61   |
| 15  | A     | 1116 | CLA  | C3B-CAB-CBB | -3.88 | 118.39      | 126.32   |
| 15  | B     | 1205 | CLA  | O1D-CGD-CBD | -3.87 | 119.08      | 124.62   |
| 14  | A     | 4002 | BCR  | C38-C26-C25 | -3.87 | 120.81      | 124.61   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15  | A     | 1121 | CLA  | O2A-CGA-O1A | -3.84 | 110.35      | 123.02   |
| 14  | B     | 4017 | BCR  | C3-C4-C5    | -3.84 | 107.77      | 113.87   |
| 14  | A     | 4008 | BCR  | C27-C26-C25 | -3.84 | 117.89      | 122.78   |
| 15  | B     | 1237 | CLA  | C4-C3-C2    | -3.83 | 115.98      | 123.50   |
| 14  | B     | 4009 | BCR  | C38-C26-C25 | -3.83 | 120.85      | 124.61   |
| 15  | B     | 1230 | CLA  | C4-C3-C2    | -3.81 | 116.03      | 123.50   |
| 14  | A     | 4001 | BCR  | C24-C23-C22 | -3.80 | 120.42      | 126.22   |
| 15  | B     | 1224 | CLA  | C3B-CAB-CBB | -3.80 | 118.55      | 126.32   |
| 14  | B     | 4006 | BCR  | C34-C9-C10  | -3.79 | 117.30      | 122.90   |
| 14  | A     | 4007 | BCR  | C33-C5-C6   | -3.79 | 120.89      | 124.61   |
| 14  | A     | 4012 | BCR  | C37-C22-C21 | -3.78 | 117.31      | 122.90   |
| 14  | A     | 4003 | BCR  | C34-C9-C10  | -3.78 | 117.32      | 122.90   |
| 15  | B     | 1204 | CLA  | O2A-CGA-O1A | -3.71 | 110.77      | 123.02   |
| 15  | B     | 1226 | CLA  | O1D-CGD-CBD | -3.70 | 119.32      | 124.62   |
| 14  | A     | 4008 | BCR  | C7-C8-C9    | -3.70 | 120.58      | 126.22   |
| 15  | A     | 1022 | CLA  | OBD-CAD-C3D | -3.69 | 120.81      | 128.35   |
| 15  | A     | 1012 | CLA  | C3B-CAB-CBB | -3.68 | 118.78      | 126.32   |
| 15  | A     | 1106 | CLA  | O1D-CGD-CBD | -3.68 | 119.35      | 124.62   |
| 15  | J     | 1303 | CLA  | O2A-CGA-O1A | -3.67 | 110.91      | 123.02   |
| 15  | A     | 1115 | CLA  | O2A-CGA-O1A | -3.67 | 110.93      | 123.02   |
| 14  | B     | 4005 | BCR  | C7-C8-C9    | -3.66 | 120.64      | 126.22   |
| 14  | B     | 4014 | BCR  | C37-C22-C21 | -3.65 | 117.51      | 122.90   |
| 15  | B     | 1201 | CLA  | O2A-CGA-O1A | -3.65 | 110.99      | 123.02   |
| 15  | A     | 1133 | CLA  | O2A-CGA-O1A | -3.65 | 110.99      | 123.02   |
| 15  | K     | 1401 | CLA  | O2A-CGA-O1A | -3.64 | 111.03      | 123.02   |
| 14  | B     | 4011 | BCR  | C37-C22-C21 | -3.64 | 117.53      | 122.90   |
| 15  | B     | 1211 | CLA  | O2A-CGA-O1A | -3.63 | 111.04      | 123.02   |
| 15  | B     | 1207 | CLA  | O2A-CGA-O1A | -3.63 | 111.06      | 123.02   |
| 15  | A     | 1118 | CLA  | O2A-CGA-O1A | -3.62 | 111.07      | 123.02   |
| 14  | B     | 4005 | BCR  | C24-C23-C22 | -3.62 | 120.70      | 126.22   |
| 15  | A     | 1124 | CLA  | C3B-CAB-CBB | -3.62 | 118.92      | 126.32   |
| 14  | A     | 4001 | BCR  | C36-C18-C17 | -3.62 | 117.56      | 122.90   |
| 14  | F     | 4016 | BCR  | C3-C4-C5    | -3.61 | 108.14      | 113.87   |
| 15  | A     | 1126 | CLA  | C3B-CAB-CBB | -3.60 | 118.95      | 126.32   |
| 15  | A     | 1129 | CLA  | O2A-CGA-O1A | -3.60 | 111.15      | 123.02   |
| 15  | B     | 1201 | CLA  | O1D-CGD-CBD | -3.59 | 119.48      | 124.62   |
| 15  | K     | 1402 | CLA  | O2A-CGA-O1A | -3.59 | 111.19      | 123.02   |
| 14  | B     | 4004 | BCR  | C36-C18-C17 | -3.58 | 117.62      | 122.90   |
| 14  | J     | 4013 | BCR  | C38-C26-C25 | -3.54 | 121.13      | 124.61   |
| 14  | B     | 4009 | BCR  | C34-C9-C10  | -3.52 | 117.69      | 122.90   |
| 15  | B     | 1202 | CLA  | C3B-CAB-CBB | -3.50 | 119.17      | 126.32   |
| 15  | B     | 1217 | CLA  | C3B-CAB-CBB | -3.49 | 119.17      | 126.32   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15  | B     | 1216 | CLA  | C3B-CAB-CBB | -3.48 | 119.19      | 126.32   |
| 15  | A     | 1135 | CLA  | C4-C3-C2    | -3.48 | 116.68      | 123.50   |
| 14  | A     | 4001 | BCR  | C37-C22-C21 | -3.48 | 117.77      | 122.90   |
| 15  | B     | 1215 | CLA  | C4-C3-C2    | -3.46 | 116.70      | 123.50   |
| 15  | K     | 1401 | CLA  | C3B-CAB-CBB | -3.46 | 119.24      | 126.32   |
| 15  | A     | 1128 | CLA  | O1D-CGD-CBD | -3.45 | 119.67      | 124.62   |
| 15  | B     | 1206 | CLA  | O2A-CGA-O1A | -3.45 | 111.66      | 123.02   |
| 15  | A     | 1134 | CLA  | O2A-CGA-O1A | -3.44 | 111.68      | 123.02   |
| 15  | A     | 1117 | CLA  | C3B-CAB-CBB | -3.43 | 119.29      | 126.32   |
| 12  | B     | 5004 | LHG  | C5-O7-C7    | -3.43 | 109.66      | 117.89   |
| 14  | A     | 4003 | BCR  | C37-C22-C21 | -3.42 | 117.85      | 122.90   |
| 15  | A     | 1110 | CLA  | C3B-CAB-CBB | -3.42 | 119.33      | 126.32   |
| 15  | F     | 1410 | CLA  | C3B-CAB-CBB | -3.40 | 119.36      | 126.32   |
| 15  | B     | 1205 | CLA  | C3B-CAB-CBB | -3.40 | 119.37      | 126.32   |
| 15  | A     | 1131 | CLA  | O1D-CGD-CBD | -3.39 | 119.76      | 124.62   |
| 14  | B     | 4009 | BCR  | C3-C4-C5    | -3.38 | 108.50      | 113.87   |
| 15  | A     | 1132 | CLA  | O1D-CGD-CBD | -3.38 | 119.78      | 124.62   |
| 14  | A     | 4012 | BCR  | C36-C18-C17 | -3.37 | 117.92      | 122.90   |
| 14  | B     | 4005 | BCR  | C36-C18-C17 | -3.37 | 117.92      | 122.90   |
| 14  | F     | 4016 | BCR  | C35-C13-C14 | -3.33 | 117.98      | 122.90   |
| 14  | A     | 4001 | BCR  | C3-C4-C5    | -3.33 | 108.58      | 113.87   |
| 15  | K     | 1402 | CLA  | C3B-CAB-CBB | -3.32 | 119.53      | 126.32   |
| 14  | B     | 4009 | BCR  | C36-C18-C17 | -3.31 | 118.02      | 122.90   |
| 14  | A     | 4007 | BCR  | C3-C4-C5    | -3.30 | 108.62      | 113.87   |
| 14  | A     | 4008 | BCR  | C38-C26-C25 | -3.28 | 121.38      | 124.61   |
| 15  | A     | 1126 | CLA  | O1D-CGD-CBD | -3.28 | 119.92      | 124.62   |
| 15  | B     | 1234 | CLA  | C3B-CAB-CBB | -3.28 | 119.62      | 126.32   |
| 14  | B     | 4004 | BCR  | C37-C22-C21 | -3.26 | 118.08      | 122.90   |
| 12  | A     | 5003 | LHG  | C5-O7-C7    | -3.25 | 110.09      | 117.89   |
| 15  | A     | 1101 | CLA  | O1D-CGD-CBD | -3.25 | 119.97      | 124.62   |
| 14  | B     | 4010 | BCR  | C3-C4-C5    | -3.24 | 108.73      | 113.87   |
| 14  | A     | 4001 | BCR  | C34-C9-C10  | -3.24 | 118.12      | 122.90   |
| 15  | A     | 1801 | CLA  | C3B-CAB-CBB | -3.23 | 119.71      | 126.32   |
| 14  | B     | 4017 | BCR  | C34-C9-C10  | -3.23 | 118.14      | 122.90   |
| 15  | B     | 1212 | CLA  | O1D-CGD-CBD | -3.22 | 120.00      | 124.62   |
| 15  | A     | 1125 | CLA  | C3B-CAB-CBB | -3.21 | 119.75      | 126.32   |
| 15  | B     | 1229 | CLA  | C3B-CAB-CBB | -3.20 | 119.77      | 126.32   |
| 14  | B     | 4005 | BCR  | C37-C22-C21 | -3.20 | 118.18      | 122.90   |
| 14  | B     | 4010 | BCR  | C24-C23-C22 | -3.20 | 121.34      | 126.22   |
| 14  | A     | 4012 | BCR  | C7-C8-C9    | -3.18 | 121.36      | 126.22   |
| 15  | A     | 1123 | CLA  | C3B-CAB-CBB | -3.18 | 119.81      | 126.32   |
| 14  | B     | 4017 | BCR  | C36-C18-C17 | -3.17 | 118.21      | 122.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15  | B     | 1240 | CLA  | C3B-CAB-CBB | -3.17 | 119.83      | 126.32   |
| 14  | J     | 4013 | BCR  | C33-C5-C6   | -3.17 | 121.50      | 124.61   |
| 15  | A     | 1125 | CLA  | O1D-CGD-CBD | -3.17 | 120.08      | 124.62   |
| 15  | B     | 1221 | CLA  | C4-C3-C2    | -3.16 | 117.31      | 123.50   |
| 15  | B     | 1218 | CLA  | C4-C3-C2    | -3.16 | 117.31      | 123.50   |
| 14  | J     | 4013 | BCR  | C30-C25-C26 | -3.15 | 118.03      | 122.66   |
| 15  | A     | 1106 | CLA  | C3B-CAB-CBB | -3.15 | 119.88      | 126.32   |
| 14  | B     | 4006 | BCR  | C7-C8-C9    | -3.14 | 121.44      | 126.22   |
| 15  | A     | 1116 | CLA  | O1D-CGD-CBD | -3.13 | 120.13      | 124.62   |
| 15  | F     | 1410 | CLA  | O1D-CGD-CBD | -3.13 | 120.13      | 124.62   |
| 14  | A     | 4002 | BCR  | C36-C18-C17 | -3.13 | 118.28      | 122.90   |
| 14  | A     | 4002 | BCR  | C34-C9-C10  | -3.13 | 118.28      | 122.90   |
| 15  | A     | 1112 | CLA  | O1D-CGD-CBD | -3.12 | 120.15      | 124.62   |
| 14  | B     | 4006 | BCR  | C36-C18-C17 | -3.12 | 118.29      | 122.90   |
| 14  | A     | 4002 | BCR  | C27-C26-C25 | -3.12 | 118.81      | 122.78   |
| 15  | B     | 1219 | CLA  | C4-C3-C2    | -3.12 | 117.38      | 123.50   |
| 15  | B     | 1227 | CLA  | O1D-CGD-CBD | -3.11 | 120.16      | 124.62   |
| 14  | A     | 4007 | BCR  | C24-C23-C22 | -3.11 | 121.47      | 126.22   |
| 14  | B     | 4011 | BCR  | C28-C27-C26 | -3.10 | 108.94      | 113.87   |
| 14  | J     | 4013 | BCR  | C4-C5-C6    | -3.10 | 118.83      | 122.78   |
| 15  | A     | 1137 | CLA  | O1D-CGD-CBD | -3.10 | 120.18      | 124.62   |
| 15  | B     | 1214 | CLA  | O1D-CGD-CBD | -3.10 | 120.18      | 124.62   |
| 15  | B     | 1211 | CLA  | O1D-CGD-CBD | -3.10 | 120.18      | 124.62   |
| 14  | B     | 4006 | BCR  | C3-C4-C5    | -3.09 | 108.96      | 113.87   |
| 15  | B     | 1209 | CLA  | C3B-CAB-CBB | -3.09 | 120.00      | 126.32   |
| 15  | A     | 1130 | CLA  | O1D-CGD-CBD | -3.08 | 120.20      | 124.62   |
| 15  | A     | 1123 | CLA  | O1D-CGD-CBD | -3.07 | 120.22      | 124.62   |
| 15  | B     | 1225 | CLA  | C3B-CAB-CBB | -3.06 | 120.06      | 126.32   |
| 15  | B     | 1234 | CLA  | C4-C3-C2    | -3.05 | 117.50      | 123.50   |
| 15  | B     | 1230 | CLA  | O1D-CGD-CBD | -3.05 | 120.25      | 124.62   |
| 14  | A     | 4002 | BCR  | C7-C8-C9    | -3.04 | 121.58      | 126.22   |
| 15  | B     | 1231 | CLA  | C4-C3-C2    | -3.04 | 117.53      | 123.50   |
| 15  | A     | 1123 | CLA  | O2D-CGD-O1D | -3.04 | 117.52      | 123.79   |
| 15  | A     | 1103 | CLA  | C3B-CAB-CBB | -3.03 | 120.11      | 126.32   |
| 15  | B     | 1217 | CLA  | O1D-CGD-CBD | -3.03 | 120.28      | 124.62   |
| 15  | A     | 1107 | CLA  | CAA-C2A-C1A | -3.03 | 101.78      | 112.47   |
| 15  | B     | 1223 | CLA  | C3B-CAB-CBB | -3.02 | 120.13      | 126.32   |
| 14  | B     | 4017 | BCR  | C27-C26-C25 | -3.01 | 118.95      | 122.78   |
| 15  | B     | 1226 | CLA  | O2D-CGD-O1D | -3.00 | 117.59      | 123.79   |
| 15  | B     | 1222 | CLA  | O2D-CGD-O1D | -3.00 | 117.60      | 123.79   |
| 14  | A     | 4002 | BCR  | C3-C4-C5    | -2.99 | 109.13      | 113.87   |
| 15  | A     | 1105 | CLA  | O1D-CGD-CBD | -2.98 | 120.35      | 124.62   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15  | A     | 1012 | CLA  | OBD-CAD-C3D | -2.97 | 122.29      | 128.35   |
| 15  | A     | 1138 | CLA  | C3B-CAB-CBB | -2.97 | 120.24      | 126.32   |
| 15  | B     | 1206 | CLA  | C3B-CAB-CBB | -2.97 | 120.25      | 126.32   |
| 15  | B     | 1207 | CLA  | C3B-CAB-CBB | -2.96 | 120.26      | 126.32   |
| 15  | A     | 1102 | CLA  | O1D-CGD-CBD | -2.95 | 120.39      | 124.62   |
| 14  | B     | 4010 | BCR  | C36-C18-C17 | -2.94 | 118.56      | 122.90   |
| 14  | A     | 4008 | BCR  | C30-C25-C26 | -2.94 | 118.34      | 122.66   |
| 14  | B     | 4005 | BCR  | C3-C4-C5    | -2.94 | 109.20      | 113.87   |
| 15  | B     | 1205 | CLA  | O2D-CGD-O1D | -2.93 | 117.74      | 123.79   |
| 15  | A     | 1136 | CLA  | O1D-CGD-CBD | -2.92 | 120.43      | 124.62   |
| 14  | B     | 4004 | BCR  | C7-C8-C9    | -2.92 | 121.77      | 126.22   |
| 14  | J     | 4013 | BCR  | C36-C18-C17 | -2.91 | 118.61      | 122.90   |
| 15  | B     | 1234 | CLA  | O1D-CGD-CBD | -2.91 | 120.46      | 124.62   |
| 14  | A     | 4008 | BCR  | C3-C4-C5    | -2.89 | 109.28      | 113.87   |
| 15  | B     | 1202 | CLA  | O2D-CGD-O1D | -2.89 | 117.82      | 123.79   |
| 15  | B     | 1218 | CLA  | O1D-CGD-CBD | -2.89 | 120.49      | 124.62   |
| 14  | A     | 4003 | BCR  | C36-C18-C17 | -2.89 | 118.64      | 122.90   |
| 14  | B     | 4009 | BCR  | C37-C22-C21 | -2.88 | 118.64      | 122.90   |
| 14  | A     | 4003 | BCR  | C3-C4-C5    | -2.88 | 109.29      | 113.87   |
| 15  | A     | 1101 | CLA  | C4-C3-C2    | -2.88 | 117.84      | 123.50   |
| 15  | B     | 1239 | CLA  | O1D-CGD-CBD | -2.88 | 120.49      | 124.62   |
| 15  | B     | 1225 | CLA  | C5-C3-C2    | -2.88 | 115.59      | 121.05   |
| 15  | A     | 1107 | CLA  | O1D-CGD-CBD | -2.88 | 120.50      | 124.62   |
| 15  | B     | 1221 | CLA  | O2D-CGD-O1D | -2.87 | 117.86      | 123.79   |
| 14  | A     | 4012 | BCR  | C3-C4-C5    | -2.87 | 109.31      | 113.87   |
| 15  | B     | 1235 | CLA  | O1D-CGD-CBD | -2.87 | 120.51      | 124.62   |
| 13  | A     | 1011 | CL0  | O1D-CGD-CBD | -2.87 | 120.51      | 124.62   |
| 15  | A     | 1128 | CLA  | O2D-CGD-O1D | -2.87 | 117.87      | 123.79   |
| 15  | A     | 1126 | CLA  | CMD-C2D-C3D | -2.85 | 119.51      | 125.09   |
| 14  | J     | 4013 | BCR  | C15-C14-C13 | -2.85 | 123.08      | 127.20   |
| 15  | B     | 1224 | CLA  | O1D-CGD-CBD | -2.85 | 120.54      | 124.62   |
| 15  | A     | 1114 | CLA  | O1D-CGD-CBD | -2.85 | 120.54      | 124.62   |
| 15  | A     | 1136 | CLA  | C3B-CAB-CBB | -2.84 | 120.50      | 126.32   |
| 15  | A     | 1101 | CLA  | O2D-CGD-O1D | -2.84 | 117.93      | 123.79   |
| 15  | B     | 1209 | CLA  | O1D-CGD-CBD | -2.84 | 120.55      | 124.62   |
| 15  | A     | 1106 | CLA  | O2D-CGD-O1D | -2.83 | 117.94      | 123.79   |
| 14  | A     | 4001 | BCR  | C30-C25-C26 | -2.83 | 118.50      | 122.66   |
| 15  | A     | 1134 | CLA  | C3B-CAB-CBB | -2.83 | 120.53      | 126.32   |
| 14  | B     | 4017 | BCR  | C38-C26-C25 | -2.83 | 121.83      | 124.61   |
| 15  | A     | 1125 | CLA  | O2D-CGD-O1D | -2.82 | 117.97      | 123.79   |
| 15  | A     | 1118 | CLA  | O1D-CGD-CBD | -2.82 | 120.58      | 124.62   |
| 15  | B     | 1238 | CLA  | O1D-CGD-CBD | -2.81 | 120.59      | 124.62   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15  | B     | 1221 | CLA  | O1D-CGD-CBD | -2.81 | 120.59      | 124.62   |
| 15  | B     | 1236 | CLA  | O1D-CGD-CBD | -2.81 | 120.60      | 124.62   |
| 15  | B     | 1219 | CLA  | O1D-CGD-CBD | -2.81 | 120.60      | 124.62   |
| 14  | J     | 4013 | BCR  | C27-C26-C25 | -2.80 | 119.21      | 122.78   |
| 15  | A     | 1111 | CLA  | C3B-CAB-CBB | -2.80 | 120.58      | 126.32   |
| 15  | A     | 1140 | CLA  | O1D-CGD-CBD | -2.80 | 120.61      | 124.62   |
| 15  | A     | 1107 | CLA  | C1-C2-C3    | -2.80 | 122.13      | 126.71   |
| 15  | A     | 1111 | CLA  | O1D-CGD-CBD | -2.80 | 120.61      | 124.62   |
| 12  | A     | 5001 | LHG  | C5-O7-C7    | -2.78 | 111.23      | 117.89   |
| 15  | A     | 1119 | CLA  | C3B-CAB-CBB | -2.77 | 120.64      | 126.32   |
| 15  | B     | 1204 | CLA  | O1D-CGD-CBD | -2.77 | 120.65      | 124.62   |
| 15  | B     | 1237 | CLA  | C3B-CAB-CBB | -2.77 | 120.65      | 126.32   |
| 15  | B     | 1215 | CLA  | O1D-CGD-CBD | -2.77 | 120.65      | 124.62   |
| 14  | J     | 4013 | BCR  | C37-C22-C21 | -2.77 | 118.81      | 122.90   |
| 15  | A     | 1109 | CLA  | C4-C3-C2    | -2.76 | 118.07      | 123.50   |
| 14  | B     | 4011 | BCR  | C3-C4-C5    | -2.76 | 109.49      | 113.87   |
| 15  | A     | 1104 | CLA  | O1D-CGD-CBD | -2.76 | 120.67      | 124.62   |
| 13  | A     | 1011 | CL0  | O2D-CGD-O1D | -2.75 | 118.10      | 123.79   |
| 15  | F     | 1301 | CLA  | O1D-CGD-CBD | -2.75 | 120.68      | 124.62   |
| 14  | B     | 4009 | BCR  | C27-C26-C25 | -2.75 | 119.28      | 122.78   |
| 14  | F     | 4016 | BCR  | C36-C18-C17 | -2.75 | 118.84      | 122.90   |
| 15  | B     | 1213 | CLA  | O1D-CGD-CBD | -2.74 | 120.70      | 124.62   |
| 15  | A     | 1012 | CLA  | O1D-CGD-CBD | -2.73 | 120.70      | 124.62   |
| 15  | B     | 1223 | CLA  | OBD-CAD-C3D | -2.73 | 122.78      | 128.35   |
| 15  | A     | 1112 | CLA  | C3B-CAB-CBB | -2.72 | 120.74      | 126.32   |
| 15  | F     | 1139 | CLA  | C4-C3-C2    | -2.72 | 118.16      | 123.50   |
| 15  | B     | 1227 | CLA  | O2D-CGD-O1D | -2.72 | 118.17      | 123.79   |
| 15  | B     | 1224 | CLA  | O2D-CGD-O1D | -2.72 | 118.17      | 123.79   |
| 14  | A     | 4012 | BCR  | C34-C9-C10  | -2.72 | 118.89      | 122.90   |
| 15  | B     | 1232 | CLA  | C3B-CAB-CBB | -2.72 | 120.76      | 126.32   |
| 15  | J     | 1303 | CLA  | O1D-CGD-CBD | -2.71 | 120.73      | 124.62   |
| 15  | A     | 1133 | CLA  | O1D-CGD-CBD | -2.71 | 120.74      | 124.62   |
| 15  | A     | 1115 | CLA  | O1D-CGD-CBD | -2.71 | 120.74      | 124.62   |
| 15  | K     | 1401 | CLA  | O1D-CGD-CBD | -2.70 | 120.75      | 124.62   |
| 14  | J     | 4013 | BCR  | C34-C9-C10  | -2.70 | 118.92      | 122.90   |
