



Full wwPDB X-ray Structure Validation Report ⓘ

May 2, 2016 – 11:39 PM EDT

PDB ID : 1JB0
Title : Crystal Structure of Photosystem I: a Photosynthetic Reaction Center and Core Antenna System from Cyanobacteria
Authors : Jordan, P.; Fromme, P.; Witt, H.T.; Klukas, O.; Saenger, W.; Krauss, N.
Deposited on : 2001-06-01
Resolution : 2.50 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

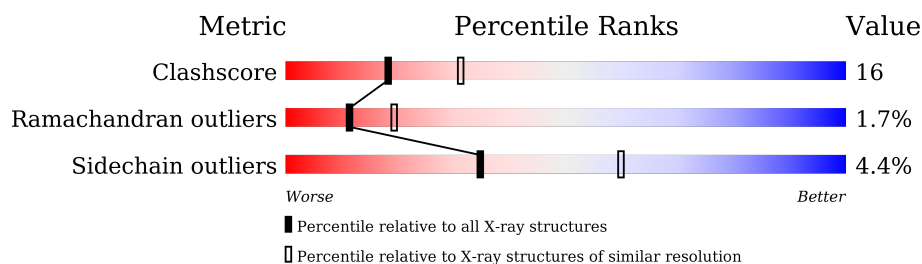
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| Clashscore | 102246 | 4242 (2.50-2.50) |
| Ramachandran outliers | 100387 | 4156 (2.50-2.50) |
| Sidechain outliers | 100360 | 4158 (2.50-2.50) |


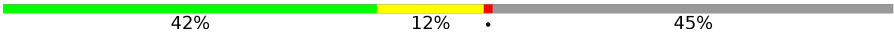



The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey 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.

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 755 | |
| 2 | B | 740 | |
| 3 | C | 80 | |
| 4 | D | 138 | |
| 5 | E | 75 | |
| 6 | F | 164 | |
| 7 | I | 38 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 8 | J | 41 |  |
| 9 | K | 83 |  |
| 10 | L | 154 |  |
| 11 | M | 31 |  |
| 12 | X | 35 |  |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 14 | CLA | A | 1011 | X | - | - | - |
| 14 | CLA | A | 1013 | X | - | - | - |
| 14 | CLA | A | 1022 | X | - | - | - |
| 14 | CLA | A | 1101 | X | - | - | - |
| 14 | CLA | A | 1102 | X | - | - | - |
| 14 | CLA | A | 1103 | X | - | - | - |
| 14 | CLA | A | 1104 | X | - | - | - |
| 14 | CLA | A | 1105 | X | - | - | - |
| 14 | CLA | A | 1106 | X | - | - | - |
| 14 | CLA | A | 1107 | X | - | - | - |
| 14 | CLA | A | 1109 | X | - | - | - |
| 14 | CLA | A | 1110 | X | - | - | - |
| 14 | CLA | A | 1111 | X | - | - | - |
| 14 | CLA | A | 1112 | X | - | - | - |
| 14 | CLA | A | 1113 | X | - | - | - |
| 14 | CLA | A | 1114 | X | - | - | - |
| 14 | CLA | A | 1115 | X | - | - | - |
| 14 | CLA | A | 1116 | X | - | - | - |
| 14 | CLA | A | 1117 | X | - | - | - |
| 14 | CLA | A | 1118 | X | - | - | - |
| 14 | CLA | A | 1119 | X | - | - | - |
| 14 | CLA | A | 1120 | X | - | - | - |
| 14 | CLA | A | 1121 | X | - | - | - |
| 14 | CLA | A | 1122 | X | - | - | - |
| 14 | CLA | A | 1123 | X | - | - | - |
| 14 | CLA | A | 1124 | X | - | - | - |
| 14 | CLA | A | 1125 | X | - | - | - |
| 14 | CLA | A | 1126 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 14 | CLA | A | 1127 | X | - | - | - |
| 14 | CLA | A | 1128 | X | - | - | - |
| 14 | CLA | A | 1129 | X | - | - | - |
| 14 | CLA | A | 1130 | X | - | - | - |
| 14 | CLA | A | 1132 | X | - | - | - |
| 14 | CLA | A | 1133 | X | - | - | - |
| 14 | CLA | A | 1134 | X | - | - | - |
| 14 | CLA | A | 1135 | X | - | - | - |
| 14 | CLA | A | 1136 | X | - | - | - |
| 14 | CLA | A | 1137 | X | - | - | - |
| 14 | CLA | A | 1138 | X | - | - | - |
| 14 | CLA | A | 1139 | X | - | - | - |
| 14 | CLA | A | 1140 | X | - | - | - |
| 14 | CLA | A | 1237 | X | - | - | - |
| 14 | CLA | A | 1402 | X | - | - | - |
| 14 | CLA | A | 1801 | X | - | - | - |
| 14 | CLA | B | 1012 | X | - | - | - |
| 14 | CLA | B | 1021 | X | - | - | - |
| 14 | CLA | B | 1023 | X | - | - | - |
| 14 | CLA | B | 1201 | X | - | - | - |
| 14 | CLA | B | 1202 | X | - | - | - |
| 14 | CLA | B | 1203 | X | - | - | - |
| 14 | CLA | B | 1204 | X | - | - | - |
| 14 | CLA | B | 1205 | X | - | - | - |
| 14 | CLA | B | 1206 | X | - | - | - |
| 14 | CLA | B | 1207 | X | - | - | - |
| 14 | CLA | B | 1208 | X | - | - | - |
| 14 | CLA | B | 1209 | X | - | - | - |
| 14 | CLA | B | 1210 | X | - | - | - |
| 14 | CLA | B | 1211 | X | - | - | - |
| 14 | CLA | B | 1212 | X | - | - | - |
| 14 | CLA | B | 1213 | X | - | - | - |
| 14 | CLA | B | 1214 | X | - | - | - |
| 14 | CLA | B | 1215 | X | - | - | - |
| 14 | CLA | B | 1216 | X | - | - | - |
| 14 | CLA | B | 1217 | X | - | - | - |
| 14 | CLA | B | 1218 | X | - | - | - |
| 14 | CLA | B | 1219 | X | - | - | - |
| 14 | CLA | B | 1220 | X | - | - | - |
| 14 | CLA | B | 1221 | X | - | - | - |
| 14 | CLA | B | 1222 | X | - | - | - |
| 14 | CLA | B | 1223 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 14 | CLA | B | 1224 | X | - | - | - |
| 14 | CLA | B | 1225 | X | - | - | - |
| 14 | CLA | B | 1226 | X | - | - | - |
| 14 | CLA | B | 1227 | X | - | - | - |
| 14 | CLA | B | 1228 | X | - | - | - |
| 14 | CLA | B | 1229 | X | - | - | - |
| 14 | CLA | B | 1230 | X | - | - | - |
| 14 | CLA | B | 1231 | X | - | - | - |
| 14 | CLA | B | 1232 | X | - | - | - |
| 14 | CLA | B | 1233 | X | - | - | - |
| 14 | CLA | B | 1234 | X | - | - | - |
| 14 | CLA | B | 1235 | X | - | - | - |
| 14 | CLA | B | 1238 | X | - | - | - |
| 14 | CLA | B | 1239 | X | - | - | - |
| 14 | CLA | F | 1301 | X | - | - | - |
| 14 | CLA | J | 1302 | X | - | - | - |
| 14 | CLA | J | 1303 | X | - | - | - |
| 14 | CLA | K | 1401 | X | - | - | - |
| 14 | CLA | L | 1501 | X | - | - | - |
| 14 | CLA | L | 1502 | X | - | - | - |
| 14 | CLA | L | 1503 | X | - | - | - |
| 14 | CLA | M | 1601 | X | - | - | - |
| 14 | CLA | X | 1701 | X | - | - | - |
| 18 | LHG | A | 5003 | X | - | - | - |

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 24198 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 | 740 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5784 | 3794 | 988 | 976 | 26 | | | |

- Molecule 2 is a protein called PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|---------|-------|
| 2 | B | 739 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5879 | 3867 | 986 | 1005 | 21 | | | |

- 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 |
| | | | 598 | 367 | 103 | 117 | 11 | | | |

- Molecule 4 is a protein called PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT II.

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

- Molecule 5 is a protein called PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT IV.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---------|---------|-------|
| 5 | E | 69 | Total | C | N | O | 0 | 0 | 0 |
| | | | 539 | 342 | 93 | 104 | | | |

- Molecule 6 is a protein called PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT III.

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

- Molecule 7 is a protein called PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT VIII.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 7 | I | 38 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 301 | 208 | 40 | 48 | 5 | | | |

- Molecule 8 is a protein called PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT IX.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 8 | J | 41 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 338 | 231 | 51 | 54 | 2 | | | |

- Molecule 9 is a protein called PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT X.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 9 | K | 46 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 222 | 130 | 46 | 46 | | | | |

- Molecule 10 is a protein called PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT XI.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | L | 151 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1119 | 735 | 179 | 201 | 4 | | | |

There are 12 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| L | 46 | ARG | PRO | CONFLICT | UNP P25902 |
| L | 144 | VAL | - | SEE REMARK 999 | UNP P25902 |
| L | 145 | VAL | - | SEE REMARK 999 | UNP P25902 |
| L | 146 | ASP | - | SEE REMARK 999 | UNP P25902 |
| L | 147 | GLY | - | SEE REMARK 999 | UNP P25902 |
| L | 148 | ILE | - | SEE REMARK 999 | UNP P25902 |
| L | 149 | MET | - | SEE REMARK 999 | UNP P25902 |
| L | 150 | THR | - | SEE REMARK 999 | UNP P25902 |
| L | 151 | GLY | - | SEE REMARK 999 | UNP P25902 |
| L | 152 | LEU | - | SEE REMARK 999 | UNP P25902 |
| L | 153 | PHE | - | SEE REMARK 999 | UNP P25902 |
| L | 154 | ASN | - | SEE REMARK 999 | UNP P25902 |

- Molecule 11 is a protein called PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT XII.

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

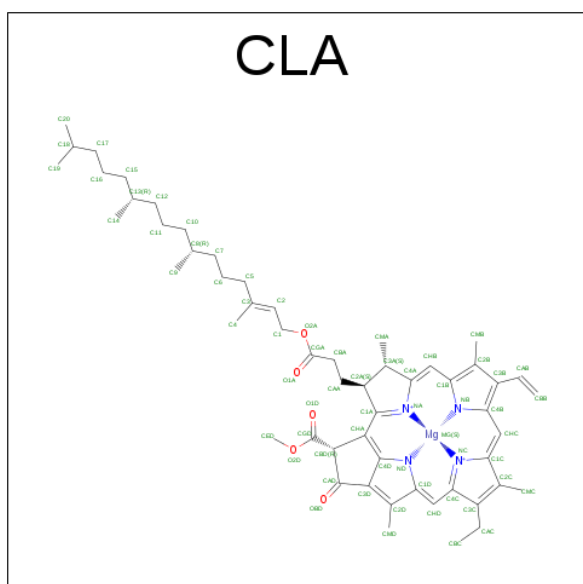
- Molecule 12 is a protein called PHOTOSYSTEM I SUBUNIT PSAX.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 12 | X | 29 | Total | C | N | O | 0 | 0 | 0 |
| | | | 233 | 164 | 34 | 35 | | | |

- Molecule 13 is CALCIUM ION (three-letter code: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 13 | L | 1 | Total | Ca | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 14 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 14 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 59 | 49 | 1 | 4 | 5 | | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 51 | 41 | 1 | 4 | 5 | | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 54 | 44 | 1 | 4 | 5 | | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 49 | 39 | 1 | 4 | 5 | | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 54 | 44 | 1 | 4 | 5 | | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 54 | 44 | 1 | 4 | 5 | | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 61 | 51 | 1 | 4 | 5 | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 14 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 49 | 39 | 1 | 4 | 5 | | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 51 | 41 | 1 | 4 | 5 | | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 59 | 49 | 1 | 4 | 5 | | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 50 | 40 | 1 | 4 | 5 | | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 54 | 44 | 1 | 4 | 5 | | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 51 | 41 | 1 | 4 | 5 | | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 47 | 37 | 1 | 4 | 5 | | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 51 | 41 | 1 | 4 | 5 | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 14 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 54 | 44 | 1 | 4 | 5 | | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 59 | 49 | 1 | 4 | 5 | | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 47 | 37 | 1 | 4 | 5 | | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | | |

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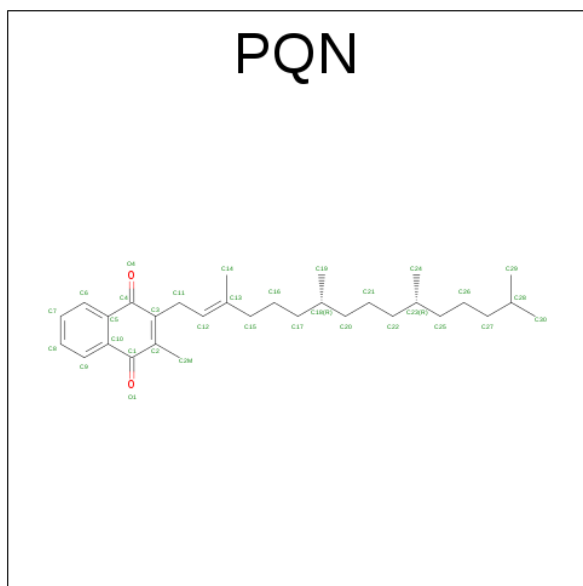
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 14 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 54 | 44 | 1 | 4 | 5 | | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 46 | 36 | 1 | 4 | 5 | | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 49 | 39 | 1 | 4 | 5 | | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 58 | 48 | 1 | 4 | 5 | | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 47 | 37 | 1 | 4 | 5 | | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 14 | F | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | | |
| 14 | J | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | | |

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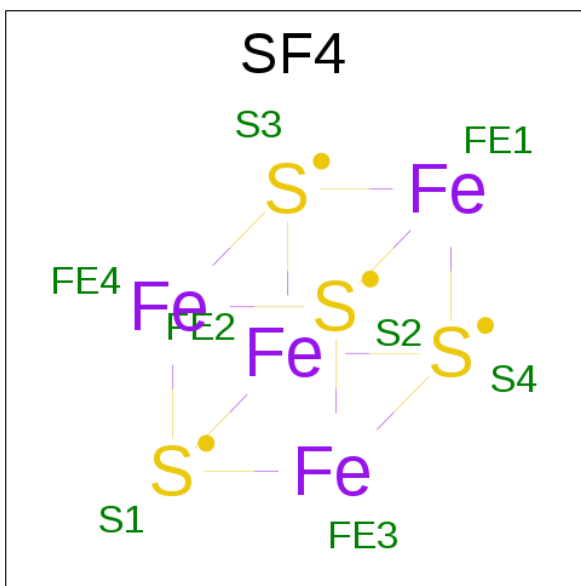
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 14 | J | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 37 | 31 | 1 | 4 | 1 | | |
| 14 | K | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 41 | 33 | 1 | 4 | 3 | | |
| 14 | L | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 14 | L | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 14 | L | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 14 | M | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | | |
| 14 | X | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 52 | 42 | 1 | 4 | 5 | | |

- Molecule 15 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



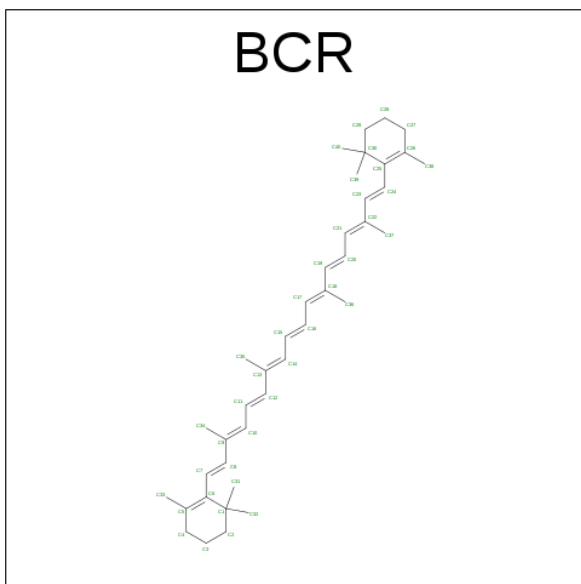
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 15 | A | 1 | Total | C | O | 0 | 0 |
| | | | 33 | 31 | 2 | | |
| 15 | B | 1 | Total | C | O | 0 | 0 |
| | | | 33 | 31 | 2 | | |

- Molecule 16 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



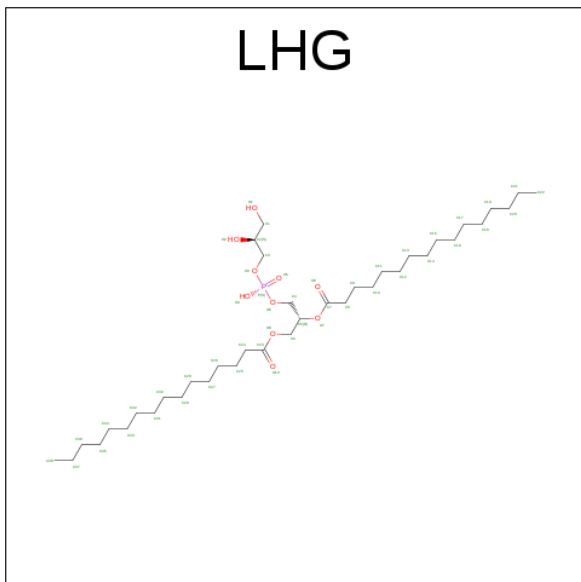
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 16 | A | 1 | Total | Fe | S | 0 | 0 |
| | | | 8 | 4 | 4 | | |
| 16 | C | 1 | Total | Fe | S | 0 | 0 |
| | | | 8 | 4 | 4 | | |
| 16 | C | 1 | Total | Fe | S | 0 | 0 |
| | | | 8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

- Molecule 17 is BETA-CAROTENE (three-letter code: BCR) (formula: $\text{C}_{40}\text{H}_{56}$).



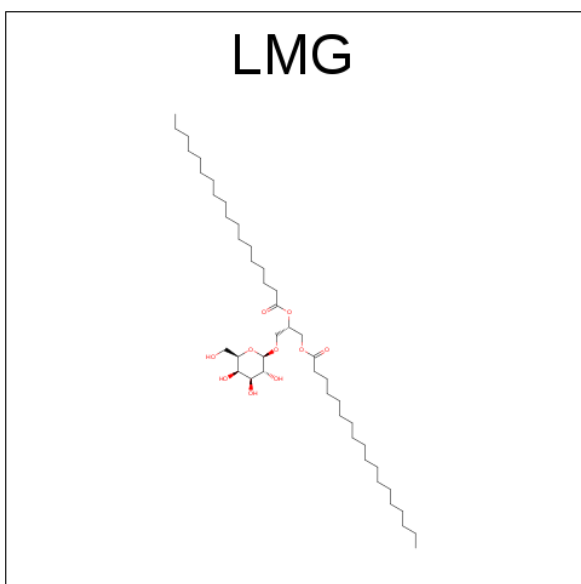
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 17 | A | 1 | Total C 40 40 | 0 | 0 |
| 17 | A | 1 | Total C 40 40 | 0 | 0 |
| 17 | A | 1 | Total C 40 40 | 0 | 0 |
| 17 | B | 1 | Total C 40 40 | 0 | 0 |
| 17 | B | 1 | Total C 40 40 | 0 | 0 |
| 17 | B | 1 | Total C 40 40 | 0 | 0 |
| 17 | A | 1 | Total C 40 40 | 0 | 0 |
| 17 | A | 1 | Total C 40 40 | 0 | 0 |
| 17 | B | 1 | Total C 25 25 | 0 | 0 |
| 17 | B | 1 | Total C 40 40 | 0 | 0 |
| 17 | A | 1 | Total C 40 40 | 0 | 0 |
| 17 | J | 1 | Total C 40 40 | 0 | 0 |
| 17 | J | 1 | Total C 40 40 | 0 | 0 |
| 17 | B | 1 | Total C 40 40 | 0 | 0 |
| 17 | J | 1 | Total C 40 40 | 0 | 0 |
| 17 | F | 1 | Total C 40 40 | 0 | 0 |
| 17 | B | 1 | Total C 40 40 | 0 | 0 |
| 17 | I | 1 | Total C 40 40 | 0 | 0 |
| 17 | L | 1 | Total C 40 40 | 0 | 0 |
| 17 | I | 1 | Total C 40 40 | 0 | 0 |
| 17 | M | 1 | Total C 40 40 | 0 | 0 |
| 17 | L | 1 | Total C 40 40 | 0 | 0 |

- Molecule 18 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 18 | A | 1 | Total | C | O | P | 0 | 0 |
| | | | 49 | 38 | 10 | 1 | | |
| 18 | A | 1 | Total | C | O | P | 0 | 0 |
| | | | 27 | 16 | 10 | 1 | | |
| 18 | B | 1 | Total | C | O | P | 0 | 0 |
| | | | 23 | 12 | 10 | 1 | | |

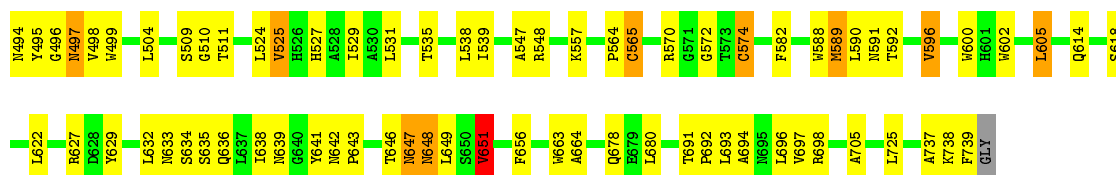
- Molecule 19 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 19 | B | 1 | Total | C | O | 0 | 0 |
| | | | 55 | 45 | 10 | | |

- Molecule 20 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 20 | A | 53 | Total | O | 0 | 0 |
| | | | 53 | 53 | | |
| 20 | B | 65 | Total | O | 0 | 0 |
| | | | 65 | 65 | | |
| 20 | C | 21 | Total | O | 0 | 0 |
| | | | 21 | 21 | | |
| 20 | D | 17 | Total | O | 0 | 0 |
| | | | 17 | 17 | | |
| 20 | E | 5 | Total | O | 0 | 0 |
| | | | 5 | 5 | | |
| 20 | F | 6 | Total | O | 0 | 0 |
| | | | 6 | 6 | | |
| 20 | I | 3 | Total | O | 0 | 0 |
| | | | 3 | 3 | | |
| 20 | J | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 20 | L | 27 | Total | O | 0 | 0 |
| | | | 27 | 27 | | |
| 20 | M | 3 | Total | O | 0 | 0 |
| | | | 3 | 3 | | |



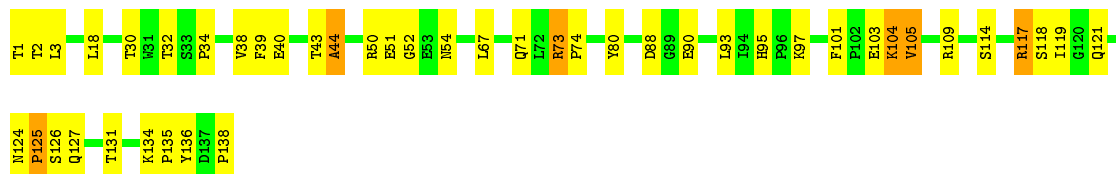
• Molecule 3: PHOTOSYSTEM I IRON-SULFUR CENTER

Chain C: 74% 25%



• Molecule 4: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT II

Chain D: 67% 28%



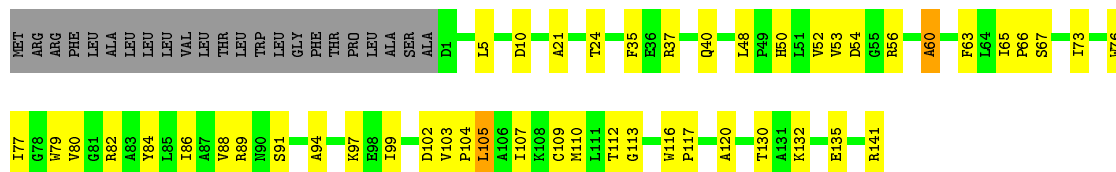
• Molecule 5: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT IV

Chain E: 72% 16% 8%



• Molecule 6: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT III

Chain F: 57% 28% 14%



• Molecule 7: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT VIII

Chain I: 74% 21% 5%

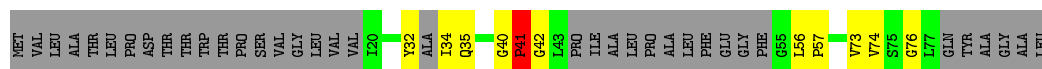


• Molecule 8: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT IX

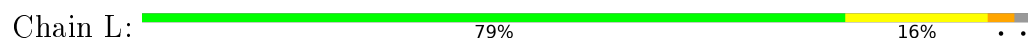
Chain J: 54% 41% 5%



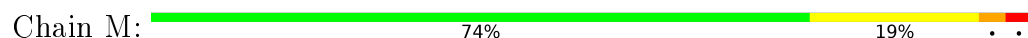
- Molecule 9: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT X



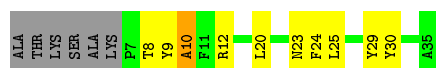
- Molecule 10: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT XI



- Molecule 11: PHOTOSYSTEM 1 REACTION CENTRE SUBUNIT XII



- Molecule 12: PHOTOSYSTEM I SUBUNIT PSAX



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

| Property | Value | Source |
|--|---|-----------|
| Space group | P 63 | Depositor |
| Cell constants a, b, c, α , β , γ | 281.00 Å 281.00 Å 165.20 Å 90.00° 90.00° 120.00° | Depositor |
| Resolution (Å) | 30.00 – 2.50 | Depositor |
| % Data completeness (in resolution range) | 93.3 (30.00-2.50) | Depositor |
| R_{merge} | 0.06 | Depositor |
| R_{sym} | (Not available) | Depositor |
| Refinement program | CNS 0.9 | Depositor |
| R, R_{free} | 0.199 , 0.217 | Depositor |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 24198 | wwPDB-VP |
| Average B, all atoms (Å ²) | 46.0 | wwPDB-VP |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, SF4, CLA, PQN, CA, 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 | 0.51 | 0/5983 | 0.66 | 2/8158 (0.0%) |
| 2 | B | 0.56 | 0/6096 | 0.67 | 2/8332 (0.0%) |
| 3 | C | 0.74 | 0/608 | 0.96 | 4/824 (0.5%) |
| 4 | D | 0.57 | 0/1101 | 0.81 | 1/1492 (0.1%) |
| 5 | E | 0.57 | 0/551 | 0.84 | 2/750 (0.3%) |
| 6 | F | 0.47 | 0/1087 | 0.66 | 0/1476 |
| 7 | I | 0.66 | 0/312 | 0.75 | 0/425 |
| 8 | J | 0.45 | 0/350 | 0.65 | 0/477 |
| 9 | K | 0.52 | 0/219 | 0.86 | 3/297 (1.0%) |
| 10 | L | 0.67 | 0/1148 | 0.75 | 0/1558 |
| 11 | M | 0.63 | 0/244 | 0.85 | 1/332 (0.3%) |
| 12 | X | 0.55 | 0/242 | 0.67 | 0/332 |
| All | All | 0.55 | 0/17941 | 0.70 | 15/24453 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 3 | C | 0 | 1 |

There are no bond length outliers.

All (15) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3 | C | 80 | TYR | CA-C-O | 9.95 | 140.99 | 120.10 |
| 11 | M | 30 | TYR | N-CA-C | 7.84 | 132.18 | 111.00 |
| 4 | D | 131 | THR | N-CA-C | -7.83 | 89.86 | 111.00 |
| 5 | E | 54 | GLY | N-CA-C | 7.52 | 131.91 | 113.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1 | A | 521 | GLY | N-CA-C | -6.39 | 97.13 | 113.10 |
| 3 | C | 60 | ASP | CA-C-N | -6.29 | 103.37 | 117.20 |
| 9 | K | 57 | PRO | N-CA-CB | 6.14 | 110.67 | 103.30 |
| 3 | C | 60 | ASP | C-N-CA | 5.89 | 136.41 | 121.70 |
| 1 | A | 114 | ALA | N-CA-C | -5.87 | 95.16 | 111.00 |
| 3 | C | 61 | PHE | N-CA-CB | 5.85 | 121.14 | 110.60 |
| 9 | K | 41 | PRO | N-CA-CB | 5.78 | 110.24 | 103.30 |
| 9 | K | 35 | GLN | N-CA-C | 5.35 | 125.45 | 111.00 |
| 2 | B | 430 | LEU | CA-CB-CG | 5.12 | 127.08 | 115.30 |
| 2 | B | 651 | VAL | CB-CA-C | -5.10 | 101.72 | 111.40 |
| 5 | E | 55 | VAL | N-CA-C | 5.01 | 124.53 | 111.00 |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 3 | C | 61 | PHE | 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 | 5784 | 0 | 5639 | 215 | 0 |
| 2 | B | 5879 | 0 | 5632 | 238 | 0 |
| 3 | C | 598 | 0 | 580 | 16 | 0 |
| 4 | D | 1075 | 0 | 1077 | 40 | 0 |
| 5 | E | 539 | 0 | 528 | 10 | 0 |
| 6 | F | 1065 | 0 | 1079 | 42 | 0 |
| 7 | I | 301 | 0 | 306 | 7 | 0 |
| 8 | J | 338 | 0 | 347 | 23 | 0 |
| 9 | K | 222 | 0 | 110 | 4 | 0 |
| 10 | L | 1119 | 0 | 1125 | 22 | 0 |
| 11 | M | 241 | 0 | 264 | 13 | 0 |
| 12 | X | 233 | 0 | 231 | 6 | 0 |
| 13 | L | 1 | 0 | 0 | 0 | 0 |
| 14 | A | 2687 | 0 | 2675 | 143 | 0 |
| 14 | B | 2349 | 0 | 2304 | 152 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 14 | F | 45 | 0 | 33 | 1 | 0 |
| 14 | J | 82 | 0 | 58 | 1 | 0 |
| 14 | K | 45 | 0 | 33 | 1 | 0 |
| 14 | L | 195 | 0 | 216 | 11 | 0 |
| 14 | M | 45 | 0 | 33 | 1 | 0 |
| 14 | X | 45 | 0 | 33 | 1 | 0 |
| 15 | A | 33 | 0 | 46 | 1 | 0 |
| 15 | B | 33 | 0 | 46 | 1 | 0 |
| 16 | A | 8 | 0 | 0 | 0 | 0 |
| 16 | C | 16 | 0 | 0 | 0 | 0 |
| 17 | A | 240 | 0 | 336 | 22 | 0 |
| 17 | B | 265 | 0 | 369 | 17 | 0 |
| 17 | F | 40 | 0 | 56 | 2 | 0 |
| 17 | I | 80 | 0 | 112 | 3 | 0 |
| 17 | J | 120 | 0 | 168 | 16 | 0 |
| 17 | L | 80 | 0 | 112 | 1 | 0 |
| 17 | M | 40 | 0 | 56 | 2 | 0 |
| 18 | A | 76 | 0 | 98 | 6 | 0 |
| 18 | B | 23 | 0 | 16 | 1 | 0 |
| 19 | B | 55 | 0 | 86 | 5 | 0 |
| 20 | A | 53 | 0 | 0 | 5 | 0 |
| 20 | B | 65 | 0 | 0 | 3 | 0 |
| 20 | C | 21 | 0 | 0 | 3 | 0 |
| 20 | D | 17 | 0 | 0 | 1 | 0 |
| 20 | E | 5 | 0 | 0 | 0 | 0 |
| 20 | F | 6 | 0 | 0 | 1 | 0 |
| 20 | I | 3 | 0 | 0 | 0 | 0 |
| 20 | J | 1 | 0 | 0 | 0 | 0 |
| 20 | L | 27 | 0 | 0 | 1 | 1 |
| 20 | M | 3 | 0 | 0 | 1 | 0 |
| All | All | 24198 | 0 | 23804 | 743 | 1 |

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 16.