| 15  | A     | 1801 | CLA  | C6-C5-C3    | -2.69 | 109.94      | 114.43   |
| 15  | A     | 1109 | CLA  | C3B-CAB-CBB | -2.69 | 120.82      | 126.32   |
| 15  | B     | 1229 | CLA  | O1D-CGD-CBD | -2.68 | 120.78      | 124.62   |
| 15  | B     | 1211 | CLA  | O2D-CGD-O1D | -2.68 | 118.26      | 123.79   |
| 15  | B     | 1223 | CLA  | O1D-CGD-CBD | -2.67 | 120.79      | 124.62   |
| 13  | A     | 1011 | CL0  | C3B-CAB-CBB | -2.67 | 120.85      | 126.32   |
| 15  | A     | 1121 | CLA  | O1D-CGD-CBD | -2.67 | 120.79      | 124.62   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | F     | 4016 | BCR  | C8-C7-C6    | -2.67 | 119.29      | 127.32   |
| 15  | A     | 1102 | CLA  | O2D-CGD-O1D | -2.67 | 118.28      | 123.79   |
| 15  | B     | 1207 | CLA  | O1D-CGD-CBD | -2.66 | 120.80      | 124.62   |
| 15  | A     | 1121 | CLA  | C3B-CAB-CBB | -2.65 | 120.91      | 126.32   |
| 14  | B     | 4010 | BCR  | C34-C9-C10  | -2.64 | 119.01      | 122.90   |
| 15  | B     | 1201 | CLA  | O2D-CGD-O1D | -2.64 | 118.35      | 123.79   |
| 15  | B     | 1203 | CLA  | C3B-CAB-CBB | -2.63 | 120.93      | 126.32   |
| 14  | F     | 4016 | BCR  | C23-C24-C25 | -2.63 | 119.43      | 127.32   |
| 15  | B     | 1215 | CLA  | C3B-CAB-CBB | -2.63 | 120.94      | 126.32   |
| 14  | B     | 4014 | BCR  | C15-C14-C13 | -2.63 | 123.40      | 127.20   |
| 14  | A     | 4007 | BCR  | C28-C27-C26 | -2.62 | 109.71      | 113.87   |
| 14  | B     | 4017 | BCR  | C37-C22-C21 | -2.62 | 119.03      | 122.90   |
| 14  | A     | 4007 | BCR  | C27-C26-C25 | -2.61 | 119.46      | 122.78   |
| 14  | A     | 4007 | BCR  | C7-C8-C9    | -2.60 | 122.25      | 126.22   |
| 14  | F     | 4016 | BCR  | C34-C9-C10  | -2.60 | 119.06      | 122.90   |
| 15  | A     | 1119 | CLA  | O1D-CGD-CBD | -2.60 | 120.90      | 124.62   |
| 15  | A     | 1138 | CLA  | O1D-CGD-CBD | -2.59 | 120.91      | 124.62   |
| 14  | B     | 4006 | BCR  | C24-C23-C22 | -2.59 | 122.27      | 126.22   |
| 14  | B     | 4004 | BCR  | C34-C9-C10  | -2.59 | 119.08      | 122.90   |
| 15  | A     | 1801 | CLA  | C4-C3-C2    | -2.59 | 118.42      | 123.50   |
| 15  | A     | 1135 | CLA  | O1D-CGD-CBD | -2.59 | 120.92      | 124.62   |
| 15  | B     | 1214 | CLA  | C3B-CAB-CBB | -2.58 | 121.03      | 126.32   |
| 15  | B     | 1209 | CLA  | O2D-CGD-O1D | -2.58 | 118.47      | 123.79   |
| 15  | A     | 1129 | CLA  | OBD-CAD-C3D | -2.58 | 123.10      | 128.35   |
| 15  | B     | 1225 | CLA  | O1D-CGD-CBD | -2.57 | 120.93      | 124.62   |
| 15  | B     | 1231 | CLA  | O1D-CGD-CBD | -2.57 | 120.93      | 124.62   |
| 15  | A     | 1117 | CLA  | O1D-CGD-CBD | -2.57 | 120.94      | 124.62   |
| 15  | A     | 1129 | CLA  | O1D-CGD-CBD | -2.57 | 120.94      | 124.62   |
| 15  | B     | 1223 | CLA  | O2D-CGD-O1D | -2.57 | 118.49      | 123.79   |
| 15  | A     | 1103 | CLA  | O2D-CGD-O1D | -2.56 | 118.50      | 123.79   |
| 15  | A     | 1124 | CLA  | O1D-CGD-CBD | -2.56 | 120.95      | 124.62   |
| 14  | A     | 4008 | BCR  | C15-C14-C13 | -2.56 | 123.50      | 127.20   |
| 15  | A     | 1118 | CLA  | C3B-CAB-CBB | -2.56 | 121.09      | 126.32   |
| 15  | A     | 1129 | CLA  | O2D-CGD-O1D | -2.55 | 118.52      | 123.79   |
| 15  | B     | 1235 | CLA  | O2D-CGD-O1D | -2.55 | 118.52      | 123.79   |
| 15  | B     | 1215 | CLA  | O2D-CGD-O1D | -2.55 | 118.52      | 123.79   |
| 15  | A     | 1137 | CLA  | O2D-CGD-O1D | -2.55 | 118.53      | 123.79   |
| 15  | B     | 1240 | CLA  | O1D-CGD-CBD | -2.55 | 120.97      | 124.62   |
| 15  | A     | 1131 | CLA  | O2D-CGD-O1D | -2.55 | 118.53      | 123.79   |
| 15  | B     | 1210 | CLA  | O1D-CGD-CBD | -2.54 | 120.98      | 124.62   |
| 15  | B     | 1212 | CLA  | O2D-CGD-O1D | -2.54 | 118.54      | 123.79   |
| 15  | B     | 1222 | CLA  | C3B-CAB-CBB | -2.54 | 121.12      | 126.32   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15  | B     | 1237 | CLA  | O1D-CGD-CBD | -2.54 | 120.98      | 124.62   |
| 12  | A     | 5005 | LHG  | C5-O7-C7    | -2.54 | 111.80      | 117.89   |
| 15  | B     | 1236 | CLA  | O2D-CGD-O1D | -2.54 | 118.55      | 123.79   |
| 15  | A     | 1122 | CLA  | O1D-CGD-CBD | -2.54 | 120.99      | 124.62   |
| 15  | B     | 1239 | CLA  | C3B-CAB-CBB | -2.53 | 121.13      | 126.32   |
| 15  | B     | 1217 | CLA  | O2D-CGD-O1D | -2.53 | 118.56      | 123.79   |
| 15  | B     | 1236 | CLA  | C1-C2-C3    | -2.53 | 122.56      | 126.71   |
| 15  | B     | 1216 | CLA  | O1D-CGD-CBD | -2.53 | 121.00      | 124.62   |
| 15  | A     | 1120 | CLA  | C3B-CAB-CBB | -2.53 | 121.15      | 126.32   |
| 15  | A     | 1022 | CLA  | O1D-CGD-CBD | -2.52 | 121.00      | 124.62   |
| 15  | B     | 1201 | CLA  | C3B-CAB-CBB | -2.52 | 121.16      | 126.32   |
| 15  | F     | 1301 | CLA  | C3B-CAB-CBB | -2.52 | 121.16      | 126.32   |
| 14  | A     | 4007 | BCR  | C23-C24-C25 | -2.52 | 119.75      | 127.32   |
| 15  | A     | 1113 | CLA  | O1D-CGD-CBD | -2.52 | 121.02      | 124.62   |
| 15  | B     | 1234 | CLA  | O2D-CGD-O1D | -2.51 | 118.60      | 123.79   |
| 15  | A     | 1127 | CLA  | OBD-CAD-C3D | -2.51 | 123.22      | 128.35   |
| 15  | A     | 1127 | CLA  | O1D-CGD-CBD | -2.51 | 121.02      | 124.62   |
| 15  | A     | 1118 | CLA  | O2D-CGD-O1D | -2.51 | 118.61      | 123.79   |
| 14  | A     | 4003 | BCR  | C28-C27-C26 | -2.51 | 109.89      | 113.87   |
| 14  | A     | 4003 | BCR  | C15-C14-C13 | -2.50 | 123.58      | 127.20   |
| 15  | A     | 1135 | CLA  | C3B-CAB-CBB | -2.50 | 121.21      | 126.32   |
| 14  | J     | 4013 | BCR  | C23-C24-C25 | -2.50 | 119.81      | 127.32   |
| 15  | A     | 1137 | CLA  | C3B-CAB-CBB | -2.50 | 121.21      | 126.32   |
| 15  | B     | 1236 | CLA  | C3B-CAB-CBB | -2.49 | 121.21      | 126.32   |
| 15  | B     | 1207 | CLA  | O2D-CGD-O1D | -2.49 | 118.64      | 123.79   |
| 14  | A     | 4002 | BCR  | C30-C25-C26 | -2.49 | 119.00      | 122.66   |
| 15  | A     | 1801 | CLA  | O2D-CGD-O1D | -2.49 | 118.65      | 123.79   |
| 15  | B     | 1220 | CLA  | O1D-CGD-CBD | -2.49 | 121.05      | 124.62   |
| 15  | A     | 1114 | CLA  | O2D-CGD-O1D | -2.48 | 118.66      | 123.79   |
| 14  | B     | 4011 | BCR  | C1-C6-C5    | -2.48 | 119.02      | 122.66   |
| 15  | A     | 1110 | CLA  | O2D-CGD-O1D | -2.48 | 118.67      | 123.79   |
| 15  | A     | 1105 | CLA  | O2D-CGD-O1D | -2.48 | 118.67      | 123.79   |
| 15  | A     | 1126 | CLA  | O2D-CGD-O1D | -2.48 | 118.68      | 123.79   |
| 14  | F     | 4015 | BCR  | C3-C4-C5    | -2.47 | 109.94      | 113.87   |
| 15  | A     | 1130 | CLA  | O2D-CGD-O1D | -2.47 | 118.69      | 123.79   |
| 15  | F     | 1139 | CLA  | O1D-CGD-CBD | -2.47 | 121.08      | 124.62   |
| 14  | F     | 4015 | BCR  | C27-C26-C25 | -2.46 | 119.64      | 122.78   |
| 15  | B     | 1206 | CLA  | O1D-CGD-CBD | -2.46 | 121.09      | 124.62   |
| 14  | A     | 4007 | BCR  | C34-C9-C10  | -2.46 | 119.27      | 122.90   |
| 14  | B     | 4010 | BCR  | C30-C25-C26 | -2.46 | 119.05      | 122.66   |
| 15  | B     | 1228 | CLA  | C3B-CAB-CBB | -2.46 | 121.28      | 126.32   |
| 15  | B     | 1203 | CLA  | O1D-CGD-CBD | -2.45 | 121.11      | 124.62   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15  | B     | 1208 | CLA  | O1D-CGD-CBD | -2.45 | 121.11      | 124.62   |
| 14  | B     | 4014 | BCR  | C34-C9-C10  | -2.45 | 119.29      | 122.90   |
| 15  | A     | 1132 | CLA  | O2D-CGD-O1D | -2.44 | 118.75      | 123.79   |
| 15  | B     | 1228 | CLA  | O1D-CGD-CBD | -2.44 | 121.13      | 124.62   |
| 15  | A     | 1022 | CLA  | O2D-CGD-O1D | -2.43 | 118.76      | 123.79   |
| 15  | B     | 1023 | CLA  | O2D-CGD-O1D | -2.43 | 118.76      | 123.79   |
| 15  | A     | 1114 | CLA  | C3B-CAB-CBB | -2.43 | 121.34      | 126.32   |
| 14  | A     | 4008 | BCR  | C23-C24-C25 | -2.43 | 120.02      | 127.32   |
| 15  | A     | 1127 | CLA  | C3B-CAB-CBB | -2.43 | 121.35      | 126.32   |
| 15  | B     | 1213 | CLA  | O2D-CGD-O1D | -2.42 | 118.79      | 123.79   |
| 15  | B     | 1211 | CLA  | C3B-CAB-CBB | -2.42 | 121.37      | 126.32   |
| 14  | A     | 4008 | BCR  | C28-C27-C26 | -2.41 | 110.04      | 113.87   |
| 15  | A     | 1012 | CLA  | O2D-CGD-O1D | -2.41 | 118.81      | 123.79   |
| 15  | B     | 1239 | CLA  | O2D-CGD-O1D | -2.41 | 118.81      | 123.79   |
| 15  | B     | 1229 | CLA  | C4-C3-C2    | -2.41 | 118.77      | 123.50   |
| 15  | A     | 1129 | CLA  | C3B-CAB-CBB | -2.40 | 121.41      | 126.32   |
| 15  | A     | 1140 | CLA  | O2D-CGD-O1D | -2.40 | 118.84      | 123.79   |
| 14  | F     | 4015 | BCR  | C36-C18-C17 | -2.40 | 119.36      | 122.90   |
| 15  | A     | 1116 | CLA  | O2D-CGD-O1D | -2.40 | 118.84      | 123.79   |
| 15  | B     | 1219 | CLA  | O2D-CGD-O1D | -2.40 | 118.84      | 123.79   |
| 15  | A     | 1136 | CLA  | O2D-CGD-O1D | -2.40 | 118.84      | 123.79   |
| 15  | A     | 1103 | CLA  | O1D-CGD-CBD | -2.39 | 121.19      | 124.62   |
| 15  | J     | 1302 | CLA  | O2D-CGD-O1D | -2.39 | 118.85      | 123.79   |
| 14  | B     | 4009 | BCR  | C30-C25-C26 | -2.39 | 119.16      | 122.66   |
| 14  | F     | 4016 | BCR  | C7-C6-C5    | -2.39 | 115.91      | 121.37   |
| 14  | B     | 4004 | BCR  | C1-C6-C5    | -2.38 | 119.16      | 122.66   |
| 15  | A     | 1125 | CLA  | CHD-C4C-C3C | -2.38 | 121.27      | 124.94   |
| 15  | A     | 1120 | CLA  | O1D-CGD-CBD | -2.37 | 121.22      | 124.62   |
| 14  | B     | 4017 | BCR  | C30-C25-C26 | -2.36 | 119.19      | 122.66   |
| 15  | B     | 1218 | CLA  | O2D-CGD-O1D | -2.36 | 118.91      | 123.79   |
| 14  | A     | 4001 | BCR  | C15-C14-C13 | -2.36 | 123.79      | 127.20   |
| 16  | B     | 1301 | LMU  | O1'-C1'-C2' | -2.36 | 105.06      | 108.04   |
| 15  | J     | 1302 | CLA  | O1D-CGD-CBD | -2.36 | 121.25      | 124.62   |
| 15  | F     | 1410 | CLA  | O2D-CGD-O1D | -2.35 | 118.93      | 123.79   |
| 14  | A     | 4007 | BCR  | C36-C18-C17 | -2.35 | 119.43      | 122.90   |
| 15  | B     | 1202 | CLA  | O1D-CGD-CBD | -2.35 | 121.25      | 124.62   |
| 14  | B     | 4006 | BCR  | C37-C22-C21 | -2.35 | 119.43      | 122.90   |
| 15  | B     | 1232 | CLA  | OBD-CAD-C3D | -2.35 | 123.56      | 128.35   |
| 15  | B     | 1230 | CLA  | O2D-CGD-O1D | -2.34 | 118.96      | 123.79   |
| 15  | B     | 1237 | CLA  | O2D-CGD-O1D | -2.33 | 118.97      | 123.79   |
| 15  | B     | 1021 | CLA  | O2D-CGD-O1D | -2.33 | 118.97      | 123.79   |
| 15  | B     | 1214 | CLA  | O2D-CGD-O1D | -2.33 | 118.98      | 123.79   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | A     | 4002 | BCR  | C37-C22-C21 | -2.33 | 119.46      | 122.90   |
| 10  | A     | 2001 | PQN  | C11-C12-C13 | -2.33 | 122.75      | 126.70   |
| 15  | A     | 1107 | CLA  | CAA-CBA-CGA | -2.33 | 106.50      | 113.32   |
| 15  | A     | 1115 | CLA  | O2D-CGD-O1D | -2.33 | 118.98      | 123.79   |
| 15  | A     | 1109 | CLA  | O2D-CGD-O1D | -2.32 | 118.99      | 123.79   |
| 15  | A     | 1107 | CLA  | O2D-CGD-O1D | -2.32 | 119.00      | 123.79   |
| 15  | A     | 1133 | CLA  | O2D-CGD-O1D | -2.32 | 119.00      | 123.79   |
| 14  | F     | 4015 | BCR  | C35-C13-C14 | -2.31 | 119.48      | 122.90   |
| 15  | B     | 1229 | CLA  | O2D-CGD-O1D | -2.31 | 119.02      | 123.79   |
| 15  | K     | 1402 | CLA  | O1D-CGD-CBD | -2.31 | 121.31      | 124.62   |
| 15  | B     | 1230 | CLA  | C3B-CAB-CBB | -2.31 | 121.60      | 126.32   |
| 14  | B     | 4005 | BCR  | C34-C9-C10  | -2.31 | 119.49      | 122.90   |
| 15  | A     | 1122 | CLA  | O2D-CGD-O1D | -2.30 | 119.03      | 123.79   |
| 15  | B     | 1208 | CLA  | O2D-CGD-O1D | -2.30 | 119.04      | 123.79   |
| 15  | B     | 1225 | CLA  | O2D-CGD-O1D | -2.29 | 119.06      | 123.79   |
| 15  | A     | 1112 | CLA  | O2D-CGD-O1D | -2.29 | 119.06      | 123.79   |
| 15  | B     | 1013 | CLA  | O2D-CGD-O1D | -2.29 | 119.06      | 123.79   |
| 14  | A     | 4008 | BCR  | C34-C9-C10  | -2.28 | 119.53      | 122.90   |
| 15  | B     | 1210 | CLA  | O2D-CGD-O1D | -2.28 | 119.08      | 123.79   |
| 15  | B     | 1220 | CLA  | O2D-CGD-O1D | -2.28 | 119.08      | 123.79   |
| 15  | B     | 1210 | CLA  | C3B-CAB-CBB | -2.28 | 121.65      | 126.32   |
| 15  | F     | 1301 | CLA  | O2D-CGD-O1D | -2.28 | 119.09      | 123.79   |
| 14  | A     | 4007 | BCR  | C30-C25-C26 | -2.27 | 119.32      | 122.66   |
| 15  | A     | 1121 | CLA  | O2D-CGD-O1D | -2.27 | 119.09      | 123.79   |
| 15  | B     | 1204 | CLA  | O2D-CGD-O1D | -2.27 | 119.10      | 123.79   |
| 14  | F     | 4015 | BCR  | C32-C1-C6   | -2.27 | 106.74      | 110.30   |
| 15  | B     | 1216 | CLA  | O2D-CGD-O1D | -2.26 | 119.11      | 123.79   |
| 15  | B     | 1203 | CLA  | O2D-CGD-O1D | -2.26 | 119.12      | 123.79   |
| 14  | A     | 4012 | BCR  | C8-C7-C6    | -2.26 | 120.52      | 127.32   |
| 15  | B     | 1021 | CLA  | CMA-C3A-C2A | -2.26 | 104.34      | 114.35   |
| 15  | B     | 1218 | CLA  | OBD-CAD-C3D | -2.26 | 123.74      | 128.35   |
| 14  | B     | 4010 | BCR  | C37-C22-C21 | -2.26 | 119.56      | 122.90   |
| 15  | A     | 1119 | CLA  | O2D-CGD-O1D | -2.26 | 119.13      | 123.79   |
| 15  | A     | 1127 | CLA  | O2D-CGD-O1D | -2.26 | 119.13      | 123.79   |
| 15  | A     | 1136 | CLA  | C4-C3-C2    | -2.26 | 119.07      | 123.50   |
| 15  | A     | 1120 | CLA  | O2D-CGD-O1D | -2.26 | 119.13      | 123.79   |
| 15  | A     | 1104 | CLA  | O2D-CGD-O1D | -2.26 | 119.13      | 123.79   |
| 14  | A     | 4001 | BCR  | C31-C1-C6   | -2.25 | 106.77      | 110.30   |
| 15  | B     | 1238 | CLA  | C3B-CAB-CBB | -2.25 | 121.71      | 126.32   |
| 15  | B     | 1235 | CLA  | C3B-CAB-CBB | -2.25 | 121.72      | 126.32   |
| 16  | J     | 1304 | LMU  | C1B-O1B-C4' | -2.24 | 112.15      | 118.01   |
| 15  | A     | 1122 | CLA  | CMD-C2D-C3D | -2.24 | 120.70      | 125.09   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | F     | 4015 | BCR  | C8-C7-C6    | -2.24 | 120.58      | 127.32   |
| 14  | A     | 4002 | BCR  | C23-C24-C25 | -2.24 | 120.58      | 127.32   |
| 14  | F     | 4015 | BCR  | C30-C25-C26 | -2.24 | 119.37      | 122.66   |
| 15  | B     | 1232 | CLA  | O1D-CGD-CBD | -2.23 | 121.42      | 124.62   |
| 15  | A     | 1117 | CLA  | O2D-CGD-O1D | -2.23 | 119.19      | 123.79   |
| 14  | B     | 4004 | BCR  | C3-C4-C5    | -2.22 | 110.34      | 113.87   |
| 15  | J     | 1303 | CLA  | O2D-CGD-O1D | -2.22 | 119.20      | 123.79   |
| 15  | B     | 1213 | CLA  | C3B-CAB-CBB | -2.22 | 121.77      | 126.32   |
| 14  | B     | 4014 | BCR  | C36-C18-C17 | -2.22 | 119.62      | 122.90   |
| 14  | B     | 4014 | BCR  | C3-C4-C5    | -2.22 | 110.35      | 113.87   |
| 15  | F     | 1139 | CLA  | O2D-CGD-O1D | -2.21 | 119.22      | 123.79   |
| 16  | B     | 1301 | LMU  | C1B-O1B-C4' | -2.21 | 112.22      | 118.01   |
| 15  | B     | 1228 | CLA  | O2D-CGD-O1D | -2.21 | 119.23      | 123.79   |
| 14  | A     | 4008 | BCR  | C36-C18-C17 | -2.21 | 119.64      | 122.90   |
| 14  | B     | 4004 | BCR  | C15-C14-C13 | -2.20 | 124.02      | 127.20   |
| 15  | K     | 1401 | CLA  | O2D-CGD-O1D | -2.20 | 119.25      | 123.79   |
| 14  | B     | 4004 | BCR  | C30-C25-C26 | -2.20 | 119.44      | 122.66   |
| 15  | B     | 1226 | CLA  | C4-C3-C2    | -2.19 | 119.20      | 123.50   |
| 14  | B     | 4011 | BCR  | C4-C5-C6    | -2.19 | 120.00      | 122.78   |
| 14  | B     | 4006 | BCR  | C23-C24-C25 | -2.18 | 120.76      | 127.32   |
| 15  | A     | 1127 | CLA  | OBD-CAD-CBD | -2.18 | 122.64      | 125.94   |
| 15  | A     | 1111 | CLA  | O2D-CGD-O1D | -2.18 | 119.29      | 123.79   |
| 15  | A     | 1140 | CLA  | C3B-CAB-CBB | -2.16 | 121.89      | 126.32   |
| 15  | B     | 1202 | CLA  | C4-C3-C2    | -2.16 | 119.26      | 123.50   |
| 15  | A     | 1104 | CLA  | C4-C3-C2    | -2.16 | 119.26      | 123.50   |
| 15  | B     | 1206 | CLA  | O2D-CGD-O1D | -2.16 | 119.34      | 123.79   |
| 10  | B     | 2002 | PQN  | C11-C12-C13 | -2.15 | 123.05      | 126.70   |
| 15  | A     | 1113 | CLA  | O2D-CGD-O1D | -2.15 | 119.35      | 123.79   |
| 15  | B     | 1220 | CLA  | C3B-CAB-CBB | -2.14 | 121.94      | 126.32   |
| 15  | A     | 1124 | CLA  | O2D-CGD-O1D | -2.14 | 119.37      | 123.79   |
| 15  | K     | 1402 | CLA  | O2D-CGD-O1D | -2.14 | 119.38      | 123.79   |
| 15  | B     | 1021 | CLA  | O1D-CGD-CBD | -2.13 | 121.56      | 124.62   |
| 14  | B     | 4017 | BCR  | C31-C1-C6   | -2.13 | 106.96      | 110.30   |
| 14  | F     | 4015 | BCR  | C23-C24-C25 | -2.13 | 120.92      | 127.32   |
| 15  | A     | 1134 | CLA  | O1D-CGD-CBD | -2.13 | 121.57      | 124.62   |
| 15  | B     | 1240 | CLA  | O2D-CGD-O1D | -2.13 | 119.39      | 123.79   |
| 15  | B     | 1232 | CLA  | O2D-CGD-O1D | -2.13 | 119.39      | 123.79   |
| 15  | A     | 1130 | CLA  | C3B-CAB-CBB | -2.12 | 121.97      | 126.32   |
| 15  | A     | 1801 | CLA  | OBD-CAD-C3D | -2.12 | 124.02      | 128.35   |
| 15  | A     | 1138 | CLA  | O2D-CGD-O1D | -2.12 | 119.41      | 123.79   |
| 15  | A     | 1125 | CLA  | C6-C5-C3    | -2.12 | 110.89      | 114.43   |
| 14  | F     | 4016 | BCR  | C7-C8-C9    | -2.12 | 122.99      | 126.22   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15  | B     | 1021 | CLA  | C3B-CAB-CBB | -2.12 | 121.99      | 126.32   |
| 15  | B     | 1230 | CLA  | CAA-C2A-C1A | -2.11 | 105.04      | 112.47   |
| 15  | A     | 1129 | CLA  | CMD-C2D-C3D | -2.10 | 120.98      | 125.09   |
| 14  | B     | 4014 | BCR  | C28-C27-C26 | -2.10 | 110.54      | 113.87   |
| 14  | F     | 4015 | BCR  | C37-C22-C21 | -2.10 | 119.80      | 122.90   |
| 15  | B     | 1212 | CLA  | C3B-CAB-CBB | -2.10 | 122.03      | 126.32   |
| 15  | B     | 1231 | CLA  | O2D-CGD-O1D | -2.09 | 119.47      | 123.79   |
| 14  | B     | 4006 | BCR  | C15-C14-C13 | -2.09 | 124.18      | 127.20   |
| 13  | A     | 1108 | CL0  | CGD-CBD-CAD | -2.09 | 103.55      | 110.62   |
| 14  | B     | 4006 | BCR  | C4-C5-C6    | -2.09 | 120.12      | 122.78   |
| 15  | A     | 1135 | CLA  | O2D-CGD-O1D | -2.08 | 119.50      | 123.79   |
| 14  | A     | 4007 | BCR  | C37-C22-C21 | -2.08 | 119.83      | 122.90   |
| 15  | A     | 1123 | CLA  | OBD-CAD-C3D | -2.08 | 124.12      | 128.35   |
| 14  | B     | 4010 | BCR  | C7-C8-C9    | -2.08 | 123.05      | 126.22   |
| 15  | A     | 1107 | CLA  | CMD-C2D-C3D | -2.07 | 121.04      | 125.09   |
| 15  | B     | 1238 | CLA  | O2D-CGD-O1D | -2.07 | 119.51      | 123.79   |
| 14  | B     | 4005 | BCR  | C23-C24-C25 | -2.07 | 121.10      | 127.32   |
| 15  | A     | 1107 | CLA  | CAA-C2A-C3A | -2.06 | 107.29      | 113.22   |
| 15  | A     | 1115 | CLA  | C3B-CAB-CBB | -2.06 | 122.11      | 126.32   |
| 14  | B     | 4004 | BCR  | C35-C13-C14 | -2.05 | 119.87      | 122.90   |
| 15  | A     | 1104 | CLA  | CBC-CAC-C3C | -2.05 | 106.13      | 112.39   |
| 15  | B     | 1227 | CLA  | OBD-CAD-C3D | -2.04 | 124.19      | 128.35   |
| 15  | B     | 1023 | CLA  | O1D-CGD-CBD | -2.04 | 121.70      | 124.62   |
| 14  | A     | 4002 | BCR  | C28-C27-C26 | -2.04 | 110.63      | 113.87   |
| 14  | B     | 4004 | BCR  | C24-C23-C22 | -2.03 | 123.11      | 126.22   |
| 15  | A     | 1109 | CLA  | O1D-CGD-CBD | -2.03 | 121.71      | 124.62   |
| 14  | B     | 4006 | BCR  | C31-C1-C6   | -2.03 | 107.12      | 110.30   |
| 15  | A     | 1128 | CLA  | OBD-CAD-C3D | -2.03 | 124.22      | 128.35   |
| 14  | J     | 4013 | BCR  | C35-C13-C14 | -2.03 | 119.91      | 122.90   |
| 14  | A     | 4007 | BCR  | C31-C1-C6   | -2.03 | 107.13      | 110.30   |
| 15  | B     | 1236 | CLA  | CHD-C4C-C3C | -2.02 | 121.82      | 124.94   |
| 15  | A     | 1012 | CLA  | C4-C3-C2    | -2.02 | 119.53      | 123.50   |
| 15  | B     | 1239 | CLA  | CHC-C1C-C2C | -2.02 | 121.04      | 126.35   |
| 14  | B     | 4004 | BCR  | C23-C24-C25 | -2.02 | 121.25      | 127.32   |
| 15  | A     | 1127 | CLA  | C4-C3-C2    | -2.01 | 119.55      | 123.50   |
| 15  | A     | 1123 | CLA  | CHC-C1C-C2C | -2.01 | 121.06      | 126.35   |
| 14  | A     | 4003 | BCR  | C23-C24-C25 | -2.01 | 121.28      | 127.32   |
| 15  | B     | 1023 | CLA  | OBD-CAD-C3D | -2.01 | 124.25      | 128.35   |
| 14  | F     | 4016 | BCR  | C32-C1-C6   | -2.00 | 107.16      | 110.30   |
| 15  | B     | 1234 | CLA  | CHB-C4A-NA  | 2.00  | 127.28      | 124.51   |
| 15  | A     | 1128 | CLA  | C4-C3-C5    | 2.00  | 118.47      | 115.41   |
| 15  | A     | 1110 | CLA  | C4A-NA-C1A  | 2.00  | 108.95      | 106.36   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 16  | B     | 1301 | LMU  | O5'-C1'-C2' | 2.01 | 114.39      | 110.28   |
| 15  | A     | 1106 | CLA  | CHB-C4A-NA  | 2.01 | 127.29      | 124.51   |
| 15  | A     | 1136 | CLA  | CHB-C4A-NA  | 2.01 | 127.29      | 124.51   |
| 15  | B     | 1226 | CLA  | CHB-C4A-NA  | 2.01 | 127.29      | 124.51   |
| 15  | A     | 1124 | CLA  | CED-O2D-CGD | 2.01 | 120.70      | 115.99   |
| 15  | A     | 1121 | CLA  | CAC-C3C-C4C | 2.01 | 127.75      | 124.83   |
| 15  | B     | 1215 | CLA  | CMB-C2B-C3B | 2.01 | 129.03      | 125.09   |
| 15  | B     | 1218 | CLA  | CMB-C2B-C3B | 2.02 | 129.03      | 125.09   |
| 15  | A     | 1129 | CLA  | CHB-C4A-NA  | 2.02 | 127.31      | 124.51   |
| 15  | A     | 1138 | CLA  | CHB-C4A-NA  | 2.03 | 127.32      | 124.51   |
| 15  | A     | 1120 | CLA  | CHB-C4A-NA  | 2.03 | 127.32      | 124.51   |
| 15  | A     | 1131 | CLA  | CED-O2D-CGD | 2.03 | 120.75      | 115.99   |
| 15  | A     | 1103 | CLA  | CMB-C2B-C3B | 2.03 | 129.06      | 125.09   |
| 15  | J     | 1303 | CLA  | CHB-C4A-NA  | 2.03 | 127.32      | 124.51   |
| 15  | A     | 1136 | CLA  | CAC-C3C-C4C | 2.03 | 127.78      | 124.83   |
| 15  | K     | 1401 | CLA  | CMB-C2B-C3B | 2.03 | 129.07      | 125.09   |
| 15  | B     | 1204 | CLA  | CHB-C4A-NA  | 2.04 | 127.34      | 124.51   |
| 15  | K     | 1401 | CLA  | CAC-C3C-C4C | 2.05 | 127.80      | 124.83   |
| 15  | A     | 1135 | CLA  | CED-O2D-CGD | 2.05 | 120.79      | 115.99   |
| 15  | A     | 1116 | CLA  | CHB-C4A-NA  | 2.05 | 127.34      | 124.51   |
| 15  | A     | 1113 | CLA  | CHB-C4A-NA  | 2.05 | 127.34      | 124.51   |
| 15  | A     | 1103 | CLA  | C4-C3-C5    | 2.05 | 118.54      | 115.41   |
| 15  | A     | 1801 | CLA  | CHB-C4A-NA  | 2.05 | 127.35      | 124.51   |
| 15  | A     | 1128 | CLA  | CHB-C4A-NA  | 2.05 | 127.35      | 124.51   |
| 15  | K     | 1401 | CLA  | CED-O2D-CGD | 2.05 | 120.81      | 115.99   |
| 15  | B     | 1204 | CLA  | CMB-C2B-C3B | 2.05 | 129.11      | 125.09   |
| 14  | A     | 4003 | BCR  | C8-C9-C10   | 2.06 | 122.30      | 118.98   |
| 15  | A     | 1117 | CLA  | C4A-NA-C1A  | 2.06 | 109.02      | 106.36   |
| 15  | F     | 1410 | CLA  | CMB-C2B-C3B | 2.06 | 129.12      | 125.09   |
| 15  | A     | 1120 | CLA  | CMB-C2B-C3B | 2.06 | 129.12      | 125.09   |
| 15  | A     | 1107 | CLA  | C5-C3-C4    | 2.06 | 119.71      | 114.64   |
| 15  | B     | 1203 | CLA  | C4-C3-C5    | 2.07 | 118.56      | 115.41   |
| 15  | A     | 1133 | CLA  | CMB-C2B-C3B | 2.07 | 129.14      | 125.09   |
| 16  | B     | 1301 | LMU  | C1'-O5'-C5' | 2.08 | 117.78      | 113.75   |
| 15  | B     | 1214 | CLA  | CHB-C4A-NA  | 2.08 | 127.39      | 124.51   |
| 15  | A     | 1801 | CLA  | C4-C3-C5    | 2.08 | 118.59      | 115.41   |
| 15  | A     | 1114 | CLA  | CMB-C2B-C3B | 2.09 | 129.17      | 125.09   |
| 15  | A     | 1123 | CLA  | CMB-C2B-C3B | 2.09 | 129.17      | 125.09   |
| 15  | B     | 1209 | CLA  | CHB-C4A-NA  | 2.09 | 127.40      | 124.51   |
| 15  | A     | 1113 | CLA  | CAC-C3C-C4C | 2.09 | 127.86      | 124.83   |
| 15  | B     | 1217 | CLA  | CMB-C2B-C3B | 2.09 | 129.17      | 125.09   |
| 15  | A     | 1122 | CLA  | CMB-C2B-C3B | 2.09 | 129.18      | 125.09   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 15  | B     | 1235 | CLA  | CHB-C4A-NA  | 2.10 | 127.42      | 124.51   |
| 15  | B     | 1023 | CLA  | CHB-C4A-NA  | 2.10 | 127.42      | 124.51   |
| 15  | B     | 1228 | CLA  | CED-O2D-CGD | 2.10 | 120.92      | 115.99   |
| 16  | B     | 1301 | LMU  | O5'-C5'-C4' | 2.10 | 114.19      | 109.75   |
| 15  | A     | 1128 | CLA  | CMC-C2C-C1C | 2.10 | 128.27      | 125.02   |
| 15  | A     | 1127 | CLA  | CED-O2D-CGD | 2.10 | 120.92      | 115.99   |
| 15  | A     | 1104 | CLA  | CMB-C2B-C3B | 2.11 | 129.21      | 125.09   |
| 15  | B     | 1239 | CLA  | CAC-C3C-C4C | 2.11 | 127.89      | 124.83   |
| 15  | A     | 1110 | CLA  | CAC-C3C-C4C | 2.11 | 127.89      | 124.83   |
| 15  | A     | 1138 | CLA  | C4A-NA-C1A  | 2.11 | 109.09      | 106.36   |
| 15  | B     | 1237 | CLA  | CAC-C3C-C4C | 2.11 | 127.89      | 124.83   |
| 15  | B     | 1202 | CLA  | CMB-C2B-C3B | 2.11 | 129.22      | 125.09   |
| 15  | B     | 1213 | CLA  | C4A-NA-C1A  | 2.11 | 109.09      | 106.36   |
| 14  | A     | 4007 | BCR  | C34-C9-C8   | 2.11 | 121.61      | 118.10   |
| 15  | A     | 1105 | CLA  | CAC-C3C-C4C | 2.12 | 127.91      | 124.83   |
| 15  | F     | 1410 | CLA  | C4A-NA-C1A  | 2.12 | 109.10      | 106.36   |
| 15  | B     | 1224 | CLA  | C4A-NA-C1A  | 2.12 | 109.10      | 106.36   |
| 15  | A     | 1126 | CLA  | CHB-C4A-NA  | 2.12 | 127.44      | 124.51   |
| 15  | A     | 1118 | CLA  | CHB-C4A-NA  | 2.12 | 127.45      | 124.51   |
| 15  | B     | 1234 | CLA  | CMB-C2B-C3B | 2.12 | 129.24      | 125.09   |
| 15  | B     | 1206 | CLA  | CHB-C4A-NA  | 2.13 | 127.45      | 124.51   |
| 15  | B     | 1222 | CLA  | CMB-C2B-C3B | 2.13 | 129.25      | 125.09   |
| 15  | B     | 1238 | CLA  | CMB-C2B-C3B | 2.13 | 129.25      | 125.09   |
| 15  | A     | 1106 | CLA  | CMB-C2B-C3B | 2.13 | 129.26      | 125.09   |
| 15  | B     | 1021 | CLA  | CED-O2D-CGD | 2.13 | 120.99      | 115.99   |
| 15  | B     | 1211 | CLA  | CMB-C2B-C3B | 2.13 | 129.26      | 125.09   |
| 15  | A     | 1105 | CLA  | C4A-NA-C1A  | 2.14 | 109.12      | 106.36   |
| 15  | B     | 1238 | CLA  | C4A-NA-C1A  | 2.14 | 109.12      | 106.36   |
| 15  | B     | 1231 | CLA  | CMB-C2B-C3B | 2.14 | 129.27      | 125.09   |
| 15  | B     | 1207 | CLA  | CHB-C4A-NA  | 2.14 | 127.47      | 124.51   |
| 15  | A     | 1103 | CLA  | CED-O2D-CGD | 2.14 | 121.01      | 115.99   |
| 15  | A     | 1119 | CLA  | CED-O2D-CGD | 2.14 | 121.01      | 115.99   |
| 15  | B     | 1206 | CLA  | C4A-NA-C1A  | 2.15 | 109.13      | 106.36   |
| 14  | J     | 4013 | BCR  | C19-C18-C17 | 2.15 | 122.44      | 118.98   |
| 15  | A     | 1113 | CLA  | CMB-C2B-C3B | 2.15 | 129.29      | 125.09   |
| 15  | A     | 1113 | CLA  | C4A-NA-C1A  | 2.15 | 109.14      | 106.36   |
| 15  | B     | 1215 | CLA  | C4A-NA-C1A  | 2.15 | 109.14      | 106.36   |
| 15  | B     | 1220 | CLA  | C4-C3-C5    | 2.15 | 118.69      | 115.41   |
| 15  | A     | 1102 | CLA  | CHB-C4A-NA  | 2.15 | 127.49      | 124.51   |
| 15  | A     | 1114 | CLA  | C4A-NA-C1A  | 2.15 | 109.14      | 106.36   |
| 15  | B     | 1221 | CLA  | CHB-C4A-NA  | 2.15 | 127.49      | 124.51   |
| 15  | A     | 1124 | CLA  | C4A-NA-C1A  | 2.15 | 109.14      | 106.36   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 15  | K     | 1401 | CLA  | CHB-C4A-NA  | 2.16 | 127.49      | 124.51   |
| 15  | A     | 1114 | CLA  | CAC-C3C-C4C | 2.16 | 127.96      | 124.83   |
| 15  | F     | 1301 | CLA  | C4A-NA-C1A  | 2.16 | 109.15      | 106.36   |
| 14  | F     | 4015 | BCR  | C19-C18-C17 | 2.16 | 122.47      | 118.98   |
| 15  | B     | 1231 | CLA  | CMC-C2C-C1C | 2.16 | 128.37      | 125.02   |
| 13  | A     | 1108 | CL0  | CHB-C4A-NA  | 2.17 | 127.51      | 124.51   |
| 15  | F     | 1410 | CLA  | C6-C5-C3    | 2.17 | 117.24      | 112.48   |
| 15  | A     | 1801 | CLA  | CAC-C3C-C2C | 2.17 | 131.31      | 127.51   |
| 14  | A     | 4001 | BCR  | C23-C22-C21 | 2.17 | 122.48      | 118.98   |
| 14  | B     | 4006 | BCR  | C38-C26-C27 | 2.17 | 117.55      | 113.43   |
| 15  | B     | 1213 | CLA  | CMB-C2B-C3B | 2.17 | 129.34      | 125.09   |
| 15  | A     | 1101 | CLA  | C4A-NA-C1A  | 2.18 | 109.17      | 106.36   |
| 15  | A     | 1104 | CLA  | C4A-NA-C1A  | 2.18 | 109.18      | 106.36   |
| 15  | A     | 1109 | CLA  | C4A-NA-C1A  | 2.18 | 109.18      | 106.36   |
| 15  | B     | 1218 | CLA  | C4A-NA-C1A  | 2.19 | 109.18      | 106.36   |
| 15  | B     | 1237 | CLA  | CMB-C2B-C3B | 2.19 | 129.36      | 125.09   |
| 15  | B     | 1235 | CLA  | CMB-C2B-C3B | 2.19 | 129.37      | 125.09   |
| 15  | B     | 1226 | CLA  | CMB-C2B-C3B | 2.19 | 129.37      | 125.09   |
| 15  | A     | 1110 | CLA  | CMB-C2B-C3B | 2.19 | 129.37      | 125.09   |
| 15  | B     | 1208 | CLA  | C4A-NA-C1A  | 2.19 | 109.19      | 106.36   |
| 15  | A     | 1116 | CLA  | C4A-NA-C1A  | 2.20 | 109.20      | 106.36   |
| 13  | A     | 1108 | CL0  | CAC-C3C-C4C | 2.20 | 128.03      | 124.83   |
| 15  | A     | 1125 | CLA  | C4A-NA-C1A  | 2.20 | 109.21      | 106.36   |
| 15  | B     | 1227 | CLA  | CHB-C4A-NA  | 2.20 | 127.56      | 124.51   |
| 15  | B     | 1217 | CLA  | C4A-NA-C1A  | 2.21 | 109.21      | 106.36   |
| 15  | A     | 1022 | CLA  | CMB-C2B-C3B | 2.21 | 129.40      | 125.09   |
| 15  | A     | 1801 | CLA  | CMB-C2B-C3B | 2.21 | 129.40      | 125.09   |
| 15  | A     | 1121 | CLA  | C4A-NA-C1A  | 2.21 | 109.21      | 106.36   |
| 15  | A     | 1135 | CLA  | C4A-NA-C1A  | 2.21 | 109.21      | 106.36   |
| 15  | B     | 1240 | CLA  | C4A-NA-C1A  | 2.21 | 109.21      | 106.36   |
| 15  | B     | 1206 | CLA  | CMB-C2B-C3B | 2.21 | 129.41      | 125.09   |
| 15  | A     | 1134 | CLA  | C4A-NA-C1A  | 2.21 | 109.22      | 106.36   |
| 15  | B     | 1211 | CLA  | C4A-NA-C1A  | 2.21 | 109.22      | 106.36   |
| 15  | B     | 1223 | CLA  | C4A-NA-C1A  | 2.22 | 109.22      | 106.36   |
| 15  | B     | 1210 | CLA  | C4A-NA-C1A  | 2.22 | 109.23      | 106.36   |
| 15  | A     | 1133 | CLA  | CAC-C3C-C4C | 2.22 | 128.05      | 124.83   |
| 15  | A     | 1112 | CLA  | CMB-C2B-C3B | 2.22 | 129.43      | 125.09   |
| 15  | A     | 1111 | CLA  | C4A-NA-C1A  | 2.22 | 109.23      | 106.36   |
| 14  | B     | 4017 | BCR  | C34-C9-C8   | 2.22 | 121.80      | 118.10   |
| 15  | B     | 1225 | CLA  | C4A-NA-C1A  | 2.22 | 109.23      | 106.36   |
| 14  | A     | 4001 | BCR  | C30-C25-C24 | 2.22 | 122.05      | 115.82   |
| 15  | A     | 1109 | CLA  | CMB-C2B-C3B | 2.23 | 129.44      | 125.09   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 15  | B     | 1219 | CLA  | C4A-NA-C1A  | 2.23 | 109.24      | 106.36   |
| 15  | B     | 1021 | CLA  | CHB-C4A-NA  | 2.23 | 127.59      | 124.51   |
| 15  | B     | 1212 | CLA  | CMB-C2B-C3B | 2.23 | 129.45      | 125.09   |
| 15  | A     | 1012 | CLA  | CMB-C2B-C3B | 2.24 | 129.46      | 125.09   |
| 14  | F     | 4015 | BCR  | C33-C5-C4   | 2.24 | 117.67      | 113.43   |
| 15  | B     | 1013 | CLA  | CHB-C4A-NA  | 2.24 | 127.61      | 124.51   |
| 15  | B     | 1230 | CLA  | CMB-C2B-C3B | 2.24 | 129.47      | 125.09   |
| 15  | B     | 1202 | CLA  | CHB-C4A-NA  | 2.24 | 127.61      | 124.51   |
| 14  | B     | 4009 | BCR  | C8-C9-C10   | 2.25 | 122.61      | 118.98   |
| 14  | A     | 4012 | BCR  | C33-C5-C4   | 2.26 | 117.71      | 113.43   |
| 15  | F     | 1301 | CLA  | CHB-C4A-NA  | 2.26 | 127.63      | 124.51   |
| 15  | A     | 1126 | CLA  | C4A-NA-C1A  | 2.26 | 109.28      | 106.36   |
| 15  | A     | 1103 | CLA  | C4A-NA-C1A  | 2.26 | 109.28      | 106.36   |
| 15  | B     | 1205 | CLA  | C4-C3-C5    | 2.26 | 118.86      | 115.41   |
| 15  | A     | 1111 | CLA  | CHB-C4A-NA  | 2.26 | 127.64      | 124.51   |
| 15  | B     | 1208 | CLA  | CMC-C2C-C1C | 2.26 | 128.52      | 125.02   |
| 15  | A     | 1123 | CLA  | C4-C3-C5    | 2.26 | 118.87      | 115.41   |
| 15  | A     | 1131 | CLA  | C4A-NA-C1A  | 2.27 | 109.29      | 106.36   |
| 14  | B     | 4014 | BCR  | C33-C5-C4   | 2.27 | 117.73      | 113.43   |
| 15  | A     | 1115 | CLA  | CMB-C2B-C3B | 2.27 | 129.53      | 125.09   |
| 15  | A     | 1129 | CLA  | C4A-NA-C1A  | 2.27 | 109.30      | 106.36   |
| 15  | A     | 1124 | CLA  | CMB-C2B-C3B | 2.27 | 129.53      | 125.09   |
| 15  | A     | 1112 | CLA  | C4A-NA-C1A  | 2.27 | 109.30      | 106.36   |
| 14  | B     | 4011 | BCR  | C35-C13-C12 | 2.27 | 121.88      | 118.10   |
| 15  | K     | 1401 | CLA  | C4A-NA-C1A  | 2.28 | 109.30      | 106.36   |
| 15  | A     | 1124 | CLA  | CHB-C4A-NA  | 2.28 | 127.66      | 124.51   |
| 15  | A     | 1117 | CLA  | CMB-C2B-C3B | 2.28 | 129.54      | 125.09   |
| 12  | A     | 5001 | LHG  | O8-C23-C24  | 2.28 | 118.86      | 111.90   |
| 13  | A     | 1108 | CL0  | CED-O2D-CGD | 2.29 | 121.35      | 115.99   |
| 15  | A     | 1102 | CLA  | C4A-NA-C1A  | 2.29 | 109.31      | 106.36   |