All (743) 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) |
|------------------|--------------------|--------------------------|-------------------|
| 8:J:31:ARG:HD3 | 17:J:4013:BCR:H312 | 1.25 | 1.17 |
| 2:B:622:LEU:HD12 | 14:B:1012:CLA:H11 | 1.29 | 1.15 |
| 1:A:508:THR:HG22 | 1:A:510:SER:H | 1.18 | 1.07 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:159:LYS:H | 2:B:159:LYS:HD2 | 1.18 | 1.05 |
| 4:D:50:ARG:H | 4:D:54:ASN:HD21 | 1.06 | 1.01 |
| 2:B:243:PHE:H | 2:B:263:GLN:HE22 | 1.07 | 1.01 |
| 2:B:231:VAL:O | 2:B:234:GLN:HG2 | 1.63 | 0.99 |
| 2:B:406:ASN:HD22 | 2:B:409:ASN:HD21 | 0.98 | 0.96 |
| 1:A:536:PHE:HA | 14:A:1136:CLA:HED1 | 1.45 | 0.96 |
| 2:B:494:ASN:HD22 | 2:B:496:GLY:H | 1.13 | 0.93 |
| 11:M:31:LYS:O | 11:M:31:LYS:HG2 | 1.70 | 0.92 |
| 1:A:353:HIS:HD2 | 1:A:411:HIS:HD1 | 1.21 | 0.88 |
| 4:D:117:ARG:HG3 | 4:D:121:GLN:HB2 | 1.54 | 0.88 |
| 17:A:4011:BCR:H362 | 14:B:1012:CLA:H42 | 1.55 | 0.87 |
| 1:A:117:VAL:HG13 | 1:A:123:GLN:HE21 | 1.42 | 0.84 |
| 2:B:406:ASN:ND2 | 2:B:409:ASN:HD21 | 1.76 | 0.83 |
| 8:J:24:GLY:HA3 | 14:J:1302:CLA:HBB1 | 1.60 | 0.83 |
| 4:D:101:PHE:HB2 | 4:D:104:LYS:HE2 | 1.59 | 0.83 |
| 8:J:31:ARG:HD3 | 17:J:4013:BCR:C31 | 2.08 | 0.83 |
| 1:A:333:LYS:O | 14:A:1801:CLA:HBC3 | 1.81 | 0.81 |
| 2:B:509:SER:O | 2:B:511:THR:N | 2.12 | 0.81 |
| 1:A:203:GLY:HA2 | 14:A:1118:CLA:HBC1 | 1.63 | 0.80 |
| 1:A:391:LEU:O | 1:A:395:THR:HG23 | 1.81 | 0.80 |
| 2:B:642:ASN:HB2 | 2:B:643:PRO:CD | 2.12 | 0.80 |
| 6:F:88:VAL:HG12 | 6:F:94:ALA:HA | 1.63 | 0.79 |
| 6:F:88:VAL:HG11 | 6:F:97:LYS:HB2 | 1.64 | 0.79 |
| 1:A:345:TYR:O | 1:A:349:THR:HB | 1.84 | 0.78 |
| 2:B:494:ASN:ND2 | 2:B:496:GLY:H | 1.80 | 0.78 |
| 2:B:459:GLU:HG3 | 6:F:5:LEU:HD11 | 1.63 | 0.78 |
| 2:B:243:PHE:H | 2:B:263:GLN:NE2 | 1.82 | 0.78 |
| 1:A:508:THR:HG22 | 1:A:510:SER:N | 1.96 | 0.77 |
| 2:B:313:LYS:O | 2:B:314:VAL:HG22 | 1.85 | 0.77 |
| 3:C:37:GLN:NE2 | 4:D:105:VAL:HG22 | 1.99 | 0.77 |
| 2:B:278:ALA:HB2 | 14:B:1214:CLA:HBB1 | 1.66 | 0.77 |
| 2:B:339:TRP:HE1 | 14:B:1221:CLA:C2B | 1.99 | 0.76 |
| 2:B:25:ALA:HB2 | 19:B:5002:LMG:H121 | 1.67 | 0.76 |
| 14:A:1011:CLA:HBB1 | 14:B:1012:CLA:HED1 | 1.67 | 0.75 |
| 1:A:231:VAL:O | 1:A:232:ALA:HB3 | 1.87 | 0.75 |
| 14:A:1126:CLA:H192 | 17:J:4012:BCR:H14C | 1.69 | 0.75 |
| 2:B:367:ASP:CG | 2:B:370:THR:HG23 | 2.07 | 0.75 |
| 2:B:647:ASN:HD22 | 2:B:649:LEU:H | 1.35 | 0.75 |
| 14:B:1215:CLA:HMB1 | 14:B:1215:CLA:HBB1 | 1.68 | 0.75 |
| 14:A:1126:CLA:H93 | 17:J:4012:BCR:H361 | 1.69 | 0.74 |
| 1:A:453:PHE:O | 14:A:1132:CLA:HBB2 | 1.88 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:B:1222:CLA:HAA2 | 14:B:1223:CLA:OBD | 1.87 | 0.74 |
| 2:B:639:ASN:HD22 | 2:B:642:ASN:HD22 | 1.36 | 0.74 |
| 2:B:229:TRP:HB2 | 14:B:1213:CLA:H12 | 1.70 | 0.73 |
| 2:B:497:ASN:O | 2:B:498:VAL:HB | 1.87 | 0.73 |
| 4:D:50:ARG:N | 4:D:54:ASN:HD21 | 1.84 | 0.73 |
| 2:B:159:LYS:H | 2:B:159:LYS:CD | 1.92 | 0.73 |
| 2:B:494:ASN:HD22 | 2:B:496:GLY:N | 1.84 | 0.72 |
| 2:B:181:LEU:HG | 14:B:1210:CLA:H43 | 1.71 | 0.72 |
| 2:B:425:LEU:HG | 14:B:1236:CLA:CBB | 2.20 | 0.72 |
| 2:B:622:LEU:HD12 | 14:B:1012:CLA:C1 | 2.15 | 0.72 |
| 2:B:725:LEU:HD11 | 14:B:1226:CLA:H203 | 1.69 | 0.72 |
| 11:M:31:LYS:O | 11:M:31:LYS:CG | 2.34 | 0.72 |
| 2:B:329:TYR:OH | 2:B:340:HIS:HE1 | 1.71 | 0.72 |
| 3:C:39:ALA:O | 20:C:3012:HOH:O | 2.07 | 0.72 |
| 2:B:343:CYS:HB3 | 14:B:1221:CLA:H42 | 1.72 | 0.71 |
| 14:B:1216:CLA:HAA2 | 14:B:1221:CLA:HBB1 | 1.72 | 0.71 |
| 2:B:36:MET:HE3 | 2:B:40:ASN:HB2 | 1.72 | 0.71 |
| 1:A:202:ALA:HB2 | 1:A:312:GLY:HA3 | 1.71 | 0.71 |
| 1:A:221:LEU:HB2 | 1:A:222:PRO:HD3 | 1.73 | 0.71 |
| 1:A:341:HIS:HE1 | 18:A:5003:LHG:HC11 | 1.56 | 0.70 |
| 5:E:68:VAL:HG23 | 5:E:69:ALA:H | 1.56 | 0.70 |
| 1:A:255:LYS:HB2 | 1:A:277:ASP:OD2 | 1.92 | 0.69 |
| 2:B:222:ALA:HB3 | 2:B:223:PRO:HD3 | 1.74 | 0.69 |
| 2:B:589:MET:HE1 | 2:B:590:LEU:HA | 1.75 | 0.69 |
| 1:A:13:ARG:HE | 1:A:15:VAL:CG2 | 2.05 | 0.68 |
| 2:B:602:TRP:HE1 | 2:B:614:GLN:HE21 | 1.40 | 0.68 |
| 14:A:1136:CLA:H101 | 14:L:1502:CLA:H191 | 1.75 | 0.68 |
| 1:A:221:LEU:HD11 | 1:A:295:SER:HA | 1.76 | 0.68 |
| 1:A:399:TRP:CD1 | 14:A:1126:CLA:HAB | 2.29 | 0.68 |
| 6:F:52:VAL:HG12 | 6:F:54:ASP:HB2 | 1.76 | 0.67 |
| 1:A:117:VAL:HG13 | 1:A:123:GLN:NE2 | 2.08 | 0.67 |
| 2:B:25:ALA:HA | 14:B:1226:CLA:H42 | 1.76 | 0.67 |
| 1:A:101:GLU:OE2 | 1:A:155:GLU:HG2 | 1.95 | 0.66 |
| 6:F:102:ASP:OD2 | 6:F:105:LEU:HB2 | 1.95 | 0.66 |
| 9:K:73:VAL:HA | 14:K:1401:CLA:HBB1 | 1.77 | 0.66 |
| 1:A:336:PHE:HB2 | 18:A:5003:LHG:HC41 | 1.78 | 0.66 |
| 2:B:339:TRP:HZ2 | 14:B:1221:CLA:HAB | 1.58 | 0.66 |
| 3:C:65:ARG:HG2 | 3:C:67:TYR:CZ | 2.31 | 0.66 |
| 15:A:2001:PQN:H172 | 17:B:4014:BCR:H382 | 1.77 | 0.66 |
| 4:D:50:ARG:H | 4:D:54:ASN:ND2 | 1.89 | 0.66 |
| 2:B:188:ALA:HA | 14:B:1212:CLA:CBB | 2.27 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:352:TRP:HB3 | 14:A:1103:CLA:HAC1 | 1.77 | 0.65 |
| 2:B:210:ASN:O | 2:B:214:THR:HG23 | 1.96 | 0.65 |
| 2:B:318:PHE:HB2 | 14:B:1220:CLA:HMA1 | 1.78 | 0.65 |
| 2:B:318:PHE:CD1 | 14:B:1219:CLA:HAB | 2.32 | 0.65 |
| 2:B:41:LEU:O | 2:B:45:ILE:HG12 | 1.97 | 0.65 |
| 6:F:63:PHE:C | 6:F:66:PRO:HD2 | 2.17 | 0.65 |
| 1:A:249:MET:O | 1:A:252:LEU:O | 2.15 | 0.65 |
| 1:A:257:ASP:OD1 | 1:A:262:SER:HB3 | 1.96 | 0.65 |
| 2:B:492:TRP:CE3 | 2:B:493:PRO:HD3 | 2.32 | 0.65 |
| 1:A:269:THR:O | 1:A:270:PHE:HB2 | 1.96 | 0.65 |
| 2:B:313:LYS:O | 2:B:314:VAL:HG13 | 1.97 | 0.65 |
| 6:F:65:ILE:HB | 6:F:66:PRO:HD3 | 1.78 | 0.65 |
| 10:L:6:LYS:HB2 | 10:L:7:PRO:HD2 | 1.79 | 0.65 |
| 14:A:1237:CLA:H191 | 14:L:1502:CLA:HBB1 | 1.78 | 0.65 |
| 6:F:54:ASP:OD2 | 12:X:30:TYR:CE2 | 2.50 | 0.64 |
| 14:B:1226:CLA:HMB1 | 14:B:1226:CLA:HBB1 | 1.78 | 0.64 |
| 2:B:304:MET:HG3 | 2:B:322:HIS:O | 1.97 | 0.64 |
| 2:B:647:ASN:ND2 | 2:B:649:LEU:H | 1.95 | 0.64 |
| 10:L:61:PRO:HB3 | 14:L:1503:CLA:HBB1 | 1.78 | 0.64 |
| 1:A:473:ASP:OD1 | 10:L:69:ARG:NH2 | 2.31 | 0.64 |
| 2:B:641:TYR:HB2 | 2:B:646:THR:HG22 | 1.79 | 0.64 |
| 8:J:12:PRO:HB2 | 17:J:4013:BCR:H391 | 1.78 | 0.64 |
| 14:B:1203:CLA:H162 | 14:B:1225:CLA:HBB2 | 1.80 | 0.64 |
| 6:F:103:VAL:HB | 6:F:104:PRO:HD3 | 1.79 | 0.63 |
| 3:C:23:ASP:OD2 | 4:D:95:HIS:HD2 | 1.81 | 0.63 |
| 14:B:1023:CLA:H111 | 17:B:4017:BCR:H362 | 1.79 | 0.63 |
| 6:F:63:PHE:O | 6:F:66:PRO:HD2 | 1.98 | 0.63 |
| 14:A:1011:CLA:HAB | 14:B:1021:CLA:NA | 2.14 | 0.63 |
| 2:B:318:PHE:HA | 14:B:1219:CLA:CAB | 2.28 | 0.63 |
| 4:D:117:ARG:HG2 | 4:D:118:SER:O | 1.98 | 0.63 |
| 2:B:622:LEU:CD1 | 14:B:1012:CLA:H11 | 2.16 | 0.63 |
| 6:F:60:ALA:O | 6:F:65:ILE:HG12 | 1.98 | 0.62 |
| 1:A:177:TRP:HB2 | 14:A:1109:CLA:HMC3 | 1.80 | 0.62 |
| 2:B:166:TRP:CZ2 | 14:B:1208:CLA:HMA1 | 2.33 | 0.62 |
| 2:B:321:PRO:HB2 | 2:B:409:ASN:HA | 1.80 | 0.62 |
| 11:M:29:LEU:O | 11:M:30:TYR:HB2 | 1.99 | 0.62 |
| 1:A:104:LEU:HD11 | 1:A:153:THR:HA | 1.81 | 0.62 |
| 1:A:651:ARG:HB2 | 2:B:638:ILE:HG23 | 1.81 | 0.62 |
| 1:A:86:TRP:HA | 14:A:1105:CLA:HBB2 | 1.82 | 0.62 |
| 2:B:136:GLN:HE22 | 2:B:208:TRP:HE1 | 1.46 | 0.62 |
| 2:B:228:ASN:O | 2:B:231:VAL:HG23 | 2.00 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:602:MET:HG2 | 14:A:1124:CLA:HBC1 | 1.80 | 0.62 |
| 2:B:647:ASN:HD21 | 2:B:649:LEU:HB2 | 1.64 | 0.62 |
| 2:B:480:LEU:C | 2:B:482:SER:H | 2.02 | 0.62 |
| 1:A:356:LEU:O | 1:A:360:LEU:HB2 | 2.00 | 0.62 |
| 1:A:353:HIS:CD2 | 1:A:411:HIS:HD1 | 2.11 | 0.61 |
| 2:B:278:ALA:CB | 14:B:1214:CLA:HBB1 | 2.29 | 0.61 |
| 14:A:1237:CLA:HMA1 | 2:B:694:ALA:CB | 2.29 | 0.61 |
| 14:A:1124:CLA:HAA2 | 14:A:1125:CLA:OBD | 2.00 | 0.61 |
| 1:A:543:ALA:HB1 | 14:A:1136:CLA:HMB3 | 1.83 | 0.61 |
| 1:A:429:VAL:O | 1:A:433:VAL:HG13 | 1.99 | 0.61 |
| 2:B:438:GLY:HA3 | 14:B:1230:CLA:CBB | 2.31 | 0.61 |
| 1:A:42:PRO:HG2 | 6:F:99:ILE:HD13 | 1.83 | 0.61 |
| 11:M:24:ARG:HG3 | 11:M:24:ARG:HH11 | 1.64 | 0.61 |
| 1:A:90:MET:HE3 | 14:A:1106:CLA:HED2 | 1.82 | 0.61 |
| 14:B:1234:CLA:HMB2 | 14:B:1236:CLA:HED1 | 1.81 | 0.61 |
| 14:A:1801:CLA:HBD | 14:A:1801:CLA:H61 | 1.83 | 0.61 |
| 1:A:453:PHE:O | 14:A:1132:CLA:CBB | 2.48 | 0.61 |
| 1:A:726:GLN:HG3 | 18:A:5001:LHG:O9 | 2.01 | 0.61 |
| 1:A:601:TRP:HH2 | 14:A:1022:CLA:HBB1 | 1.66 | 0.60 |
| 1:A:518:VAL:HG22 | 1:A:525:ALA:HB3 | 1.82 | 0.60 |
| 10:L:153:PHE:O | 10:L:154:ASN:HB2 | 1.99 | 0.60 |
| 14:B:1203:CLA:H151 | 14:B:1203:CLA:H102 | 1.84 | 0.60 |
| 3:C:30:TRP:O | 3:C:36:GLY:HA2 | 2.00 | 0.60 |
| 1:A:303:ALA:HB2 | 14:A:1116:CLA:HBB1 | 1.83 | 0.60 |
| 9:K:32:TYR:O | 9:K:34:ILE:N | 2.34 | 0.60 |
| 1:A:484:PRO:HB3 | 14:A:1136:CLA:HED3 | 1.83 | 0.60 |
| 14:A:1011:CLA:HBB1 | 14:B:1012:CLA:CED | 2.31 | 0.60 |
| 1:A:168:MET:CE | 1:A:171:LEU:HD23 | 2.31 | 0.60 |
| 14:A:1013:CLA:H71 | 14:A:1140:CLA:HMC3 | 1.83 | 0.59 |
| 1:A:210:LEU:HD21 | 17:A:4001:BCR:H342 | 1.84 | 0.59 |
| 1:A:300:HIS:O | 1:A:304:ILE:HG12 | 2.03 | 0.59 |
| 1:A:19:ASP:HA | 1:A:181:HIS:O | 2.02 | 0.59 |
| 1:A:231:VAL:O | 1:A:232:ALA:CB | 2.50 | 0.59 |
| 14:B:1227:CLA:HBC1 | 17:B:4009:BCR:H23C | 1.83 | 0.59 |
| 1:A:259:GLY:O | 1:A:261:PHE:N | 2.35 | 0.59 |
| 2:B:181:LEU:HD21 | 14:B:1210:CLA:H12 | 1.85 | 0.59 |
| 14:A:1138:CLA:H43 | 14:B:1229:CLA:HAA2 | 1.84 | 0.59 |
| 2:B:36:MET:CE | 2:B:41:LEU:N | 2.66 | 0.59 |
| 2:B:642:ASN:HB2 | 2:B:643:PRO:HD2 | 1.84 | 0.59 |
| 4:D:40:GLU:H | 4:D:71:GLN:NE2 | 2.01 | 0.59 |
| 1:A:257:ASP:CG | 1:A:258:TRP:N | 2.56 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:I:7:ALA:HB1 | 7:I:10:LEU:HD22 | 1.83 | 0.59 |
| 2:B:591:ASN:HB2 | 14:B:1012:CLA:HBC2 | 1.83 | 0.58 |
| 7:I:37:GLU:C | 7:I:38:ALA:OXT | 2.41 | 0.58 |
| 1:A:16:VAL:HG12 | 1:A:17:ASP:N | 2.17 | 0.58 |
| 1:A:207:LEU:HD22 | 17:A:4002:BCR:H361 | 1.84 | 0.58 |
| 2:B:438:GLY:HA3 | 14:B:1230:CLA:HBB1 | 1.85 | 0.58 |
| 10:L:36:ALA:HB2 | 14:L:1502:CLA:HMD1 | 1.84 | 0.58 |
| 1:A:86:TRP:HA | 14:A:1105:CLA:CBB | 2.33 | 0.58 |
| 14:A:1121:CLA:HMA1 | 14:A:1801:CLA:HAC2 | 1.85 | 0.58 |
| 2:B:589:MET:HE2 | 2:B:589:MET:O | 2.02 | 0.58 |
| 14:B:1230:CLA:O1D | 8:J:35:ASP:HA | 2.02 | 0.58 |
| 2:B:243:PHE:N | 2:B:263:GLN:HE22 | 1.90 | 0.58 |
| 14:A:1106:CLA:HMC2 | 14:A:1126:CLA:H142 | 1.84 | 0.58 |
| 1:A:145:GLN:NE2 | 1:A:145:GLN:H | 2.02 | 0.58 |
| 1:A:744:TRP:HB2 | 14:A:1126:CLA:HBB1 | 1.86 | 0.58 |
| 2:B:367:ASP:OD1 | 2:B:370:THR:HG23 | 2.03 | 0.58 |
| 2:B:648:ASN:HD22 | 2:B:648:ASN:N | 2.02 | 0.58 |
| 17:A:4011:BCR:H321 | 17:A:4011:BCR:HC8 | 1.83 | 0.58 |
| 2:B:380:TYR:CD1 | 14:B:1224:CLA:HBB1 | 2.39 | 0.57 |
| 1:A:91:TYR:CZ | 1:A:147:TRP:CZ3 | 2.91 | 0.57 |
| 1:A:392:SER:HB3 | 14:A:1126:CLA:HMA1 | 1.87 | 0.57 |
| 2:B:414:VAL:HG11 | 17:B:4009:BCR:H401 | 1.85 | 0.57 |
| 6:F:82:ARG:O | 6:F:86:ILE:HG12 | 2.04 | 0.57 |
| 14:A:1013:CLA:H12 | 2:B:430:LEU:HD12 | 1.85 | 0.57 |
| 1:A:542:HIS:HB3 | 14:A:1135:CLA:HBB1 | 1.87 | 0.57 |
| 2:B:557:LYS:HD2 | 4:D:124:ASN:OD1 | 2.04 | 0.57 |
| 2:B:279:ILE:HD11 | 14:B:1214:CLA:CBC | 2.35 | 0.57 |
| 5:E:24:ALA:O | 5:E:25:SER:HB3 | 2.05 | 0.57 |
| 14:A:1106:CLA:H112 | 14:A:1128:CLA:H203 | 1.87 | 0.56 |
| 1:A:355:GLN:HG3 | 14:A:1123:CLA:H152 | 1.87 | 0.56 |
| 1:A:349:THR:HG22 | 1:A:350:THR:HG23 | 1.87 | 0.56 |
| 1:A:694:ARG:HD3 | 2:B:572:GLY:HA3 | 1.86 | 0.56 |
| 2:B:678:GLN:NE2 | 2:B:705:ALA:H | 2.03 | 0.56 |
| 6:F:37:ARG:O | 6:F:40:GLN:HG2 | 2.04 | 0.56 |
| 1:A:189:TRP:CZ2 | 14:A:1108:CLA:HMA1 | 2.40 | 0.56 |
| 1:A:67:ASP:O | 1:A:71:LYS:HG3 | 2.05 | 0.56 |
| 2:B:282:LEU:HD12 | 14:B:1216:CLA:HMC1 | 1.87 | 0.56 |
| 8:J:15:ALA:O | 8:J:19:MET:HB2 | 2.06 | 0.56 |
| 1:A:233:ALA:O | 1:A:235:ASP:N | 2.36 | 0.56 |
| 2:B:234:GLN:OE1 | 2:B:234:GLN:HA | 2.06 | 0.56 |
| 2:B:339:TRP:CH2 | 17:B:4009:BCR:H372 | 2.40 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:X:20:LEU:HD11 | 12:X:24:PHE:HE1 | 1.71 | 0.56 |
| 2:B:279:ILE:HG23 | 2:B:283:PHE:CE2 | 2.41 | 0.56 |
| 2:B:339:TRP:CZ2 | 14:B:1221:CLA:HAB | 2.39 | 0.56 |
| 2:B:480:LEU:O | 2:B:482:SER:N | 2.38 | 0.56 |
| 6:F:76:TRP:CE2 | 6:F:113:GLY:HA3 | 2.40 | 0.56 |
| 1:A:66:GLU:OE2 | 1:A:186:LYS:HG3 | 2.05 | 0.56 |
| 14:A:1011:CLA:HAB | 14:B:1021:CLA:C1A | 2.36 | 0.56 |
| 12:X:9:TYR:O | 12:X:10:ALA:HB2 | 2.05 | 0.56 |
| 1:A:366:LEU:HD11 | 14:A:1117:CLA:H71 | 1.87 | 0.56 |
| 1:A:297:THR:O | 1:A:300:HIS:HB3 | 2.06 | 0.56 |
| 1:A:741:ALA:HB2 | 17:A:4011:BCR:H323 | 1.88 | 0.56 |
| 14:A:1102:CLA:HMC3 | 14:A:1104:CLA:HED2 | 1.86 | 0.55 |
| 14:A:1130:CLA:H12 | 14:L:1502:CLA:H93 | 1.86 | 0.55 |
| 4:D:117:ARG:CG | 4:D:121:GLN:HB2 | 2.33 | 0.55 |
| 2:B:588:TRP:HH2 | 14:B:1012:CLA:CBB | 2.19 | 0.55 |
| 2:B:589:MET:HE1 | 2:B:590:LEU:CA | 2.36 | 0.55 |
| 9:K:40:GLY:O | 9:K:41:PRO:C | 2.44 | 0.55 |
| 1:A:433:VAL:HA | 1:A:436:HIS:CE1 | 2.41 | 0.55 |
| 2:B:398:VAL:CG2 | 2:B:547:ALA:HB1 | 2.36 | 0.55 |
| 2:B:425:LEU:HD13 | 2:B:538:LEU:HA | 1.89 | 0.55 |
| 1:A:681:PHE:CD2 | 17:A:4011:BCR:H363 | 2.42 | 0.55 |
| 14:B:1225:CLA:H51 | 17:B:4006:BCR:H392 | 1.88 | 0.55 |
| 14:B:1224:CLA:HBC3 | 19:B:5002:LMG:H421 | 1.88 | 0.55 |
| 2:B:261:HIS:CD2 | 2:B:264:THR:H | 2.25 | 0.55 |
| 1:A:372:GLN:HG3 | 14:A:1124:CLA:CED | 2.37 | 0.55 |
| 2:B:233:ALA:O | 2:B:234:GLN:O | 2.25 | 0.55 |
| 14:A:1116:CLA:H41 | 14:A:1133:CLA:HAA2 | 1.88 | 0.54 |
| 1:A:244:LEU:O | 1:A:246:PRO:HD3 | 2.06 | 0.54 |
| 1:A:681:PHE:CG | 17:A:4011:BCR:H363 | 2.43 | 0.54 |
| 14:B:1238:CLA:H18 | 17:I:4018:BCR:H362 | 1.89 | 0.54 |
| 14:A:1237:CLA:HMA1 | 2:B:694:ALA:HB1 | 1.88 | 0.54 |
| 17:A:4007:BCR:H333 | 17:A:4008:BCR:H333 | 1.89 | 0.54 |
| 2:B:179:ALA:HB2 | 2:B:287:GLY:HA3 | 1.89 | 0.54 |
| 2:B:525:VAL:HG13 | 14:B:1021:CLA:H141 | 1.89 | 0.54 |
| 1:A:390:GLN:HA | 1:A:390:GLN:HE21 | 1.71 | 0.54 |
| 1:A:403:PHE:HB3 | 14:A:1104:CLA:H112 | 1.90 | 0.54 |
| 2:B:205:HIS:ND1 | 20:B:5051:HOH:O | 2.24 | 0.54 |
| 4:D:43:THR:O | 4:D:44:ALA:HB3 | 2.07 | 0.54 |
| 10:L:35:PRO:HG3 | 14:L:1502:CLA:HED2 | 1.88 | 0.54 |
| 2:B:413:ARG:HD3 | 14:B:1227:CLA:OBD | 2.07 | 0.54 |
| 14:B:1216:CLA:HMB2 | 14:B:1221:CLA:HMA3 | 1.89 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:157:GLN:O | 2:B:161:ARG:HG3 | 2.08 | 0.54 |
| 2:B:318:PHE:HA | 14:B:1219:CLA:HAB | 1.88 | 0.54 |
| 2:B:592:THR:O | 2:B:596:VAL:HG13 | 2.08 | 0.54 |
| 1:A:308:PHE:HE2 | 14:A:1119:CLA:HAB | 1.72 | 0.54 |
| 2:B:171:GLU:HB3 | 2:B:290:TYR:HB3 | 1.90 | 0.54 |
| 12:X:25:LEU:O | 12:X:29:TYR:HD1 | 1.89 | 0.54 |
| 1:A:42:PRO:HG3 | 1:A:47:TRP:CE3 | 2.42 | 0.54 |
| 2:B:589:MET:HE2 | 2:B:589:MET:C | 2.29 | 0.54 |
| 2:B:103:PHE:CZ | 2:B:651:VAL:HG22 | 2.42 | 0.54 |
| 2:B:614:GLN:O | 2:B:618:SER:HB2 | 2.08 | 0.54 |
| 5:E:6:LYS:HD3 | 5:E:22:THR:HG22 | 1.89 | 0.54 |
| 14:A:1022:CLA:OBD | 14:B:1021:CLA:HMB3 | 2.08 | 0.53 |
| 2:B:212:LEU:HD21 | 17:B:4006:BCR:H341 | 1.90 | 0.53 |
| 1:A:305:ALA:O | 1:A:309:ILE:HG12 | 2.08 | 0.53 |
| 6:F:52:VAL:CG1 | 6:F:54:ASP:HB2 | 2.37 | 0.53 |
| 11:M:24:ARG:HH11 | 11:M:24:ARG:CG | 2.20 | 0.53 |
| 14:A:1125:CLA:HBB1 | 14:A:1133:CLA:HMA2 | 1.89 | 0.53 |
| 14:A:1011:CLA:HMB3 | 14:B:1012:CLA:OBD | 2.09 | 0.53 |
| 14:A:1013:CLA:H142 | 17:A:4011:BCR:H402 | 1.90 | 0.53 |
| 14:A:1101:CLA:HED1 | 8:J:12:PRO:HA | 1.90 | 0.53 |
| 1:A:466:ARG:O | 2:B:646:THR:HG21 | 2.09 | 0.53 |
| 2:B:479:THR:O | 2:B:480:LEU:O | 2.27 | 0.53 |
| 14:B:1226:CLA:H143 | 19:B:5002:LMG:H231 | 1.89 | 0.53 |
| 6:F:53:VAL:HG12 | 6:F:63:PHE:HB2 | 1.90 | 0.53 |
| 6:F:88:VAL:HG11 | 6:F:97:LYS:CB | 2.37 | 0.53 |
| 14:A:1124:CLA:H162 | 17:A:4007:BCR:H272 | 1.91 | 0.53 |
| 14:A:1128:CLA:H111 | 18:A:5001:LHG:H202 | 1.90 | 0.53 |
| 1:A:622:TRP:O | 1:A:633:HIS:HD2 | 1.92 | 0.53 |
| 8:J:19:MET:CE | 8:J:19:MET:HA | 2.38 | 0.53 |
| 10:L:16:HIS:CD2 | 10:L:17:LEU:H | 2.27 | 0.53 |
| 1:A:13:ARG:HE | 1:A:15:VAL:HG22 | 1.72 | 0.53 |
| 1:A:168:MET:HE1 | 1:A:171:LEU:HD23 | 1.91 | 0.53 |
| 14:A:1013:CLA:O1A | 2:B:531:LEU:HD11 | 2.10 | 0.52 |
| 14:A:1119:CLA:HMB2 | 14:A:1123:CLA:HMA3 | 1.92 | 0.52 |
| 1:A:221:LEU:HD11 | 1:A:295:SER:CA | 2.39 | 0.52 |
| 1:A:59:ASP:OD2 | 1:A:353:HIS:HE1 | 1.91 | 0.52 |
| 2:B:406:ASN:HD22 | 2:B:409:ASN:ND2 | 1.84 | 0.52 |
| 1:A:296:ASP:HB3 | 14:A:1116:CLA:HMA1 | 1.90 | 0.52 |
| 1:A:244:LEU:C | 1:A:246:PRO:HD3 | 2.30 | 0.52 |
| 2:B:430:LEU:HB3 | 14:B:1229:CLA:HED3 | 1.90 | 0.52 |
| 6:F:40:GLN:OE1 | 8:J:40:PRO:O | 2.26 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:90:MET:CE | 14:A:1106:CLA:HED2 | 2.39 | 0.52 |
| 2:B:78:GLN:OE1 | 2:B:78:GLN:HA | 2.10 | 0.52 |
| 1:A:356:LEU:HG | 1:A:360:LEU:HD22 | 1.91 | 0.52 |
| 2:B:90:ILE:HB | 2:B:111:PRO:HB2 | 1.91 | 0.52 |
| 6:F:79:TRP:CH2 | 6:F:120:ALA:HA | 2.44 | 0.52 |
| 2:B:217:HIS:CG | 2:B:218:PRO:HD2 | 2.44 | 0.52 |
| 2:B:36:MET:HE2 | 2:B:41:LEU:N | 2.25 | 0.52 |
| 1:A:744:TRP:CZ2 | 14:A:1126:CLA:H43 | 2.44 | 0.52 |
| 14:A:1133:CLA:HMD2 | 14:A:1134:CLA:HBB1 | 1.92 | 0.52 |
| 1:A:578:CYS:HB3 | 1:A:587:CYS:HA | 1.91 | 0.52 |
| 8:J:28:GLU:OE1 | 8:J:28:GLU:HA | 2.09 | 0.52 |
| 2:B:634:SER:O | 2:B:638:ILE:HB | 2.10 | 0.52 |
| 1:A:77:PHE:CE2 | 14:A:1108:CLA:HBB1 | 2.45 | 0.52 |
| 1:A:718:GLN:NE2 | 5:E:42:LYS:HD3 | 2.25 | 0.52 |
| 2:B:294:PHE:HE1 | 14:B:1209:CLA:HMA1 | 1.75 | 0.52 |
| 1:A:83:VAL:HG11 | 14:A:1103:CLA:H72 | 1.92 | 0.51 |
| 1:A:16:VAL:HG11 | 1:A:183:ARG:HB3 | 1.92 | 0.51 |
| 2:B:279:ILE:HD11 | 14:B:1214:CLA:HBC2 | 1.92 | 0.51 |
| 1:A:226:LEU:HD22 | 1:A:231:VAL:HG21 | 1.93 | 0.51 |
| 1:A:259:GLY:C | 1:A:261:PHE:H | 2.14 | 0.51 |
| 2:B:398:VAL:HG23 | 2:B:547:ALA:HB1 | 1.93 | 0.51 |
| 10:L:31:ILE:HA | 10:L:34:LEU:HD22 | 1.92 | 0.51 |
| 1:A:542:HIS:HE1 | 1:A:612:HIS:ND1 | 2.09 | 0.51 |
| 1:A:71:LYS:NZ | 20:A:5034:HOH:O | 2.43 | 0.51 |
| 14:A:1125:CLA:HMB3 | 14:A:1133:CLA:H12 | 1.93 | 0.51 |
| 1:A:257:ASP:O | 1:A:258:TRP:HB2 | 2.11 | 0.51 |
| 2:B:456:ILE:HG22 | 2:B:458:ILE:CD1 | 2.40 | 0.51 |
| 2:B:159:LYS:HD2 | 2:B:159:LYS:N | 2.03 | 0.51 |
| 1:A:303:ALA:CB | 14:A:1116:CLA:HBB1 | 2.40 | 0.51 |
| 1:A:444:LEU:HB2 | 14:A:1137:CLA:CBB | 2.40 | 0.51 |
| 1:A:453:PHE:C | 14:A:1132:CLA:HBB2 | 2.31 | 0.51 |
| 14:B:1238:CLA:HBB2 | 15:B:2002:PQN:H141 | 1.91 | 0.51 |
| 2:B:379:GLN:HA | 2:B:379:GLN:OE1 | 2.11 | 0.51 |
| 2:B:453:GLU:HA | 6:F:48:LEU:HD22 | 1.93 | 0.51 |
| 1:A:118:TRP:CB | 17:J:4013:BCR:H323 | 2.41 | 0.51 |
| 14:B:1216:CLA:HMD1 | 14:B:1218:CLA:HBB1 | 1.93 | 0.50 |
| 4:D:117:ARG:HG2 | 4:D:118:SER:N | 2.26 | 0.50 |
| 7:I:30:LEU:O | 7:I:34:ILE:HG12 | 2.11 | 0.50 |
| 1:A:16:VAL:CG1 | 1:A:17:ASP:N | 2.74 | 0.50 |
| 3:C:14:THR:HG22 | 3:C:27:MET:HG3 | 1.93 | 0.50 |
| 2:B:638:ILE:HD11 | 2:B:656:PHE:CE2 | 2.46 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:464:GLN:HG2 | 2:B:475:TYR:CE2 | 2.47 | 0.50 |
| 11:M:30:TYR:O | 11:M:31:LYS:OXT | 2.29 | 0.50 |
| 2:B:339:TRP:HE1 | 14:B:1221:CLA:C3B | 2.23 | 0.50 |
| 14:B:1220:CLA:HBB1 | 14:B:1227:CLA:HMD2 | 1.94 | 0.50 |
| 2:B:588:TRP:HH2 | 14:B:1012:CLA:HBB1 | 1.77 | 0.50 |
| 4:D:32:THR:HA | 4:D:52:GLY:O | 2.12 | 0.50 |
| 14:A:1013:CLA:HBB1 | 14:B:1012:CLA:NB | 2.27 | 0.50 |
| 14:B:1221:CLA:H61 | 14:B:1223:CLA:H42 | 1.94 | 0.50 |
| 14:B:1226:CLA:H8 | 19:B:5002:LMG:H242 | 1.94 | 0.50 |
| 2:B:431:PHE:CZ | 17:J:4015:BCR:HC41 | 2.46 | 0.50 |
| 5:E:68:VAL:O | 5:E:69:ALA:O | 2.30 | 0.49 |
| 7:I:9:PHE:CE1 | 7:I:10:LEU:HD13 | 2.46 | 0.49 |
| 1:A:691:PHE:HB2 | 14:A:1013:CLA:HBC2 | 1.95 | 0.49 |
| 2:B:340:HIS:HD2 | 14:B:1202:CLA:OBD | 1.95 | 0.49 |
| 4:D:101:PHE:HB3 | 4:D:103:GLU:OE2 | 2.11 | 0.49 |
| 2:B:459:GLU:OE2 | 6:F:50:HIS:ND1 | 2.40 | 0.49 |
| 2:B:548:ARG:HH22 | 4:D:124:ASN:ND2 | 2.10 | 0.49 |
| 2:B:548:ARG:HH22 | 4:D:124:ASN:CG | 2.15 | 0.49 |
| 2:B:664:ALA:C | 14:B:1023:CLA:HBB1 | 2.31 | 0.49 |
| 6:F:80:VAL:HG22 | 6:F:109:CYS:O | 2.13 | 0.49 |
| 14:A:1237:CLA:H52 | 14:B:1238:CLA:H43 | 1.93 | 0.49 |
| 10:L:105:GLY:O | 10:L:106:SER:HB2 | 2.11 | 0.49 |
| 14:A:1117:CLA:HMB1 | 14:A:1117:CLA:HBB1 | 1.93 | 0.49 |
| 2:B:114:ILE:O | 14:B:1205:CLA:HMD3 | 2.13 | 0.49 |
| 2:B:425:LEU:HG | 14:B:1236:CLA:HBB1 | 1.94 | 0.49 |
| 2:B:458:ILE:HD12 | 2:B:458:ILE:N | 2.28 | 0.49 |
| 4:D:30:THR:O | 4:D:80:TYR:HA | 2.13 | 0.49 |
| 2:B:162:PRO:HB2 | 2:B:167:PHE:CE1 | 2.48 | 0.49 |
| 14:B:1021:CLA:H72 | 14:B:1012:CLA:CED | 2.41 | 0.49 |
| 14:B:1216:CLA:CMB | 14:B:1221:CLA:HMA3 | 2.42 | 0.49 |
| 5:E:7:VAL:O | 5:E:20:VAL:HA | 2.13 | 0.49 |
| 6:F:84:TYR:O | 6:F:88:VAL:HG23 | 2.13 | 0.49 |
| 1:A:293:TRP:O | 1:A:296:ASP:HB2 | 2.13 | 0.49 |
| 1:A:662:ILE:HD12 | 2:B:627:ARG:HG3 | 1.95 | 0.49 |
| 2:B:261:HIS:CD2 | 2:B:263:GLN:H | 2.31 | 0.49 |
| 2:B:487:ILE:HG12 | 14:B:1232:CLA:HMD3 | 1.94 | 0.49 |
| 10:L:143:LEU:HD12 | 10:L:143:LEU:HA | 1.61 | 0.49 |
| 2:B:294:PHE:O | 2:B:296:ILE:HG22 | 2.13 | 0.48 |
| 2:B:390:PHE:CE1 | 17:B:4010:BCR:H373 | 2.48 | 0.48 |
| 14:B:1203:CLA:H143 | 14:B:1225:CLA:HBB2 | 1.95 | 0.48 |