| 15  | A     | 1140 | CLA  | CMB-C2B-C3B | 2.29 | 129.56      | 125.09   |
| 15  | J     | 1302 | CLA  | C4A-NA-C1A  | 2.29 | 109.32      | 106.36   |
| 15  | B     | 1021 | CLA  | C4-C3-C5    | 2.29 | 118.90      | 115.41   |
| 15  | B     | 1013 | CLA  | C4-C3-C5    | 2.29 | 118.90      | 115.41   |
| 14  | A     | 4003 | BCR  | C19-C18-C17 | 2.29 | 122.67      | 118.98   |
| 15  | A     | 1112 | CLA  | CHB-C4A-NA  | 2.30 | 127.69      | 124.51   |
| 15  | B     | 1023 | CLA  | CMC-C2C-C1C | 2.30 | 128.58      | 125.02   |
| 15  | B     | 1202 | CLA  | C4A-NA-C1A  | 2.30 | 109.33      | 106.36   |
| 15  | B     | 1204 | CLA  | C4A-NA-C1A  | 2.30 | 109.34      | 106.36   |
| 15  | B     | 1239 | CLA  | CMC-C2C-C1C | 2.31 | 128.59      | 125.02   |
| 15  | A     | 1012 | CLA  | CHB-C4A-NA  | 2.31 | 127.70      | 124.51   |
| 15  | A     | 1131 | CLA  | CAC-C3C-C4C | 2.31 | 128.18      | 124.83   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 15  | F     | 1301 | CLA  | CMB-C2B-C3B | 2.31 | 129.61      | 125.09   |
| 15  | A     | 1106 | CLA  | C4A-NA-C1A  | 2.31 | 109.35      | 106.36   |
| 15  | A     | 1127 | CLA  | C4A-NA-C1A  | 2.31 | 109.35      | 106.36   |
| 15  | B     | 1232 | CLA  | C4A-NA-C1A  | 2.32 | 109.35      | 106.36   |
| 15  | A     | 1111 | CLA  | CMB-C2B-C3B | 2.32 | 129.62      | 125.09   |
| 15  | A     | 1126 | CLA  | C4-C3-C5    | 2.32 | 118.95      | 115.41   |
| 15  | B     | 1230 | CLA  | C4A-NA-C1A  | 2.32 | 109.36      | 106.36   |
| 15  | A     | 1133 | CLA  | C4A-NA-C1A  | 2.32 | 109.36      | 106.36   |
| 15  | B     | 1227 | CLA  | C4A-NA-C1A  | 2.33 | 109.37      | 106.36   |
| 15  | A     | 1103 | CLA  | CHB-C4A-NA  | 2.33 | 127.74      | 124.51   |
| 15  | B     | 1237 | CLA  | C4A-NA-C1A  | 2.33 | 109.38      | 106.36   |
| 10  | B     | 2002 | PQN  | C2M-C2-C1   | 2.33 | 120.06      | 116.27   |
| 15  | B     | 1207 | CLA  | C4A-NA-C1A  | 2.34 | 109.38      | 106.36   |
| 15  | B     | 1023 | CLA  | C4A-NA-C1A  | 2.34 | 109.38      | 106.36   |
| 15  | A     | 1135 | CLA  | CMB-C2B-C3B | 2.34 | 129.67      | 125.09   |
| 15  | A     | 1116 | CLA  | C4-C3-C5    | 2.34 | 118.99      | 115.41   |
| 15  | B     | 1212 | CLA  | C4A-NA-C1A  | 2.35 | 109.39      | 106.36   |
| 15  | J     | 1303 | CLA  | C4A-NA-C1A  | 2.35 | 109.39      | 106.36   |
| 15  | A     | 1137 | CLA  | C4A-NA-C1A  | 2.35 | 109.40      | 106.36   |
| 15  | A     | 1140 | CLA  | C4A-NA-C1A  | 2.35 | 109.40      | 106.36   |
| 15  | B     | 1209 | CLA  | C4A-NA-C1A  | 2.36 | 109.40      | 106.36   |
| 15  | B     | 1236 | CLA  | CMB-C2B-C3B | 2.36 | 129.70      | 125.09   |
| 14  | A     | 4002 | BCR  | C35-C13-C12 | 2.36 | 122.02      | 118.10   |
| 10  | A     | 2001 | PQN  | C2M-C2-C1   | 2.36 | 120.10      | 116.27   |
| 14  | A     | 4002 | BCR  | C33-C5-C4   | 2.36 | 117.91      | 113.43   |
| 15  | A     | 1120 | CLA  | C4A-NA-C1A  | 2.36 | 109.41      | 106.36   |
| 15  | B     | 1231 | CLA  | CED-O2D-CGD | 2.37 | 121.54      | 115.99   |
| 15  | A     | 1125 | CLA  | CMB-C2B-C3B | 2.37 | 129.72      | 125.09   |
| 15  | B     | 1201 | CLA  | C4A-NA-C1A  | 2.37 | 109.43      | 106.36   |
| 15  | B     | 1013 | CLA  | CMC-C2C-C1C | 2.38 | 128.69      | 125.02   |
| 15  | A     | 1128 | CLA  | C4A-NA-C1A  | 2.38 | 109.44      | 106.36   |
| 15  | B     | 1231 | CLA  | C4A-NA-C1A  | 2.38 | 109.44      | 106.36   |
| 15  | B     | 1222 | CLA  | CMC-C2C-C1C | 2.38 | 128.71      | 125.02   |
| 14  | B     | 4005 | BCR  | C33-C5-C4   | 2.39 | 117.95      | 113.43   |
| 15  | B     | 1240 | CLA  | CMB-C2B-C3B | 2.39 | 129.76      | 125.09   |
| 14  | B     | 4014 | BCR  | C38-C26-C27 | 2.39 | 117.96      | 113.43   |
| 15  | B     | 1013 | CLA  | CMB-C2B-C3B | 2.39 | 129.76      | 125.09   |
| 15  | A     | 1140 | CLA  | C4-C3-C5    | 2.39 | 119.06      | 115.41   |
| 15  | A     | 1123 | CLA  | C4A-NA-C1A  | 2.39 | 109.45      | 106.36   |
| 15  | B     | 1202 | CLA  | CMC-C2C-C1C | 2.40 | 128.73      | 125.02   |
| 15  | F     | 1139 | CLA  | C4A-NA-C1A  | 2.40 | 109.46      | 106.36   |
| 15  | B     | 1013 | CLA  | C4A-NA-C1A  | 2.40 | 109.46      | 106.36   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 15  | A     | 1101 | CLA  | CMB-C2B-C3B | 2.40 | 129.79      | 125.09   |
| 14  | B     | 4005 | BCR  | C38-C26-C27 | 2.40 | 117.98      | 113.43   |
| 15  | B     | 1209 | CLA  | CAC-C3C-C4C | 2.40 | 128.32      | 124.83   |
| 15  | B     | 1013 | CLA  | CED-O2D-CGD | 2.40 | 121.63      | 115.99   |
| 15  | B     | 1235 | CLA  | C4A-NA-C1A  | 2.40 | 109.47      | 106.36   |
| 15  | A     | 1132 | CLA  | CMC-C2C-C1C | 2.41 | 128.75      | 125.02   |
| 15  | B     | 1023 | CLA  | C4-C3-C5    | 2.41 | 119.08      | 115.41   |
| 15  | B     | 1226 | CLA  | C4A-NA-C1A  | 2.41 | 109.48      | 106.36   |
| 15  | A     | 1115 | CLA  | C4A-NA-C1A  | 2.42 | 109.48      | 106.36   |
| 15  | K     | 1402 | CLA  | C4A-NA-C1A  | 2.42 | 109.49      | 106.36   |
| 13  | A     | 1108 | CL0  | C4A-NA-C1A  | 2.42 | 109.49      | 106.36   |
| 14  | F     | 4016 | BCR  | C33-C5-C4   | 2.42 | 118.03      | 113.43   |
| 15  | A     | 1117 | CLA  | C4-C3-C5    | 2.43 | 119.11      | 115.41   |
| 15  | B     | 1234 | CLA  | C4A-NA-C1A  | 2.43 | 109.50      | 106.36   |
| 15  | B     | 1206 | CLA  | CAC-C3C-C4C | 2.43 | 128.36      | 124.83   |
| 15  | B     | 1234 | CLA  | CMC-C2C-C1C | 2.43 | 128.78      | 125.02   |
| 15  | A     | 1132 | CLA  | C4A-NA-C1A  | 2.43 | 109.50      | 106.36   |
| 15  | B     | 1225 | CLA  | CMB-C2B-C3B | 2.45 | 129.88      | 125.09   |
| 15  | B     | 1209 | CLA  | CMB-C2B-C3B | 2.45 | 129.88      | 125.09   |
| 15  | A     | 1137 | CLA  | CMB-C2B-C3B | 2.46 | 129.90      | 125.09   |
| 15  | B     | 1235 | CLA  | C4-C3-C5    | 2.47 | 119.18      | 115.41   |
| 15  | A     | 1137 | CLA  | CMC-C2C-C1C | 2.47 | 128.85      | 125.02   |
| 15  | A     | 1012 | CLA  | C4A-NA-C1A  | 2.48 | 109.56      | 106.36   |
| 15  | B     | 1239 | CLA  | C4A-NA-C1A  | 2.48 | 109.56      | 106.36   |
| 14  | A     | 4001 | BCR  | C33-C5-C4   | 2.48 | 118.14      | 113.43   |
| 15  | A     | 1801 | CLA  | C4A-NA-C1A  | 2.49 | 109.58      | 106.36   |
| 14  | F     | 4016 | BCR  | C34-C9-C8   | 2.50 | 122.25      | 118.10   |
| 15  | A     | 1134 | CLA  | CMB-C2B-C3B | 2.50 | 129.98      | 125.09   |
| 15  | B     | 1021 | CLA  | CBA-CAA-C2A | 2.50 | 120.80      | 113.73   |
| 14  | B     | 4005 | BCR  | C23-C22-C21 | 2.50 | 123.02      | 118.98   |
| 15  | A     | 1111 | CLA  | CAC-C3C-C4C | 2.51 | 128.47      | 124.83   |
| 15  | B     | 1203 | CLA  | C4A-NA-C1A  | 2.52 | 109.61      | 106.36   |
| 15  | B     | 1222 | CLA  | CHB-C4A-NA  | 2.52 | 128.00      | 124.51   |
| 14  | J     | 4013 | BCR  | C2-C1-C6    | 2.52 | 114.36      | 110.36   |
| 15  | B     | 1209 | CLA  | CMC-C2C-C1C | 2.53 | 128.93      | 125.02   |
| 15  | B     | 1201 | CLA  | CMB-C2B-C3B | 2.54 | 130.06      | 125.09   |
| 15  | B     | 1203 | CLA  | CMC-C2C-C1C | 2.54 | 128.95      | 125.02   |
| 12  | A     | 5003 | LHG  | O8-C23-C24  | 2.54 | 119.65      | 111.90   |
| 15  | B     | 1225 | CLA  | CBA-CAA-C2A | 2.55 | 120.93      | 113.73   |
| 14  | B     | 4004 | BCR  | C23-C22-C21 | 2.55 | 123.10      | 118.98   |
| 15  | B     | 1232 | CLA  | CMC-C2C-C1C | 2.56 | 128.98      | 125.02   |
| 15  | A     | 1118 | CLA  | C4A-NA-C1A  | 2.56 | 109.67      | 106.36   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 13  | A     | 1011 | CL0  | C4A-NA-C1A  | 2.56 | 109.67      | 106.36   |
| 15  | B     | 1229 | CLA  | C4A-NA-C1A  | 2.57 | 109.68      | 106.36   |
| 15  | B     | 1205 | CLA  | C4A-NA-C1A  | 2.57 | 109.68      | 106.36   |
| 15  | B     | 1226 | CLA  | CMC-C2C-C1C | 2.57 | 129.00      | 125.02   |
| 15  | B     | 1207 | CLA  | CMC-C2C-C1C | 2.57 | 129.00      | 125.02   |
| 15  | B     | 1221 | CLA  | CMB-C2B-C3B | 2.58 | 130.13      | 125.09   |
| 15  | B     | 1220 | CLA  | CED-O2D-CGD | 2.58 | 122.03      | 115.99   |
| 14  | B     | 4010 | BCR  | C34-C9-C8   | 2.58 | 122.39      | 118.10   |
| 15  | B     | 1227 | CLA  | CMC-C2C-C1C | 2.58 | 129.01      | 125.02   |
| 15  | B     | 1021 | CLA  | C4A-NA-C1A  | 2.58 | 109.70      | 106.36   |
| 15  | B     | 1222 | CLA  | C4A-NA-C1A  | 2.58 | 109.70      | 106.36   |
| 15  | B     | 1223 | CLA  | CMB-C2B-C3B | 2.59 | 130.15      | 125.09   |
| 15  | A     | 1101 | CLA  | CHB-C4A-NA  | 2.59 | 128.09      | 124.51   |
| 14  | B     | 4010 | BCR  | C38-C26-C27 | 2.59 | 118.34      | 113.43   |
| 15  | B     | 1210 | CLA  | CAC-C3C-C4C | 2.59 | 128.59      | 124.83   |
| 14  | A     | 4012 | BCR  | C38-C26-C27 | 2.59 | 118.34      | 113.43   |
| 15  | B     | 1224 | CLA  | CMB-C2B-C3B | 2.59 | 130.16      | 125.09   |
| 15  | A     | 1103 | CLA  | CMC-C2C-C1C | 2.60 | 129.04      | 125.02   |
| 15  | A     | 1136 | CLA  | CMC-C2C-C1C | 2.60 | 129.05      | 125.02   |
| 15  | B     | 1216 | CLA  | CMC-C2C-C1C | 2.60 | 129.05      | 125.02   |
| 15  | A     | 1114 | CLA  | CMC-C2C-C1C | 2.61 | 129.05      | 125.02   |
| 15  | B     | 1216 | CLA  | C4-C3-C5    | 2.61 | 119.39      | 115.41   |
| 15  | A     | 1101 | CLA  | CBA-CAA-C2A | 2.62 | 121.13      | 113.73   |
| 15  | K     | 1401 | CLA  | CMC-C2C-C1C | 2.63 | 129.08      | 125.02   |
| 15  | A     | 1120 | CLA  | CMC-C2C-C1C | 2.63 | 129.09      | 125.02   |
| 14  | B     | 4010 | BCR  | C33-C5-C4   | 2.63 | 118.42      | 113.43   |
| 15  | B     | 1228 | CLA  | CMC-C2C-C1C | 2.63 | 129.09      | 125.02   |
| 15  | A     | 1136 | CLA  | C4A-NA-C1A  | 2.64 | 109.77      | 106.36   |
| 15  | A     | 1127 | CLA  | CMB-C2B-C3B | 2.65 | 130.26      | 125.09   |
| 15  | A     | 1107 | CLA  | CMB-C2B-C3B | 2.65 | 130.26      | 125.09   |
| 15  | J     | 1303 | CLA  | CMC-C2C-C1C | 2.65 | 129.12      | 125.02   |
| 15  | A     | 1110 | CLA  | C4-C3-C5    | 2.65 | 119.45      | 115.41   |
| 15  | A     | 1116 | CLA  | CMC-C2C-C1C | 2.65 | 129.12      | 125.02   |
| 15  | B     | 1206 | CLA  | O2A-CGA-CBA | 2.65 | 123.42      | 112.36   |
| 15  | B     | 1221 | CLA  | C4A-NA-C1A  | 2.66 | 109.79      | 106.36   |
| 15  | A     | 1129 | CLA  | CMC-C2C-C1C | 2.66 | 129.13      | 125.02   |
| 15  | B     | 1214 | CLA  | CMB-C2B-C3B | 2.66 | 130.29      | 125.09   |
| 14  | B     | 4006 | BCR  | C34-C9-C8   | 2.66 | 122.53      | 118.10   |
| 15  | A     | 1107 | CLA  | CMC-C2C-C1C | 2.66 | 129.14      | 125.02   |
| 17  | B     | 5002 | LMG  | O8-C28-C29  | 2.66 | 120.02      | 111.90   |
| 14  | A     | 4003 | BCR  | C38-C26-C27 | 2.67 | 118.49      | 113.43   |
| 15  | B     | 1234 | CLA  | C5-C3-C2    | 2.67 | 126.12      | 121.05   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 14  | B     | 4009 | BCR  | C33-C5-C4   | 2.68 | 118.51      | 113.43   |
| 14  | A     | 4007 | BCR  | C33-C5-C4   | 2.69 | 118.52      | 113.43   |
| 15  | A     | 1135 | CLA  | CMC-C2C-C1C | 2.69 | 129.18      | 125.02   |
| 15  | A     | 1119 | CLA  | CMC-C2C-C1C | 2.69 | 129.18      | 125.02   |
| 15  | B     | 1224 | CLA  | CMC-C2C-C1C | 2.69 | 129.19      | 125.02   |
| 15  | A     | 1115 | CLA  | CMC-C2C-C1C | 2.70 | 129.19      | 125.02   |
| 14  | A     | 4003 | BCR  | C23-C22-C21 | 2.70 | 123.33      | 118.98   |
| 15  | B     | 1207 | CLA  | O2A-CGA-CBA | 2.70 | 123.62      | 112.36   |
| 15  | B     | 1215 | CLA  | CMC-C2C-C1C | 2.71 | 129.21      | 125.02   |
| 12  | B     | 5004 | LHG  | O8-C23-C24  | 2.71 | 120.16      | 111.90   |
| 14  | A     | 4002 | BCR  | C34-C9-C8   | 2.72 | 122.61      | 118.10   |
| 15  | B     | 1240 | CLA  | CMC-C2C-C1C | 2.72 | 129.22      | 125.02   |
| 15  | A     | 1133 | CLA  | O2A-CGA-CBA | 2.72 | 123.69      | 112.36   |
| 15  | A     | 1126 | CLA  | CMB-C2B-C3B | 2.73 | 130.44      | 125.09   |
| 15  | A     | 1133 | CLA  | CMC-C2C-C1C | 2.74 | 129.25      | 125.02   |
| 14  | A     | 4012 | BCR  | C23-C22-C21 | 2.74 | 123.39      | 118.98   |
| 15  | B     | 1204 | CLA  | CMC-C2C-C1C | 2.74 | 129.26      | 125.02   |
| 15  | B     | 1218 | CLA  | CMC-C2C-C1C | 2.74 | 129.26      | 125.02   |
| 12  | A     | 5005 | LHG  | O8-C23-C24  | 2.74 | 120.25      | 111.90   |
| 15  | A     | 1110 | CLA  | CMC-C2C-C1C | 2.74 | 129.26      | 125.02   |
| 15  | A     | 1102 | CLA  | C4-C3-C5    | 2.74 | 119.59      | 115.41   |
| 15  | B     | 1205 | CLA  | CMC-C2C-C1C | 2.74 | 129.26      | 125.02   |
| 15  | A     | 1117 | CLA  | CMC-C2C-C1C | 2.75 | 129.27      | 125.02   |
| 15  | B     | 1221 | CLA  | CMC-C2C-C1C | 2.75 | 129.27      | 125.02   |
| 15  | A     | 1113 | CLA  | CMC-C2C-C1C | 2.75 | 129.27      | 125.02   |
| 15  | A     | 1111 | CLA  | CMC-C2C-C1C | 2.75 | 129.28      | 125.02   |
| 15  | A     | 1124 | CLA  | CMC-C2C-C1C | 2.75 | 129.28      | 125.02   |
| 15  | B     | 1201 | CLA  | O2A-CGA-CBA | 2.77 | 123.89      | 112.36   |
| 15  | K     | 1402 | CLA  | CMC-C2C-C1C | 2.77 | 129.30      | 125.02   |
| 15  | A     | 1102 | CLA  | CMC-C2C-C1C | 2.77 | 129.31      | 125.02   |
| 15  | A     | 1118 | CLA  | O2A-CGA-CBA | 2.78 | 123.94      | 112.36   |
| 15  | A     | 1129 | CLA  | O2A-CGA-CBA | 2.78 | 123.96      | 112.36   |
| 15  | B     | 1211 | CLA  | O2A-CGA-CBA | 2.79 | 123.99      | 112.36   |
| 15  | A     | 1118 | CLA  | CMC-C2C-C1C | 2.79 | 129.34      | 125.02   |
| 14  | F     | 4016 | BCR  | C38-C26-C27 | 2.79 | 118.72      | 113.43   |
| 15  | A     | 1123 | CLA  | CMC-C2C-C1C | 2.80 | 129.35      | 125.02   |
| 15  | A     | 1134 | CLA  | CMC-C2C-C1C | 2.81 | 129.37      | 125.02   |
| 15  | A     | 1127 | CLA  | CMC-C2C-C1C | 2.81 | 129.37      | 125.02   |
| 15  | A     | 1012 | CLA  | CMC-C2C-C1C | 2.81 | 129.37      | 125.02   |
| 15  | B     | 1212 | CLA  | CMC-C2C-C1C | 2.82 | 129.38      | 125.02   |
| 15  | A     | 1140 | CLA  | CMC-C2C-C1C | 2.82 | 129.38      | 125.02   |
| 15  | B     | 1021 | CLA  | CMC-C2C-C1C | 2.84 | 129.42      | 125.02   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 15  | A     | 1022 | CLA  | C4-C3-C5    | 2.84 | 119.75      | 115.41   |
| 15  | B     | 1222 | CLA  | C4-C3-C5    | 2.85 | 119.76      | 115.41   |
| 15  | K     | 1402 | CLA  | O2A-CGA-CBA | 2.85 | 124.26      | 112.36   |
| 15  | J     | 1302 | CLA  | CMC-C2C-C1C | 2.86 | 129.45      | 125.02   |
| 15  | A     | 1134 | CLA  | O2A-CGA-CBA | 2.86 | 124.30      | 112.36   |
| 15  | B     | 1206 | CLA  | CMC-C2C-C1C | 2.87 | 129.45      | 125.02   |
| 15  | A     | 1121 | CLA  | CMC-C2C-C1C | 2.87 | 129.46      | 125.02   |
| 15  | A     | 1131 | CLA  | CMC-C2C-C1C | 2.87 | 129.46      | 125.02   |
| 15  | B     | 1223 | CLA  | C4-C3-C5    | 2.87 | 119.80      | 115.41   |
| 14  | A     | 4012 | BCR  | C19-C18-C17 | 2.88 | 123.62      | 118.98   |
| 15  | A     | 1138 | CLA  | CMB-C2B-C3B | 2.88 | 130.72      | 125.09   |
| 15  | B     | 1238 | CLA  | CMC-C2C-C1C | 2.88 | 129.48      | 125.02   |
| 15  | A     | 1101 | CLA  | CMC-C2C-C1C | 2.88 | 129.48      | 125.02   |
| 15  | B     | 1204 | CLA  | O2A-CGA-CBA | 2.89 | 124.42      | 112.36   |
| 15  | B     | 1210 | CLA  | CMC-C2C-C1C | 2.90 | 129.50      | 125.02   |
| 15  | B     | 1229 | CLA  | CMC-C2C-C1C | 2.91 | 129.52      | 125.02   |
| 15  | B     | 1220 | CLA  | CMC-C2C-C1C | 2.91 | 129.53      | 125.02   |
| 14  | A     | 4008 | BCR  | C33-C5-C4   | 2.91 | 118.95      | 113.43   |
| 15  | A     | 1124 | CLA  | O2A-CGA-CBA | 2.92 | 120.79      | 111.90   |
| 15  | B     | 1219 | CLA  | CMC-C2C-C1C | 2.92 | 129.53      | 125.02   |
| 15  | A     | 1130 | CLA  | CMC-C2C-C1C | 2.92 | 129.54      | 125.02   |
| 13  | A     | 1011 | CL0  | CMC-C2C-C1C | 2.92 | 129.54      | 125.02   |
| 15  | A     | 1115 | CLA  | O2A-CGA-CBA | 2.93 | 124.56      | 112.36   |
| 15  | B     | 1214 | CLA  | CMC-C2C-C1C | 2.93 | 129.55      | 125.02   |
| 15  | B     | 1222 | CLA  | O2A-CGA-CBA | 2.93 | 120.83      | 111.90   |
| 15  | J     | 1303 | CLA  | O2A-CGA-CBA | 2.93 | 124.58      | 112.36   |
| 15  | A     | 1104 | CLA  | C4-C3-C5    | 2.94 | 119.90      | 115.41   |
| 15  | A     | 1130 | CLA  | CMB-C2B-C3B | 2.95 | 130.86      | 125.09   |
| 14  | B     | 4004 | BCR  | C38-C26-C27 | 2.95 | 119.02      | 113.43   |
| 13  | A     | 1011 | CL0  | CHB-C4A-NA  | 2.96 | 128.61      | 124.51   |