| 2:B:182:PHE:CE2 | 14:B:1210:CLA:H61 | 2.48 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:446:VAL:HG13 | 2:B:451:THR:O | 2.13 | 0.48 |
| 14:A:1013:CLA:H71 | 14:A:1140:CLA:CMC | 2.42 | 0.48 |
| 1:A:399:TRP:NE1 | 14:A:1126:CLA:HAB | 2.27 | 0.48 |
| 1:A:120:ILE:C | 1:A:122:GLY:H | 2.16 | 0.48 |
| 1:A:444:LEU:HB2 | 14:A:1137:CLA:HBB1 | 1.96 | 0.48 |
| 2:B:261:HIS:HD2 | 2:B:263:GLN:H | 1.62 | 0.48 |
| 14:B:1221:CLA:H61 | 14:B:1221:CLA:H41 | 1.68 | 0.48 |
| 1:A:651:ARG:HG3 | 2:B:638:ILE:CG2 | 2.43 | 0.48 |
| 8:J:33:TYR:N | 8:J:34:PRO:HD3 | 2.28 | 0.48 |
| 1:A:118:TRP:HB3 | 17:J:4013:BCR:H323 | 1.94 | 0.48 |
| 1:A:658:ALA:O | 1:A:662:ILE:HG12 | 2.14 | 0.48 |
| 14:B:1203:CLA:H91 | 19:B:5002:LMG:H401 | 1.96 | 0.48 |
| 2:B:271:ASP:HB3 | 14:B:1214:CLA:HMA1 | 1.96 | 0.48 |
| 6:F:109:CYS:O | 6:F:112:THR:HB | 2.12 | 0.48 |
| 6:F:73:ILE:O | 6:F:76:TRP:HB3 | 2.14 | 0.48 |
| 14:A:1107:CLA:HMA1 | 8:J:27:ILE:HD13 | 1.95 | 0.48 |
| 1:A:283:GLY:O | 1:A:508:THR:O | 2.32 | 0.48 |
| 6:F:88:VAL:HG13 | 6:F:97:LYS:HD2 | 1.95 | 0.48 |
| 8:J:31:ARG:CD | 17:J:4013:BCR:H312 | 2.19 | 0.48 |
| 1:A:360:LEU:CD1 | 14:A:1128:CLA:HBB1 | 2.44 | 0.48 |
| 1:A:497:ALA:N | 1:A:498:PRO:CD | 2.76 | 0.48 |
| 1:A:693:GLY:HA3 | 2:B:574:CYS:HB2 | 1.95 | 0.48 |
| 2:B:180:GLY:HA3 | 14:B:1210:CLA:HBB1 | 1.96 | 0.48 |
| 9:K:74:VAL:C | 9:K:76:GLY:H | 2.16 | 0.48 |
| 1:A:203:GLY:O | 1:A:207:LEU:HB2 | 2.14 | 0.47 |
| 1:A:577:PRO:O | 1:A:578:CYS:HB3 | 2.14 | 0.47 |
| 11:M:24:ARG:NH1 | 20:M:155:HOH:O | 2.46 | 0.47 |
| 1:A:686:SER:HB3 | 1:A:734:HIS:HB2 | 1.95 | 0.47 |
| 6:F:10:ASP:HB3 | 20:F:4022:HOH:O | 2.14 | 0.47 |
| 1:A:168:MET:O | 1:A:172:MET:HB2 | 2.14 | 0.47 |
| 1:A:74:SER:OG | 1:A:180:TYR:HB2 | 2.15 | 0.47 |
| 1:A:691:PHE:HB2 | 14:A:1013:CLA:CBC | 2.44 | 0.47 |
| 14:B:1211:CLA:HAB | 14:B:1225:CLA:H13 | 1.96 | 0.47 |
| 2:B:329:TYR:OH | 2:B:340:HIS:CE1 | 2.61 | 0.47 |
| 14:A:1101:CLA:H8 | 8:J:16:ALA:HA | 1.96 | 0.47 |
| 2:B:647:ASN:HD22 | 2:B:649:LEU:N | 2.08 | 0.47 |
| 4:D:124:ASN:O | 4:D:127:GLN:HB2 | 2.13 | 0.47 |
| 14:B:1205:CLA:HMB2 | 14:B:1205:CLA:H142 | 1.96 | 0.47 |
| 14:A:1112:CLA:HBA2 | 14:A:1114:CLA:HMB3 | 1.96 | 0.47 |
| 1:A:121:VAL:HB | 14:B:1230:CLA:HMD1 | 1.96 | 0.47 |
| 1:A:399:TRP:HB3 | 14:A:1126:CLA:HMC3 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:56:HIS:CG | 14:A:1103:CLA:HAB | 2.49 | 0.47 |
| 2:B:525:VAL:CG1 | 14:B:1021:CLA:H141 | 2.45 | 0.47 |
| 2:B:589:MET:CE | 2:B:589:MET:C | 2.83 | 0.47 |
| 2:B:693:LEU:HD12 | 14:L:1502:CLA:H11 | 1.97 | 0.47 |
| 1:A:174:PHE:HD2 | 14:A:1108:CLA:CBC | 2.28 | 0.47 |
| 2:B:313:LYS:O | 2:B:314:VAL:CG2 | 2.60 | 0.47 |
| 11:M:24:ARG:CG | 11:M:24:ARG:NH1 | 2.78 | 0.47 |
| 14:A:1103:CLA:HMC3 | 14:A:1128:CLA:HMA1 | 1.97 | 0.47 |
| 8:J:40:PRO:O | 8:J:41:LEU:HB2 | 2.14 | 0.47 |
| 1:A:447:VAL:HG21 | 14:A:1137:CLA:C2C | 2.45 | 0.47 |
| 1:A:379:PRO:HB2 | 14:A:1117:CLA:HAA2 | 1.96 | 0.47 |
| 2:B:641:TYR:CB | 2:B:646:THR:HG22 | 2.42 | 0.47 |
| 2:B:696:LEU:HD11 | 10:L:36:ALA:HB1 | 1.97 | 0.47 |
| 14:B:1217:CLA:HBB1 | 17:B:4004:BCR:H14C | 1.97 | 0.46 |
| 2:B:198:ILE:HB | 2:B:199:PRO:HD3 | 1.96 | 0.46 |
| 3:C:65:ARG:HG2 | 3:C:67:TYR:OH | 2.15 | 0.46 |
| 6:F:88:VAL:CG1 | 6:F:97:LYS:HB2 | 2.41 | 0.46 |
| 14:A:1140:CLA:H172 | 8:J:19:MET:HG3 | 1.98 | 0.46 |
| 14:B:1207:CLA:H42 | 10:L:81:SER:HA | 1.96 | 0.46 |
| 1:A:638:ASN:O | 1:A:642:SER:HB2 | 2.16 | 0.46 |
| 14:A:1140:CLA:H2 | 14:A:1140:CLA:O1A | 2.15 | 0.46 |
| 1:A:603:TYR:OH | 14:A:1011:CLA:HED1 | 2.15 | 0.46 |
| 14:B:1225:CLA:H3A | 14:B:1225:CLA:HBA2 | 1.64 | 0.46 |
| 2:B:39:GLU:O | 2:B:43:GLN:HG3 | 2.15 | 0.46 |
| 3:C:57:CYS:HA | 3:C:58:PRO:HD3 | 1.71 | 0.46 |
| 14:A:1119:CLA:CMB | 14:A:1123:CLA:HMA3 | 2.46 | 0.46 |
| 4:D:34:PRO:O | 4:D:51:GLU:HG3 | 2.16 | 0.46 |
| 14:B:1235:CLA:H203 | 6:F:67:SER:HB3 | 1.98 | 0.46 |
| 2:B:386:MET:HE1 | 17:B:4010:BCR:H361 | 1.98 | 0.46 |
| 10:L:33:ASN:HB3 | 14:L:1501:CLA:HAC1 | 1.97 | 0.46 |
| 14:A:1118:CLA:HBC2 | 14:A:1118:CLA:HMC1 | 1.97 | 0.46 |
| 1:A:656:ALA:O | 1:A:659:SER:HB2 | 2.16 | 0.46 |
| 1:A:90:MET:HE1 | 14:A:1106:CLA:HAA2 | 1.98 | 0.46 |
| 14:B:1012:CLA:H41 | 14:B:1012:CLA:H61 | 1.56 | 0.46 |
| 2:B:361:TYR:O | 2:B:364:ILE:HG22 | 2.15 | 0.46 |
| 3:C:61:PHE:HD2 | 4:D:119:ILE:HG21 | 1.81 | 0.46 |
| 11:M:17:LEU:HB3 | 11:M:18:PRO:CD | 2.46 | 0.46 |
| 14:A:1011:CLA:HED1 | 20:A:5011:HOH:O | 2.14 | 0.46 |
| 1:A:686:SER:HB3 | 1:A:734:HIS:CB | 2.46 | 0.46 |
| 6:F:80:VAL:HG11 | 6:F:110:MET:HG2 | 1.97 | 0.46 |
| 1:A:19:ASP:N | 1:A:20:PRO:HD3 | 2.31 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:B:1207:CLA:HHC | 14:B:1207:CLA:HBB1 | 1.97 | 0.46 |
| 2:B:479:THR:H | 2:B:482:SER:HB3 | 1.79 | 0.46 |
| 1:A:744:TRP:CG | 17:A:4011:BCR:HC22 | 2.51 | 0.46 |
| 1:A:445:ASN:ND2 | 14:B:1023:CLA:HED2 | 2.31 | 0.46 |
| 3:C:23:ASP:OD2 | 4:D:95:HIS:CD2 | 2.67 | 0.46 |
| 1:A:91:TYR:CZ | 1:A:147:TRP:HZ3 | 2.33 | 0.46 |
| 2:B:189:TRP:CA | 14:B:1211:CLA:HBB1 | 2.45 | 0.46 |
| 17:A:4011:BCR:H381 | 14:B:1229:CLA:HMA1 | 1.97 | 0.46 |
| 2:B:642:ASN:HB2 | 2:B:643:PRO:HD3 | 1.95 | 0.46 |
| 2:B:738:LYS:O | 2:B:739:PHE:CB | 2.64 | 0.46 |
| 14:B:1204:CLA:H102 | 17:I:4018:BCR:HC31 | 1.98 | 0.46 |
| 11:M:13:VAL:HG23 | 17:M:4021:BCR:H402 | 1.98 | 0.46 |
| 1:A:257:ASP:OD2 | 1:A:262:SER:C | 2.55 | 0.45 |
| 1:A:539:HIS:CG | 14:A:1136:CLA:HED2 | 2.51 | 0.45 |
| 4:D:124:ASN:HB2 | 4:D:127:GLN:NE2 | 2.31 | 0.45 |
| 1:A:44:THR:HB | 1:A:720:ARG:HG2 | 1.98 | 0.45 |
| 1:A:475:PHE:HA | 1:A:480:ILE:O | 2.16 | 0.45 |
| 1:A:508:THR:HG21 | 20:A:5033:HOH:O | 2.15 | 0.45 |
| 2:B:468:ALA:O | 2:B:482:SER:HB2 | 2.16 | 0.45 |
| 14:B:1217:CLA:H3A | 14:B:1217:CLA:HBA2 | 1.64 | 0.45 |
| 14:B:1225:CLA:H12 | 17:B:4005:BCR:H393 | 1.97 | 0.45 |
| 14:B:1227:CLA:HBA2 | 14:B:1227:CLA:H3A | 1.49 | 0.45 |
| 2:B:339:TRP:CZ3 | 17:B:4009:BCR:H372 | 2.51 | 0.45 |
| 2:B:36:MET:CE | 2:B:40:ASN:HB2 | 2.45 | 0.45 |
| 2:B:509:SER:O | 2:B:509:SER:OG | 2.25 | 0.45 |
| 2:B:589:MET:HE1 | 2:B:590:LEU:HD23 | 1.97 | 0.45 |
| 14:L:1501:CLA:C1B | 14:L:1502:CLA:HED1 | 2.46 | 0.45 |
| 14:A:1120:CLA:H3A | 14:A:1120:CLA:HBA2 | 1.44 | 0.45 |
| 1:A:91:TYR:CE2 | 1:A:161:THR:HG21 | 2.52 | 0.45 |
| 1:A:313:HIS:CE1 | 17:A:4001:BCR:H363 | 2.51 | 0.45 |
| 14:A:1123:CLA:HAB | 17:A:4007:BCR:H341 | 1.98 | 0.45 |
| 2:B:64:LEU:HD11 | 17:B:4006:BCR:H271 | 1.98 | 0.45 |
| 2:B:471:GLY:HA3 | 2:B:504:LEU:CD2 | 2.47 | 0.45 |
| 8:J:22:THR:O | 8:J:26:LEU:HD13 | 2.15 | 0.45 |
| 10:L:115:GLU:O | 10:L:119:GLN:HG3 | 2.17 | 0.45 |
| 2:B:220:GLY:HA3 | 14:B:1212:CLA:HMD1 | 1.98 | 0.45 |
| 14:B:1215:CLA:H41 | 14:B:1215:CLA:H62 | 1.70 | 0.45 |
| 14:A:1118:CLA:H3A | 14:A:1118:CLA:HBA2 | 1.83 | 0.45 |
| 1:A:112:PRO:HB3 | 1:A:144:PHE:CD1 | 2.51 | 0.45 |
| 14:B:1213:CLA:H41 | 14:B:1213:CLA:H62 | 1.71 | 0.45 |
| 2:B:570:ARG:HH11 | 2:B:570:ARG:HG3 | 1.81 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:D:39:PHE:HB2 | 4:D:71:GLN:HE21 | 1.81 | 0.45 |
| 1:A:168:MET:HE2 | 1:A:171:LEU:HD23 | 1.97 | 0.45 |
| 1:A:508:THR:HG22 | 1:A:509:ALA:N | 2.31 | 0.45 |
| 14:B:1229:CLA:HBB1 | 14:B:1230:CLA:HMB2 | 1.98 | 0.45 |
| 2:B:50:PHE:HB3 | 2:B:148:ALA:O | 2.17 | 0.45 |
| 11:M:17:LEU:HB3 | 11:M:18:PRO:HD3 | 1.98 | 0.45 |
| 1:A:321:ILE:HD11 | 14:A:1118:CLA:H2A | 1.99 | 0.45 |
| 14:A:1011:CLA:NA | 14:B:1021:CLA:HAB | 2.31 | 0.45 |
| 2:B:445:VAL:HG21 | 14:B:1230:CLA:HAC2 | 1.97 | 0.45 |
| 1:A:445:ASN:ND2 | 2:B:680:LEU:HD21 | 2.32 | 0.45 |
| 1:A:90:MET:HE2 | 14:A:1126:CLA:HED1 | 1.99 | 0.45 |
| 4:D:134:LYS:HG2 | 4:D:136:TYR:CZ | 2.52 | 0.45 |
| 1:A:711:LEU:HD23 | 6:F:130:THR:HG22 | 1.98 | 0.45 |
| 8:J:1:MET:O | 8:J:1:MET:HE2 | 2.17 | 0.45 |
| 1:A:250:ALA:HA | 1:A:258:TRP:CD1 | 2.52 | 0.45 |
| 1:A:737:LEU:HD22 | 14:A:1140:CLA:HMA1 | 1.99 | 0.45 |
| 1:A:86:TRP:HE1 | 14:A:1106:CLA:HBA1 | 1.82 | 0.45 |
| 2:B:497:ASN:O | 2:B:499:TRP:CE3 | 2.70 | 0.45 |
| 4:D:114:SER:N | 20:D:144:HOH:O | 2.50 | 0.45 |
| 2:B:557:LYS:NZ | 4:D:124:ASN:OD1 | 2.43 | 0.45 |
| 1:A:75:ALA:HB1 | 14:A:1103:CLA:HBB1 | 1.99 | 0.44 |
| 14:A:1104:CLA:H3A | 14:A:1128:CLA:HAB | 1.99 | 0.44 |
| 14:B:1224:CLA:CGA | 14:B:1224:CLA:H3A | 2.47 | 0.44 |
| 2:B:215:MET:HA | 2:B:216:PRO:HD3 | 1.83 | 0.44 |
| 1:A:92:PHE:CZ | 1:A:96:LYS:HG3 | 2.53 | 0.44 |
| 14:B:1207:CLA:H43 | 14:B:1207:CLA:CED | 2.47 | 0.44 |
| 2:B:531:LEU:HD21 | 14:B:1012:CLA:HBB1 | 1.99 | 0.44 |
| 1:A:212:TRP:N | 14:A:1112:CLA:HBB1 | 2.32 | 0.44 |
| 2:B:370:THR:HG21 | 20:B:5026:HOH:O | 2.16 | 0.44 |
| 14:B:1211:CLA:HBA1 | 17:B:4006:BCR:H383 | 2.00 | 0.44 |
| 2:B:480:LEU:C | 2:B:482:SER:N | 2.70 | 0.44 |
| 3:C:6:ILE:HD12 | 3:C:6:ILE:N | 2.33 | 0.44 |
| 5:E:6:LYS:CD | 5:E:22:THR:HG22 | 2.47 | 0.44 |
| 14:B:1228:CLA:HBC3 | 17:F:4016:BCR:H362 | 1.99 | 0.44 |
| 14:B:1232:CLA:HMB1 | 17:B:4010:BCR:HC31 | 1.98 | 0.44 |
| 2:B:441:VAL:O | 2:B:445:VAL:HG23 | 2.17 | 0.44 |
| 2:B:48:SER:HB3 | 14:B:1202:CLA:HBB1 | 1.98 | 0.44 |
| 2:B:79:ASP:OD2 | 2:B:82:ASN:HB2 | 2.18 | 0.44 |
| 14:M:1601:CLA:H3A | 14:M:1601:CLA:HBA2 | 1.69 | 0.44 |
| 1:A:111:LYS:HB2 | 1:A:130:VAL:HB | 2.00 | 0.44 |
| 1:A:484:PRO:HB3 | 14:A:1136:CLA:CED | 2.47 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:D:125:PRO:HG3 | 4:D:135:PRO:HG3 | 2.00 | 0.44 |
| 14:A:1103:CLA:H71 | 17:A:4003:BCR:H402 | 2.00 | 0.44 |
| 3:C:65:ARG:HD2 | 4:D:119:ILE:CD1 | 2.48 | 0.44 |
| 6:F:132:LYS:HB2 | 6:F:135:GLU:HG3 | 1.99 | 0.44 |
| 10:L:56:TYR:OH | 14:L:1503:CLA:HED2 | 2.18 | 0.44 |
| 14:A:1107:CLA:HBC2 | 14:A:1126:CLA:H141 | 1.99 | 0.44 |
| 1:A:98:SER:HB2 | 1:A:113:SER:O | 2.18 | 0.44 |
| 17:A:4011:BCR:H23C | 17:A:4011:BCR:H403 | 1.99 | 0.44 |
| 1:A:462:ASN:HB3 | 1:A:645:THR:HG22 | 1.99 | 0.44 |
| 1:A:642:SER:O | 1:A:648:GLY:HA3 | 2.17 | 0.44 |
| 2:B:430:LEU:HB3 | 14:B:1229:CLA:CED | 2.48 | 0.44 |
| 2:B:181:LEU:HD13 | 14:B:1210:CLA:HBB | 2.00 | 0.44 |
| 5:E:17:TYR:O | 5:E:18:ASN:HB2 | 2.18 | 0.44 |
| 14:A:1140:CLA:H41 | 14:A:1140:CLA:H62 | 1.73 | 0.43 |
| 14:B:1206:CLA:H102 | 14:B:1224:CLA:H193 | 1.99 | 0.43 |
| 2:B:427:TRP:CE2 | 14:B:1228:CLA:HBB1 | 2.53 | 0.43 |
| 2:B:211:PHE:CE2 | 2:B:212:LEU:HG | 2.53 | 0.43 |
| 1:A:221:LEU:CB | 1:A:222:PRO:HD3 | 2.44 | 0.43 |
| 1:A:519:ALA:HB2 | 1:A:625:VAL:HG21 | 2.00 | 0.43 |
| 14:B:1232:CLA:HBA2 | 14:B:1233:CLA:HMB3 | 2.00 | 0.43 |
| 2:B:236:PRO:O | 2:B:250:GLY:HA3 | 2.18 | 0.43 |
| 2:B:317:PRO:HB3 | 20:B:5053:HOH:O | 2.18 | 0.43 |
| 2:B:529:ILE:HG21 | 14:B:1234:CLA:HAB | 1.99 | 0.43 |
| 2:B:439:LEU:HD11 | 17:J:4015:BCR:H342 | 2.00 | 0.43 |
| 8:J:1:MET:HE2 | 8:J:5:LEU:HG | 2.01 | 0.43 |
| 10:L:7:PRO:HB3 | 10:L:12:PRO:HA | 2.00 | 0.43 |
| 2:B:531:LEU:HD21 | 14:B:1012:CLA:CBB | 2.48 | 0.43 |
| 2:B:431:PHE:HD2 | 14:B:1235:CLA:HBB2 | 1.84 | 0.43 |
| 2:B:36:MET:HE1 | 2:B:41:LEU:N | 2.33 | 0.43 |
| 14:B:1203:CLA:H41 | 14:B:1203:CLA:H61 | 1.60 | 0.43 |
| 2:B:305:ASP:OD1 | 2:B:323:GLN:HA | 2.18 | 0.43 |
| 2:B:339:TRP:CE2 | 14:B:1223:CLA:H91 | 2.54 | 0.43 |
| 2:B:636:GLN:HG3 | 2:B:737:ALA:CB | 2.49 | 0.43 |
| 1:A:212:TRP:CA | 14:A:1112:CLA:HBB1 | 2.49 | 0.43 |
| 14:A:1117:CLA:HMB1 | 14:A:1117:CLA:CBB | 2.48 | 0.43 |
| 1:A:91:TYR:CE2 | 1:A:147:TRP:CZ3 | 3.07 | 0.43 |
| 14:B:1215:CLA:H3A | 14:B:1215:CLA:HBA2 | 1.92 | 0.43 |
| 2:B:234:GLN:O | 2:B:236:PRO:HD3 | 2.19 | 0.43 |
| 6:F:116:TRP:CG | 6:F:117:PRO:HD3 | 2.54 | 0.43 |
| 1:A:215:HIS:HB2 | 14:A:1112:CLA:C1C | 2.48 | 0.43 |
| 1:A:261:PHE:CD2 | 1:A:261:PHE:O | 2.72 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:443:HIS:CD2 | 14:A:1129:CLA:HMB1 | 2.53 | 0.43 |
| 14:B:1236:CLA:HBC2 | 14:X:1701:CLA:HBC3 | 2.00 | 0.43 |
| 2:B:231:VAL:C | 2:B:234:GLN:HG2 | 2.36 | 0.43 |
| 6:F:21:ALA:HB2 | 6:F:35:PHE:CD1 | 2.54 | 0.43 |
| 17:J:4015:BCR:H361 | 17:J:4015:BCR:H20C | 1.89 | 0.43 |
| 1:A:231:VAL:HG11 | 1:A:236:ILE:HG12 | 1.99 | 0.43 |
| 14:B:1205:CLA:O1A | 14:B:1224:CLA:HBD | 2.19 | 0.43 |
| 2:B:24:ILE:HA | 14:B:1201:CLA:HMD3 | 2.01 | 0.43 |
| 4:D:18:LEU:HA | 4:D:18:LEU:HD23 | 1.86 | 0.43 |
| 5:E:6:LYS:NZ | 5:E:22:THR:HG21 | 2.34 | 0.43 |
| 14:A:1237:CLA:H41 | 14:A:1237:CLA:H62 | 1.62 | 0.42 |
| 14:A:1402:CLA:H3A | 14:A:1402:CLA:HBA2 | 1.74 | 0.42 |
| 2:B:325:ILE:HD12 | 2:B:409:ASN:ND2 | 2.34 | 0.42 |
| 2:B:36:MET:HE1 | 2:B:40:ASN:C | 2.39 | 0.42 |
| 4:D:73:ARG:HB2 | 4:D:74:PRO:HD3 | 2.00 | 0.42 |
| 14:A:1117:CLA:O1A | 14:A:1127:CLA:HMD1 | 2.20 | 0.42 |
| 1:A:257:ASP:OD1 | 1:A:262:SER:CB | 2.66 | 0.42 |
| 1:A:514:GLY:HA2 | 1:A:528:PRO:HB3 | 2.01 | 0.42 |
| 2:B:360:PRO:HG3 | 14:B:1215:CLA:HBA1 | 2.00 | 0.42 |
| 14:B:1207:CLA:CBB | 7:I:19:CYS:HB3 | 2.50 | 0.42 |
| 8:J:39:HIS:HA | 17:J:4015:BCR:H21C | 2.00 | 0.42 |
| 1:A:683:TRP:CE3 | 14:A:1011:CLA:HMA1 | 2.54 | 0.42 |
| 1:A:403:PHE:CB | 14:A:1104:CLA:H112 | 2.49 | 0.42 |
| 1:A:215:HIS:CD2 | 1:A:215:HIS:C | 2.92 | 0.42 |
| 1:A:711:LEU:O | 1:A:713:VAL:HG22 | 2.20 | 0.42 |
| 14:B:1214:CLA:HBA2 | 14:B:1214:CLA:H3A | 1.39 | 0.42 |
| 14:B:1229:CLA:H61 | 17:F:4016:BCR:H312 | 2.00 | 0.42 |
| 2:B:357:SER:C | 2:B:359:PRO:HD3 | 2.39 | 0.42 |
| 2:B:103:PHE:HZ | 2:B:651:VAL:HG22 | 1.82 | 0.42 |
| 1:A:360:LEU:HD11 | 14:A:1128:CLA:HBB1 | 2.01 | 0.42 |
| 1:A:234:LYS:H | 1:A:234:LYS:HG2 | 1.68 | 0.42 |
| 14:A:1107:CLA:H11 | 17:J:4012:BCR:H19C | 2.01 | 0.42 |
| 14:A:1124:CLA:H51 | 14:A:1135:CLA:H43 | 2.00 | 0.42 |
| 1:A:679:ALA:HB1 | 1:A:738:GLY:O | 2.20 | 0.42 |
| 2:B:588:TRP:CH2 | 14:B:1012:CLA:CBB | 3.02 | 0.42 |
| 14:B:1226:CLA:CBB | 14:B:1226:CLA:HMB1 | 2.48 | 0.42 |
| 2:B:325:ILE:CD1 | 2:B:409:ASN:ND2 | 2.82 | 0.42 |
| 2:B:535:THR:O | 2:B:539:ILE:HG13 | 2.20 | 0.42 |
| 10:L:4:LEU:HD22 | 10:L:4:LEU:N | 2.35 | 0.42 |
| 2:B:341:LEU:HD21 | 14:B:1226:CLA:HAB | 2.02 | 0.42 |
| 2:B:458:ILE:CD1 | 2:B:458:ILE:N | 2.82 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:492:TRP:CZ3 | 14:B:1233:CLA:HMD3 | 2.54 | 0.42 |
| 2:B:6:LYS:HD2 | 11:M:31:LYS:HB3 | 2.02 | 0.42 |
| 4:D:95:HIS:HA | 4:D:97:LYS:N | 2.35 | 0.42 |
| 14:A:1128:CLA:H41 | 14:A:1128:CLA:H62 | 1.90 | 0.42 |
| 1:A:120:ILE:O | 1:A:122:GLY:N | 2.52 | 0.42 |
| 1:A:256:VAL:HG12 | 1:A:257:ASP:N | 2.35 | 0.42 |
| 1:A:542:HIS:HD2 | 20:A:5029:HOH:O | 2.03 | 0.42 |
| 14:A:1122:CLA:H92 | 17:A:4007:BCR:H14C | 2.01 | 0.42 |
| 1:A:145:GLN:CD | 1:A:145:GLN:H | 2.22 | 0.42 |
| 17:A:4011:BCR:H362 | 14:B:1012:CLA:C4 | 2.38 | 0.42 |
| 2:B:372:ALA:HA | 2:B:600:TRP:CZ3 | 2.55 | 0.42 |
| 18:B:5004:LHG:HC5 | 12:X:12:ARG:HB3 | 2.02 | 0.42 |
| 2:B:589:MET:HE1 | 2:B:590:LEU:N | 2.35 | 0.42 |
| 14:A:1126:CLA:H93 | 17:J:4012:BCR:H20C | 2.01 | 0.42 |
| 2:B:527:HIS:CD2 | 17:J:4015:BCR:H322 | 2.55 | 0.42 |
| 1:A:483:GLN:HA | 1:A:484:PRO:HD3 | 1.70 | 0.42 |
| 1:A:47:TRP:CZ3 | 1:A:51:LEU:HD12 | 2.54 | 0.42 |
| 1:A:511:VAL:HB | 1:A:526:MET:HG3 | 2.02 | 0.42 |
| 14:B:1203:CLA:H143 | 14:B:1225:CLA:CBB | 2.50 | 0.42 |
| 2:B:261:HIS:HD2 | 2:B:264:THR:H | 1.67 | 0.42 |
| 2:B:414:VAL:HG11 | 17:B:4009:BCR:C40 | 2.50 | 0.42 |
| 6:F:103:VAL:O | 6:F:107:ILE:HG13 | 2.20 | 0.42 |
| 14:A:1108:CLA:HBA2 | 14:A:1108:CLA:H3A | 1.64 | 0.42 |
| 1:A:346:GLU:N | 1:A:346:GLU:OE1 | 2.47 | 0.42 |
| 1:A:741:ALA:CB | 17:A:4011:BCR:H323 | 2.50 | 0.42 |
| 2:B:136:GLN:HE21 | 14:B:1211:CLA:HAA1 | 1.85 | 0.42 |
| 8:J:19:MET:HE2 | 8:J:19:MET:HA | 2.00 | 0.42 |
| 3:C:28:VAL:HG12 | 4:D:109:ARG:HB3 | 2.02 | 0.41 |
| 1:A:423:ALA:HA | 4:D:38:VAL:HG11 | 2.02 | 0.41 |
| 1:A:42:PRO:CG | 6:F:99:ILE:HD13 | 2.50 | 0.41 |
| 1:A:336:PHE:CD2 | 10:L:4:LEU:HD21 | 2.55 | 0.41 |
| 1:A:203:GLY:HA3 | 14:A:1111:CLA:HBB1 | 2.02 | 0.41 |
| 1:A:156:PHE:CE2 | 14:A:1114:CLA:HAA2 | 2.55 | 0.41 |
| 1:A:686:SER:HB2 | 1:A:731:GLY:O | 2.20 | 0.41 |
| 1:A:744:TRP:NE1 | 14:A:1126:CLA:H11 | 2.35 | 0.41 |
| 2:B:189:TRP:HA | 14:B:1211:CLA:HBB1 | 2.02 | 0.41 |
| 3:C:25:LEU:HA | 3:C:40:SER:O | 2.20 | 0.41 |
| 7:I:22:MET:O | 7:I:26:VAL:HG13 | 2.19 | 0.41 |
| 11:M:9:TYR:HB3 | 17:M:4021:BCR:H401 | 2.02 | 0.41 |
| 1:A:685:PHE:HA | 14:A:1013:CLA:HAB | 2.01 | 0.41 |
| 14:A:1801:CLA:H12 | 14:A:1801:CLA:HBA2 | 1.86 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:212:TRP:HA | 14:A:1112:CLA:HBB1 | 2.01 | 0.41 |
| 1:A:710:LYS:O | 1:A:710:LYS:HD2 | 2.20 | 0.41 |
| 2:B:663:TRP:CE3 | 14:B:1021:CLA:HMA1 | 2.56 | 0.41 |
| 2:B:178:LEU:O | 2:B:283:PHE:HB3 | 2.21 | 0.41 |
| 4:D:50:ARG:HG3 | 4:D:50:ARG:NH1 | 2.35 | 0.41 |
| 14:A:1134:CLA:H3A | 14:A:1134:CLA:HBA2 | 1.73 | 0.41 |
| 1:A:202:ALA:C | 14:A:1118:CLA:HBC3 | 2.41 | 0.41 |
| 1:A:378:PRO:HA | 1:A:379:PRO:HD3 | 1.83 | 0.41 |
| 1:A:49:TRP:CZ3 | 18:A:5001:LHG:H121 | 2.56 | 0.41 |
| 2:B:691:THR:HA | 2:B:692:PRO:HD3 | 1.90 | 0.41 |
| 6:F:54:ASP:OD2 | 12:X:30:TYR:HE2 | 1.98 | 0.41 |
| 1:A:49:TRP:HZ3 | 18:A:5001:LHG:H121 | 1.86 | 0.41 |
| 14:B:1213:CLA:HBA2 | 14:B:1213:CLA:H3A | 1.68 | 0.41 |
| 2:B:529:ILE:HG21 | 14:B:1234:CLA:CAB | 2.51 | 0.41 |
| 1:A:161:THR:HG22 | 17:A:4002:BCR:HC32 | 2.01 | 0.41 |
| 14:L:1502:CLA:H111 | 14:L:1502:CLA:H152 | 1.99 | 0.41 |
| 14:A:1119:CLA:HMD1 | 14:A:1120:CLA:HBB1 | 2.02 | 0.41 |
| 1:A:112:PRO:HA | 1:A:144:PHE:CE1 | 2.55 | 0.41 |
| 1:A:360:LEU:HD12 | 1:A:360:LEU:HA | 1.93 | 0.41 |
| 14:B:1202:CLA:HBA1 | 14:B:1202:CLA:H3A | 1.74 | 0.41 |
| 14:B:1222:CLA:HBA2 | 14:B:1222:CLA:H3A | 1.69 | 0.41 |
| 4:D:104:LYS:H | 4:D:104:LYS:HG2 | 1.51 | 0.41 |
| 6:F:73:ILE:O | 6:F:77:ILE:HG13 | 2.21 | 0.41 |
| 14:B:1023:CLA:H122 | 17:I:4018:BCR:H281 | 2.03 | 0.41 |
| 14:A:1022:CLA:H3A | 14:A:1022:CLA:O1A | 2.21 | 0.41 |
| 14:A:1117:CLA:H3A | 14:A:1117:CLA:HBA2 | 1.89 | 0.41 |
| 1:A:80:LEU:HD23 | 1:A:80:LEU:HA | 1.82 | 0.41 |
| 2:B:442:HIS:CD2 | 2:B:456:ILE:HG13 | 2.56 | 0.41 |
| 3:C:13:CYS:SG | 3:C:15:GLN:HB2 | 2.61 | 0.41 |
| 6:F:24:THR:HG21 | 8:J:35:ASP:OD1 | 2.20 | 0.41 |
| 10:L:44:ILE:HG23 | 10:L:45:LEU:N | 2.36 | 0.41 |
| 14:A:1140:CLA:H52 | 14:A:1140:CLA:NC | 2.36 | 0.41 |
| 1:A:260:PHE:O | 1:A:261:PHE:HB2 | 2.21 | 0.41 |
| 14:B:1207:CLA:H2A | 14:B:1207:CLA:O2A | 2.20 | 0.41 |
| 2:B:30:PHE:CD1 | 2:B:45:ILE:HD13 | 2.56 | 0.41 |
| 2:B:440:TYR:CZ | 2:B:524:LEU:HB3 | 2.56 | 0.41 |
| 14:B:1206:CLA:H203 | 7:I:26:VAL:CG2 | 2.51 | 0.41 |
| 1:A:118:TRP:HB3 | 17:J:4013:BCR:C32 | 2.51 | 0.41 |
| 14:A:1013:CLA:C14 | 17:A:4011:BCR:H402 | 2.51 | 0.41 |
| 2:B:459:GLU:HA | 2:B:460:PRO:HD3 | 1.81 | 0.41 |
| 2:B:629:TYR:O | 2:B:633:ASN:HB2 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:D:43:THR:O | 4:D:44:ALA:CB | 2.68 | 0.41 |
| 14:A:1132:CLA:HED2 | 10:L:65:LEU:O | 2.21 | 0.41 |
| 14:A:1140:CLA:H203 | 14:F:1301:CLA:CBB | 2.52 | 0.40 |
| 1:A:502:ALA:N | 1:A:503:PRO:HD3 | 2.36 | 0.40 |
| 14:B:1214:CLA:O1D | 14:B:1215:CLA:HMA1 | 2.21 | 0.40 |
| 14:B:1215:CLA:H3A | 14:B:1215:CLA:CGA | 2.51 | 0.40 |
| 14:B:1211:CLA:HMA2 | 17:B:4006:BCR:H282 | 2.03 | 0.40 |
| 6:F:80:VAL:HG21 | 6:F:110:MET:HA | 2.03 | 0.40 |
| 20:A:5047:HOH:O | 10:L:16:HIS:HE1 | 2.04 | 0.40 |
| 1:A:713:VAL:HG11 | 14:A:1138:CLA:HMB3 | 2.03 | 0.40 |
| 1:A:114:ALA:O | 1:A:115:GLN:O | 2.39 | 0.40 |
| 2:B:279:ILE:HD11 | 14:B:1214:CLA:HBC3 | 2.02 | 0.40 |
| 2:B:33:HIS:HE1 | 14:B:1201:CLA:HED1 | 1.85 | 0.40 |
| 2:B:490:THR:O | 2:B:495:TYR:HA | 2.21 | 0.40 |
| 2:B:53:LEU:HD12 | 2:B:53:LEU:HA | 1.83 | 0.40 |
| 2:B:605:LEU:HA | 2:B:605:LEU:HD12 | 1.80 | 0.40 |
| 5:E:19:GLU:OE1 | 5:E:42:LYS:NZ | 2.52 | 0.40 |
| 14:A:1126:CLA:H62 | 14:A:1126:CLA:H41 | 1.75 | 0.40 |
| 14:A:1130:CLA:HMC2 | 14:A:1136:CLA:H203 | 2.03 | 0.40 |
| 14:A:1122:CLA:HHB | 14:A:1801:CLA:HBB1 | 2.02 | 0.40 |
| 1:A:212:TRP:O | 1:A:216:GLN:HG3 | 2.22 | 0.40 |
| 2:B:176:HIS:CG | 14:B:1210:CLA:HMC2 | 2.56 | 0.40 |
| 2:B:193:LEU:HA | 2:B:197:ALA:HB3 | 2.03 | 0.40 |
| 2:B:269:LEU:HD23 | 2:B:272:MET:HE3 | 2.02 | 0.40 |
| 2:B:377:HIS:HE2 | 14:B:1225:CLA:C1B | 2.35 | 0.40 |
| 2:B:564:PRO:O | 2:B:565:CYS:HB3 | 2.22 | 0.40 |
| 17:L:4022:BCR:H361 | 17:L:4022:BCR:H20C | 1.88 | 0.40 |
| 10:L:44:ILE:HB | 20:L:4045:HOH:O | 2.21 | 0.40 |
| 14:A:1116:CLA:H3A | 14:A:1116:CLA:CGA | 2.52 | 0.40 |
| 2:B:318:PHE:H | 14:B:1219:CLA:C2B | 2.34 | 0.40 |
| 2:B:313:LYS:O | 2:B:314:VAL:CG1 | 2.68 | 0.40 |
| 2:B:548:ARG:HD3 | 6:F:141:ARG:O | 2.21 | 0.40 |
| 3:C:40:SER:HA | 20:C:3012:HOH:O | 2.21 | 0.40 |
| 4:D:67:LEU:HD12 | 4:D:71:GLN:HG3 | 2.03 | 0.40 |
| 8:J:30:ASN:O | 8:J:34:PRO:HG3 | 2.22 | 0.40 |
| 1:A:120:ILE:HG12 | 1:A:121:VAL:N | 2.36 | 0.40 |
| 1:A:741:ALA:CB | 17:A:4011:BCR:C32 | 2.99 | 0.40 |
| 14:B:1220:CLA:CBB | 14:B:1227:CLA:HMD2 | 2.51 | 0.40 |
| 14:A:1107:CLA:CBB | 14:B:1230:CLA:HMD2 | 2.51 | 0.40 |
| 2:B:36:MET:HE3 | 2:B:40:ASN:CB | 2.47 | 0.40 |
| 2:B:496:GLY:O | 2:B:497:ASN:C | 2.59 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 20:C:3013:HOH:O | 4:D:138:PRO:HG3 | 2.21 | 0.40 |
| 4:D:88:ASP:HB3 | 4:D:90:GLU:H | 1.86 | 0.40 |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 20:L:4048:HOH:O | 20:L:4048:HOH:O[2_655] | 1.94 | 0.26 |