| 15  | A     | 1126 | CLA  | CMC-C2C-C1C | 2.96 | 129.61      | 125.02   |
| 15  | A     | 1138 | CLA  | C4-C3-C5    | 2.97 | 119.95      | 115.41   |
| 15  | A     | 1112 | CLA  | CMC-C2C-C1C | 2.98 | 129.63      | 125.02   |
| 15  | A     | 1022 | CLA  | CMC-C2C-C1C | 2.98 | 129.63      | 125.02   |
| 15  | B     | 1217 | CLA  | CMC-C2C-C1C | 2.98 | 129.64      | 125.02   |
| 15  | A     | 1105 | CLA  | CMC-C2C-C1C | 2.99 | 129.64      | 125.02   |
| 15  | B     | 1216 | CLA  | CMB-C2B-C3B | 2.99 | 130.93      | 125.09   |
| 14  | B     | 4017 | BCR  | C33-C5-C4   | 2.99 | 119.10      | 113.43   |
| 15  | B     | 1217 | CLA  | O2A-C1-C2   | 3.00 | 119.70      | 108.42   |
| 15  | B     | 1201 | CLA  | CMC-C2C-C1C | 3.01 | 129.68      | 125.02   |
| 14  | B     | 4014 | BCR  | C23-C22-C21 | 3.02 | 123.84      | 118.98   |
| 15  | B     | 1223 | CLA  | CMC-C2C-C1C | 3.02 | 129.70      | 125.02   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 15  | A     | 1106 | CLA  | CMC-C2C-C1C | 3.03 | 129.71      | 125.02   |
| 15  | F     | 1301 | CLA  | CMC-C2C-C1C | 3.04 | 129.73      | 125.02   |
| 14  | B     | 4004 | BCR  | C33-C5-C4   | 3.05 | 119.20      | 113.43   |
| 14  | B     | 4017 | BCR  | C38-C26-C27 | 3.05 | 119.21      | 113.43   |
| 15  | A     | 1109 | CLA  | CMC-C2C-C1C | 3.06 | 129.76      | 125.02   |
| 15  | B     | 1239 | CLA  | O2A-CGA-CBA | 3.07 | 125.16      | 112.36   |
| 15  | F     | 1139 | CLA  | CMC-C2C-C1C | 3.07 | 129.77      | 125.02   |
| 15  | A     | 1102 | CLA  | CMB-C2B-C3B | 3.08 | 131.12      | 125.09   |
| 15  | A     | 1122 | CLA  | CMC-C2C-C1C | 3.09 | 129.79      | 125.02   |
| 14  | B     | 4011 | BCR  | C23-C22-C21 | 3.09 | 123.96      | 118.98   |
| 15  | B     | 1213 | CLA  | CMC-C2C-C1C | 3.09 | 129.80      | 125.02   |
| 15  | A     | 1132 | CLA  | C4-C3-C5    | 3.10 | 120.14      | 115.41   |
| 15  | A     | 1103 | CLA  | O2A-CGA-CBA | 3.11 | 121.36      | 111.90   |
| 14  | B     | 4011 | BCR  | C8-C9-C10   | 3.11 | 124.00      | 118.98   |
| 15  | B     | 1237 | CLA  | CMC-C2C-C1C | 3.13 | 129.87      | 125.02   |
| 15  | K     | 1401 | CLA  | O2A-CGA-CBA | 3.14 | 125.44      | 112.36   |
| 15  | B     | 1230 | CLA  | CMC-C2C-C1C | 3.14 | 129.88      | 125.02   |
| 15  | B     | 1219 | CLA  | C4-C3-C5    | 3.15 | 120.22      | 115.41   |
| 15  | B     | 1225 | CLA  | CMC-C2C-C1C | 3.15 | 129.89      | 125.02   |
| 15  | B     | 1210 | CLA  | CMB-C2B-C3B | 3.16 | 131.26      | 125.09   |
| 14  | A     | 4001 | BCR  | C38-C26-C27 | 3.16 | 119.42      | 113.43   |
| 15  | A     | 1121 | CLA  | O2A-CGA-CBA | 3.17 | 125.56      | 112.36   |
| 15  | B     | 1231 | CLA  | C4-C3-C5    | 3.17 | 120.25      | 115.41   |
| 15  | A     | 1012 | CLA  | C4-C3-C5    | 3.17 | 120.25      | 115.41   |
| 15  | A     | 1119 | CLA  | CMB-C2B-C3B | 3.17 | 131.29      | 125.09   |
| 15  | F     | 1410 | CLA  | CMC-C2C-C1C | 3.18 | 129.94      | 125.02   |
| 14  | B     | 4011 | BCR  | C38-C26-C27 | 3.19 | 119.47      | 113.43   |
| 14  | A     | 4002 | BCR  | C19-C18-C17 | 3.19 | 124.12      | 118.98   |
| 10  | A     | 2001 | PQN  | C14-C13-C15 | 3.21 | 120.31      | 115.41   |
| 15  | A     | 1138 | CLA  | CED-O2D-CGD | 3.21 | 123.53      | 115.99   |
| 15  | B     | 1208 | CLA  | CMB-C2B-C3B | 3.22 | 131.39      | 125.09   |
| 15  | A     | 1123 | CLA  | CAC-C3C-C4C | 3.23 | 129.52      | 124.83   |
| 14  | B     | 4006 | BCR  | C33-C5-C4   | 3.23 | 119.56      | 113.43   |
| 14  | F     | 4015 | BCR  | C38-C26-C27 | 3.24 | 119.56      | 113.43   |
| 14  | B     | 4017 | BCR  | C19-C18-C17 | 3.24 | 124.20      | 118.98   |
| 14  | A     | 4003 | BCR  | C33-C5-C4   | 3.26 | 119.61      | 113.43   |
| 14  | F     | 4016 | BCR  | C12-C13-C14 | 3.27 | 124.26      | 118.98   |
| 14  | B     | 4005 | BCR  | C19-C18-C17 | 3.29 | 124.28      | 118.98   |
| 14  | J     | 4013 | BCR  | C38-C26-C27 | 3.29 | 119.66      | 113.43   |
| 14  | J     | 4013 | BCR  | C33-C5-C4   | 3.29 | 119.67      | 113.43   |
| 15  | B     | 1235 | CLA  | CMC-C2C-C1C | 3.30 | 130.13      | 125.02   |
| 14  | B     | 4009 | BCR  | C19-C18-C17 | 3.30 | 124.31      | 118.98   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 15  | A     | 1122 | CLA  | O2A-CGA-CBA | 3.30 | 121.97      | 111.90   |
| 15  | B     | 1220 | CLA  | CMB-C2B-C3B | 3.32 | 131.59      | 125.09   |
| 15  | B     | 1211 | CLA  | CMC-C2C-C1C | 3.35 | 130.21      | 125.02   |
| 15  | A     | 1125 | CLA  | CMC-C2C-C1C | 3.36 | 130.21      | 125.02   |
| 14  | A     | 4001 | BCR  | C19-C18-C17 | 3.36 | 124.39      | 118.98   |
| 14  | B     | 4009 | BCR  | C38-C26-C27 | 3.40 | 119.88      | 113.43   |
| 15  | B     | 1203 | CLA  | O2A-CGA-CBA | 3.43 | 122.35      | 111.90   |
| 15  | A     | 1101 | CLA  | O2A-CGA-CBA | 3.44 | 122.37      | 111.90   |
| 15  | B     | 1216 | CLA  | O2A-CGA-CBA | 3.45 | 122.40      | 111.90   |
| 15  | A     | 1104 | CLA  | CMC-C2C-C1C | 3.46 | 130.38      | 125.02   |
| 15  | B     | 1225 | CLA  | O2A-CGA-CBA | 3.46 | 122.46      | 111.90   |
| 15  | B     | 1228 | CLA  | CMB-C2B-C3B | 3.47 | 131.87      | 125.09   |
| 14  | B     | 4011 | BCR  | C33-C5-C4   | 3.55 | 120.16      | 113.43   |
| 15  | A     | 1138 | CLA  | CMC-C2C-C1C | 3.56 | 130.52      | 125.02   |
| 15  | F     | 1139 | CLA  | O2A-CGA-CBA | 3.57 | 122.79      | 111.90   |
| 14  | A     | 4007 | BCR  | C38-C26-C27 | 3.60 | 120.26      | 113.43   |
| 15  | A     | 1135 | CLA  | C4-C3-C5    | 3.64 | 120.97      | 115.41   |
| 15  | A     | 1126 | CLA  | O2A-CGA-CBA | 3.65 | 123.01      | 111.90   |
| 14  | A     | 4002 | BCR  | C38-C26-C27 | 3.67 | 120.38      | 113.43   |
| 14  | B     | 4004 | BCR  | C19-C18-C17 | 3.69 | 124.92      | 118.98   |
| 15  | B     | 1237 | CLA  | O2A-CGA-CBA | 3.69 | 123.15      | 111.90   |
| 15  | A     | 1138 | CLA  | O2A-CGA-CBA | 3.70 | 123.18      | 111.90   |
| 15  | F     | 1410 | CLA  | O2A-CGA-CBA | 3.72 | 123.22      | 111.90   |
| 15  | A     | 1105 | CLA  | O2A-CGA-CBA | 3.74 | 123.28      | 111.90   |
| 15  | A     | 1106 | CLA  | O2A-CGA-CBA | 3.74 | 123.30      | 111.90   |
| 15  | A     | 1128 | CLA  | O2A-CGA-CBA | 3.75 | 123.33      | 111.90   |
| 15  | A     | 1123 | CLA  | O2A-CGA-CBA | 3.75 | 123.34      | 111.90   |
| 15  | B     | 1219 | CLA  | CMB-C2B-C3B | 3.76 | 132.45      | 125.09   |
| 15  | A     | 1012 | CLA  | O2A-CGA-CBA | 3.77 | 123.39      | 111.90   |
| 15  | B     | 1213 | CLA  | O2A-CGA-CBA | 3.80 | 123.47      | 111.90   |
| 15  | B     | 1237 | CLA  | C4-C3-C5    | 3.83 | 121.25      | 115.41   |
| 15  | B     | 1229 | CLA  | O2A-CGA-CBA | 3.84 | 123.59      | 111.90   |
| 15  | A     | 1022 | CLA  | O2A-CGA-CBA | 3.84 | 123.61      | 111.90   |
| 14  | A     | 4008 | BCR  | C38-C26-C27 | 3.85 | 120.73      | 113.43   |
| 12  | A     | 5005 | LHG  | O7-C7-C8    | 3.86 | 119.91      | 111.53   |
| 15  | B     | 1023 | CLA  | O2A-CGA-CBA | 3.87 | 123.69      | 111.90   |
| 15  | B     | 1228 | CLA  | O2A-CGA-CBA | 3.87 | 123.70      | 111.90   |
| 15  | B     | 1220 | CLA  | O2A-CGA-CBA | 3.88 | 123.72      | 111.90   |
| 15  | A     | 1125 | CLA  | O2A-CGA-CBA | 3.90 | 123.80      | 111.90   |
| 15  | A     | 1114 | CLA  | O2A-CGA-CBA | 3.91 | 123.80      | 111.90   |
| 17  | B     | 5002 | LMG  | O7-C10-C11  | 3.95 | 120.11      | 111.53   |
| 13  | A     | 1011 | CL0  | O2A-CGA-CBA | 3.97 | 124.00      | 111.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 15  | A     | 1140 | CLA  | O2A-CGA-CBA | 3.99 | 124.07      | 111.90   |
| 15  | B     | 1234 | CLA  | O2A-CGA-CBA | 4.00 | 124.08      | 111.90   |
| 15  | A     | 1127 | CLA  | O2A-CGA-CBA | 4.00 | 124.08      | 111.90   |
| 13  | A     | 1108 | CL0  | CMC-C2C-C1C | 4.00 | 131.21      | 125.02   |
| 15  | B     | 1236 | CLA  | O2A-CGA-CBA | 4.00 | 124.09      | 111.90   |
| 12  | A     | 5001 | LHG  | O7-C7-C8    | 4.00 | 120.23      | 111.53   |
| 15  | A     | 1117 | CLA  | O2A-CGA-CBA | 4.01 | 124.10      | 111.90   |
| 15  | B     | 1215 | CLA  | O2A-CGA-CBA | 4.02 | 124.14      | 111.90   |
| 15  | B     | 1226 | CLA  | O2A-CGA-CBA | 4.02 | 124.15      | 111.90   |
| 15  | A     | 1110 | CLA  | O2A-CGA-CBA | 4.03 | 124.17      | 111.90   |
| 15  | B     | 1219 | CLA  | O2A-CGA-CBA | 4.04 | 124.20      | 111.90   |
| 15  | B     | 1223 | CLA  | O2A-CGA-CBA | 4.05 | 124.22      | 111.90   |
| 15  | A     | 1127 | CLA  | C4-C3-C5    | 4.07 | 121.62      | 115.41   |
| 15  | A     | 1137 | CLA  | O2A-CGA-CBA | 4.08 | 124.32      | 111.90   |
| 15  | B     | 1202 | CLA  | O2A-CGA-CBA | 4.09 | 124.35      | 111.90   |
| 15  | B     | 1205 | CLA  | O2A-CGA-CBA | 4.10 | 124.39      | 111.90   |
| 15  | A     | 1135 | CLA  | O2A-CGA-CBA | 4.11 | 124.41      | 111.90   |
| 15  | A     | 1107 | CLA  | O2A-CGA-CBA | 4.11 | 124.42      | 111.90   |
| 15  | A     | 1130 | CLA  | O2A-CGA-CBA | 4.18 | 124.63      | 111.90   |
| 15  | B     | 1217 | CLA  | O2A-CGA-CBA | 4.19 | 124.65      | 111.90   |
| 15  | A     | 1109 | CLA  | O2A-CGA-CBA | 4.19 | 124.67      | 111.90   |
| 15  | A     | 1120 | CLA  | O2A-CGA-CBA | 4.20 | 124.71      | 111.90   |
| 15  | A     | 1116 | CLA  | O2A-CGA-CBA | 4.23 | 124.79      | 111.90   |
| 15  | A     | 1102 | CLA  | O2A-CGA-CBA | 4.24 | 124.81      | 111.90   |
| 15  | B     | 1236 | CLA  | CMC-C2C-C1C | 4.25 | 131.60      | 125.02   |
| 15  | B     | 1214 | CLA  | O2A-CGA-CBA | 4.27 | 124.92      | 111.90   |
| 15  | B     | 1235 | CLA  | O2A-CGA-CBA | 4.28 | 124.95      | 111.90   |
| 15  | B     | 1210 | CLA  | O2A-CGA-CBA | 4.29 | 124.96      | 111.90   |
| 15  | B     | 1231 | CLA  | O2A-CGA-CBA | 4.29 | 124.98      | 111.90   |
| 15  | A     | 1114 | CLA  | O2A-C1-C2   | 4.29 | 119.89      | 109.05   |
| 15  | B     | 1021 | CLA  | O2A-CGA-CBA | 4.30 | 125.00      | 111.90   |
| 15  | A     | 1119 | CLA  | O2A-CGA-CBA | 4.34 | 125.11      | 111.90   |
| 10  | B     | 2002 | PQN  | C14-C13-C15 | 4.36 | 122.06      | 115.41   |
| 15  | B     | 1230 | CLA  | O2A-CGA-CBA | 4.36 | 125.19      | 111.90   |
| 15  | B     | 1013 | CLA  | O2A-CGA-CBA | 4.37 | 125.22      | 111.90   |
| 15  | A     | 1111 | CLA  | O2A-CGA-CBA | 4.38 | 125.23      | 111.90   |
| 15  | A     | 1119 | CLA  | O2A-C1-C2   | 4.42 | 120.21      | 109.05   |
| 15  | A     | 1104 | CLA  | O2A-CGA-CBA | 4.42 | 125.38      | 111.90   |
| 15  | A     | 1801 | CLA  | O2A-CGA-CBA | 4.42 | 125.38      | 111.90   |
| 15  | B     | 1218 | CLA  | O2A-CGA-CBA | 4.43 | 125.39      | 111.90   |
| 12  | A     | 5003 | LHG  | O7-C7-C8    | 4.45 | 121.21      | 111.53   |
| 15  | A     | 1120 | CLA  | O2A-C1-C2   | 4.46 | 120.29      | 109.05   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 12  | B     | 5004 | LHG  | O7-C7-C8    | 4.53 | 121.38      | 111.53   |
| 15  | B     | 1224 | CLA  | O2A-CGA-CBA | 4.54 | 125.72      | 111.90   |
| 15  | B     | 1214 | CLA  | C4-C3-C5    | 4.57 | 122.39      | 115.41   |
| 15  | A     | 1132 | CLA  | O2A-CGA-CBA | 4.58 | 125.86      | 111.90   |
| 15  | A     | 1131 | CLA  | O2A-CGA-CBA | 4.59 | 125.89      | 111.90   |
| 15  | A     | 1136 | CLA  | O2A-CGA-CBA | 4.68 | 126.17      | 111.90   |
| 15  | B     | 1221 | CLA  | O2A-CGA-CBA | 4.80 | 126.52      | 111.90   |
| 15  | A     | 1122 | CLA  | C4-C3-C5    | 4.86 | 122.83      | 115.41   |
| 13  | A     | 1108 | CL0  | O2D-CGD-CBD | 4.93 | 118.06      | 111.30   |
| 15  | B     | 1215 | CLA  | C4-C3-C5    | 5.23 | 123.40      | 115.41   |
| 15  | A     | 1134 | CLA  | O2D-CGD-CBD | 5.26 | 118.52      | 111.30   |
| 15  | B     | 1225 | CLA  | C4-C3-C5    | 5.29 | 123.49      | 115.41   |
| 15  | A     | 1109 | CLA  | C4-C3-C5    | 5.39 | 123.63      | 115.41   |
| 15  | F     | 1410 | CLA  | C4-C3-C5    | 5.56 | 123.90      | 115.41   |
| 15  | B     | 1013 | CLA  | O2D-CGD-CBD | 5.68 | 119.08      | 111.30   |
| 15  | B     | 1232 | CLA  | O2D-CGD-CBD | 5.74 | 119.18      | 111.30   |
| 15  | A     | 1138 | CLA  | C2C-C1C-NC  | 5.76 | 114.53      | 110.24   |
| 15  | A     | 1109 | CLA  | O2D-CGD-CBD | 5.83 | 119.30      | 111.30   |
| 15  | K     | 1402 | CLA  | O2D-CGD-CBD | 5.84 | 119.31      | 111.30   |
| 15  | B     | 1230 | CLA  | C4-C3-C5    | 5.87 | 124.37      | 115.41   |
| 15  | B     | 1021 | CLA  | O2D-CGD-CBD | 5.95 | 119.46      | 111.30   |
| 15  | B     | 1023 | CLA  | O2D-CGD-CBD | 6.00 | 119.53      | 111.30   |
| 15  | A     | 1801 | CLA  | O2D-CGD-CBD | 6.00 | 119.53      | 111.30   |
| 15  | A     | 1110 | CLA  | O2D-CGD-CBD | 6.01 | 119.55      | 111.30   |
| 15  | A     | 1135 | CLA  | O2D-CGD-CBD | 6.03 | 119.57      | 111.30   |
| 15  | B     | 1206 | CLA  | O2D-CGD-CBD | 6.03 | 119.57      | 111.30   |
| 14  | B     | 4004 | BCR  | C20-C19-C18 | 6.05 | 144.12      | 126.32   |
| 15  | B     | 1231 | CLA  | O2D-CGD-CBD | 6.05 | 119.60      | 111.30   |
| 15  | A     | 1124 | CLA  | O2D-CGD-CBD | 6.06 | 119.62      | 111.30   |
| 15  | A     | 1113 | CLA  | O2D-CGD-CBD | 6.07 | 119.63      | 111.30   |
| 15  | B     | 1240 | CLA  | O2D-CGD-CBD | 6.08 | 119.64      | 111.30   |
| 15  | B     | 1228 | CLA  | O2D-CGD-CBD | 6.08 | 119.64      | 111.30   |
| 15  | A     | 1120 | CLA  | O2D-CGD-CBD | 6.08 | 119.64      | 111.30   |
| 15  | B     | 1218 | CLA  | C4-C3-C5    | 6.11 | 122.60      | 115.68   |
| 15  | A     | 1138 | CLA  | O2D-CGD-CBD | 6.11 | 119.68      | 111.30   |
| 15  | F     | 1139 | CLA  | O2D-CGD-CBD | 6.12 | 119.69      | 111.30   |
| 15  | B     | 1203 | CLA  | O2D-CGD-CBD | 6.17 | 119.77      | 111.30   |
| 15  | B     | 1208 | CLA  | O2D-CGD-CBD | 6.23 | 119.84      | 111.30   |
| 14  | A     | 4001 | BCR  | C20-C19-C18 | 6.23 | 144.66      | 126.32   |
| 15  | A     | 1127 | CLA  | O2D-CGD-CBD | 6.23 | 119.85      | 111.30   |
| 15  | B     | 1220 | CLA  | O2D-CGD-CBD | 6.24 | 119.86      | 111.30   |
| 15  | A     | 1117 | CLA  | O2D-CGD-CBD | 6.25 | 119.87      | 111.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 15  | B     | 1216 | CLA  | O2D-CGD-CBD | 6.26 | 119.89      | 111.30   |
| 15  | J     | 1302 | CLA  | O2D-CGD-CBD | 6.27 | 119.89      | 111.30   |
| 15  | B     | 1238 | CLA  | O2D-CGD-CBD | 6.27 | 119.90      | 111.30   |
| 15  | B     | 1210 | CLA  | O2D-CGD-CBD | 6.30 | 119.94      | 111.30   |
| 15  | A     | 1119 | CLA  | O2D-CGD-CBD | 6.32 | 119.97      | 111.30   |
| 15  | A     | 1122 | CLA  | O2D-CGD-CBD | 6.33 | 119.98      | 111.30   |
| 15  | K     | 1401 | CLA  | O2D-CGD-CBD | 6.34 | 119.99      | 111.30   |
| 15  | B     | 1225 | CLA  | O2D-CGD-CBD | 6.35 | 120.01      | 111.30   |
| 15  | B     | 1237 | CLA  | O2D-CGD-CBD | 6.38 | 120.05      | 111.30   |
| 14  | B     | 4005 | BCR  | C20-C19-C18 | 6.38 | 145.09      | 126.32   |
| 14  | A     | 4012 | BCR  | C20-C19-C18 | 6.38 | 145.10      | 126.32   |
| 15  | J     | 1303 | CLA  | O2D-CGD-CBD | 6.38 | 120.06      | 111.30   |
| 14  | A     | 4002 | BCR  | C20-C19-C18 | 6.40 | 145.15      | 126.32   |
| 15  | A     | 1111 | CLA  | O2D-CGD-CBD | 6.41 | 120.09      | 111.30   |
| 14  | B     | 4017 | BCR  | C20-C19-C18 | 6.41 | 145.18      | 126.32   |
| 14  | B     | 4009 | BCR  | C20-C19-C18 | 6.41 | 145.19      | 126.32   |
| 15  | A     | 1121 | CLA  | O2D-CGD-CBD | 6.42 | 120.11      | 111.30   |
| 15  | A     | 1126 | CLA  | C2C-C1C-NC  | 6.45 | 115.05      | 110.24   |
| 15  | A     | 1125 | CLA  | C2C-C1C-NC  | 6.46 | 115.05      | 110.24   |
| 15  | A     | 1104 | CLA  | O2D-CGD-CBD | 6.49 | 120.20      | 111.30   |
| 15  | B     | 1229 | CLA  | O2D-CGD-CBD | 6.49 | 120.20      | 111.30   |
| 15  | A     | 1022 | CLA  | O2D-CGD-CBD | 6.50 | 120.22      | 111.30   |
| 15  | F     | 1301 | CLA  | O2D-CGD-CBD | 6.51 | 120.23      | 111.30   |
| 15  | B     | 1204 | CLA  | O2D-CGD-CBD | 6.52 | 120.25      | 111.30   |
| 15  | A     | 1133 | CLA  | O2D-CGD-CBD | 6.53 | 120.26      | 111.30   |
| 15  | A     | 1115 | CLA  | O2D-CGD-CBD | 6.54 | 120.27      | 111.30   |
| 15  | A     | 1103 | CLA  | O2D-CGD-CBD | 6.57 | 120.31      | 111.30   |
| 15  | B     | 1236 | CLA  | C2C-C1C-NC  | 6.57 | 115.14      | 110.24   |
| 14  | A     | 4003 | BCR  | C20-C19-C18 | 6.61 | 145.77      | 126.32   |