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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 | 736/755 (98%) | 695 (94%) | 31 (4%) | 10 (1%) | 14 | 24 |
| 2 | B | 737/740 (100%) | 691 (94%) | 37 (5%) | 9 (1%) | 16 | 29 |
| 3 | C | 78/80 (98%) | 73 (94%) | 4 (5%) | 1 (1%) | 15 | 26 |
| 4 | D | 136/138 (99%) | 125 (92%) | 8 (6%) | 3 (2%) | 8 | 13 |
| 5 | E | 67/75 (89%) | 59 (88%) | 4 (6%) | 4 (6%) | 2 | 2 |
| 6 | F | 139/164 (85%) | 128 (92%) | 8 (6%) | 3 (2%) | 8 | 13 |
| 7 | I | 36/38 (95%) | 35 (97%) | 1 (3%) | 0 | 100 | 100 |
| 8 | J | 39/41 (95%) | 37 (95%) | 2 (5%) | 0 | 100 | 100 |
| 9 | K | 40/83 (48%) | 32 (80%) | 5 (12%) | 3 (8%) | 1 | 1 |
| 10 | L | 149/154 (97%) | 140 (94%) | 7 (5%) | 2 (1%) | 15 | 26 |
| 11 | M | 29/31 (94%) | 28 (97%) | 0 | 1 (3%) | 5 | 6 |
| 12 | X | 27/35 (77%) | 22 (82%) | 4 (15%) | 1 (4%) | 4 | 5 |
| All | All | 2213/2334 (95%) | 2065 (93%) | 111 (5%) | 37 (2%) | 11 | 19 |

All (37) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 115 | GLN |
| 1 | A | 235 | ASP |
| 1 | A | 260 | PHE |
| 1 | A | 261 | PHE |
| 2 | B | 234 | GLN |
| 2 | B | 313 | LYS |
| 2 | B | 314 | VAL |
| 2 | B | 480 | LEU |
| 2 | B | 492 | TRP |
| 2 | B | 497 | ASN |
| 2 | B | 510 | GLY |
| 3 | C | 62 | LEU |
| 4 | D | 2 | THR |
| 6 | F | 91 | SER |
| 9 | K | 41 | PRO |
| 9 | K | 42 | GLY |
| 11 | M | 30 | TYR |
| 12 | X | 10 | ALA |
| 1 | A | 121 | VAL |
| 1 | A | 578 | CYS |
| 2 | B | 565 | CYS |
| 4 | D | 3 | LEU |
| 6 | F | 60 | ALA |
| 6 | F | 89 | ARG |
| 10 | L | 106 | SER |
| 1 | A | 234 | LYS |
| 4 | D | 44 | ALA |
| 5 | E | 53 | SER |
| 10 | L | 104 | GLY |
| 1 | A | 42 | PRO |
| 1 | A | 232 | ALA |
| 2 | B | 481 | LEU |
| 5 | E | 25 | SER |
| 5 | E | 54 | GLY |
| 1 | A | 276 | SER |
| 5 | E | 55 | VAL |
| 9 | K | 56 | LEU |

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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 | 589/603 (98%) | 565 (96%) | 24 (4%) | 37 | 63 |
| 2 | B | 595/597 (100%) | 567 (95%) | 28 (5%) | 32 | 56 |
| 3 | C | 67/67 (100%) | 66 (98%) | 1 (2%) | 72 | 91 |
| 4 | D | 115/115 (100%) | 107 (93%) | 8 (7%) | 19 | 34 |
| 5 | E | 59/64 (92%) | 59 (100%) | 0 | 100 | 100 |
| 6 | F | 109/128 (85%) | 107 (98%) | 2 (2%) | 66 | 88 |
| 7 | I | 32/32 (100%) | 30 (94%) | 2 (6%) | 22 | 40 |
| 8 | J | 36/36 (100%) | 34 (94%) | 2 (6%) | 26 | 47 |
| 10 | L | 117/119 (98%) | 109 (93%) | 8 (7%) | 20 | 36 |
| 11 | M | 26/26 (100%) | 25 (96%) | 1 (4%) | 40 | 67 |
| 12 | X | 20/24 (83%) | 18 (90%) | 2 (10%) | 9 | 18 |
| All | All | 1765/1811 (98%) | 1687 (96%) | 78 (4%) | 35 | 60 |

All (78) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 145 | GLN |
| 1 | A | 147 | TRP |
| 1 | A | 155 | GLU |
| 1 | A | 172 | MET |
| 1 | A | 186 | LYS |
| 1 | A | 210 | LEU |
| 1 | A | 221 | LEU |
| 1 | A | 235 | ASP |
| 1 | A | 252 | LEU |
| 1 | A | 253 | TYR |
| 1 | A | 257 | ASP |
| 1 | A | 260 | PHE |
| 1 | A | 281 | PHE |
| 1 | A | 349 | THR |
| 1 | A | 360 | LEU |
| 1 | A | 372 | GLN |
| 1 | A | 395 | THR |
| 1 | A | 433 | VAL |
| 1 | A | 466 | ARG |
| 1 | A | 538 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 587 | CYS |
| 1 | A | 632 | SER |
| 1 | A | 675 | LEU |
| 1 | A | 713 | VAL |
| 2 | B | 53 | LEU |
| 2 | B | 142 | LEU |
| 2 | B | 159 | LYS |
| 2 | B | 171 | GLU |
| 2 | B | 211 | PHE |
| 2 | B | 214 | THR |
| 2 | B | 256 | PHE |
| 2 | B | 279 | ILE |
| 2 | B | 318 | PHE |
| 2 | B | 349 | SER |
| 2 | B | 370 | THR |
| 2 | B | 411 | LEU |
| 2 | B | 430 | LEU |
| 2 | B | 446 | VAL |
| 2 | B | 479 | THR |
| 2 | B | 525 | VAL |
| 2 | B | 574 | CYS |
| 2 | B | 582 | PHE |
| 2 | B | 589 | MET |
| 2 | B | 596 | VAL |
| 2 | B | 605 | LEU |
| 2 | B | 632 | LEU |
| 2 | B | 635 | SER |
| 2 | B | 647 | ASN |
| 2 | B | 648 | ASN |
| 2 | B | 651 | VAL |
| 2 | B | 697 | VAL |
| 2 | B | 698 | ARG |
| 3 | C | 61 | PHE |
| 4 | D | 1 | THR |
| 4 | D | 73 | ARG |
| 4 | D | 93 | LEU |
| 4 | D | 104 | LYS |
| 4 | D | 105 | VAL |
| 4 | D | 117 | ARG |
| 4 | D | 125 | PRO |
| 4 | D | 126 | SER |
| 6 | F | 56 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | F | 105 | LEU |
| 7 | I | 10 | LEU |
| 7 | I | 26 | VAL |
| 8 | J | 1 | MET |
| 8 | J | 19 | MET |
| 10 | L | 4 | LEU |
| 10 | L | 34 | LEU |
| 10 | L | 42 | SER |
| 10 | L | 44 | ILE |
| 10 | L | 48 | LEU |
| 10 | L | 69 | ARG |
| 10 | L | 85 | LEU |
| 10 | L | 134 | VAL |
| 11 | M | 17 | LEU |
| 12 | X | 8 | THR |
| 12 | X | 23 | ASN |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 33 | HIS |
| 1 | A | 50 | ASN |
| 1 | A | 145 | GLN |
| 1 | A | 353 | HIS |
| 1 | A | 359 | ASN |
| 1 | A | 372 | GLN |
| 1 | A | 390 | GLN |
| 1 | A | 426 | GLN |
| 1 | A | 445 | ASN |
| 1 | A | 542 | HIS |
| 1 | A | 633 | HIS |
| 1 | A | 647 | ASN |
| 1 | A | 718 | GLN |
| 2 | B | 33 | HIS |
| 2 | B | 40 | ASN |
| 2 | B | 136 | GLN |
| 2 | B | 261 | HIS |
| 2 | B | 263 | GLN |
| 2 | B | 336 | GLN |
| 2 | B | 340 | HIS |
| 2 | B | 406 | ASN |
| 2 | B | 494 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 611 | ASN |
| 2 | B | 614 | GLN |
| 2 | B | 616 | ASN |
| 2 | B | 639 | ASN |
| 2 | B | 647 | ASN |
| 2 | B | 648 | ASN |
| 2 | B | 678 | GLN |
| 2 | B | 688 | HIS |
| 3 | C | 37 | GLN |
| 4 | D | 54 | ASN |
| 4 | D | 71 | GLN |
| 4 | D | 95 | HIS |
| 5 | E | 18 | ASN |
| 6 | F | 40 | GLN |
| 6 | F | 95 | ASN |
| 10 | L | 16 | HIS |