| 15  | A     | 1012 | CLA  | O2D-CGD-CBD | 6.69 | 120.48      | 111.30   |
| 15  | A     | 1107 | CLA  | C2C-C1C-NC  | 6.70 | 115.23      | 110.24   |
| 15  | A     | 1107 | CLA  | O2D-CGD-CBD | 6.71 | 120.50      | 111.30   |
| 15  | B     | 1213 | CLA  | O2D-CGD-CBD | 6.72 | 120.51      | 111.30   |
| 15  | A     | 1129 | CLA  | O2D-CGD-CBD | 6.73 | 120.54      | 111.30   |
| 15  | A     | 1140 | CLA  | O2D-CGD-CBD | 6.74 | 120.55      | 111.30   |
| 15  | B     | 1207 | CLA  | O2D-CGD-CBD | 6.74 | 120.55      | 111.30   |
| 15  | B     | 1219 | CLA  | O2D-CGD-CBD | 6.75 | 120.56      | 111.30   |
| 15  | B     | 1218 | CLA  | O2D-CGD-CBD | 6.78 | 120.60      | 111.30   |
| 15  | A     | 1122 | CLA  | C2C-C1C-NC  | 6.80 | 115.30      | 110.24   |
| 15  | B     | 1228 | CLA  | C2C-C1C-NC  | 6.81 | 115.31      | 110.24   |
| 15  | B     | 1239 | CLA  | O2D-CGD-CBD | 6.84 | 120.68      | 111.30   |
| 15  | A     | 1109 | CLA  | C2C-C1C-NC  | 6.84 | 115.33      | 110.24   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 15  | B     | 1223 | CLA  | O2D-CGD-CBD | 6.87 | 120.72      | 111.30   |
| 15  | A     | 1136 | CLA  | O2D-CGD-CBD | 6.87 | 120.72      | 111.30   |
| 15  | B     | 1235 | CLA  | C2C-C1C-NC  | 6.89 | 115.37      | 110.24   |
| 15  | B     | 1230 | CLA  | O2D-CGD-CBD | 6.91 | 120.78      | 111.30   |
| 15  | A     | 1103 | CLA  | C2C-C1C-NC  | 6.91 | 115.39      | 110.24   |
| 15  | A     | 1114 | CLA  | O2D-CGD-CBD | 6.92 | 120.79      | 111.30   |
| 15  | A     | 1112 | CLA  | O2D-CGD-CBD | 6.92 | 120.80      | 111.30   |
| 15  | A     | 1118 | CLA  | O2D-CGD-CBD | 6.93 | 120.81      | 111.30   |
| 15  | B     | 1215 | CLA  | O2D-CGD-CBD | 6.94 | 120.82      | 111.30   |
| 15  | B     | 1214 | CLA  | O2D-CGD-CBD | 6.95 | 120.84      | 111.30   |
| 15  | B     | 1236 | CLA  | O2D-CGD-CBD | 6.96 | 120.84      | 111.30   |
| 15  | A     | 1101 | CLA  | C2C-C1C-NC  | 6.97 | 115.43      | 110.24   |
| 15  | A     | 1140 | CLA  | C2C-C1C-NC  | 6.97 | 115.43      | 110.24   |
| 15  | A     | 1130 | CLA  | C2C-C1C-NC  | 6.97 | 115.43      | 110.24   |
| 14  | B     | 4014 | BCR  | C20-C19-C18 | 7.02 | 146.97      | 126.32   |
| 15  | B     | 1202 | CLA  | O2D-CGD-CBD | 7.02 | 120.93      | 111.30   |
| 15  | F     | 1410 | CLA  | O2D-CGD-CBD | 7.02 | 120.93      | 111.30   |
| 15  | B     | 1234 | CLA  | O2D-CGD-CBD | 7.03 | 120.94      | 111.30   |
| 15  | B     | 1220 | CLA  | C2C-C1C-NC  | 7.04 | 115.48      | 110.24   |
| 15  | A     | 1111 | CLA  | C2C-C1C-NC  | 7.05 | 115.49      | 110.24   |
| 15  | B     | 1210 | CLA  | C2C-C1C-NC  | 7.05 | 115.49      | 110.24   |
| 15  | B     | 1235 | CLA  | O2D-CGD-CBD | 7.05 | 120.97      | 111.30   |
| 15  | A     | 1105 | CLA  | O2D-CGD-CBD | 7.05 | 120.97      | 111.30   |
| 15  | B     | 1209 | CLA  | O2D-CGD-CBD | 7.05 | 120.98      | 111.30   |
| 15  | B     | 1013 | CLA  | C2C-C1C-NC  | 7.06 | 115.50      | 110.24   |
| 15  | A     | 1116 | CLA  | O2D-CGD-CBD | 7.09 | 121.03      | 111.30   |
| 15  | A     | 1130 | CLA  | O2D-CGD-CBD | 7.15 | 121.11      | 111.30   |
| 15  | A     | 1104 | CLA  | C2C-C1C-NC  | 7.16 | 115.58      | 110.24   |
| 15  | B     | 1211 | CLA  | C2C-C1C-NC  | 7.17 | 115.58      | 110.24   |
| 15  | A     | 1117 | CLA  | C2C-C1C-NC  | 7.17 | 115.58      | 110.24   |
| 15  | B     | 1217 | CLA  | O2D-CGD-CBD | 7.18 | 121.16      | 111.30   |
| 15  | B     | 1214 | CLA  | C2C-C1C-NC  | 7.20 | 115.60      | 110.24   |
| 15  | B     | 1224 | CLA  | O2D-CGD-CBD | 7.25 | 121.24      | 111.30   |
| 15  | B     | 1223 | CLA  | C2C-C1C-NC  | 7.25 | 115.64      | 110.24   |
| 14  | F     | 4015 | BCR  | C20-C19-C18 | 7.25 | 147.67      | 126.32   |
| 15  | A     | 1115 | CLA  | C2C-C1C-NC  | 7.25 | 115.64      | 110.24   |
| 15  | F     | 1301 | CLA  | C2C-C1C-NC  | 7.28 | 115.66      | 110.24   |
| 15  | A     | 1137 | CLA  | O2D-CGD-CBD | 7.28 | 121.29      | 111.30   |
| 15  | A     | 1102 | CLA  | O2D-CGD-CBD | 7.30 | 121.32      | 111.30   |
| 15  | A     | 1126 | CLA  | O2D-CGD-CBD | 7.33 | 121.36      | 111.30   |
| 15  | A     | 1106 | CLA  | C2C-C1C-NC  | 7.34 | 115.70      | 110.24   |
| 15  | B     | 1213 | CLA  | C2C-C1C-NC  | 7.34 | 115.70      | 110.24   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 13  | A     | 1011 | CL0  | O2D-CGD-CBD | 7.35 | 121.38      | 111.30   |
| 15  | A     | 1102 | CLA  | C2C-C1C-NC  | 7.36 | 115.72      | 110.24   |
| 15  | B     | 1212 | CLA  | O2D-CGD-CBD | 7.40 | 121.45      | 111.30   |
| 15  | A     | 1132 | CLA  | C2C-C1C-NC  | 7.41 | 115.76      | 110.24   |
| 15  | A     | 1132 | CLA  | O2D-CGD-CBD | 7.41 | 121.46      | 111.30   |
| 15  | B     | 1230 | CLA  | C2C-C1C-NC  | 7.41 | 115.76      | 110.24   |
| 15  | A     | 1112 | CLA  | C2C-C1C-NC  | 7.42 | 115.76      | 110.24   |
| 15  | A     | 1119 | CLA  | C2C-C1C-NC  | 7.43 | 115.77      | 110.24   |
| 15  | B     | 1202 | CLA  | C2C-C1C-NC  | 7.46 | 115.79      | 110.24   |
| 15  | B     | 1221 | CLA  | O2D-CGD-CBD | 7.46 | 121.54      | 111.30   |
| 15  | B     | 1211 | CLA  | O2D-CGD-CBD | 7.47 | 121.55      | 111.30   |
| 15  | B     | 1021 | CLA  | C2C-C1C-NC  | 7.48 | 115.81      | 110.24   |
| 15  | B     | 1240 | CLA  | C2C-C1C-NC  | 7.48 | 115.81      | 110.24   |
| 15  | B     | 1208 | CLA  | C2C-C1C-NC  | 7.50 | 115.83      | 110.24   |
| 15  | F     | 1410 | CLA  | C2C-C1C-NC  | 7.52 | 115.84      | 110.24   |
| 15  | A     | 1134 | CLA  | C2C-C1C-NC  | 7.52 | 115.84      | 110.24   |
| 15  | B     | 1023 | CLA  | C2C-C1C-NC  | 7.53 | 115.85      | 110.24   |
| 15  | B     | 1237 | CLA  | C2C-C1C-NC  | 7.55 | 115.86      | 110.24   |
| 15  | F     | 1139 | CLA  | C2C-C1C-NC  | 7.55 | 115.86      | 110.24   |
| 13  | A     | 1108 | CL0  | C2C-C1C-NC  | 7.55 | 115.87      | 110.24   |
| 15  | B     | 1227 | CLA  | O2D-CGD-CBD | 7.55 | 121.66      | 111.30   |
| 15  | B     | 1218 | CLA  | C2C-C1C-NC  | 7.56 | 115.87      | 110.24   |
| 15  | B     | 1219 | CLA  | C2C-C1C-NC  | 7.56 | 115.87      | 110.24   |
| 15  | B     | 1224 | CLA  | C2C-C1C-NC  | 7.56 | 115.88      | 110.24   |
| 15  | B     | 1201 | CLA  | C2C-C1C-NC  | 7.57 | 115.88      | 110.24   |
| 15  | B     | 1216 | CLA  | C2C-C1C-NC  | 7.57 | 115.88      | 110.24   |
| 15  | A     | 1131 | CLA  | O2D-CGD-CBD | 7.58 | 121.70      | 111.30   |
| 15  | B     | 1217 | CLA  | C2C-C1C-NC  | 7.59 | 115.89      | 110.24   |
| 15  | B     | 1212 | CLA  | C2C-C1C-NC  | 7.59 | 115.89      | 110.24   |
| 15  | B     | 1229 | CLA  | C2C-C1C-NC  | 7.60 | 115.90      | 110.24   |
| 14  | B     | 4011 | BCR  | C20-C19-C18 | 7.60 | 148.69      | 126.32   |
| 15  | A     | 1022 | CLA  | C2C-C1C-NC  | 7.62 | 115.92      | 110.24   |
| 15  | A     | 1124 | CLA  | C2C-C1C-NC  | 7.66 | 115.94      | 110.24   |
| 15  | B     | 1206 | CLA  | C2C-C1C-NC  | 7.66 | 115.94      | 110.24   |
| 14  | J     | 4013 | BCR  | C20-C19-C18 | 7.66 | 148.86      | 126.32   |
| 15  | A     | 1118 | CLA  | C2C-C1C-NC  | 7.66 | 115.95      | 110.24   |
| 15  | K     | 1401 | CLA  | C2C-C1C-NC  | 7.68 | 115.96      | 110.24   |
| 14  | B     | 4006 | BCR  | C20-C19-C18 | 7.69 | 148.96      | 126.32   |
| 15  | B     | 1234 | CLA  | C2C-C1C-NC  | 7.70 | 115.98      | 110.24   |
| 15  | A     | 1129 | CLA  | C2C-C1C-NC  | 7.72 | 115.99      | 110.24   |
| 15  | A     | 1121 | CLA  | C2C-C1C-NC  | 7.74 | 116.00      | 110.24   |
| 15  | A     | 1125 | CLA  | O2D-CGD-CBD | 7.76 | 121.94      | 111.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 15  | B     | 1238 | CLA  | C2C-C1C-NC  | 7.76 | 116.02      | 110.24   |
| 15  | K     | 1402 | CLA  | C2C-C1C-NC  | 7.76 | 116.02      | 110.24   |
| 15  | A     | 1116 | CLA  | C2C-C1C-NC  | 7.77 | 116.03      | 110.24   |
| 15  | A     | 1127 | CLA  | C2C-C1C-NC  | 7.77 | 116.03      | 110.24   |
| 15  | A     | 1114 | CLA  | C2C-C1C-NC  | 7.78 | 116.04      | 110.24   |
| 15  | B     | 1226 | CLA  | C2C-C1C-NC  | 7.78 | 116.04      | 110.24   |
| 15  | B     | 1225 | CLA  | C2C-C1C-NC  | 7.79 | 116.04      | 110.24   |
| 15  | A     | 1110 | CLA  | C2C-C1C-NC  | 7.79 | 116.05      | 110.24   |
| 15  | B     | 1222 | CLA  | C2C-C1C-NC  | 7.81 | 116.05      | 110.24   |
| 15  | J     | 1303 | CLA  | C2C-C1C-NC  | 7.84 | 116.08      | 110.24   |
| 15  | B     | 1204 | CLA  | C2C-C1C-NC  | 7.85 | 116.09      | 110.24   |
| 15  | A     | 1012 | CLA  | C2C-C1C-NC  | 7.87 | 116.10      | 110.24   |
| 15  | A     | 1101 | CLA  | O2D-CGD-CBD | 7.87 | 122.10      | 111.30   |
| 15  | B     | 1205 | CLA  | C2C-C1C-NC  | 7.90 | 116.12      | 110.24   |
| 15  | B     | 1227 | CLA  | C2C-C1C-NC  | 7.90 | 116.13      | 110.24   |
| 15  | A     | 1105 | CLA  | C2C-C1C-NC  | 7.91 | 116.13      | 110.24   |
| 15  | A     | 1113 | CLA  | C2C-C1C-NC  | 7.92 | 116.14      | 110.24   |
| 15  | B     | 1201 | CLA  | O2D-CGD-CBD | 7.92 | 122.17      | 111.30   |
| 15  | B     | 1221 | CLA  | C2C-C1C-NC  | 7.93 | 116.14      | 110.24   |
| 15  | A     | 1120 | CLA  | C2C-C1C-NC  | 7.93 | 116.15      | 110.24   |
| 15  | B     | 1209 | CLA  | C2C-C1C-NC  | 7.97 | 116.17      | 110.24   |
| 15  | A     | 1123 | CLA  | O2D-CGD-CBD | 7.98 | 122.25      | 111.30   |
| 15  | J     | 1302 | CLA  | C2C-C1C-NC  | 8.00 | 116.20      | 110.24   |
| 15  | B     | 1232 | CLA  | C2C-C1C-NC  | 8.01 | 116.21      | 110.24   |
| 15  | A     | 1133 | CLA  | C2C-C1C-NC  | 8.02 | 116.21      | 110.24   |
| 15  | A     | 1801 | CLA  | C2C-C1C-NC  | 8.02 | 116.21      | 110.24   |
| 15  | B     | 1231 | CLA  | C2C-C1C-NC  | 8.04 | 116.23      | 110.24   |
| 15  | A     | 1137 | CLA  | C2C-C1C-NC  | 8.06 | 116.24      | 110.24   |
| 15  | A     | 1136 | CLA  | C2C-C1C-NC  | 8.08 | 116.26      | 110.24   |
| 15  | A     | 1123 | CLA  | C2C-C1C-NC  | 8.10 | 116.27      | 110.24   |
| 15  | A     | 1128 | CLA  | C2C-C1C-NC  | 8.13 | 116.30      | 110.24   |
| 15  | A     | 1128 | CLA  | O2D-CGD-CBD | 8.13 | 122.46      | 111.30   |
| 14  | B     | 4010 | BCR  | C20-C19-C18 | 8.14 | 150.28      | 126.32   |
| 14  | A     | 4008 | BCR  | C20-C19-C18 | 8.15 | 150.30      | 126.32   |
| 15  | A     | 1131 | CLA  | C2C-C1C-NC  | 8.17 | 116.32      | 110.24   |
| 15  | B     | 1203 | CLA  | C2C-C1C-NC  | 8.17 | 116.33      | 110.24   |
| 15  | B     | 1207 | CLA  | C2C-C1C-NC  | 8.18 | 116.33      | 110.24   |
| 15  | A     | 1135 | CLA  | C2C-C1C-NC  | 8.20 | 116.35      | 110.24   |
| 14  | A     | 4007 | BCR  | C20-C19-C18 | 8.24 | 150.57      | 126.32   |
| 14  | F     | 4016 | BCR  | C20-C19-C18 | 8.24 | 150.57      | 126.32   |
| 13  | A     | 1011 | CL0  | C2C-C1C-NC  | 8.25 | 116.38      | 110.24   |
| 15  | A     | 1106 | CLA  | O2D-CGD-CBD | 8.32 | 122.71      | 111.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15  | B     | 1239 | CLA  | C2C-C1C-NC  | 8.33  | 116.45      | 110.24   |
| 15  | B     | 1215 | CLA  | C2C-C1C-NC  | 8.34  | 116.45      | 110.24   |
| 14  | F     | 4016 | BCR  | C11-C12-C13 | 8.48  | 151.27      | 126.32   |
| 15  | B     | 1226 | CLA  | O2D-CGD-CBD | 8.59  | 123.08      | 111.30   |
| 15  | B     | 1205 | CLA  | O2D-CGD-CBD | 8.66  | 123.18      | 111.30   |
| 15  | B     | 1222 | CLA  | O2D-CGD-CBD | 8.79  | 123.35      | 111.30   |
| 14  | B     | 4009 | BCR  | C11-C12-C13 | 9.11  | 153.13      | 126.32   |
| 14  | A     | 4001 | BCR  | C11-C12-C13 | 9.23  | 153.49      | 126.32   |
| 14  | B     | 4014 | BCR  | C11-C12-C13 | 9.94  | 155.58      | 126.32   |
| 14  | A     | 4003 | BCR  | C11-C12-C13 | 10.05 | 155.91      | 126.32   |
| 14  | B     | 4017 | BCR  | C11-C12-C13 | 10.08 | 155.99      | 126.32   |
| 14  | B     | 4004 | BCR  | C11-C12-C13 | 10.27 | 156.54      | 126.32   |
| 14  | B     | 4006 | BCR  | C11-C12-C13 | 10.37 | 156.85      | 126.32   |
| 14  | B     | 4010 | BCR  | C11-C12-C13 | 10.37 | 156.85      | 126.32   |
| 14  | A     | 4001 | BCR  | C11-C10-C9  | 10.37 | 142.18      | 127.20   |
| 14  | A     | 4012 | BCR  | C11-C12-C13 | 10.43 | 157.01      | 126.32   |
| 14  | F     | 4015 | BCR  | C11-C12-C13 | 10.44 | 157.06      | 126.32   |
| 14  | A     | 4008 | BCR  | C11-C12-C13 | 10.50 | 157.22      | 126.32   |
| 14  | J     | 4013 | BCR  | C11-C12-C13 | 10.51 | 157.25      | 126.32   |
| 14  | A     | 4012 | BCR  | C11-C10-C9  | 10.55 | 142.44      | 127.20   |
| 14  | B     | 4005 | BCR  | C11-C12-C13 | 10.62 | 157.59      | 126.32   |
| 14  | A     | 4007 | BCR  | C11-C12-C13 | 10.84 | 158.23      | 126.32   |
| 14  | A     | 4002 | BCR  | C11-C12-C13 | 10.99 | 158.66      | 126.32   |
| 14  | A     | 4002 | BCR  | C16-C15-C14 | 11.06 | 147.85      | 123.39   |
| 14  | A     | 4012 | BCR  | C16-C15-C14 | 11.15 | 148.06      | 123.39   |
| 14  | F     | 4016 | BCR  | C16-C15-C14 | 11.33 | 148.45      | 123.39   |
| 14  | A     | 4003 | BCR  | C11-C10-C9  | 11.44 | 143.73      | 127.20   |
| 14  | B     | 4009 | BCR  | C11-C10-C9  | 11.51 | 143.82      | 127.20   |
| 14  | F     | 4016 | BCR  | C11-C10-C9  | 11.52 | 143.84      | 127.20   |
| 14  | B     | 4005 | BCR  | C16-C15-C14 | 11.53 | 148.90      | 123.39   |
| 14  | B     | 4006 | BCR  | C16-C15-C14 | 11.64 | 149.13      | 123.39   |
| 14  | B     | 4011 | BCR  | C11-C12-C13 | 11.80 | 161.04      | 126.32   |
| 14  | F     | 4015 | BCR  | C11-C10-C9  | 11.97 | 144.48      | 127.20   |
| 14  | B     | 4017 | BCR  | C16-C15-C14 | 12.00 | 149.93      | 123.39   |
| 14  | J     | 4013 | BCR  | C21-C20-C19 | 12.03 | 159.80      | 123.13   |
| 14  | B     | 4011 | BCR  | C16-C15-C14 | 12.17 | 150.29      | 123.39   |
| 14  | A     | 4001 | BCR  | C16-C15-C14 | 12.20 | 150.36      | 123.39   |
| 14  | B     | 4006 | BCR  | C21-C20-C19 | 12.25 | 160.47      | 123.13   |
| 14  | A     | 4007 | BCR  | C16-C15-C14 | 12.38 | 150.78      | 123.39   |
| 14  | B     | 4010 | BCR  | C21-C20-C19 | 12.41 | 160.97      | 123.13   |
| 14  | B     | 4004 | BCR  | C11-C10-C9  | 12.45 | 145.18      | 127.20   |
| 14  | A     | 4007 | BCR  | C21-C20-C19 | 12.45 | 161.09      | 123.13   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | A     | 4002 | BCR  | C11-C10-C9  | 12.49 | 145.23      | 127.20   |
| 14  | B     | 4004 | BCR  | C16-C15-C14 | 12.53 | 151.10      | 123.39   |
| 14  | A     | 4003 | BCR  | C16-C15-C14 | 12.58 | 151.22      | 123.39   |
| 14  | A     | 4008 | BCR  | C21-C20-C19 | 12.59 | 161.50      | 123.13   |
| 14  | B     | 4010 | BCR  | C16-C15-C14 | 12.64 | 151.35      | 123.39   |
| 14  | J     | 4013 | BCR  | C16-C15-C14 | 12.66 | 151.38      | 123.39   |
| 14  | B     | 4005 | BCR  | C11-C10-C9  | 12.72 | 145.57      | 127.20   |
| 14  | F     | 4015 | BCR  | C21-C20-C19 | 12.72 | 161.92      | 123.13   |
| 14  | F     | 4016 | BCR  | C21-C20-C19 | 12.84 | 162.28      | 123.13   |
| 14  | A     | 4008 | BCR  | C16-C15-C14 | 12.92 | 151.97      | 123.39   |
| 14  | A     | 4007 | BCR  | C11-C10-C9  | 12.98 | 145.94      | 127.20   |
| 14  | B     | 4011 | BCR  | C21-C20-C19 | 12.98 | 162.71      | 123.13   |
| 14  | J     | 4013 | BCR  | C11-C10-C9  | 12.99 | 145.96      | 127.20   |
| 14  | A     | 4008 | BCR  | C11-C10-C9  | 13.16 | 146.20      | 127.20   |
| 14  | B     | 4010 | BCR  | C11-C10-C9  | 13.24 | 146.32      | 127.20   |
| 14  | B     | 4006 | BCR  | C11-C10-C9  | 13.24 | 146.32      | 127.20   |
| 14  | A     | 4002 | BCR  | C21-C20-C19 | 13.32 | 163.73      | 123.13   |
| 14  | B     | 4017 | BCR  | C21-C20-C19 | 13.47 | 164.19      | 123.13   |
| 14  | B     | 4009 | BCR  | C21-C20-C19 | 13.51 | 164.32      | 123.13   |
| 14  | B     | 4014 | BCR  | C11-C10-C9  | 13.54 | 146.75      | 127.20   |
| 14  | B     | 4005 | BCR  | C21-C20-C19 | 13.64 | 164.70      | 123.13   |
| 14  | A     | 4003 | BCR  | C21-C20-C19 | 13.67 | 164.79      | 123.13   |
| 14  | B     | 4014 | BCR  | C21-C20-C19 | 13.71 | 164.92      | 123.13   |
| 14  | A     | 4012 | BCR  | C21-C20-C19 | 13.80 | 165.18      | 123.13   |
| 14  | B     | 4017 | BCR  | C11-C10-C9  | 13.84 | 147.18      | 127.20   |
| 14  | A     | 4001 | BCR  | C21-C20-C19 | 13.94 | 165.64      | 123.13   |
| 14  | B     | 4014 | BCR  | C16-C15-C14 | 13.95 | 154.24      | 123.39   |