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 128 ligands modelled in this entry, 1 is monoatomic - leaving 127 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 14 | CLA | A | 1011 | 1 | 57,73,73 | 1.20 | 2 (3%) | 61,113,113 | 2.30 | 10 (16%) |
| 14 | CLA | A | 1013 | 1 | 57,73,73 | 1.21 | 4 (7%) | 61,113,113 | 1.48 | 10 (16%) |
| 14 | CLA | A | 1022 | 20 | 57,73,73 | 1.09 | 4 (7%) | 61,113,113 | 1.45 | 10 (16%) |
| 14 | CLA | A | 1101 | 1 | 57,73,73 | 1.11 | 4 (7%) | 61,113,113 | 1.49 | 9 (14%) |
| 14 | CLA | A | 1102 | 1,14 | 51,67,73 | 1.19 | 3 (5%) | 53,105,113 | 1.69 | 13 (24%) |
| 14 | CLA | A | 1103 | 1 | 57,73,73 | 1.15 | 3 (5%) | 61,113,113 | 1.61 | 12 (19%) |
| 14 | CLA | A | 1104 | 1 | 57,73,73 | 1.16 | 3 (5%) | 61,113,113 | 1.76 | 15 (24%) |
| 14 | CLA | A | 1105 | 1 | 43,59,73 | 1.44 | 4 (9%) | 43,96,113 | 1.63 | 9 (20%) |
| 14 | CLA | A | 1106 | 1 | 57,73,73 | 1.30 | 5 (8%) | 61,113,113 | 1.56 | 11 (18%) |
| 14 | CLA | A | 1107 | 1 | 57,73,73 | 1.11 | 3 (5%) | 61,113,113 | 1.52 | 12 (19%) |
| 14 | CLA | A | 1108 | 1 | 34,53,73 | 1.38 | 5 (14%) | 37,89,113 | 1.63 | 9 (24%) |
| 14 | CLA | A | 1109 | 1,14 | 57,73,73 | 1.15 | 5 (8%) | 61,113,113 | 1.39 | 9 (14%) |
| 14 | CLA | A | 1110 | 1 | 46,62,73 | 1.36 | 5 (10%) | 47,99,113 | 1.62 | 11 (23%) |
| 14 | CLA | A | 1111 | 1 | 52,68,73 | 1.17 | 3 (5%) | 55,107,113 | 1.58 | 10 (18%) |
| 14 | CLA | A | 1112 | 1 | 34,53,73 | 1.39 | 4 (11%) | 37,89,113 | 1.72 | 9 (24%) |
| 14 | CLA | A | 1113 | 1 | 34,53,73 | 1.46 | 2 (5%) | 37,89,113 | 1.84 | 11 (29%) |
| 14 | CLA | A | 1114 | 20 | 41,57,73 | 1.29 | 4 (9%) | 43,93,113 | 1.70 | 9 (20%) |
| 14 | CLA | A | 1115 | 1 | 46,62,73 | 1.25 | 4 (8%) | 47,99,113 | 1.55 | 8 (17%) |
| 14 | CLA | A | 1116 | 1 | 46,62,73 | 1.39 | 5 (10%) | 47,99,113 | 1.69 | 13 (27%) |
| 14 | CLA | A | 1117 | 1 | 57,73,73 | 1.16 | 7 (12%) | 61,113,113 | 1.56 | 15 (24%) |
| 14 | CLA | A | 1118 | 1 | 53,69,73 | 1.33 | 5 (9%) | 55,108,113 | 1.62 | 11 (20%) |
| 14 | CLA | A | 1119 | 20 | 57,73,73 | 1.14 | 5 (8%) | 61,113,113 | 1.58 | 13 (21%) |
| 14 | CLA | A | 1120 | 1 | 41,57,73 | 1.35 | 4 (9%) | 43,93,113 | 1.84 | 12 (27%) |
| 14 | CLA | A | 1121 | 1 | 43,59,73 | 1.35 | 6 (13%) | 43,96,113 | 1.71 | 9 (20%) |
| 14 | CLA | A | 1122 | 1 | 51,67,73 | 1.21 | 3 (5%) | 53,105,113 | 1.54 | 11 (20%) |
| 14 | CLA | A | 1123 | 20 | 57,73,73 | 1.19 | 3 (5%) | 61,113,113 | 1.49 | 10 (16%) |
| 14 | CLA | A | 1124 | 20 | 57,73,73 | 1.14 | 4 (7%) | 61,113,113 | 1.39 | 8 (13%) |
| 14 | CLA | A | 1125 | 1 | 57,73,73 | 1.25 | 4 (7%) | 61,113,113 | 1.52 | 10 (16%) |
| 14 | CLA | A | 1126 | 1 | 57,73,73 | 1.02 | 3 (5%) | 61,113,113 | 1.37 | 12 (19%) |
| 14 | CLA | A | 1127 | 1 | 57,73,73 | 1.20 | 2 (3%) | 61,113,113 | 1.51 | 9 (14%) |
| 14 | CLA | A | 1128 | 1 | 57,73,73 | 1.20 | 5 (8%) | 61,113,113 | 1.51 | 11 (18%) |
| 14 | CLA | A | 1129 | 1 | 42,58,73 | 1.37 | 4 (9%) | 44,95,113 | 1.85 | 13 (29%) |
| 14 | CLA | A | 1130 | 1 | 57,73,73 | 1.18 | 1 (1%) | 61,113,113 | 1.50 | 12 (19%) |
| 14 | CLA | A | 1131 | 1 | 57,73,73 | 1.05 | 1 (1%) | 61,113,113 | 1.47 | 11 (18%) |
| 14 | CLA | A | 1132 | 1 | 57,73,73 | 1.17 | 5 (8%) | 61,113,113 | 1.58 | 10 (16%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 14 | CLA | A | 1133 | 1 | 46,62,73 | 1.35 | 5 (10%) | 47,99,113 | 1.68 | 13 (27%) |
| 14 | CLA | A | 1134 | 1 | 34,53,73 | 1.48 | 4 (11%) | 37,89,113 | 1.69 | 9 (24%) |
| 14 | CLA | A | 1135 | 1 | 43,59,73 | 1.40 | 1 (2%) | 43,96,113 | 1.68 | 10 (23%) |
| 14 | CLA | A | 1136 | 1 | 57,73,73 | 1.15 | 5 (8%) | 61,113,113 | 1.32 | 7 (11%) |
| 14 | CLA | A | 1137 | 1 | 39,55,73 | 1.45 | 4 (10%) | 42,91,113 | 1.75 | 10 (23%) |
| 14 | CLA | A | 1138 | 1 | 57,73,73 | 1.12 | 4 (7%) | 61,113,113 | 1.43 | 12 (19%) |
| 14 | CLA | A | 1139 | 20 | 43,59,73 | 1.48 | 4 (9%) | 43,96,113 | 1.67 | 11 (25%) |
| 14 | CLA | A | 1140 | 1 | 57,73,73 | 1.26 | 3 (5%) | 61,113,113 | 1.50 | 11 (18%) |
| 14 | CLA | A | 1237 | 20 | 57,73,73 | 1.25 | 6 (10%) | 61,113,113 | 1.43 | 11 (18%) |
| 14 | CLA | A | 1402 | - | 31,49,73 | 1.59 | 5 (16%) | 30,83,113 | 1.60 | 7 (23%) |
| 14 | CLA | A | 1801 | 18 | 44,60,73 | 1.38 | 6 (13%) | 45,97,113 | 1.87 | 11 (24%) |
| 15 | PQN | A | 2001 | - | 34,34,34 | 3.38 | 17 (50%) | 45,45,45 | 2.21 | 3 (6%) |
| 16 | SF4 | A | 3001 | 1,2 | 0,12,12 | 0.00 | - | 0,24,24 | 0.00 | - |
| 17 | BCR | A | 4001 | - | 41,41,41 | 1.33 | 5 (12%) | 56,56,56 | 1.89 | 15 (26%) |
| 17 | BCR | A | 4002 | - | 41,41,41 | 1.23 | 4 (9%) | 56,56,56 | 1.79 | 16 (28%) |
| 17 | BCR | A | 4003 | - | 41,41,41 | 1.37 | 6 (14%) | 56,56,56 | 1.96 | 18 (32%) |
| 17 | BCR | A | 4007 | - | 41,41,41 | 1.33 | 4 (9%) | 56,56,56 | 1.81 | 15 (26%) |
| 17 | BCR | A | 4008 | - | 41,41,41 | 1.24 | 6 (14%) | 56,56,56 | 1.91 | 18 (32%) |
| 17 | BCR | A | 4011 | - | 41,41,41 | 1.35 | 6 (14%) | 56,56,56 | 2.06 | 20 (35%) |
| 18 | LHG | A | 5001 | - | 48,48,48 | 1.70 | 6 (12%) | 49,54,54 | 1.26 | 3 (6%) |
| 18 | LHG | A | 5003 | 14 | 26,26,48 | 2.24 | 5 (19%) | 27,32,54 | 1.49 | 4 (14%) |
| 14 | CLA | B | 1012 | 20 | 57,73,73 | 1.16 | 2 (3%) | 61,113,113 | 1.60 | 10 (16%) |
| 14 | CLA | B | 1021 | 2 | 57,73,73 | 1.22 | 3 (5%) | 61,113,113 | 1.42 | 9 (14%) |
| 14 | CLA | B | 1023 | 2 | 57,73,73 | 1.24 | 4 (7%) | 61,113,113 | 1.39 | 10 (16%) |
| 14 | CLA | B | 1201 | 2 | 46,62,73 | 1.31 | 5 (10%) | 47,99,113 | 1.75 | 9 (19%) |
| 14 | CLA | B | 1202 | 2 | 57,73,73 | 1.17 | 4 (7%) | 61,113,113 | 1.48 | 10 (16%) |
| 14 | CLA | B | 1203 | 2 | 57,73,73 | 1.09 | 2 (3%) | 61,113,113 | 1.37 | 8 (13%) |
| 14 | CLA | B | 1204 | 2 | 57,73,73 | 1.26 | 4 (7%) | 61,113,113 | 1.49 | 10 (16%) |
| 14 | CLA | B | 1205 | 2 | 57,73,73 | 1.05 | 4 (7%) | 61,113,113 | 1.64 | 12 (19%) |
| 14 | CLA | B | 1206 | 2 | 57,73,73 | 1.03 | 1 (1%) | 61,113,113 | 1.44 | 10 (16%) |
| 14 | CLA | B | 1207 | 2 | 57,73,73 | 1.18 | 3 (5%) | 61,113,113 | 1.38 | 8 (13%) |
| 14 | CLA | B | 1208 | 2 | 34,53,73 | 1.37 | 5 (14%) | 37,89,113 | 1.66 | 9 (24%) |
| 14 | CLA | B | 1209 | 2 | 34,53,73 | 1.51 | 2 (5%) | 37,89,113 | 1.67 | 8 (21%) |
| 14 | CLA | B | 1210 | 2 | 57,73,73 | 1.06 | 3 (5%) | 61,113,113 | 1.48 | 10 (16%) |
| 14 | CLA | B | 1211 | 2 | 57,73,73 | 1.20 | 5 (8%) | 61,113,113 | 1.54 | 9 (14%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 14 | CLA | B | 1212 | 2 | 34,53,73 | 1.37 | 4 (11%) | 37,89,113 | 1.74 | 8 (21%) |
| 14 | CLA | B | 1213 | 2 | 47,63,73 | 1.36 | 8 (17%) | 49,101,113 | 1.61 | 11 (22%) |
| 14 | CLA | B | 1214 | 2 | 51,67,73 | 1.25 | 5 (9%) | 53,105,113 | 1.60 | 12 (22%) |
| 14 | CLA | B | 1215 | 2 | 52,68,73 | 1.27 | 4 (7%) | 55,107,113 | 1.67 | 12 (21%) |
| 14 | CLA | B | 1216 | 20 | 57,73,73 | 1.16 | 4 (7%) | 61,113,113 | 1.43 | 11 (18%) |
| 14 | CLA | B | 1217 | 2 | 39,55,73 | 1.41 | 3 (7%) | 42,91,113 | 1.85 | 13 (30%) |
| 14 | CLA | B | 1218 | 2 | 34,53,73 | 1.42 | 2 (5%) | 37,89,113 | 1.83 | 9 (24%) |
| 14 | CLA | B | 1219 | 20 | 47,63,73 | 1.36 | 3 (6%) | 49,101,113 | 1.54 | 12 (24%) |
| 14 | CLA | B | 1220 | 2 | 34,53,73 | 1.37 | 3 (8%) | 37,89,113 | 1.64 | 8 (21%) |
| 14 | CLA | B | 1221 | 2 | 46,62,73 | 1.33 | 6 (13%) | 47,99,113 | 1.71 | 11 (23%) |
| 14 | CLA | B | 1222 | 20 | 38,54,73 | 1.27 | 3 (7%) | 41,90,113 | 1.87 | 11 (26%) |
| 14 | CLA | B | 1223 | 2 | 57,73,73 | 1.25 | 3 (5%) | 61,113,113 | 1.50 | 11 (18%) |
| 14 | CLA | B | 1224 | 2 | 57,73,73 | 1.26 | 4 (7%) | 61,113,113 | 1.62 | 12 (19%) |
| 14 | CLA | B | 1225 | 2 | 57,73,73 | 1.31 | 8 (14%) | 61,113,113 | 1.52 | 12 (19%) |
| 14 | CLA | B | 1226 | 2 | 57,73,73 | 1.22 | 5 (8%) | 61,113,113 | 1.62 | 10 (16%) |
| 14 | CLA | B | 1227 | 2 | 34,53,73 | 1.47 | 5 (14%) | 37,89,113 | 1.79 | 10 (27%) |
| 14 | CLA | B | 1228 | 2 | 41,57,73 | 1.31 | 4 (9%) | 43,93,113 | 1.66 | 9 (20%) |
| 14 | CLA | B | 1229 | 2 | 57,73,73 | 1.16 | 4 (7%) | 61,113,113 | 1.51 | 9 (14%) |
| 14 | CLA | B | 1230 | 2 | 50,66,73 | 1.42 | 4 (8%) | 52,104,113 | 1.65 | 10 (19%) |
| 14 | CLA | B | 1231 | 2 | 34,53,73 | 1.55 | 5 (14%) | 37,89,113 | 1.75 | 9 (24%) |
| 14 | CLA | B | 1232 | 20 | 34,53,73 | 1.43 | 5 (14%) | 37,89,113 | 1.65 | 9 (24%) |
| 14 | CLA | B | 1233 | 20 | 34,53,73 | 1.47 | 3 (8%) | 37,89,113 | 1.61 | 8 (21%) |
| 14 | CLA | B | 1234 | 2 | 52,68,73 | 1.37 | 3 (5%) | 55,107,113 | 1.51 | 11 (20%) |
| 14 | CLA | B | 1235 | 2 | 57,73,73 | 1.22 | 4 (7%) | 61,113,113 | 1.53 | 14 (22%) |
| 14 | CLA | B | 1236 | 2 | 39,55,73 | 1.30 | 4 (10%) | 42,91,113 | 1.61 | 9 (21%) |
| 14 | CLA | B | 1238 | 20 | 57,73,73 | 1.17 | 5 (8%) | 61,113,113 | 1.36 | 9 (14%) |
| 14 | CLA | B | 1239 | 2 | 57,73,73 | 1.20 | 5 (8%) | 61,113,113 | 1.46 | 12 (19%) |
| 15 | PQN | B | 2002 | - | 34,34,34 | 3.30 | 15 (44%) | 45,45,45 | 2.06 | 3 (6%) |
| 17 | BCR | B | 4004 | - | 41,41,41 | 1.48 | 5 (12%) | 56,56,56 | 2.04 | 17 (30%) |
| 17 | BCR | B | 4005 | - | 41,41,41 | 1.53 | 7 (17%) | 56,56,56 | 2.11 | 18 (32%) |
| 17 | BCR | B | 4006 | - | 41,41,41 | 1.22 | 5 (12%) | 56,56,56 | 2.04 | 20 (35%) |
| 17 | BCR | B | 4009 | - | 25,25,41 | 1.33 | 4 (16%) | 32,33,56 | 1.87 | 10 (31%) |
| 17 | BCR | B | 4010 | - | 41,41,41 | 1.21 | 4 (9%) | 56,56,56 | 1.90 | 19 (33%) |
| 17 | BCR | B | 4014 | - | 41,41,41 | 1.20 | 4 (9%) | 56,56,56 | 2.01 | 20 (35%) |
| 17 | BCR | B | 4017 | - | 41,41,41 | 1.24 | 4 (9%) | 56,56,56 | 1.75 | 16 (28%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 19 | LMG | B | 5002 | - | 55,55,55 | 0.86 | 2 (3%) | 63,63,63 | 1.27 | 3 (4%) |
| 18 | LHG | B | 5004 | - | 22,22,48 | 2.70 | 4 (18%) | 23,28,54 | 1.08 | 1 (4%) |
| 16 | SF4 | C | 3002 | 3 | 0,12,12 | 0.00 | - | 0,24,24 | 0.00 | - |
| 16 | SF4 | C | 3003 | 3 | 0,12,12 | 0.00 | - | 0,24,24 | 0.00 | - |
| 14 | CLA | F | 1301 | 20 | 34,53,73 | 1.42 | 3 (8%) | 37,89,113 | 1.64 | 10 (27%) |
| 17 | BCR | F | 4016 | - | 41,41,41 | 1.23 | 3 (7%) | 56,56,56 | 1.83 | 15 (26%) |
| 17 | BCR | I | 4018 | - | 41,41,41 | 1.28 | 6 (14%) | 56,56,56 | 1.81 | 15 (26%) |
| 17 | BCR | I | 4020 | - | 41,41,41 | 1.24 | 6 (14%) | 56,56,56 | 1.84 | 16 (28%) |
| 14 | CLA | J | 1302 | 8 | 34,53,73 | 1.54 | 4 (11%) | 37,89,113 | 1.80 | 9 (24%) |
| 14 | CLA | J | 1303 | 8 | 29,45,73 | 1.72 | 3 (10%) | 28,78,113 | 1.75 | 9 (32%) |
| 17 | BCR | J | 4012 | - | 41,41,41 | 1.25 | 5 (12%) | 56,56,56 | 1.92 | 16 (28%) |
| 17 | BCR | J | 4013 | - | 41,41,41 | 1.24 | 3 (7%) | 56,56,56 | 1.85 | 21 (37%) |
| 17 | BCR | J | 4015 | - | 41,41,41 | 1.36 | 5 (12%) | 56,56,56 | 1.90 | 13 (23%) |
| 14 | CLA | K | 1401 | - | 34,53,73 | 1.43 | 4 (11%) | 37,89,113 | 1.65 | 9 (24%) |
| 14 | CLA | L | 1501 | 10 | 57,73,73 | 1.18 | 4 (7%) | 61,113,113 | 1.54 | 11 (18%) |
| 14 | CLA | L | 1502 | 10 | 57,73,73 | 1.17 | 6 (10%) | 61,113,113 | 1.48 | 12 (19%) |
| 14 | CLA | L | 1503 | 20 | 57,73,73 | 1.15 | 3 (5%) | 61,113,113 | 1.44 | 9 (14%) |
| 17 | BCR | L | 4019 | - | 41,41,41 | 1.39 | 7 (17%) | 56,56,56 | 1.83 | 15 (26%) |
| 17 | BCR | L | 4022 | - | 41,41,41 | 1.57 | 7 (17%) | 56,56,56 | 1.75 | 11 (19%) |
| 14 | CLA | M | 1601 | 20 | 34,53,73 | 1.53 | 3 (8%) | 37,89,113 | 1.78 | 9 (24%) |
| 17 | BCR | M | 4021 | - | 41,41,41 | 1.30 | 6 (14%) | 56,56,56 | 1.80 | 14 (25%) |
| 14 | CLA | X | 1701 | 12 | 34,53,73 | 1.48 | 2 (5%) | 37,89,113 | 1.72 | 10 (27%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|--------------|---------|
| 14 | CLA | A | 1011 | 1 | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 14 | CLA | A | 1013 | 1 | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 14 | CLA | A | 1022 | 20 | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 14 | CLA | A | 1101 | 1 | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 14 | CLA | A | 1102 | 1,14 | 3/3/18/25 | 0/30/128/135 | 0/0/9/9 |
| 14 | CLA | A | 1103 | 1 | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 14 | CLA | A | 1104 | 1 | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|--------------|---------|
| 14 | CLA | A | 1105 | 1 | 2/2/17/25 | 0/21/119/135 | 0/0/9/9 |
| 14 | CLA | A | 1106 | 1 | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 14 | CLA | A | 1107 | 1 | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 14 | CLA | A | 1108 | 1 | - | 0/11/111/135 | 0/0/9/9 |
| 14 | CLA | A | 1109 | 1,14 | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 14 | CLA | A | 1110 | 1 | 3/3/17/25 | 0/24/122/135 | 0/0/9/9 |
| 14 | CLA | A | 1111 | 1 | 3/3/19/25 | 0/31/129/135 | 0/0/9/9 |
| 14 | CLA | A | 1112 | 1 | 3/3/16/25 | 0/11/111/135 | 0/0/9/9 |
| 14 | CLA | A | 1113 | 1 | 3/3/16/25 | 0/11/111/135 | 0/0/9/9 |
| 14 | CLA | A | 1114 | 20 | 3/3/16/25 | 1/18/116/135 | 0/0/9/9 |
| 14 | CLA | A | 1115 | 1 | 1/1/17/25 | 0/24/122/135 | 0/0/9/9 |
| 14 | CLA | A | 1116 | 1 | 3/3/17/25 | 0/24/122/135 | 0/0/9/9 |
| 14 | CLA | A | 1117 | 1 | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 14 | CLA | A | 1118 | 1 | 3/3/19/25 | 0/33/131/135 | 0/0/9/9 |
| 14 | CLA | A | 1119 | 20 | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 14 | CLA | A | 1120 | 1 | 3/3/16/25 | 0/18/116/135 | 0/0/9/9 |
| 14 | CLA | A | 1121 | 1 | 2/2/17/25 | 0/21/119/135 | 0/0/9/9 |
| 14 | CLA | A | 1122 | 1 | 3/3/18/25 | 0/30/128/135 | 0/0/9/9 |
| 14 | CLA | A | 1123 | 20 | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 14 | CLA | A | 1124 | 20 | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 14 | CLA | A | 1125 | 1 | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 14 | CLA | A | 1126 | 1 | 1/1/20/25 | 0/37/135/135 | 0/0/9/9 |
| 14 | CLA | A | 1127 | 1 | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 14 | CLA | A | 1128 | 1 | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 14 | CLA | A | 1129 | 1 | 3/3/17/25 | 0/19/117/135 | 0/0/9/9 |
| 14 | CLA | A | 1130 | 1 | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 14 | CLA | A | 1131 | 1 | - | 0/37/135/135 | 0/0/9/9 |
| 14 | CLA | A | 1132 | 1 | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 14 | CLA | A | 1133 | 1 | 3/3/17/25 | 0/24/122/135 | 0/0/9/9 |
| 14 | CLA | A | 1134 | 1 | 3/3/16/25 | 0/11/111/135 | 0/0/9/9 |
| 14 | CLA | A | 1135 | 1 | 3/3/17/25 | 0/21/119/135 | 0/0/9/9 |
| 14 | CLA | A | 1136 | 1 | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 14 | CLA | A | 1137 | 1 | 1/1/16/25 | 0/16/114/135 | 0/0/9/9 |
| 14 | CLA | A | 1138 | 1 | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 14 | CLA | A | 1139 | 20 | 3/3/17/25 | 0/21/119/135 | 0/0/9/9 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|--------------|---------|
| 14 | CLA | A | 1140 | 1 | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 14 | CLA | A | 1237 | 20 | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 14 | CLA | A | 1402 | - | 3/3/14/25 | 0/5/101/135 | 0/0/9/9 |
| 14 | CLA | A | 1801 | 18 | 3/3/17/25 | 0/22/120/135 | 0/0/9/9 |
| 15 | PQN | A | 2001 | - | - | 0/23/43/43 | 0/2/2/2 |
| 16 | SF4 | A | 3001 | 1,2 | - | 0/0/48/48 | 0/6/5/5 |
| 17 | BCR | A | 4001 | - | - | 0/29/63/63 | 0/2/2/2 |
| 17 | BCR | A | 4002 | - | - | 0/29/63/63 | 0/2/2/2 |
| 17 | BCR | A | 4003 | - | - | 0/29/63/63 | 0/2/2/2 |
| 17 | BCR | A | 4007 | - | - | 0/29/63/63 | 0/2/2/2 |
| 17 | BCR | A | 4008 | - | - | 0/29/63/63 | 0/2/2/2 |
| 17 | BCR | A | 4011 | - | - | 0/29/63/63 | 0/2/2/2 |
| 18 | LHG | A | 5001 | - | - | 0/53/53/53 | 0/0/0/0 |
| 18 | LHG | A | 5003 | 14 | 1/1/5/5 | 0/31/31/53 | 0/0/0/0 |
| 14 | CLA | B | 1012 | 20 | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 14 | CLA | B | 1021 | 2 | 1/1/20/25 | 0/37/135/135 | 0/0/9/9 |
| 14 | CLA | B | 1023 | 2 | 1/1/20/25 | 0/37/135/135 | 0/0/9/9 |
| 14 | CLA | B | 1201 | 2 | 2/2/17/25 | 0/24/122/135 | 0/0/9/9 |
| 14 | CLA | B | 1202 | 2 | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 14 | CLA | B | 1203 | 2 | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 14 | CLA | B | 1204 | 2 | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 14 | CLA | B | 1205 | 2 | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 14 | CLA | B | 1206 | 2 | 1/1/20/25 | 0/37/135/135 | 0/0/9/9 |
| 14 | CLA | B | 1207 | 2 | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 14 | CLA | B | 1208 | 2 | 2/2/16/25 | 0/11/111/135 | 0/0/9/9 |
| 14 | CLA | B | 1209 | 2 | 3/3/16/25 | 0/11/111/135 | 0/0/9/9 |
| 14 | CLA | B | 1210 | 2 | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 14 | CLA | B | 1211 | 2 | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 14 | CLA | B | 1212 | 2 | 2/2/16/25 | 0/11/111/135 | 0/0/9/9 |
| 14 | CLA | B | 1213 | 2 | 3/3/18/25 | 0/25/123/135 | 0/0/9/9 |
| 14 | CLA | B | 1214 | 2 | 3/3/18/25 | 0/30/128/135 | 0/0/9/9 |
| 14 | CLA | B | 1215 | 2 | 3/3/19/25 | 0/31/129/135 | 0/0/9/9 |
| 14 | CLA | B | 1216 | 20 | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 14 | CLA | B | 1217 | 2 | 3/3/16/25 | 0/16/114/135 | 0/0/9/9 |
| 14 | CLA | B | 1218 | 2 | 3/3/16/25 | 0/11/111/135 | 0/0/9/9 |
| 14 | CLA | B | 1219 | 20 | 3/3/18/25 | 0/25/123/135 | 0/0/9/9 |
| 14 | CLA | B | 1220 | 2 | 3/3/16/25 | 0/11/111/135 | 0/0/9/9 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|--------------|---------|
| 14 | CLA | B | 1221 | 2 | 3/3/17/25 | 0/24/122/135 | 0/0/9/9 |
| 14 | CLA | B | 1222 | 20 | 3/3/16/25 | 0/15/113/135 | 0/0/9/9 |
| 14 | CLA | B | 1223 | 2 | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 14 | CLA | B | 1224 | 2 | 1/1/20/25 | 0/37/135/135 | 0/0/9/9 |
| 14 | CLA | B | 1225 | 2 | 1/1/20/25 | 0/37/135/135 | 0/0/9/9 |
| 14 | CLA | B | 1226 | 2 | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 14 | CLA | B | 1227 | 2 | 3/3/16/25 | 0/11/111/135 | 0/0/9/9 |
| 14 | CLA | B | 1228 | 2 | 3/3/16/25 | 0/18/116/135 | 0/0/9/9 |
| 14 | CLA | B | 1229 | 2 | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 14 | CLA | B | 1230 | 2 | 3/3/18/25 | 0/29/127/135 | 0/0/9/9 |
| 14 | CLA | B | 1231 | 2 | 3/3/16/25 | 0/11/111/135 | 0/0/9/9 |
| 14 | CLA | B | 1232 | 20 | 3/3/16/25 | 0/11/111/135 | 0/0/9/9 |
| 14 | CLA | B | 1233 | 20 | 3/3/16/25 | 0/11/111/135 | 0/0/9/9 |
| 14 | CLA | B | 1234 | 2 | 3/3/19/25 | 0/31/129/135 | 0/0/9/9 |
| 14 | CLA | B | 1235 | 2 | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 14 | CLA | B | 1236 | 2 | - | 0/16/114/135 | 0/0/9/9 |
| 14 | CLA | B | 1238 | 20 | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 14 | CLA | B | 1239 | 2 | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 15 | PQN | B | 2002 | - | - | 0/23/43/43 | 0/2/2/2 |
| 17 | BCR | B | 4004 | - | - | 0/29/63/63 | 0/2/2/2 |
| 17 | BCR | B | 4005 | - | - | 0/29/63/63 | 0/2/2/2 |
| 17 | BCR | B | 4006 | - | - | 0/29/63/63 | 0/2/2/2 |
| 17 | BCR | B | 4009 | - | - | 0/18/35/63 | 0/1/1/2 |
| 17 | BCR | B | 4010 | - | - | 0/29/63/63 | 0/2/2/2 |
| 17 | BCR | B | 4014 | - | - | 0/29/63/63 | 0/2/2/2 |
| 17 | BCR | B | 4017 | - | - | 0/29/63/63 | 0/2/2/2 |
| 19 | LMG | B | 5002 | - | - | 0/50/70/70 | 0/1/1/1 |
| 18 | LHG | B | 5004 | - | - | 0/26/26/53 | 0/0/0/0 |
| 16 | SF4 | C | 3002 | 3 | - | 0/0/48/48 | 0/6/5/5 |
| 16 | SF4 | C | 3003 | 3 | - | 0/0/48/48 | 0/6/5/5 |
| 14 | CLA | F | 1301 | 20 | 3/3/16/25 | 0/11/111/135 | 0/0/9/9 |
| 17 | BCR | F | 4016 | - | - | 0/29/63/63 | 0/2/2/2 |
| 17 | BCR | I | 4018 | - | - | 0/29/63/63 | 0/2/2/2 |
| 17 | BCR | I | 4020 | - | - | 0/29/63/63 | 0/2/2/2 |
| 14 | CLA | J | 1302 | 8 | 3/3/16/25 | 0/11/111/135 | 0/0/9/9 |
| 14 | CLA | J | 1303 | 8 | 3/3/13/25 | 0/2/96/135 | 0/0/9/9 |
| 17 | BCR | J | 4012 | - | - | 0/29/63/63 | 0/2/2/2 |
| 17 | BCR | J | 4013 | - | - | 0/29/63/63 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|--------------|---------|
| 17 | BCR | J | 4015 | - | - | 0/29/63/63 | 0/2/2/2 |
| 14 | CLA | K | 1401 | - | 2/2/16/25 | 0/11/111/135 | 0/0/9/9 |
| 14 | CLA | L | 1501 | 10 | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 14 | CLA | L | 1502 | 10 | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 14 | CLA | L | 1503 | 20 | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 17 | BCR | L | 4019 | - | - | 0/29/63/63 | 0/2/2/2 |
| 17 | BCR | L | 4022 | - | - | 0/29/63/63 | 0/2/2/2 |
| 14 | CLA | M | 1601 | 20 | 3/3/16/25 | 0/11/111/135 | 0/0/9/9 |
| 17 | BCR | M | 4021 | - | - | 0/29/63/63 | 0/2/2/2 |
| 14 | CLA | X | 1701 | 12 | 3/3/16/25 | 0/11/111/135 | 0/0/9/9 |