| 14  | F     | 4015 | BCR  | C16-C15-C14 | 13.96 | 154.25      | 123.39   |
| 14  | B     | 4004 | BCR  | C21-C20-C19 | 14.12 | 166.17      | 123.13   |
| 14  | B     | 4009 | BCR  | C15-C16-C17 | 14.79 | 156.10      | 123.39   |
| 14  | A     | 4001 | BCR  | C10-C11-C12 | 15.32 | 169.83      | 123.13   |
| 14  | B     | 4009 | BCR  | C16-C15-C14 | 15.33 | 157.29      | 123.39   |
| 14  | B     | 4009 | BCR  | C10-C11-C12 | 15.58 | 170.63      | 123.13   |
| 14  | A     | 4012 | BCR  | C10-C11-C12 | 15.71 | 171.03      | 123.13   |
| 14  | B     | 4011 | BCR  | C10-C11-C12 | 15.99 | 171.87      | 123.13   |
| 14  | F     | 4015 | BCR  | C15-C16-C17 | 16.49 | 159.85      | 123.39   |
| 14  | B     | 4011 | BCR  | C11-C10-C9  | 16.99 | 151.74      | 127.20   |
| 14  | A     | 4003 | BCR  | C10-C11-C12 | 17.00 | 174.95      | 123.13   |
| 14  | F     | 4016 | BCR  | C10-C11-C12 | 17.11 | 175.29      | 123.13   |
| 14  | B     | 4004 | BCR  | C10-C11-C12 | 17.20 | 175.56      | 123.13   |
| 14  | B     | 4014 | BCR  | C15-C16-C17 | 17.27 | 161.57      | 123.39   |
| 14  | B     | 4010 | BCR  | C10-C11-C12 | 17.35 | 176.01      | 123.13   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | A     | 4007 | BCR  | C10-C11-C12 | 17.38 | 176.12      | 123.13   |
| 14  | A     | 4008 | BCR  | C15-C16-C17 | 17.47 | 162.01      | 123.39   |
| 14  | A     | 4002 | BCR  | C10-C11-C12 | 17.55 | 176.64      | 123.13   |
| 14  | B     | 4006 | BCR  | C10-C11-C12 | 17.61 | 176.83      | 123.13   |
| 14  | B     | 4017 | BCR  | C10-C11-C12 | 17.64 | 176.89      | 123.13   |
| 14  | A     | 4008 | BCR  | C10-C11-C12 | 17.64 | 176.90      | 123.13   |
| 14  | B     | 4010 | BCR  | C15-C16-C17 | 17.69 | 162.50      | 123.39   |
| 14  | J     | 4013 | BCR  | C10-C11-C12 | 17.70 | 177.10      | 123.13   |
| 14  | B     | 4014 | BCR  | C10-C11-C12 | 17.71 | 177.11      | 123.13   |
| 14  | B     | 4005 | BCR  | C10-C11-C12 | 17.73 | 177.17      | 123.13   |
| 14  | A     | 4007 | BCR  | C15-C16-C17 | 17.90 | 162.96      | 123.39   |
| 14  | F     | 4015 | BCR  | C10-C11-C12 | 17.91 | 177.72      | 123.13   |
| 14  | B     | 4011 | BCR  | C15-C16-C17 | 17.95 | 163.09      | 123.39   |
| 14  | J     | 4013 | BCR  | C15-C16-C17 | 18.03 | 163.25      | 123.39   |
| 14  | B     | 4004 | BCR  | C16-C17-C18 | 18.26 | 153.56      | 127.20   |
| 14  | B     | 4006 | BCR  | C15-C16-C17 | 18.31 | 163.88      | 123.39   |
| 14  | A     | 4001 | BCR  | C15-C16-C17 | 18.36 | 163.98      | 123.39   |
| 14  | B     | 4004 | BCR  | C15-C16-C17 | 18.59 | 164.51      | 123.39   |
| 14  | A     | 4003 | BCR  | C15-C16-C17 | 18.61 | 164.55      | 123.39   |
| 14  | A     | 4012 | BCR  | C15-C16-C17 | 18.73 | 164.81      | 123.39   |
| 14  | A     | 4012 | BCR  | C20-C21-C22 | 18.74 | 154.26      | 127.20   |
| 14  | B     | 4017 | BCR  | C15-C16-C17 | 18.80 | 164.95      | 123.39   |
| 14  | A     | 4002 | BCR  | C16-C17-C18 | 18.83 | 154.39      | 127.20   |
| 14  | B     | 4005 | BCR  | C16-C17-C18 | 18.94 | 154.56      | 127.20   |
| 14  | B     | 4005 | BCR  | C15-C16-C17 | 19.05 | 165.52      | 123.39   |
| 14  | F     | 4016 | BCR  | C15-C16-C17 | 19.18 | 165.79      | 123.39   |
| 14  | B     | 4011 | BCR  | C20-C21-C22 | 19.18 | 154.90      | 127.20   |
| 14  | A     | 4001 | BCR  | C16-C17-C18 | 19.22 | 154.96      | 127.20   |
| 14  | A     | 4012 | BCR  | C16-C17-C18 | 19.27 | 155.03      | 127.20   |
| 14  | A     | 4002 | BCR  | C15-C16-C17 | 19.27 | 166.01      | 123.39   |
| 14  | B     | 4004 | BCR  | C20-C21-C22 | 19.53 | 155.40      | 127.20   |
| 14  | B     | 4014 | BCR  | C20-C21-C22 | 19.58 | 155.48      | 127.20   |
| 14  | A     | 4003 | BCR  | C20-C21-C22 | 19.61 | 155.53      | 127.20   |
| 14  | B     | 4017 | BCR  | C16-C17-C18 | 19.79 | 155.78      | 127.20   |
| 14  | B     | 4009 | BCR  | C20-C21-C22 | 19.99 | 156.06      | 127.20   |
| 14  | A     | 4001 | BCR  | C20-C21-C22 | 20.04 | 156.15      | 127.20   |
| 14  | B     | 4005 | BCR  | C20-C21-C22 | 20.14 | 156.28      | 127.20   |
| 14  | B     | 4006 | BCR  | C16-C17-C18 | 20.28 | 156.48      | 127.20   |
| 14  | J     | 4013 | BCR  | C16-C17-C18 | 20.35 | 156.59      | 127.20   |
| 14  | F     | 4016 | BCR  | C16-C17-C18 | 20.50 | 156.80      | 127.20   |
| 14  | B     | 4017 | BCR  | C20-C21-C22 | 20.79 | 157.23      | 127.20   |
| 14  | A     | 4002 | BCR  | C20-C21-C22 | 20.89 | 157.36      | 127.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | B     | 4010 | BCR  | C16-C17-C18 | 21.01 | 157.54      | 127.20   |
| 14  | A     | 4003 | BCR  | C16-C17-C18 | 21.10 | 157.67      | 127.20   |
| 14  | B     | 4011 | BCR  | C16-C17-C18 | 21.63 | 158.44      | 127.20   |
| 14  | F     | 4015 | BCR  | C16-C17-C18 | 21.63 | 158.44      | 127.20   |
| 14  | J     | 4013 | BCR  | C20-C21-C22 | 21.68 | 158.50      | 127.20   |
| 14  | A     | 4007 | BCR  | C16-C17-C18 | 21.71 | 158.55      | 127.20   |
| 14  | A     | 4008 | BCR  | C16-C17-C18 | 22.00 | 158.97      | 127.20   |
| 14  | F     | 4015 | BCR  | C20-C21-C22 | 22.00 | 158.97      | 127.20   |
| 14  | B     | 4010 | BCR  | C20-C21-C22 | 22.85 | 160.21      | 127.20   |
| 14  | B     | 4014 | BCR  | C16-C17-C18 | 22.88 | 160.24      | 127.20   |
| 14  | A     | 4007 | BCR  | C20-C21-C22 | 23.04 | 160.48      | 127.20   |
| 14  | A     | 4008 | BCR  | C20-C21-C22 | 23.04 | 160.48      | 127.20   |
| 14  | B     | 4006 | BCR  | C20-C21-C22 | 23.74 | 161.49      | 127.20   |
| 14  | F     | 4016 | BCR  | C20-C21-C22 | 25.12 | 163.47      | 127.20   |
| 14  | B     | 4009 | BCR  | C16-C17-C18 | 26.52 | 165.49      | 127.20   |

All (258) chirality outliers are listed below:

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 15  | B     | 1213 | CLA  | NC   |
| 15  | B     | 1213 | CLA  | NA   |
| 15  | A     | 1118 | CLA  | NC   |
| 15  | A     | 1118 | CLA  | ND   |
| 15  | A     | 1118 | CLA  | NA   |
| 15  | B     | 1204 | CLA  | NC   |
| 15  | B     | 1204 | CLA  | ND   |
| 15  | B     | 1204 | CLA  | NA   |
| 15  | B     | 1227 | CLA  | NC   |
| 15  | B     | 1227 | CLA  | NA   |
| 15  | A     | 1022 | CLA  | ND   |
| 15  | A     | 1022 | CLA  | NA   |
| 15  | J     | 1302 | CLA  | NC   |
| 15  | J     | 1302 | CLA  | ND   |
| 15  | J     | 1302 | CLA  | NA   |
| 15  | B     | 1207 | CLA  | NC   |
| 15  | B     | 1207 | CLA  | ND   |
| 15  | B     | 1207 | CLA  | NA   |
| 15  | F     | 1410 | CLA  | ND   |
| 15  | F     | 1410 | CLA  | NA   |
| 15  | A     | 1134 | CLA  | NC   |
| 15  | A     | 1134 | CLA  | ND   |
| 15  | A     | 1134 | CLA  | NA   |

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| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 15  | A     | 1114 | CLA  | NC   |
| 15  | A     | 1114 | CLA  | ND   |
| 15  | A     | 1114 | CLA  | NA   |
| 15  | A     | 1110 | CLA  | NC   |
| 15  | A     | 1110 | CLA  | ND   |
| 15  | A     | 1110 | CLA  | NA   |
| 15  | B     | 1220 | CLA  | NC   |
| 15  | B     | 1220 | CLA  | ND   |
| 15  | B     | 1220 | CLA  | NA   |
| 15  | B     | 1240 | CLA  | NC   |
| 15  | B     | 1240 | CLA  | ND   |
| 15  | B     | 1240 | CLA  | NA   |
| 15  | B     | 1225 | CLA  | NC   |
| 15  | B     | 1225 | CLA  | ND   |
| 15  | B     | 1225 | CLA  | NA   |
| 15  | A     | 1128 | CLA  | NC   |
| 15  | A     | 1128 | CLA  | ND   |
| 15  | A     | 1128 | CLA  | NA   |
| 15  | A     | 1105 | CLA  | NC   |
| 15  | A     | 1105 | CLA  | ND   |
| 15  | A     | 1105 | CLA  | NA   |
| 15  | B     | 1209 | CLA  | NC   |
| 15  | B     | 1209 | CLA  | ND   |
| 15  | B     | 1209 | CLA  | NA   |
| 15  | B     | 1234 | CLA  | NC   |
| 15  | B     | 1234 | CLA  | ND   |
| 15  | B     | 1234 | CLA  | NA   |
| 15  | A     | 1124 | CLA  | NC   |
| 15  | A     | 1124 | CLA  | ND   |
| 15  | A     | 1124 | CLA  | NA   |
| 15  | A     | 1121 | CLA  | NC   |
| 15  | A     | 1121 | CLA  | ND   |
| 15  | A     | 1121 | CLA  | NA   |
| 15  | A     | 1104 | CLA  | NC   |
| 15  | A     | 1104 | CLA  | ND   |
| 15  | A     | 1104 | CLA  | NA   |
| 15  | B     | 1203 | CLA  | ND   |
| 15  | B     | 1203 | CLA  | NA   |
| 15  | B     | 1217 | CLA  | NC   |
| 15  | B     | 1217 | CLA  | ND   |
| 15  | B     | 1217 | CLA  | NA   |
| 15  | B     | 1218 | CLA  | NC   |

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| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 15  | B     | 1218 | CLA  | ND   |
| 15  | B     | 1218 | CLA  | NA   |
| 15  | B     | 1201 | CLA  | NC   |
| 15  | B     | 1201 | CLA  | ND   |
| 15  | B     | 1201 | CLA  | NA   |
| 15  | A     | 1137 | CLA  | NC   |
| 15  | A     | 1137 | CLA  | NA   |
| 15  | A     | 1137 | CLA  | ND   |
| 15  | B     | 1232 | CLA  | NC   |
| 15  | B     | 1232 | CLA  | ND   |
| 15  | B     | 1232 | CLA  | NA   |
| 15  | A     | 1138 | CLA  | NC   |
| 15  | A     | 1138 | CLA  | ND   |
| 15  | A     | 1138 | CLA  | NA   |
| 15  | B     | 1222 | CLA  | NC   |
| 15  | B     | 1222 | CLA  | NA   |
| 15  | A     | 1101 | CLA  | NC   |
| 15  | A     | 1101 | CLA  | ND   |
| 15  | A     | 1101 | CLA  | NA   |
| 15  | A     | 1115 | CLA  | NC   |
| 15  | A     | 1115 | CLA  | ND   |
| 15  | A     | 1115 | CLA  | NA   |
| 15  | A     | 1123 | CLA  | NC   |
| 15  | A     | 1123 | CLA  | ND   |
| 15  | A     | 1123 | CLA  | NA   |
| 15  | F     | 1139 | CLA  | NC   |
| 15  | F     | 1139 | CLA  | ND   |
| 15  | F     | 1139 | CLA  | NA   |
| 15  | B     | 1224 | CLA  | NC   |
| 15  | B     | 1224 | CLA  | NA   |
| 15  | B     | 1224 | CLA  | ND   |
| 15  | B     | 1205 | CLA  | NC   |
| 15  | B     | 1205 | CLA  | ND   |
| 15  | B     | 1205 | CLA  | NA   |
| 15  | A     | 1126 | CLA  | NA   |
| 15  | A     | 1801 | CLA  | NC   |
| 15  | A     | 1801 | CLA  | ND   |
| 15  | A     | 1801 | CLA  | NA   |
| 15  | B     | 1236 | CLA  | ND   |
| 15  | B     | 1236 | CLA  | NA   |
| 15  | B     | 1212 | CLA  | NC   |
| 15  | B     | 1212 | CLA  | ND   |

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| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 15  | B     | 1212 | CLA  | NA   |
| 15  | B     | 1238 | CLA  | NC   |
| 15  | B     | 1238 | CLA  | ND   |
| 15  | B     | 1238 | CLA  | NA   |
| 15  | A     | 1120 | CLA  | NC   |
| 15  | A     | 1120 | CLA  | ND   |
| 15  | A     | 1120 | CLA  | NA   |
| 15  | B     | 1219 | CLA  | NC   |
| 15  | B     | 1219 | CLA  | ND   |
| 15  | B     | 1219 | CLA  | NA   |
| 15  | A     | 1116 | CLA  | NC   |
| 15  | A     | 1116 | CLA  | ND   |
| 15  | A     | 1116 | CLA  | NA   |
| 15  | A     | 1122 | CLA  | NC   |
| 15  | A     | 1122 | CLA  | ND   |
| 15  | A     | 1122 | CLA  | NA   |
| 15  | A     | 1127 | CLA  | NC   |
| 15  | A     | 1127 | CLA  | ND   |
| 15  | A     | 1127 | CLA  | NA   |
| 15  | A     | 1107 | CLA  | NC   |
| 15  | A     | 1107 | CLA  | NA   |
| 15  | B     | 1023 | CLA  | NC   |
| 15  | B     | 1023 | CLA  | ND   |
| 15  | B     | 1023 | CLA  | NA   |
| 15  | A     | 1135 | CLA  | NC   |
| 15  | A     | 1135 | CLA  | ND   |
| 15  | A     | 1135 | CLA  | NA   |
| 15  | A     | 1119 | CLA  | NC   |
| 15  | A     | 1119 | CLA  | NA   |
| 15  | B     | 1239 | CLA  | NC   |
| 15  | B     | 1239 | CLA  | ND   |
| 15  | B     | 1239 | CLA  | NA   |
| 15  | B     | 1230 | CLA  | NC   |
| 15  | B     | 1230 | CLA  | ND   |
| 15  | B     | 1230 | CLA  | NA   |
| 15  | K     | 1401 | CLA  | NC   |
| 15  | K     | 1401 | CLA  | NA   |
| 15  | K     | 1401 | CLA  | ND   |
| 15  | B     | 1228 | CLA  | NC   |
| 15  | B     | 1228 | CLA  | ND   |
| 15  | B     | 1228 | CLA  | NA   |
| 15  | B     | 1214 | CLA  | NC   |

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| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 15  | B     | 1214 | CLA  | NA   |
| 15  | A     | 1133 | CLA  | NC   |
| 15  | A     | 1133 | CLA  | ND   |
| 15  | A     | 1133 | CLA  | NA   |
| 15  | A     | 1117 | CLA  | NC   |
| 15  | A     | 1117 | CLA  | ND   |
| 15  | A     | 1117 | CLA  | NA   |
| 15  | J     | 1303 | CLA  | NC   |
| 15  | J     | 1303 | CLA  | NA   |
| 15  | J     | 1303 | CLA  | ND   |
| 15  | B     | 1208 | CLA  | NC   |
| 15  | B     | 1208 | CLA  | ND   |
| 15  | B     | 1208 | CLA  | NA   |
| 15  | A     | 1131 | CLA  | NC   |
| 15  | A     | 1131 | CLA  | NA   |
| 15  | A     | 1131 | CLA  | ND   |
| 15  | A     | 1111 | CLA  | NC   |
| 15  | A     | 1111 | CLA  | ND   |
| 15  | A     | 1111 | CLA  | NA   |
| 15  | A     | 1136 | CLA  | NC   |
| 15  | A     | 1136 | CLA  | ND   |
| 15  | A     | 1136 | CLA  | NA   |
| 15  | B     | 1226 | CLA  | NC   |
| 15  | B     | 1226 | CLA  | ND   |
| 15  | B     | 1226 | CLA  | NA   |
| 15  | B     | 1221 | CLA  | NC   |
| 15  | B     | 1221 | CLA  | NA   |
| 15  | B     | 1221 | CLA  | ND   |
| 15  | B     | 1202 | CLA  | NC   |
| 15  | B     | 1202 | CLA  | NA   |
| 15  | B     | 1202 | CLA  | ND   |
| 13  | A     | 1108 | CL0  | NC   |
| 13  | A     | 1108 | CL0  | ND   |
| 13  | A     | 1108 | CL0  | NA   |
| 15  | A     | 1102 | CLA  | NC   |
| 15  | A     | 1102 | CLA  | ND   |
| 15  | A     | 1102 | CLA  | NA   |
| 15  | B     | 1211 | CLA  | NC   |
| 15  | B     | 1211 | CLA  | ND   |
| 15  | B     | 1211 | CLA  | NA   |
| 15  | B     | 1021 | CLA  | NC   |
| 15  | B     | 1021 | CLA  | ND   |

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| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 15  | B     | 1021 | CLA  | NA   |
| 15  | B     | 1235 | CLA  | NC   |
| 15  | B     | 1235 | CLA  | ND   |
| 15  | B     | 1235 | CLA  | NA   |
| 15  | A     | 1112 | CLA  | NC   |
| 15  | A     | 1112 | CLA  | ND   |
| 15  | A     | 1112 | CLA  | NA   |
| 15  | B     | 1216 | CLA  | NC   |
| 15  | B     | 1216 | CLA  | NA   |
| 15  | A     | 1132 | CLA  | NC   |
| 15  | A     | 1132 | CLA  | ND   |
| 15  | A     | 1132 | CLA  | NA   |
| 15  | A     | 1113 | CLA  | NC   |
| 15  | A     | 1113 | CLA  | ND   |
| 15  | A     | 1113 | CLA  | NA   |
| 15  | B     | 1206 | CLA  | NC   |
| 15  | B     | 1206 | CLA  | ND   |
| 15  | B     | 1206 | CLA  | NA   |
| 15  | A     | 1140 | CLA  | NC   |
| 15  | A     | 1140 | CLA  | ND   |
| 15  | A     | 1140 | CLA  | NA   |
| 15  | A     | 1012 | CLA  | ND   |
| 15  | A     | 1012 | CLA  | NA   |
| 15  | A     | 1125 | CLA  | ND   |
| 15  | A     | 1125 | CLA  | NA   |
| 15  | B     | 1237 | CLA  | NC   |
| 15  | B     | 1237 | CLA  | ND   |
| 15  | B     | 1237 | CLA  | NA   |
| 15  | A     | 1129 | CLA  | NC   |
| 15  | A     | 1129 | CLA  | ND   |
| 15  | A     | 1129 | CLA  | NA   |
| 15  | B     | 1013 | CLA  | NC   |
| 15  | B     | 1013 | CLA  | NA   |
| 15  | B     | 1223 | CLA  | NC   |
| 15  | B     | 1223 | CLA  | ND   |
| 15  | B     | 1223 | CLA  | NA   |
| 13  | A     | 1011 | CL0  | NC   |
| 13  | A     | 1011 | CL0  | ND   |
| 13  | A     | 1011 | CL0  | NA   |
| 15  | A     | 1109 | CLA  | NC   |
| 15  | A     | 1109 | CLA  | NA   |
| 15  | B     | 1229 | CLA  | NC   |

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| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 15  | B     | 1229 | CLA  | ND   |
| 15  | B     | 1229 | CLA  | NA   |
| 15  | B     | 1231 | CLA  | NC   |
| 15  | B     | 1231 | CLA  | ND   |
| 15  | B     | 1231 | CLA  | NA   |
| 15  | F     | 1301 | CLA  | NC   |
| 15  | F     | 1301 | CLA  | ND   |
| 15  | F     | 1301 | CLA  | NA   |
| 15  | K     | 1402 | CLA  | NC   |
| 15  | K     | 1402 | CLA  | NA   |
| 15  | K     | 1402 | CLA  | ND   |
| 15  | A     | 1103 | CLA  | NC   |
| 15  | A     | 1103 | CLA  | NA   |
| 15  | A     | 1103 | CLA  | ND   |
| 15  | A     | 1106 | CLA  | NC   |
| 15  | A     | 1106 | CLA  | ND   |
| 15  | A     | 1106 | CLA  | NA   |
| 15  | A     | 1130 | CLA  | NC   |
| 15  | A     | 1130 | CLA  | ND   |
| 15  | A     | 1130 | CLA  | NA   |
| 15  | B     | 1215 | CLA  | ND   |
| 15  | B     | 1215 | CLA  | NA   |
| 15  | B     | 1210 | CLA  | NC   |
| 15  | B     | 1210 | CLA  | ND   |
| 15  | B     | 1210 | CLA  | NA   |

All (2) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms          |
|-----|-------|------|------|----------------|
| 14  | B     | 4009 | BCR  | C11-C10-C9-C8  |
| 14  | B     | 4009 | BCR  | C11-C10-C9-C34 |

There are no ring outliers.

91 monomers are involved in 200 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 13  | A     | 1011 | CL0  | 9       | 0            |
| 15  | A     | 1012 | CLA  | 2       | 0            |
| 15  | A     | 1022 | CLA  | 3       | 0            |
| 15  | A     | 1101 | CLA  | 3       | 0            |
| 15  | A     | 1102 | CLA  | 3       | 0            |
| 15  | A     | 1103 | CLA  | 5       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 15  | A     | 1104 | CLA  | 1       | 0            |
| 15  | A     | 1105 | CLA  | 2       | 0            |
| 15  | A     | 1106 | CLA  | 2       | 0            |
| 15  | A     | 1107 | CLA  | 1       | 0            |
| 13  | A     | 1108 | CL0  | 3       | 0            |
| 15  | A     | 1109 | CLA  | 3       | 0            |
| 15  | A     | 1110 | CLA  | 13      | 0            |
| 15  | A     | 1111 | CLA  | 1       | 0            |
| 15  | A     | 1112 | CLA  | 1       | 0            |
| 15  | A     | 1113 | CLA  | 1       | 0            |
| 15  | A     | 1114 | CLA  | 2       | 0            |
| 15  | A     | 1118 | CLA  | 3       | 0            |
| 15  | A     | 1119 | CLA  | 1       | 0            |
| 15  | A     | 1120 | CLA  | 1       | 0            |
| 15  | A     | 1121 | CLA  | 2       | 0            |
| 15  | A     | 1122 | CLA  | 4       | 0            |
| 15  | A     | 1123 | CLA  | 2       | 0            |
| 15  | A     | 1124 | CLA  | 3       | 0            |
| 15  | A     | 1126 | CLA  | 8       | 0            |
| 15  | A     | 1127 | CLA  | 4       | 0            |
| 15  | A     | 1128 | CLA  | 2       | 0            |
| 15  | A     | 1129 | CLA  | 2       | 0            |
| 15  | A     | 1131 | CLA  | 2       | 0            |
| 15  | A     | 1133 | CLA  | 2       | 0            |
| 15  | A     | 1135 | CLA  | 1       | 0            |
| 15  | A     | 1137 | CLA  | 1       | 0            |
| 15  | A     | 1138 | CLA  | 1       | 0            |
| 15  | A     | 1801 | CLA  | 1       | 0            |
| 10  | A     | 2001 | PQN  | 1       | 0            |
| 14  | A     | 4001 | BCR  | 3       | 0            |
| 14  | A     | 4002 | BCR  | 3       | 0            |
| 14  | A     | 4003 | BCR  | 3       | 0            |
| 14  | A     | 4007 | BCR  | 1       | 0            |
| 14  | A     | 4008 | BCR  | 5       | 0            |
| 14  | A     | 4012 | BCR  | 2       | 0            |
| 12  | A     | 5001 | LHG  | 1       | 0            |
| 12  | A     | 5003 | LHG  | 7       | 0            |
| 12  | A     | 5005 | LHG  | 10      | 0            |
| 15  | B     | 1013 | CLA  | 8       | 0            |
| 15  | B     | 1021 | CLA  | 2       | 0            |
| 15  | B     | 1023 | CLA  | 3       | 0            |
| 15  | B     | 1201 | CLA  | 1       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 15  | B     | 1203 | CLA  | 2       | 0            |
| 15  | B     | 1205 | CLA  | 1       | 0            |
| 15  | B     | 1206 | CLA  | 1       | 0            |
| 15  | B     | 1210 | CLA  | 2       | 0            |
| 15  | B     | 1211 | CLA  | 2       | 0            |
| 15  | B     | 1212 | CLA  | 2       | 0            |
| 15  | B     | 1213 | CLA  | 1       | 0            |
| 15  | B     | 1215 | CLA  | 4       | 0            |
| 15  | B     | 1216 | CLA  | 2       | 0            |
| 15  | B     | 1218 | CLA  | 2       | 0            |
| 15  | B     | 1220 | CLA  | 1       | 0            |
| 15  | B     | 1221 | CLA  | 4       | 0            |
| 15  | B     | 1222 | CLA  | 4       | 0            |
| 15  | B     | 1224 | CLA  | 2       | 0            |
| 15  | B     | 1226 | CLA  | 3       | 0            |
| 15  | B     | 1227 | CLA  | 2       | 0            |
| 15  | B     | 1229 | CLA  | 4       | 0            |
| 15  | B     | 1230 | CLA  | 2       | 0            |
| 15  | B     | 1231 | CLA  | 3       | 0            |
| 15  | B     | 1232 | CLA  | 1       | 0            |
| 15  | B     | 1235 | CLA  | 4       | 0            |
| 15  | B     | 1236 | CLA  | 3       | 0            |
| 15  | B     | 1237 | CLA  | 1       | 0            |
| 15  | B     | 1239 | CLA  | 2       | 0            |
| 10  | B     | 2002 | PQN  | 3       | 0            |
| 14  | B     | 4004 | BCR  | 3       | 0            |
| 14  | B     | 4005 | BCR  | 1       | 0            |
| 14  | B     | 4006 | BCR  | 1       | 0            |
| 14  | B     | 4009 | BCR  | 1       | 0            |
| 14  | B     | 4010 | BCR  | 5       | 0            |
| 14  | B     | 4011 | BCR  | 7       | 0            |
| 14  | B     | 4014 | BCR  | 2       | 0            |
| 14  | B     | 4017 | BCR  | 6       | 0            |
| 17  | B     | 5002 | LMG  | 2       | 0            |
| 12  | B     | 5004 | LHG  | 2       | 0            |
| 15  | F     | 1139 | CLA  | 3       | 0            |
| 14  | F     | 4015 | BCR  | 6       | 0            |
| 14  | F     | 4016 | BCR  | 2       | 0            |
| 15  | J     | 1302 | CLA  | 2       | 0            |
| 16  | J     | 1304 | LMU  | 2       | 0            |
| 14  | J     | 4013 | BCR  | 3       | 0            |
| 15  | K     | 1401 | CLA  | 1       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 15  | K     | 1402 | CLA  | 1       | 0            |

## 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 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 1   | A     | 739/751 (98%)   | 0.20   | 58 (7%) 16 8   | 43, 90, 141, 226      | 0     |
| 2   | B     | 728/731 (99%)   | -0.09  | 23 (3%) 51 39  | 53, 83, 126, 179      | 0     |
| 3   | C     | 80/81 (98%)     | -0.30  | 0 100 100      | 60, 72, 95, 105       | 0     |
| 4   | D     | 138/141 (97%)   | 0.49   | 24 (17%) 2 1   | 72, 90, 125, 161      | 0     |
| 5   | E     | 68/74 (91%)     | 0.01   | 3 (4%) 38 26   | 59, 75, 109, 138      | 0     |
| 6   | F     | 141/165 (85%)   | -0.26  | 4 (2%) 56 44   | 64, 82, 111, 169      | 0     |
| 7   | J     | 40/40 (100%)    | -0.45  | 2 (5%) 32 21   | 66, 76, 124, 149      | 0     |
| 8   | K     | 53/128 (41%)    | 1.50   | 17 (32%) 1 0   | 134, 160, 207, 253    | 0     |
| 9   | M     | 30/31 (96%)     | 2.00   | 9 (30%) 1 0    | 109, 132, 158, 172    | 0     |
| All | All   | 2017/2142 (94%) | 0.11   | 140 (6%) 20 11 | 43, 86, 145, 253      | 0     |

All (140) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 9   | M     | 2   | ALA  | 21.6 |
| 9   | M     | 3   | LEU  | 12.7 |
| 8   | K     | 127 | ILE  | 10.4 |
| 1   | A     | 751 | GLY  | 8.4  |
| 1   | A     | 238 | LEU  | 5.9  |
| 1   | A     | 257 | ALA  | 5.8  |
| 1   | A     | 260 | LEU  | 5.8  |
| 1   | A     | 241 | GLU  | 5.8  |
| 8   | K     | 100 | GLY  | 5.8  |
| 9   | M     | 4   | SER  | 5.7  |
| 8   | K     | 64  | MET  | 5.7  |
| 1   | A     | 239 | PRO  | 5.6  |
| 8   | K     | 60  | VAL  | 5.6  |
| 8   | K     | 101 | LEU  | 5.4  |
| 1   | A     | 488 | HIS  | 5.2  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 4          | D            | 113        | GLU         | 5.1         |
| 4          | D            | 36         | SER         | 4.9         |
| 2          | B            | 96         | PHE         | 4.8         |
| 5          | E            | 31         | SER         | 4.8         |
| 1          | A            | 485        | TRP         | 4.8         |
| 9          | M            | 6          | THR         | 4.7         |
| 8          | K            | 126        | GLY         | 4.7         |
| 4          | D            | 52         | GLU         | 4.6         |
| 1          | A            | 511        | GLY         | 4.5         |
| 1          | A            | 237        | PRO         | 4.4         |
| 1          | A            | 235        | ASP         | 4.4         |
| 4          | D            | 130        | THR         | 4.3         |
| 1          | A            | 256        | PHE         | 4.3         |
| 1          | A            | 244        | LEU         | 4.1         |
| 1          | A            | 236        | ILE         | 4.1         |
| 1          | A            | 154        | ASP         | 4.1         |
| 4          | D            | 37         | GLU         | 4.0         |
| 1          | A            | 156        | TYR         | 4.0         |
| 2          | B            | 92         | TRP         | 4.0         |
| 1          | A            | 233        | PRO         | 3.9         |
| 6          | F            | 94         | LYS         | 3.8         |
| 1          | A            | 622        | SER         | 3.8         |
| 4          | D            | 49         | ILE         | 3.8         |
| 2          | B            | 216        | PRO         | 3.8         |
| 1          | A            | 304        | PHE         | 3.8         |
| 2          | B            | 111        | ASN         | 3.7         |
| 2          | B            | 294        | ASN         | 3.7         |
| 2          | B            | 214        | SER         | 3.6         |
| 5          | E            | 3          | LEU         | 3.6         |
| 1          | A            | 300        | ILE         | 3.6         |
| 1          | A            | 623        | PRO         | 3.6         |
| 1          | A            | 59         | ASP         | 3.6         |
| 2          | B            | 248        | GLU         | 3.5         |
| 6          | F            | 15         | ALA         | 3.5         |
| 8          | K            | 108        | MET         | 3.5         |
| 8          | K            | 59         | SER         | 3.5         |
| 4          | D            | 77         | LYS         | 3.4         |
| 1          | A            | 240        | HIS         | 3.3         |
| 2          | B            | 486        | THR         | 3.3         |
| 9          | M            | 7          | GLN         | 3.2         |
| 9          | M            | 8          | ILE         | 3.2         |
| 1          | A            | 234        | LYS         | 3.2         |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 620 | THR  | 3.2  |
| 1   | A     | 361 | SER  | 3.2  |
| 8   | K     | 76  | TYR  | 3.1  |
| 2   | B     | 165 | LEU  | 3.1  |
| 4   | D     | 54  | GLU  | 3.1  |
| 1   | A     | 63  | SER  | 3.1  |
| 1   | A     | 489 | LEU  | 3.1  |
| 9   | M     | 5   | ASP  | 3.1  |
| 2   | B     | 215 | THR  | 3.0  |
| 6   | F     | 14  | PRO  | 3.0  |
| 4   | D     | 35  | ALA  | 2.9  |
| 4   | D     | 140 | GLU  | 2.9  |
| 1   | A     | 369 | HIS  | 2.9  |
| 1   | A     | 259 | GLY  | 2.9  |
| 9   | M     | 11  | ALA  | 2.9  |
| 4   | D     | 51  | ASN  | 2.9  |
| 4   | D     | 50  | MET  | 2.8  |
| 6   | F     | 92  | GLU  | 2.8  |
| 4   | D     | 10  | LYS  | 2.8  |
| 1   | A     | 297 | HIS  | 2.8  |
| 1   | A     | 64  | ASP  | 2.8  |
| 8   | K     | 125 | SER  | 2.7  |
| 8   | K     | 77  | PHE  | 2.7  |
| 2   | B     | 375 | TYR  | 2.7  |
| 1   | A     | 296 | HIS  | 2.7  |
| 4   | D     | 3   | GLU  | 2.7  |
| 4   | D     | 114 | ALA  | 2.7  |
| 4   | D     | 139 | TYR  | 2.7  |
| 1   | A     | 62  | THR  | 2.7  |
| 4   | D     | 134 | SER  | 2.7  |
| 9   | M     | 10  | ALA  | 2.6  |
| 4   | D     | 34  | SER  | 2.6  |
| 2   | B     | 297 | ILE  | 2.6  |
| 5   | E     | 30  | LYS  | 2.6  |
| 4   | D     | 126 | PRO  | 2.6  |
| 8   | K     | 75  | GLY  | 2.5  |
| 4   | D     | 131 | ILE  | 2.5  |
| 1   | A     | 242 | PHE  | 2.5  |
| 1   | A     | 332 | PHE  | 2.5  |
| 2   | B     | 157 | LEU  | 2.5  |
| 2   | B     | 293 | THR  | 2.5  |
| 1   | A     | 624 | ASP  | 2.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 303 | LEU  | 2.5  |
| 2   | B     | 136 | TYR  | 2.5  |
| 8   | K     | 63  | ILE  | 2.5  |
| 1   | A     | 370 | MET  | 2.5  |
| 2   | B     | 313 | THR  | 2.5  |
| 1   | A     | 365 | ILE  | 2.4  |
| 1   | A     | 628 | THR  | 2.4  |
| 4   | D     | 38  | GLN  | 2.4  |
| 1   | A     | 355 | ASN  | 2.4  |
| 1   | A     | 205 | LEU  | 2.4  |
| 1   | A     | 67  | ASP  | 2.3  |
| 1   | A     | 299 | ALA  | 2.3  |
| 1   | A     | 155 | SER  | 2.3  |
| 7   | J     | 1   | MET  | 2.3  |
| 7   | J     | 2   | ASP  | 2.3  |
| 2   | B     | 488 | ALA  | 2.3  |
| 1   | A     | 251 | GLU  | 2.3  |
| 1   | A     | 101 | GLU  | 2.3  |
| 1   | A     | 532 | PHE  | 2.3  |
| 8   | K     | 62  | ILE  | 2.3  |
| 8   | K     | 74  | ILE  | 2.3  |
| 1   | A     | 243 | ILE  | 2.2  |
| 1   | A     | 362 | LEU  | 2.2  |
| 2   | B     | 112 | PRO  | 2.2  |
| 2   | B     | 44  | GLN  | 2.2  |
| 4   | D     | 4   | LEU  | 2.2  |
| 2   | B     | 379 | PHE  | 2.2  |
| 1   | A     | 625 | GLY  | 2.2  |
| 4   | D     | 100 | ALA  | 2.2  |
| 1   | A     | 209 | SER  | 2.1  |
| 8   | K     | 124 | SER  | 2.1  |
| 1   | A     | 17  | ASP  | 2.1  |
| 1   | A     | 94  | GLY  | 2.1  |
| 8   | K     | 65  | CYS  | 2.1  |
| 1   | A     | 477 | GLN  | 2.1  |
| 2   | B     | 339 | LEU  | 2.1  |
| 4   | D     | 127 | GLU  | 2.1  |
| 2   | B     | 343 | THR  | 2.0  |
| 1   | A     | 157 | GLN  | 2.0  |
| 1   | A     | 496 | ALA  | 2.0  |
| 2   | B     | 94  | PRO  | 2.0  |

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|----------------------------|-------|
| 15  | CLA  | J     | 1303 | 46/65 | 0.87 | 0.35 | 11.08 | 94,114,141,159             | 0     |
| 14  | BCR  | A     | 4007 | 40/40 | 0.69 | 0.39 | 4.00  | 69,86,137,139              | 0     |
| 15  | CLA  | A     | 1121 | 46/65 | 0.94 | 0.25 | 3.70  | 91,114,141,163             | 0     |
| 14  | BCR  | A     | 4012 | 40/40 | 0.94 | 0.18 | 3.55  | 55,77,87,91                | 0     |
| 15  | CLA  | J     | 1302 | 45/65 | 0.89 | 0.30 | 3.12  | 82,93,138,150              | 0     |
| 10  | PQN  | B     | 2002 | 33/33 | 0.91 | 0.26 | 3.04  | 59,79,99,105               | 0     |
| 14  | BCR  | B     | 4009 | 40/40 | 0.77 | 0.27 | 2.79  | 72,103,147,151             | 0     |
| 14  | BCR  | A     | 4003 | 40/40 | 0.75 | 0.39 | 2.57  | 69,111,146,146             | 0     |
| 15  | CLA  | F     | 1410 | 65/65 | 0.92 | 0.23 | 2.49  | 69,96,135,147              | 0     |
| 14  | BCR  | F     | 4015 | 40/40 | 0.91 | 0.22 | 2.44  | 52,73,107,111              | 0     |
| 11  | SF4  | A     | 3001 | 8/8   | 0.93 | 0.23 | 2.44  | 50,62,210,290              | 0     |
| 14  | BCR  | J     | 4013 | 40/40 | 0.82 | 0.29 | 2.37  | 78,97,112,121              | 0     |
| 15  | CLA  | A     | 1801 | 52/65 | 0.90 | 0.43 | 1.96  | 100,122,154,158            | 0     |
| 15  | CLA  | A     | 1127 | 65/65 | 0.93 | 0.42 | 1.92  | 67,79,100,106              | 0     |
| 14  | BCR  | B     | 4005 | 40/40 | 0.83 | 0.27 | 1.89  | 73,93,125,128              | 0     |
| 15  | CLA  | A     | 1012 | 65/65 | 0.95 | 0.27 | 1.79  | 47,60,86,93                | 0     |
| 15  | CLA  | A     | 1122 | 65/65 | 0.93 | 0.19 | 1.76  | 74,91,119,129              | 0     |
| 15  | CLA  | A     | 1110 | 54/65 | 0.87 | 0.22 | 1.68  | 96,121,150,154             | 0     |
| 14  | BCR  | B     | 4011 | 40/40 | 0.94 | 0.26 | 1.66  | 49,67,84,91                | 0     |
| 15  | CLA  | B     | 1215 | 65/65 | 0.94 | 0.30 | 1.54  | 72,85,104,106              | 0     |
| 17  | LMG  | B     | 5002 | 55/55 | 0.84 | 0.29 | 1.47  | 71,101,130,137             | 0     |
| 15  | CLA  | B     | 1229 | 65/65 | 0.96 | 0.17 | 1.45  | 50,62,86,107               | 0     |
| 15  | CLA  | B     | 1230 | 65/65 | 0.95 | 0.17 | 1.38  | 53,68,118,125              | 0     |
| 15  | CLA  | A     | 1126 | 65/65 | 0.94 | 0.23 | 1.37  | 63,80,101,116              | 0     |
| 15  | CLA  | A     | 1106 | 65/65 | 0.94 | 0.20 | 1.31  | 59,79,98,109               | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 15  | CLA  | A     | 1111 | 60/65 | 0.88 | 0.24 | 1.19 | 78,96,107,112               | 0     |
| 15  | CLA  | B     | 1210 | 65/65 | 0.86 | 0.26 | 1.18 | 75,95,108,120               | 0     |
| 14  | BCR  | A     | 4002 | 40/40 | 0.92 | 0.21 | 1.16 | 88,109,128,130              | 0     |
| 14  | BCR  | B     | 4004 | 40/40 | 0.67 | 0.31 | 1.16 | 101,115,147,151             | 0     |
| 15  | CLA  | A     | 1022 | 65/65 | 0.92 | 0.25 | 1.15 | 53,78,96,103                | 0     |
| 15  | CLA  | A     | 1101 | 65/65 | 0.93 | 0.17 | 1.14 | 55,73,89,96                 | 0     |
| 15  | CLA  | K     | 1401 | 46/65 | 0.67 | 0.34 | 1.14 | 120,155,169,173             | 0     |
| 15  | CLA  | A     | 1138 | 65/65 | 0.94 | 0.22 | 1.09 | 47,55,69,77                 | 0     |
| 11  | SF4  | C     | 3003 | 8/8   | 0.97 | 0.19 | 1.04 | 60,67,100,115               | 0     |
| 12  | LHG  | A     | 5003 | 49/49 | 0.87 | 0.30 | 1.04 | 91,121,142,143              | 0     |
| 14  | BCR  | B     | 4006 | 40/40 | 0.84 | 0.22 | 1.03 | 86,109,141,142              | 0     |
| 15  | CLA  | B     | 1021 | 65/65 | 0.95 | 0.26 | 1.00 | 49,69,80,84                 | 0     |
| 15  | CLA  | A     | 1117 | 65/65 | 0.95 | 0.43 | 0.99 | 80,100,111,113              | 0     |
| 14  | BCR  | F     | 4016 | 40/40 | 0.92 | 0.16 | 0.98 | 59,72,89,94                 | 0     |
| 15  | CLA  | B     | 1214 | 65/65 | 0.88 | 0.24 | 0.92 | 72,89,119,133               | 0     |
| 15  | CLA  | F     | 1139 | 65/65 | 0.93 | 0.22 | 0.92 | 47,58,90,98                 | 0     |
| 15  | CLA  | B     | 1228 | 65/65 | 0.92 | 0.18 | 0.89 | 54,74,105,114               | 0     |
| 10  | PQN  | A     | 2001 | 33/33 | 0.94 | 0.20 | 0.87 | 45,57,68,74                 | 0     |
| 15  | CLA  | B     | 1023 | 65/65 | 0.92 | 0.24 | 0.86 | 55,79,111,119               | 0     |
| 15  | CLA  | B     | 1240 | 45/65 | 0.93 | 0.30 | 0.78 | 71,83,124,151               | 0     |
| 15  | CLA  | A     | 1116 | 54/65 | 0.89 | 0.37 | 0.77 | 84,113,130,141              | 0     |
| 15  | CLA  | B     | 1234 | 65/65 | 0.93 | 0.21 | 0.72 | 56,73,108,120               | 0     |
| 15  | CLA  | A     | 1140 | 65/65 | 0.96 | 0.22 | 0.71 | 52,73,103,116               | 0     |
| 11  | SF4  | C     | 3002 | 8/8   | 0.89 | 0.20 | 0.66 | 60,88,151,152               | 0     |
| 15  | CLA  | A     | 1135 | 55/65 | 0.82 | 0.26 | 0.65 | 70,98,132,135               | 0     |
| 15  | CLA  | B     | 1225 | 65/65 | 0.95 | 0.29 | 0.62 | 66,80,100,104               | 0     |
| 15  | CLA  | A     | 1132 | 62/65 | 0.90 | 0.24 | 0.61 | 74,105,153,156              | 0     |
| 16  | LMU  | J     | 1304 | 35/35 | 0.69 | 0.27 | 0.60 | 91,159,172,173              | 0     |
| 15  | CLA  | A     | 1105 | 65/65 | 0.90 | 0.21 | 0.59 | 70,96,111,120               | 0     |
| 12  | LHG  | A     | 5005 | 36/49 | 0.84 | 0.35 | 0.58 | 103,143,182,188             | 0     |
| 15  | CLA  | B     | 1013 | 65/65 | 0.94 | 0.22 | 0.57 | 46,53,77,89                 | 0     |
| 15  | CLA  | A     | 1118 | 46/65 | 0.88 | 0.22 | 0.56 | 99,113,135,154              | 0     |
| 15  | CLA  | A     | 1123 | 65/65 | 0.90 | 0.27 | 0.55 | 75,88,98,104                | 0     |
| 15  | CLA  | B     | 1224 | 65/65 | 0.89 | 0.26 | 0.55 | 60,78,98,108                | 0     |
| 14  | BCR  | B     | 4014 | 40/40 | 0.93 | 0.19 | 0.51 | 46,62,88,89                 | 0     |
| 13  | CL0  | A     | 1108 | 45/65 | 0.87 | 0.23 | 0.50 | 86,113,154,170              | 0     |
| 15  | CLA  | K     | 1402 | 46/65 | 0.79 | 0.30 | 0.49 | 163,187,214,221             | 0     |
| 13  | CL0  | A     | 1011 | 65/65 | 0.94 | 0.20 | 0.47 | 51,69,81,99                 | 0     |
| 15  | CLA  | A     | 1136 | 65/65 | 0.93 | 0.26 | 0.45 | 78,105,139,142              | 0     |
| 14  | BCR  | B     | 4017 | 40/40 | 0.95 | 0.18 | 0.44 | 70,87,101,104               | 0     |
| 15  | CLA  | B     | 1231 | 65/65 | 0.91 | 0.22 | 0.43 | 66,89,115,138               | 0     |
| 14  | BCR  | B     | 4010 | 40/40 | 0.92 | 0.21 | 0.42 | 55,74,102,113               | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 15  | CLA  | A     | 1104 | 65/65 | 0.94 | 0.23 | 0.41  | 58,72,83,96                 | 0     |
| 15  | CLA  | A     | 1134 | 46/65 | 0.88 | 0.23 | 0.34  | 109,127,151,186             | 0     |
| 15  | CLA  | A     | 1119 | 64/65 | 0.89 | 0.27 | 0.33  | 78,97,115,137               | 0     |
| 15  | CLA  | A     | 1133 | 46/65 | 0.85 | 0.29 | 0.32  | 86,103,118,128              | 0     |
| 15  | CLA  | B     | 1219 | 55/65 | 0.93 | 0.19 | 0.31  | 74,86,119,142               | 0     |
| 14  | BCR  | A     | 4008 | 40/40 | 0.82 | 0.29 | 0.30  | 67,93,105,115               | 0     |
| 15  | CLA  | A     | 1103 | 65/65 | 0.90 | 0.24 | 0.29  | 61,80,108,118               | 0     |
| 15  | CLA  | B     | 1239 | 46/65 | 0.96 | 0.21 | 0.29  | 62,78,107,141               | 0     |
| 15  | CLA  | A     | 1129 | 46/65 | 0.91 | 0.21 | 0.22  | 76,92,115,151               | 0     |
| 15  | CLA  | A     | 1125 | 52/65 | 0.93 | 0.29 | 0.21  | 76,98,124,133               | 0     |
| 12  | LHG  | B     | 5004 | 49/49 | 0.85 | 0.24 | 0.17  | 59,88,99,106                | 0     |
| 15  | CLA  | A     | 1130 | 55/65 | 0.96 | 0.20 | 0.16  | 82,106,133,139              | 0     |
| 15  | CLA  | B     | 1236 | 50/65 | 0.94 | 0.20 | 0.15  | 52,72,106,114               | 0     |
| 15  | CLA  | B     | 1217 | 47/65 | 0.91 | 0.25 | 0.15  | 96,114,132,157              | 0     |
| 15  | CLA  | B     | 1237 | 55/65 | 0.94 | 0.19 | 0.09  | 71,82,117,132               | 0     |
| 12  | LHG  | A     | 5001 | 49/49 | 0.94 | 0.20 | 0.05  | 49,70,91,100                | 0     |
| 15  | CLA  | F     | 1301 | 45/65 | 0.94 | 0.16 | 0.04  | 54,75,97,131                | 0     |
| 15  | CLA  | A     | 1102 | 65/65 | 0.92 | 0.17 | 0.04  | 55,81,107,112               | 0     |
| 15  | CLA  | B     | 1235 | 65/65 | 0.94 | 0.16 | 0.02  | 55,66,85,92                 | 0     |
| 15  | CLA  | B     | 1208 | 45/65 | 0.90 | 0.19 | 0.01  | 88,114,130,140              | 0     |
| 15  | CLA  | B     | 1211 | 46/65 | 0.91 | 0.17 | -0.03 | 90,106,116,133              | 0     |
| 14  | BCR  | A     | 4001 | 40/40 | 0.86 | 0.23 | -0.03 | 111,127,138,140             | 0     |
| 15  | CLA  | B     | 1227 | 45/65 | 0.93 | 0.16 | -0.08 | 54,72,94,98                 | 0     |
| 15  | CLA  | B     | 1226 | 65/65 | 0.93 | 0.20 | -0.09 | 54,79,133,144               | 0     |
| 15  | CLA  | B     | 1202 | 65/65 | 0.93 | 0.20 | -0.09 | 67,82,99,106                | 0     |
| 15  | CLA  | B     | 1201 | 46/65 | 0.92 | 0.21 | -0.16 | 72,83,107,123               | 0     |
| 15  | CLA  | B     | 1203 | 65/65 | 0.92 | 0.22 | -0.16 | 62,83,99,104                | 0     |
| 15  | CLA  | B     | 1212 | 45/65 | 0.83 | 0.20 | -0.17 | 101,117,128,143             | 0     |
| 15  | CLA  | A     | 1124 | 55/65 | 0.87 | 0.27 | -0.19 | 61,92,120,129               | 0     |
| 15  | CLA  | A     | 1128 | 65/65 | 0.91 | 0.20 | -0.19 | 54,74,90,101                | 0     |
| 18  | CL   | B     | 6000 | 1/1   | 0.95 | 0.12 | -0.20 | 82,82,82,82                 | 0     |
| 15  | CLA  | A     | 1109 | 65/65 | 0.94 | 0.18 | -0.21 | 66,81,105,112               | 0     |
| 15  | CLA  | B     | 1213 | 50/65 | 0.89 | 0.16 | -0.21 | 89,104,128,136              | 0     |
| 15  | CLA  | B     | 1221 | 65/65 | 0.90 | 0.19 | -0.26 | 68,79,105,125               | 0     |
| 15  | CLA  | A     | 1115 | 46/65 | 0.94 | 0.21 | -0.26 | 109,129,140,151             | 0     |
| 15  | CLA  | B     | 1220 | 56/65 | 0.94 | 0.15 | -0.28 | 61,77,111,119               | 0     |
| 15  | CLA  | B     | 1218 | 51/65 | 0.92 | 0.21 | -0.29 | 86,98,125,159               | 0     |
| 15  | CLA  | B     | 1223 | 65/65 | 0.93 | 0.22 | -0.32 | 59,77,94,98                 | 0     |
| 15  | CLA  | A     | 1120 | 49/65 | 0.91 | 0.19 | -0.32 | 101,116,140,156             | 0     |
| 15  | CLA  | B     | 1205 | 55/65 | 0.96 | 0.16 | -0.32 | 68,87,100,112               | 0     |
| 15  | CLA  | B     | 1216 | 65/65 | 0.89 | 0.18 | -0.33 | 67,91,106,118               | 0     |
| 16  | LMU  | B     | 1301 | 35/35 | 0.82 | 0.21 | -0.36 | 120,136,148,154             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 15  | CLA  | A     | 1107 | 50/65 | 0.96 | 0.15 | -0.37 | 56,64,98,112                | 0     |
| 15  | CLA  | A     | 1113 | 45/65 | 0.88 | 0.23 | -0.43 | 112,129,158,162             | 0     |
| 15  | CLA  | A     | 1114 | 49/65 | 0.85 | 0.35 | -0.51 | 98,124,137,150              | 0     |
| 15  | CLA  | B     | 1238 | 44/65 | 0.94 | 0.13 | -0.52 | 68,80,92,111                | 0     |
| 15  | CLA  | A     | 1137 | 50/65 | 0.94 | 0.18 | -0.57 | 72,94,128,134               | 0     |
| 15  | CLA  | B     | 1206 | 46/65 | 0.95 | 0.18 | -0.57 | 78,100,119,149              | 0     |
| 15  | CLA  | B     | 1232 | 45/65 | 0.92 | 0.17 | -0.64 | 72,89,109,115               | 0     |
| 15  | CLA  | A     | 1112 | 45/65 | 0.91 | 0.17 | -0.65 | 89,115,127,130              | 0     |
| 15  | CLA  | B     | 1204 | 46/65 | 0.94 | 0.17 | -0.89 | 79,96,115,137               | 0     |
| 15  | CLA  | B     | 1209 | 45/65 | 0.96 | 0.19 | -0.89 | 102,113,134,148             | 0     |
| 15  | CLA  | B     | 1222 | 56/65 | 0.93 | 0.21 | -1.04 | 52,66,101,108               | 0     |
| 15  | CLA  | A     | 1131 | 55/65 | 0.94 | 0.26 | -     | 78,107,126,140              | 0     |
| 15  | CLA  | B     | 1207 | 46/65 | 0.82 | 0.39 | -     | 118,164,185,189             | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.