All (537) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 15 | A | 2001 | PQN | C2M-C2 | -6.78 | 1.36 | 1.50 |
| 15 | B | 2002 | PQN | C2M-C2 | -6.43 | 1.37 | 1.50 |
| 15 | B | 2002 | PQN | C16-C15 | -4.56 | 1.34 | 1.52 |
| 15 | A | 2001 | PQN | C16-C15 | -4.44 | 1.35 | 1.52 |
| 14 | B | 1204 | CLA | C3B-C2B | -3.89 | 1.35 | 1.40 |
| 14 | A | 1132 | CLA | C3B-C2B | -3.78 | 1.35 | 1.40 |
| 14 | B | 1227 | CLA | C3B-C2B | -3.73 | 1.35 | 1.40 |
| 14 | B | 1235 | CLA | C3B-C2B | -3.44 | 1.36 | 1.40 |
| 14 | B | 1234 | CLA | C3B-C2B | -3.33 | 1.36 | 1.40 |
| 14 | B | 1228 | CLA | C3B-C2B | -3.30 | 1.36 | 1.40 |
| 14 | B | 1229 | CLA | C3B-C2B | -3.25 | 1.36 | 1.40 |
| 14 | A | 1116 | CLA | C3B-C2B | -3.22 | 1.36 | 1.40 |
| 14 | A | 1129 | CLA | C3B-C2B | -3.14 | 1.36 | 1.40 |
| 14 | B | 1023 | CLA | C3B-C2B | -3.04 | 1.36 | 1.40 |
| 14 | A | 1123 | CLA | C3B-C2B | -3.04 | 1.36 | 1.40 |
| 14 | A | 1136 | CLA | C3B-C2B | -2.99 | 1.36 | 1.40 |
| 14 | A | 1106 | CLA | C3B-C2B | -2.99 | 1.36 | 1.40 |
| 14 | B | 1208 | CLA | C3B-C2B | -2.97 | 1.36 | 1.40 |
| 14 | A | 1128 | CLA | C3B-C2B | -2.96 | 1.36 | 1.40 |
| 14 | B | 1205 | CLA | C3B-C2B | -2.90 | 1.36 | 1.40 |
| 14 | A | 1105 | CLA | C3B-C2B | -2.88 | 1.36 | 1.40 |
| 14 | B | 1236 | CLA | C3B-C2B | -2.85 | 1.36 | 1.40 |
| 14 | A | 1108 | CLA | C3B-C2B | -2.84 | 1.36 | 1.40 |
| 14 | B | 1231 | CLA | C3B-C2B | -2.83 | 1.36 | 1.40 |
| 14 | B | 1232 | CLA | C3B-C2B | -2.82 | 1.36 | 1.40 |
| 14 | A | 1121 | CLA | C3B-C2B | -2.81 | 1.36 | 1.40 |
| 14 | B | 1216 | CLA | C3B-C2B | -2.76 | 1.36 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | B | 1225 | CLA | C3B-C2B | -2.75 | 1.36 | 1.40 |
| 14 | B | 1238 | CLA | C3B-C2B | -2.74 | 1.36 | 1.40 |
| 14 | B | 1205 | CLA | C1B-CHB | -2.70 | 1.32 | 1.40 |
| 14 | B | 1207 | CLA | C3B-C2B | -2.69 | 1.36 | 1.40 |
| 14 | B | 1228 | CLA | C1B-CHB | -2.67 | 1.32 | 1.40 |
| 14 | A | 1120 | CLA | C3B-C2B | -2.64 | 1.37 | 1.40 |
| 14 | B | 1214 | CLA | C3B-C2B | -2.64 | 1.37 | 1.40 |
| 14 | A | 1112 | CLA | C3B-C2B | -2.63 | 1.37 | 1.40 |
| 14 | A | 1137 | CLA | C3B-C2B | -2.62 | 1.37 | 1.40 |
| 14 | A | 1237 | CLA | C3B-C2B | -2.62 | 1.37 | 1.40 |
| 14 | A | 1013 | CLA | C1B-CHB | -2.62 | 1.33 | 1.40 |
| 14 | B | 1212 | CLA | C3B-C2B | -2.58 | 1.37 | 1.40 |
| 14 | A | 1129 | CLA | C1B-CHB | -2.58 | 1.33 | 1.40 |
| 14 | A | 1119 | CLA | C1B-CHB | -2.58 | 1.33 | 1.40 |
| 14 | B | 1221 | CLA | C3B-C2B | -2.57 | 1.37 | 1.40 |
| 14 | A | 1801 | CLA | C3B-C2B | -2.57 | 1.37 | 1.40 |
| 14 | A | 1022 | CLA | C3B-C2B | -2.56 | 1.37 | 1.40 |
| 14 | B | 1023 | CLA | C1B-CHB | -2.54 | 1.33 | 1.40 |
| 17 | A | 4011 | BCR | C23-C22 | -2.53 | 1.40 | 1.45 |
| 15 | A | 2001 | PQN | C10-C1 | -2.52 | 1.43 | 1.48 |
| 14 | A | 1109 | CLA | C3B-C2B | -2.52 | 1.37 | 1.40 |
| 14 | B | 1213 | CLA | C3B-C2B | -2.51 | 1.37 | 1.40 |
| 14 | B | 1204 | CLA | C1B-CHB | -2.51 | 1.33 | 1.40 |
| 14 | A | 1110 | CLA | C3B-C2B | -2.49 | 1.37 | 1.40 |
| 14 | A | 1101 | CLA | C3B-C2B | -2.49 | 1.37 | 1.40 |
| 14 | A | 1118 | CLA | C3B-C2B | -2.48 | 1.37 | 1.40 |
| 14 | A | 1124 | CLA | C1B-CHB | -2.46 | 1.33 | 1.40 |
| 14 | B | 1021 | CLA | C1B-CHB | -2.46 | 1.33 | 1.40 |
| 14 | L | 1502 | CLA | C1B-CHB | -2.45 | 1.33 | 1.40 |
| 14 | B | 1214 | CLA | C1B-CHB | -2.43 | 1.33 | 1.40 |
| 14 | B | 1236 | CLA | C1B-CHB | -2.43 | 1.33 | 1.40 |
| 14 | B | 1208 | CLA | C1B-CHB | -2.43 | 1.33 | 1.40 |
| 14 | A | 1106 | CLA | C1B-CHB | -2.43 | 1.33 | 1.40 |
| 14 | K | 1401 | CLA | C3B-C2B | -2.41 | 1.37 | 1.40 |
| 14 | A | 1138 | CLA | C1B-CHB | -2.40 | 1.33 | 1.40 |
| 14 | B | 1221 | CLA | C1B-CHB | -2.39 | 1.33 | 1.40 |
| 14 | A | 1139 | CLA | C3B-C2B | -2.39 | 1.37 | 1.40 |
| 14 | A | 1133 | CLA | C3B-C2B | -2.37 | 1.37 | 1.40 |
| 17 | M | 4021 | BCR | C23-C22 | -2.36 | 1.40 | 1.45 |
| 17 | L | 4019 | BCR | C19-C18 | -2.35 | 1.40 | 1.45 |
| 14 | A | 1112 | CLA | C1B-CHB | -2.34 | 1.33 | 1.40 |
| 14 | A | 1101 | CLA | C1B-CHB | -2.34 | 1.33 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | B | 1235 | CLA | C1B-CHB | -2.34 | 1.33 | 1.40 |
| 14 | A | 1132 | CLA | C1B-CHB | -2.33 | 1.33 | 1.40 |
| 19 | B | 5002 | LMG | O7-C8 | -2.33 | 1.40 | 1.46 |
| 14 | A | 1136 | CLA | C1B-CHB | -2.31 | 1.33 | 1.40 |
| 14 | A | 1111 | CLA | C1B-CHB | -2.30 | 1.33 | 1.40 |
| 14 | B | 1232 | CLA | C1B-CHB | -2.30 | 1.34 | 1.40 |
| 14 | B | 1210 | CLA | C1B-CHB | -2.30 | 1.34 | 1.40 |
| 14 | A | 1103 | CLA | C1B-CHB | -2.30 | 1.34 | 1.40 |
| 14 | A | 1115 | CLA | C3B-C2B | -2.29 | 1.37 | 1.40 |
| 14 | A | 1115 | CLA | C1B-CHB | -2.28 | 1.34 | 1.40 |
| 14 | A | 1109 | CLA | C1B-CHB | -2.28 | 1.34 | 1.40 |
| 14 | B | 1211 | CLA | C3B-C2B | -2.28 | 1.37 | 1.40 |
| 14 | A | 1122 | CLA | C1B-CHB | -2.27 | 1.34 | 1.40 |
| 14 | B | 1216 | CLA | C1B-CHB | -2.27 | 1.34 | 1.40 |
| 17 | B | 4009 | BCR | C23-C22 | -2.27 | 1.40 | 1.45 |
| 17 | B | 4017 | BCR | C23-C22 | -2.27 | 1.40 | 1.45 |
| 14 | B | 1233 | CLA | C3B-C2B | -2.26 | 1.37 | 1.40 |
| 14 | B | 1231 | CLA | C1B-CHB | -2.26 | 1.34 | 1.40 |
| 14 | A | 1114 | CLA | C3B-C2B | -2.26 | 1.37 | 1.40 |
| 17 | B | 4014 | BCR | C23-C22 | -2.25 | 1.40 | 1.45 |
| 14 | B | 1227 | CLA | C1B-CHB | -2.25 | 1.34 | 1.40 |
| 14 | B | 1220 | CLA | C3B-C2B | -2.25 | 1.37 | 1.40 |
| 14 | B | 1239 | CLA | C3B-C2B | -2.25 | 1.37 | 1.40 |
| 15 | B | 2002 | PQN | C5-C4 | -2.24 | 1.43 | 1.48 |
| 14 | B | 1211 | CLA | C1B-CHB | -2.23 | 1.34 | 1.40 |
| 14 | K | 1401 | CLA | C1B-CHB | -2.21 | 1.34 | 1.40 |
| 14 | A | 1022 | CLA | C1B-CHB | -2.19 | 1.34 | 1.40 |
| 14 | A | 1126 | CLA | C1B-CHB | -2.19 | 1.34 | 1.40 |
| 17 | I | 4020 | BCR | C19-C18 | -2.19 | 1.41 | 1.45 |
| 14 | A | 1237 | CLA | C1B-CHB | -2.18 | 1.34 | 1.40 |
| 14 | B | 1212 | CLA | C1B-CHB | -2.18 | 1.34 | 1.40 |
| 14 | A | 1801 | CLA | C1B-CHB | -2.18 | 1.34 | 1.40 |
| 14 | A | 1134 | CLA | C3B-C2B | -2.16 | 1.37 | 1.40 |
| 14 | F | 1301 | CLA | C3B-C2B | -2.14 | 1.37 | 1.40 |
| 14 | B | 1239 | CLA | C1C-NC | -2.13 | 1.34 | 1.37 |
| 17 | L | 4022 | BCR | C23-C22 | -2.13 | 1.41 | 1.45 |
| 15 | A | 2001 | PQN | C5-C4 | -2.12 | 1.43 | 1.48 |
| 14 | A | 1114 | CLA | C1B-CHB | -2.12 | 1.34 | 1.40 |
| 14 | J | 1302 | CLA | C3B-C2B | -2.12 | 1.37 | 1.40 |
| 14 | B | 1239 | CLA | CAA-CBA | -2.12 | 1.45 | 1.52 |
| 14 | A | 1121 | CLA | C1B-CHB | -2.11 | 1.34 | 1.40 |
| 17 | B | 4005 | BCR | C29-C28 | -2.11 | 1.47 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 17 | I | 4018 | BCR | C19-C18 | -2.11 | 1.41 | 1.45 |
| 17 | I | 4018 | BCR | C2-C3 | -2.10 | 1.47 | 1.52 |
| 14 | B | 1229 | CLA | C1B-CHB | -2.09 | 1.34 | 1.40 |
| 14 | A | 1120 | CLA | C1B-CHB | -2.09 | 1.34 | 1.40 |
| 14 | B | 1213 | CLA | C1B-CHB | -2.09 | 1.34 | 1.40 |
| 14 | B | 1225 | CLA | C1B-CHB | -2.09 | 1.34 | 1.40 |
| 15 | B | 2002 | PQN | C10-C1 | -2.08 | 1.44 | 1.48 |
| 14 | A | 1110 | CLA | C1B-CHB | -2.08 | 1.34 | 1.40 |
| 14 | L | 1502 | CLA | C3B-C2B | -2.07 | 1.37 | 1.40 |
| 14 | A | 1108 | CLA | C1B-CHB | -2.07 | 1.34 | 1.40 |
| 14 | A | 1117 | CLA | C1B-CHB | -2.07 | 1.34 | 1.40 |
| 14 | B | 1201 | CLA | C3B-C2B | -2.05 | 1.37 | 1.40 |
| 17 | A | 4008 | BCR | C19-C18 | -2.05 | 1.41 | 1.45 |
| 14 | A | 1107 | CLA | C1B-CHB | -2.05 | 1.34 | 1.40 |
| 18 | A | 5001 | LHG | O8-C6 | -2.05 | 1.40 | 1.45 |
| 14 | L | 1503 | CLA | CBA-CGA | -2.04 | 1.44 | 1.50 |
| 14 | A | 1125 | CLA | C3B-C2B | -2.04 | 1.37 | 1.40 |
| 14 | B | 1207 | CLA | C1B-CHB | -2.04 | 1.34 | 1.40 |
| 14 | A | 1104 | CLA | CAA-CBA | -2.02 | 1.46 | 1.52 |
| 14 | A | 1402 | CLA | C3B-C2B | -2.02 | 1.37 | 1.40 |
| 17 | A | 4003 | BCR | C29-C28 | -2.02 | 1.47 | 1.52 |
| 17 | L | 4019 | BCR | C29-C28 | -2.01 | 1.47 | 1.52 |
| 17 | M | 4021 | BCR | C2-C3 | -2.00 | 1.47 | 1.52 |
| 14 | B | 1201 | CLA | CAA-C2A | 2.01 | 1.58 | 1.54 |
| 14 | B | 1226 | CLA | C3B-CAB | 2.01 | 1.52 | 1.47 |
| 14 | B | 1238 | CLA | C1-C2 | 2.01 | 1.55 | 1.49 |
| 14 | B | 1202 | CLA | C5-C3 | 2.01 | 1.55 | 1.51 |
| 14 | B | 1238 | CLA | CHC-C1C | 2.01 | 1.41 | 1.35 |
| 14 | A | 1402 | CLA | CAA-C2A | 2.01 | 1.58 | 1.54 |
| 14 | A | 1136 | CLA | CAA-C2A | 2.01 | 1.58 | 1.54 |
| 14 | L | 1501 | CLA | C1C-C2C | 2.02 | 1.48 | 1.44 |
| 14 | A | 1117 | CLA | C3B-CAB | 2.02 | 1.52 | 1.47 |
| 14 | A | 1121 | CLA | C1-C2 | 2.02 | 1.55 | 1.49 |
| 14 | A | 1128 | CLA | CAA-C2A | 2.02 | 1.58 | 1.54 |
| 14 | A | 1117 | CLA | CHC-C1C | 2.03 | 1.41 | 1.35 |
| 14 | B | 1231 | CLA | CAA-C2A | 2.03 | 1.58 | 1.54 |
| 14 | B | 1222 | CLA | CAA-C2A | 2.04 | 1.58 | 1.54 |
| 14 | A | 1132 | CLA | C1-C2 | 2.04 | 1.55 | 1.49 |
| 14 | B | 1227 | CLA | CAA-C2A | 2.04 | 1.58 | 1.54 |
| 14 | B | 1202 | CLA | CMD-C2D | 2.04 | 1.56 | 1.51 |
| 14 | A | 1109 | CLA | CAA-C2A | 2.04 | 1.58 | 1.54 |
| 14 | B | 1201 | CLA | C1-C2 | 2.06 | 1.55 | 1.49 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 14 | J | 1302 | CLA | CAA-C2A | 2.06 | 1.58 | 1.54 |
| 17 | A | 4003 | BCR | C26-C25 | 2.07 | 1.38 | 1.34 |
| 17 | I | 4020 | BCR | C26-C25 | 2.07 | 1.38 | 1.34 |
| 14 | A | 1134 | CLA | CAA-C2A | 2.08 | 1.58 | 1.54 |
| 14 | B | 1213 | CLA | C4-C3 | 2.09 | 1.56 | 1.50 |
| 14 | B | 1211 | CLA | C5-C3 | 2.09 | 1.56 | 1.51 |
| 17 | B | 4006 | BCR | C5-C6 | 2.09 | 1.38 | 1.34 |
| 14 | A | 1801 | CLA | C5-C3 | 2.10 | 1.56 | 1.51 |
| 14 | A | 1126 | CLA | CHC-C1C | 2.10 | 1.41 | 1.35 |
| 17 | L | 4019 | BCR | C26-C25 | 2.10 | 1.38 | 1.34 |
| 17 | J | 4012 | BCR | C26-C25 | 2.11 | 1.38 | 1.34 |
| 14 | A | 1124 | CLA | CHC-C1C | 2.11 | 1.41 | 1.35 |
| 14 | L | 1502 | CLA | CMD-C2D | 2.12 | 1.56 | 1.51 |
| 14 | A | 1124 | CLA | CAA-C2A | 2.12 | 1.58 | 1.54 |
| 14 | A | 1138 | CLA | CAA-C2A | 2.12 | 1.58 | 1.54 |
| 14 | B | 1226 | CLA | OBD-CAD | 2.13 | 1.25 | 1.22 |
| 14 | B | 1221 | CLA | C1-C2 | 2.13 | 1.55 | 1.49 |
| 14 | A | 1119 | CLA | C1-C2 | 2.13 | 1.55 | 1.49 |
| 14 | B | 1213 | CLA | C1-C2 | 2.13 | 1.55 | 1.49 |
| 14 | A | 1132 | CLA | CHC-C1C | 2.14 | 1.41 | 1.35 |
| 17 | A | 4008 | BCR | C2-C1 | 2.14 | 1.59 | 1.54 |
| 14 | A | 1139 | CLA | CHC-C1C | 2.14 | 1.41 | 1.35 |
| 14 | A | 1105 | CLA | C1-C2 | 2.15 | 1.55 | 1.49 |
| 14 | A | 1133 | CLA | C1-C2 | 2.15 | 1.55 | 1.49 |
| 17 | A | 4008 | BCR | C33-C5 | 2.16 | 1.54 | 1.51 |
| 14 | B | 1208 | CLA | CAA-C2A | 2.16 | 1.58 | 1.54 |
| 14 | B | 1203 | CLA | CHC-C1C | 2.16 | 1.41 | 1.35 |
| 14 | B | 1021 | CLA | CHC-C1C | 2.16 | 1.41 | 1.35 |
| 14 | A | 1139 | CLA | C5-C3 | 2.17 | 1.58 | 1.51 |
| 14 | B | 1238 | CLA | CAA-C2A | 2.17 | 1.58 | 1.54 |
| 14 | B | 1223 | CLA | C3B-CAB | 2.17 | 1.52 | 1.47 |
| 14 | B | 1215 | CLA | CHC-C1C | 2.18 | 1.41 | 1.35 |
| 14 | A | 1237 | CLA | C4-C3 | 2.19 | 1.56 | 1.50 |
| 17 | B | 4014 | BCR | C5-C6 | 2.19 | 1.38 | 1.34 |
| 14 | B | 1202 | CLA | CHC-C1C | 2.20 | 1.41 | 1.35 |
| 14 | B | 1230 | CLA | CAA-C2A | 2.20 | 1.58 | 1.54 |
| 14 | L | 1501 | CLA | CAA-C2A | 2.23 | 1.58 | 1.54 |
| 17 | I | 4020 | BCR | C33-C5 | 2.23 | 1.54 | 1.51 |
| 14 | B | 1239 | CLA | CHC-C1C | 2.23 | 1.41 | 1.35 |
| 17 | B | 4009 | BCR | C14-C13 | 2.24 | 1.40 | 1.34 |
| 14 | A | 1118 | CLA | CAA-C2A | 2.24 | 1.58 | 1.54 |
| 14 | A | 1118 | CLA | C5-C3 | 2.25 | 1.56 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 15 | A | 2001 | PQN | C11-C3 | 2.25 | 1.55 | 1.51 |
| 17 | L | 4019 | BCR | C38-C26 | 2.25 | 1.54 | 1.51 |
| 14 | A | 1110 | CLA | CAA-C2A | 2.25 | 1.58 | 1.54 |
| 14 | B | 1204 | CLA | CAA-C2A | 2.25 | 1.58 | 1.54 |
| 15 | A | 2001 | PQN | C9-C10 | 2.26 | 1.43 | 1.39 |
| 15 | A | 2001 | PQN | C7-C6 | 2.26 | 1.43 | 1.38 |
| 14 | A | 1128 | CLA | C5-C3 | 2.26 | 1.56 | 1.51 |
| 15 | B | 2002 | PQN | C8-C7 | 2.27 | 1.43 | 1.38 |
| 14 | A | 1133 | CLA | C5-C3 | 2.28 | 1.56 | 1.51 |
| 17 | L | 4022 | BCR | C26-C25 | 2.28 | 1.38 | 1.34 |
| 14 | B | 1225 | CLA | CAA-C2A | 2.29 | 1.58 | 1.54 |
| 14 | B | 1226 | CLA | CHC-C1C | 2.29 | 1.42 | 1.35 |
| 14 | A | 1116 | CLA | C5-C3 | 2.29 | 1.56 | 1.51 |
| 14 | B | 1215 | CLA | C3B-CAB | 2.29 | 1.52 | 1.47 |
| 14 | A | 1121 | CLA | CAA-C2A | 2.29 | 1.58 | 1.54 |
| 14 | B | 1225 | CLA | C1-C2 | 2.30 | 1.56 | 1.49 |
| 17 | A | 4003 | BCR | C29-C30 | 2.30 | 1.59 | 1.54 |
| 14 | A | 1117 | CLA | CAA-C2A | 2.30 | 1.58 | 1.54 |
| 14 | L | 1502 | CLA | CAA-C2A | 2.30 | 1.58 | 1.54 |
| 14 | A | 1108 | CLA | CAA-C2A | 2.31 | 1.58 | 1.54 |
| 17 | I | 4018 | BCR | C33-C5 | 2.32 | 1.54 | 1.51 |
| 17 | B | 4010 | BCR | C29-C30 | 2.33 | 1.59 | 1.54 |
| 17 | A | 4001 | BCR | C26-C25 | 2.33 | 1.38 | 1.34 |
| 17 | I | 4018 | BCR | C30-C25 | 2.33 | 1.57 | 1.53 |
| 14 | B | 1225 | CLA | CHC-C1C | 2.35 | 1.42 | 1.35 |
| 14 | B | 1217 | CLA | CAA-C2A | 2.35 | 1.58 | 1.54 |
| 14 | M | 1601 | CLA | CAA-C2A | 2.36 | 1.58 | 1.54 |
| 14 | A | 1117 | CLA | C2-C3 | 2.36 | 1.38 | 1.32 |
| 14 | A | 1013 | CLA | CAA-C2A | 2.36 | 1.58 | 1.54 |
| 17 | B | 4005 | BCR | C29-C30 | 2.37 | 1.59 | 1.54 |
| 17 | I | 4018 | BCR | C2-C1 | 2.37 | 1.59 | 1.54 |
| 17 | L | 4019 | BCR | C2-C1 | 2.37 | 1.59 | 1.54 |
| 14 | A | 1110 | CLA | CHC-C1C | 2.37 | 1.42 | 1.35 |
| 14 | B | 1225 | CLA | C5-C3 | 2.38 | 1.56 | 1.51 |
| 15 | B | 2002 | PQN | C8-C9 | 2.38 | 1.43 | 1.38 |
| 15 | A | 2001 | PQN | C8-C7 | 2.39 | 1.44 | 1.38 |
| 14 | A | 1108 | CLA | CHC-C1C | 2.39 | 1.42 | 1.35 |
| 14 | A | 1237 | CLA | CMD-C2D | 2.39 | 1.56 | 1.51 |
| 17 | B | 4005 | BCR | C38-C26 | 2.40 | 1.54 | 1.51 |
| 17 | L | 4022 | BCR | C38-C26 | 2.40 | 1.54 | 1.51 |
| 15 | B | 2002 | PQN | C9-C10 | 2.41 | 1.43 | 1.39 |
| 14 | A | 1117 | CLA | C1-C2 | 2.42 | 1.56 | 1.49 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 15 | A | 2001 | PQN | C8-C9 | 2.42 | 1.43 | 1.38 |
| 14 | A | 1127 | CLA | CHC-C1C | 2.42 | 1.42 | 1.35 |
| 17 | A | 4011 | BCR | C14-C13 | 2.43 | 1.39 | 1.35 |
| 14 | A | 1102 | CLA | CAA-C2A | 2.43 | 1.58 | 1.54 |
| 17 | A | 4008 | BCR | C29-C30 | 2.43 | 1.60 | 1.54 |
| 14 | A | 1402 | CLA | CHC-C1C | 2.44 | 1.42 | 1.35 |
| 17 | J | 4015 | BCR | C5-C6 | 2.44 | 1.38 | 1.34 |
| 15 | A | 2001 | PQN | C15-C13 | 2.45 | 1.56 | 1.51 |
| 14 | B | 1230 | CLA | C5-C3 | 2.45 | 1.57 | 1.51 |
| 14 | A | 1237 | CLA | CAA-C2A | 2.45 | 1.58 | 1.54 |
| 14 | A | 1109 | CLA | CHC-C1C | 2.46 | 1.42 | 1.35 |
| 14 | B | 1222 | CLA | CHC-C1C | 2.46 | 1.42 | 1.35 |
| 15 | A | 2001 | PQN | C11-C12 | 2.46 | 1.54 | 1.50 |
| 15 | B | 2002 | PQN | C11-C3 | 2.49 | 1.55 | 1.51 |
| 14 | A | 1111 | CLA | CHC-C1C | 2.50 | 1.42 | 1.35 |
| 14 | J | 1303 | CLA | CBD-CAD | 2.50 | 1.57 | 1.51 |
| 14 | B | 1215 | CLA | CAA-C2A | 2.51 | 1.59 | 1.54 |
| 14 | A | 1121 | CLA | CHC-C1C | 2.51 | 1.42 | 1.35 |
| 17 | B | 4014 | BCR | C2-C1 | 2.52 | 1.60 | 1.54 |
| 14 | A | 1114 | CLA | CHC-C1C | 2.52 | 1.42 | 1.35 |
| 14 | A | 1013 | CLA | CHC-C1C | 2.52 | 1.42 | 1.35 |
| 17 | A | 4007 | BCR | C2-C1 | 2.52 | 1.60 | 1.54 |
| 14 | B | 1230 | CLA | CHC-C1C | 2.53 | 1.42 | 1.35 |
| 14 | A | 1133 | CLA | CHC-C1C | 2.53 | 1.42 | 1.35 |
| 14 | B | 1205 | CLA | CHC-C1C | 2.54 | 1.42 | 1.35 |
| 18 | A | 5001 | LHG | O7-C7 | 2.55 | 1.41 | 1.34 |
| 17 | L | 4022 | BCR | C29-C30 | 2.56 | 1.60 | 1.54 |
| 14 | A | 1101 | CLA | CHC-C1C | 2.56 | 1.42 | 1.35 |
| 14 | B | 1210 | CLA | CHC-C1C | 2.56 | 1.42 | 1.35 |
| 17 | B | 4010 | BCR | C1-C6 | 2.56 | 1.57 | 1.53 |
| 14 | A | 1140 | CLA | C1-C2 | 2.56 | 1.57 | 1.49 |
| 14 | B | 1233 | CLA | CHC-C1C | 2.57 | 1.42 | 1.35 |
| 14 | A | 1113 | CLA | CHC-C1C | 2.57 | 1.42 | 1.35 |
| 14 | B | 1214 | CLA | CAA-C2A | 2.57 | 1.59 | 1.54 |
| 14 | A | 1011 | CLA | CHC-C1C | 2.57 | 1.42 | 1.35 |
| 17 | I | 4020 | BCR | C29-C30 | 2.57 | 1.60 | 1.54 |
| 17 | A | 4001 | BCR | C2-C1 | 2.60 | 1.60 | 1.54 |
| 14 | B | 1208 | CLA | CHC-C1C | 2.61 | 1.43 | 1.35 |
| 14 | A | 1107 | CLA | CHC-C1C | 2.61 | 1.43 | 1.35 |
| 14 | B | 1216 | CLA | CHC-C1C | 2.61 | 1.43 | 1.35 |
| 14 | B | 1221 | CLA | C5-C3 | 2.62 | 1.57 | 1.51 |
| 17 | A | 4008 | BCR | C30-C25 | 2.62 | 1.57 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 17 | I | 4018 | BCR | C29-C30 | 2.63 | 1.60 | 1.54 |
| 14 | B | 1226 | CLA | CAA-C2A | 2.63 | 1.59 | 1.54 |
| 14 | B | 1213 | CLA | CHC-C1C | 2.63 | 1.43 | 1.35 |
| 17 | A | 4007 | BCR | C1-C6 | 2.64 | 1.57 | 1.53 |
| 14 | A | 1119 | CLA | CAA-C2A | 2.64 | 1.59 | 1.54 |
| 14 | K | 1401 | CLA | CHC-C1C | 2.64 | 1.43 | 1.35 |
| 14 | B | 1213 | CLA | C5-C3 | 2.65 | 1.57 | 1.51 |
| 17 | A | 4002 | BCR | C1-C6 | 2.65 | 1.57 | 1.53 |
| 14 | B | 1236 | CLA | CHC-C1C | 2.65 | 1.43 | 1.35 |
| 14 | B | 1211 | CLA | CHC-C1C | 2.66 | 1.43 | 1.35 |
| 17 | L | 4019 | BCR | C29-C30 | 2.67 | 1.60 | 1.54 |
| 14 | B | 1224 | CLA | CAA-C2A | 2.67 | 1.59 | 1.54 |
| 14 | B | 1232 | CLA | CAA-C2A | 2.67 | 1.59 | 1.54 |
| 14 | A | 1022 | CLA | CHC-C1C | 2.67 | 1.43 | 1.35 |
| 14 | B | 1209 | CLA | CHC-C1C | 2.68 | 1.43 | 1.35 |
| 14 | A | 1122 | CLA | CHC-C1C | 2.68 | 1.43 | 1.35 |
| 17 | M | 4021 | BCR | C30-C25 | 2.68 | 1.57 | 1.53 |
| 17 | J | 4012 | BCR | C2-C1 | 2.68 | 1.60 | 1.54 |
| 14 | A | 1801 | CLA | CAA-C2A | 2.69 | 1.59 | 1.54 |
| 14 | A | 1402 | CLA | CBD-CAD | 2.69 | 1.57 | 1.51 |
| 14 | B | 1213 | CLA | CAA-C2A | 2.69 | 1.59 | 1.54 |
| 18 | A | 5001 | LHG | O8-C23 | 2.70 | 1.41 | 1.33 |
| 17 | B | 4009 | BCR | C30-C25 | 2.70 | 1.57 | 1.53 |
| 14 | A | 1104 | CLA | CHC-C1C | 2.70 | 1.43 | 1.35 |
| 14 | A | 1115 | CLA | CHC-C1C | 2.71 | 1.43 | 1.35 |
| 17 | A | 4011 | BCR | C29-C30 | 2.72 | 1.60 | 1.54 |
| 17 | I | 4020 | BCR | C2-C1 | 2.72 | 1.60 | 1.54 |
| 19 | B | 5002 | LMG | O8-C28 | 2.72 | 1.41 | 1.33 |
| 14 | B | 1224 | CLA | OBD-CAD | 2.72 | 1.26 | 1.22 |
| 14 | A | 1137 | CLA | CAA-C2A | 2.73 | 1.59 | 1.54 |
| 14 | B | 1229 | CLA | CHC-C1C | 2.73 | 1.43 | 1.35 |
| 14 | A | 1134 | CLA | CHC-C1C | 2.73 | 1.43 | 1.35 |
| 14 | B | 1227 | CLA | CHC-C1C | 2.73 | 1.43 | 1.35 |
| 17 | B | 4005 | BCR | C26-C25 | 2.74 | 1.39 | 1.34 |
| 17 | B | 4004 | BCR | C29-C30 | 2.74 | 1.60 | 1.54 |
| 14 | J | 1303 | CLA | CHC-C1C | 2.74 | 1.43 | 1.35 |
| 14 | B | 1219 | CLA | CHC-C1C | 2.74 | 1.43 | 1.35 |
| 14 | B | 1217 | CLA | CHC-C1C | 2.74 | 1.43 | 1.35 |
| 14 | B | 1219 | CLA | CAA-C2A | 2.75 | 1.59 | 1.54 |
| 14 | A | 1125 | CLA | C5-C3 | 2.76 | 1.57 | 1.51 |
| 17 | B | 4006 | BCR | C29-C30 | 2.76 | 1.60 | 1.54 |
| 17 | J | 4012 | BCR | C30-C25 | 2.76 | 1.57 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 17 | B | 4006 | BCR | C30-C25 | 2.76 | 1.57 | 1.53 |
| 17 | J | 4015 | BCR | C29-C30 | 2.77 | 1.60 | 1.54 |
| 17 | B | 4006 | BCR | C1-C6 | 2.77 | 1.57 | 1.53 |
| 17 | A | 4001 | BCR | C29-C30 | 2.78 | 1.60 | 1.54 |
| 17 | B | 4010 | BCR | C2-C1 | 2.78 | 1.60 | 1.54 |
| 14 | A | 1103 | CLA | CHC-C1C | 2.78 | 1.43 | 1.35 |
| 14 | A | 1105 | CLA | CHC-C1C | 2.78 | 1.43 | 1.35 |
| 17 | B | 4017 | BCR | C30-C25 | 2.79 | 1.57 | 1.53 |
| 17 | B | 4006 | BCR | C2-C1 | 2.80 | 1.60 | 1.54 |
| 14 | A | 1116 | CLA | CAA-C2A | 2.80 | 1.59 | 1.54 |
| 14 | B | 1214 | CLA | CHC-C1C | 2.80 | 1.43 | 1.35 |
| 17 | F | 4016 | BCR | C29-C30 | 2.81 | 1.60 | 1.54 |
| 14 | A | 1116 | CLA | CHC-C1C | 2.81 | 1.43 | 1.35 |
| 17 | B | 4017 | BCR | C29-C30 | 2.81 | 1.60 | 1.54 |
| 17 | B | 4009 | BCR | C29-C30 | 2.81 | 1.60 | 1.54 |
| 14 | M | 1601 | CLA | CHC-C1C | 2.81 | 1.43 | 1.35 |
| 17 | B | 4005 | BCR | C2-C1 | 2.82 | 1.60 | 1.54 |
| 18 | A | 5003 | LHG | O8-C23 | 2.83 | 1.41 | 1.33 |
| 14 | B | 1228 | CLA | CHC-C1C | 2.84 | 1.43 | 1.35 |
| 17 | M | 4021 | BCR | C29-C30 | 2.85 | 1.61 | 1.54 |
| 14 | A | 1140 | CLA | CHC-C1C | 2.85 | 1.43 | 1.35 |
| 14 | B | 1201 | CLA | CHC-C1C | 2.86 | 1.43 | 1.35 |
| 14 | B | 1223 | CLA | CHC-C1C | 2.86 | 1.43 | 1.35 |
| 17 | J | 4012 | BCR | C1-C6 | 2.86 | 1.57 | 1.53 |
| 17 | M | 4021 | BCR | C2-C1 | 2.86 | 1.61 | 1.54 |
| 14 | A | 1106 | CLA | CAA-C2A | 2.88 | 1.59 | 1.54 |
| 14 | A | 1136 | CLA | CHC-C1C | 2.89 | 1.43 | 1.35 |
| 17 | A | 4002 | BCR | C29-C30 | 2.89 | 1.61 | 1.54 |
| 17 | B | 4014 | BCR | C29-C30 | 2.89 | 1.61 | 1.54 |
| 14 | A | 1137 | CLA | CHC-C1C | 2.89 | 1.43 | 1.35 |
| 17 | A | 4003 | BCR | C2-C1 | 2.89 | 1.61 | 1.54 |
| 14 | A | 1102 | CLA | CHC-C1C | 2.90 | 1.43 | 1.35 |
| 17 | B | 4005 | BCR | C30-C25 | 2.91 | 1.57 | 1.53 |
| 14 | F | 1301 | CLA | CHC-C1C | 2.91 | 1.43 | 1.35 |
| 14 | J | 1302 | CLA | CHC-C1C | 2.94 | 1.44 | 1.35 |
| 14 | B | 1012 | CLA | CHC-C1C | 2.95 | 1.44 | 1.35 |
| 14 | L | 1503 | CLA | CHC-C1C | 2.95 | 1.44 | 1.35 |
| 17 | A | 4011 | BCR | C2-C1 | 2.95 | 1.61 | 1.54 |
| 15 | A | 2001 | PQN | C6-C5 | 2.96 | 1.44 | 1.39 |
| 17 | A | 4002 | BCR | C2-C1 | 2.96 | 1.61 | 1.54 |
| 14 | A | 1129 | CLA | CHC-C1C | 2.97 | 1.44 | 1.35 |
| 17 | J | 4015 | BCR | C2-C1 | 2.98 | 1.61 | 1.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 14 | B | 1234 | CLA | CHC-C1C | 2.99 | 1.44 | 1.35 |
| 17 | B | 4017 | BCR | C2-C1 | 3.00 | 1.61 | 1.54 |
| 14 | A | 1120 | CLA | CHC-C1C | 3.00 | 1.44 | 1.35 |
| 14 | A | 1123 | CLA | CHC-C1C | 3.00 | 1.44 | 1.35 |
| 17 | F | 4016 | BCR | C30-C25 | 3.01 | 1.58 | 1.53 |
| 14 | B | 1225 | CLA | C2-C3 | 3.01 | 1.40 | 1.32 |
| 17 | J | 4012 | BCR | C29-C30 | 3.01 | 1.61 | 1.54 |
| 17 | A | 4007 | BCR | C29-C30 | 3.01 | 1.61 | 1.54 |
| 15 | B | 2002 | PQN | C6-C5 | 3.02 | 1.44 | 1.39 |
| 14 | A | 1119 | CLA | CHC-C1C | 3.02 | 1.44 | 1.35 |
| 14 | B | 1232 | CLA | CHC-C1C | 3.02 | 1.44 | 1.35 |
| 14 | A | 1118 | CLA | CHC-C1C | 3.04 | 1.44 | 1.35 |
| 14 | B | 1212 | CLA | CHC-C1C | 3.04 | 1.44 | 1.35 |
| 14 | B | 1220 | CLA | CHC-C1C | 3.06 | 1.44 | 1.35 |
| 14 | A | 1112 | CLA | CHC-C1C | 3.07 | 1.44 | 1.35 |
| 14 | X | 1701 | CLA | CHC-C1C | 3.08 | 1.44 | 1.35 |
| 17 | B | 4010 | BCR | C30-C25 | 3.08 | 1.58 | 1.53 |
| 17 | J | 4013 | BCR | C30-C25 | 3.09 | 1.58 | 1.53 |
| 17 | B | 4004 | BCR | C2-C1 | 3.09 | 1.61 | 1.54 |
| 14 | A | 1125 | CLA | CHC-C1C | 3.10 | 1.44 | 1.35 |
| 14 | B | 1231 | CLA | CHC-C1C | 3.10 | 1.44 | 1.35 |
| 17 | B | 4004 | BCR | C26-C25 | 3.11 | 1.40 | 1.34 |
| 14 | A | 1106 | CLA | CHC-C1C | 3.12 | 1.44 | 1.35 |
| 14 | A | 1801 | CLA | CHC-C1C | 3.12 | 1.44 | 1.35 |
| 14 | B | 1221 | CLA | CHC-C1C | 3.13 | 1.44 | 1.35 |
| 14 | L | 1502 | CLA | CHC-C1C | 3.13 | 1.44 | 1.35 |
| 14 | B | 1224 | CLA | CHC-C1C | 3.13 | 1.44 | 1.35 |
| 14 | A | 1138 | CLA | CHC-C1C | 3.14 | 1.44 | 1.35 |
| 15 | B | 2002 | PQN | C11-C12 | 3.15 | 1.55 | 1.50 |
| 14 | A | 1128 | CLA | CHC-C1C | 3.16 | 1.44 | 1.35 |
| 17 | A | 4008 | BCR | C1-C6 | 3.18 | 1.58 | 1.53 |
| 17 | J | 4015 | BCR | C1-C6 | 3.18 | 1.58 | 1.53 |
| 17 | I | 4020 | BCR | C30-C25 | 3.18 | 1.58 | 1.53 |
| 17 | A | 4011 | BCR | C1-C6 | 3.21 | 1.58 | 1.53 |
| 14 | B | 1218 | CLA | CHC-C1C | 3.22 | 1.44 | 1.35 |
| 17 | L | 4022 | BCR | C2-C1 | 3.22 | 1.61 | 1.54 |
| 17 | B | 4004 | BCR | C1-C6 | 3.23 | 1.58 | 1.53 |
| 14 | B | 1023 | CLA | CHC-C1C | 3.26 | 1.44 | 1.35 |
| 17 | M | 4021 | BCR | C1-C6 | 3.30 | 1.58 | 1.53 |
| 14 | L | 1501 | CLA | CHC-C1C | 3.33 | 1.45 | 1.35 |
| 17 | A | 4002 | BCR | C30-C25 | 3.36 | 1.58 | 1.53 |
| 17 | F | 4016 | BCR | C2-C1 | 3.38 | 1.62 | 1.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 14 | B | 1235 | CLA | CHC-C1C | 3.40 | 1.45 | 1.35 |
| 17 | A | 4011 | BCR | C30-C25 | 3.41 | 1.58 | 1.53 |
| 17 | A | 4001 | BCR | C1-C6 | 3.44 | 1.58 | 1.53 |
| 18 | B | 5004 | LHG | O7-C7 | 3.45 | 1.44 | 1.34 |
| 17 | J | 4013 | BCR | C2-C1 | 3.47 | 1.62 | 1.54 |
| 15 | A | 2001 | PQN | C10-C5 | 3.48 | 1.46 | 1.40 |
| 17 | A | 4001 | BCR | C30-C25 | 3.51 | 1.58 | 1.53 |
| 17 | J | 4015 | BCR | C30-C25 | 3.55 | 1.58 | 1.53 |
| 17 | A | 4003 | BCR | C30-C25 | 3.58 | 1.58 | 1.53 |
| 17 | J | 4013 | BCR | C29-C30 | 3.60 | 1.62 | 1.54 |
| 17 | A | 4003 | BCR | C1-C6 | 3.62 | 1.58 | 1.53 |
| 18 | A | 5003 | LHG | O7-C7 | 3.65 | 1.45 | 1.34 |
| 14 | B | 1205 | CLA | CHB-C4A | 3.95 | 1.38 | 1.33 |
| 18 | A | 5001 | LHG | P-O6 | 3.95 | 1.76 | 1.59 |
| 15 | B | 2002 | PQN | C10-C5 | 3.99 | 1.46 | 1.40 |
| 14 | B | 1023 | CLA | CHB-C4A | 4.13 | 1.39 | 1.33 |
| 14 | L | 1502 | CLA | CHB-C4A | 4.23 | 1.39 | 1.33 |
| 18 | A | 5003 | LHG | P-O3 | 4.27 | 1.77 | 1.59 |
| 14 | A | 1126 | CLA | CHB-C4A | 4.34 | 1.39 | 1.33 |
| 17 | A | 4007 | BCR | C30-C25 | 4.39 | 1.59 | 1.53 |
| 14 | B | 1221 | CLA | CHB-C4A | 4.42 | 1.39 | 1.33 |
| 17 | L | 4022 | BCR | C30-C25 | 4.50 | 1.60 | 1.53 |
| 14 | A | 1132 | CLA | CHB-C4A | 4.55 | 1.39 | 1.33 |
| 17 | B | 4004 | BCR | C30-C25 | 4.63 | 1.60 | 1.53 |
| 17 | L | 4019 | BCR | C30-C25 | 4.67 | 1.60 | 1.53 |
| 14 | B | 1228 | CLA | CHB-C4A | 4.68 | 1.39 | 1.33 |
| 14 | A | 1136 | CLA | CHB-C4A | 4.69 | 1.39 | 1.33 |
| 14 | B | 1210 | CLA | CHB-C4A | 4.70 | 1.39 | 1.33 |
| 18 | A | 5003 | LHG | P-O6 | 4.72 | 1.79 | 1.59 |
| 17 | B | 4005 | BCR | C1-C6 | 4.73 | 1.60 | 1.53 |
| 14 | A | 1022 | CLA | CHB-C4A | 4.77 | 1.39 | 1.33 |
| 14 | A | 1117 | CLA | CHB-C4A | 4.82 | 1.40 | 1.33 |
| 14 | B | 1229 | CLA | CHB-C4A | 4.83 | 1.40 | 1.33 |
| 14 | B | 1232 | CLA | CHB-C4A | 4.86 | 1.40 | 1.33 |
| 17 | L | 4022 | BCR | C1-C6 | 4.88 | 1.60 | 1.53 |
| 15 | B | 2002 | PQN | C3-C2 | 4.92 | 1.46 | 1.35 |
| 14 | B | 1208 | CLA | CHB-C4A | 4.93 | 1.40 | 1.33 |
| 14 | B | 1236 | CLA | CHB-C4A | 4.95 | 1.40 | 1.33 |
| 15 | A | 2001 | PQN | C3-C2 | 4.96 | 1.46 | 1.35 |
| 14 | A | 1112 | CLA | CHB-C4A | 4.96 | 1.40 | 1.33 |
| 14 | B | 1214 | CLA | CHB-C4A | 4.97 | 1.40 | 1.33 |
| 18 | A | 5001 | LHG | P-O3 | 4.99 | 1.80 | 1.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 14 | A | 1119 | CLA | CHB-C4A | 5.03 | 1.40 | 1.33 |
| 14 | A | 1129 | CLA | CHB-C4A | 5.05 | 1.40 | 1.33 |
| 18 | B | 5004 | LHG | P-O3 | 5.07 | 1.80 | 1.59 |
| 14 | A | 1138 | CLA | CHB-C4A | 5.08 | 1.40 | 1.33 |
| 14 | A | 1128 | CLA | CHB-C4A | 5.08 | 1.40 | 1.33 |
| 14 | A | 1115 | CLA | CHB-C4A | 5.09 | 1.40 | 1.33 |
| 14 | B | 1212 | CLA | CHB-C4A | 5.10 | 1.40 | 1.33 |
| 14 | B | 1238 | CLA | CHB-C4A | 5.12 | 1.40 | 1.33 |
| 14 | A | 1801 | CLA | CHB-C4A | 5.12 | 1.40 | 1.33 |
| 14 | A | 1101 | CLA | CHB-C4A | 5.26 | 1.40 | 1.33 |
| 14 | B | 1216 | CLA | CHB-C4A | 5.29 | 1.40 | 1.33 |
| 14 | A | 1114 | CLA | CHB-C4A | 5.34 | 1.40 | 1.33 |
| 14 | L | 1503 | CLA | CHB-C4A | 5.34 | 1.40 | 1.33 |
| 14 | B | 1201 | CLA | CHB-C4A | 5.37 | 1.40 | 1.33 |
| 14 | A | 1124 | CLA | CHB-C4A | 5.38 | 1.40 | 1.33 |
| 14 | A | 1237 | CLA | CHB-C4A | 5.39 | 1.40 | 1.33 |
| 14 | B | 1224 | CLA | CHB-C4A | 5.40 | 1.40 | 1.33 |
| 14 | B | 1213 | CLA | CHB-C4A | 5.43 | 1.40 | 1.33 |
| 14 | A | 1109 | CLA | CHB-C4A | 5.44 | 1.40 | 1.33 |
| 14 | B | 1206 | CLA | CHB-C4A | 5.47 | 1.40 | 1.33 |
| 14 | A | 1106 | CLA | CHB-C4A | 5.48 | 1.40 | 1.33 |
| 14 | B | 1203 | CLA | CHB-C4A | 5.49 | 1.40 | 1.33 |
| 14 | A | 1013 | CLA | CHB-C4A | 5.51 | 1.40 | 1.33 |
| 14 | A | 1108 | CLA | CHB-C4A | 5.51 | 1.40 | 1.33 |
| 14 | B | 1211 | CLA | CHB-C4A | 5.52 | 1.40 | 1.33 |
| 14 | A | 1102 | CLA | CHB-C4A | 5.53 | 1.40 | 1.33 |
| 14 | K | 1401 | CLA | CHB-C4A | 5.57 | 1.41 | 1.33 |
| 14 | B | 1215 | CLA | CHB-C4A | 5.57 | 1.41 | 1.33 |
| 14 | A | 1111 | CLA | CHB-C4A | 5.57 | 1.41 | 1.33 |
| 14 | B | 1220 | CLA | CHB-C4A | 5.59 | 1.41 | 1.33 |
| 14 | A | 1140 | CLA | CHB-C4A | 5.63 | 1.41 | 1.33 |
| 14 | A | 1131 | CLA | CHB-C4A | 5.63 | 1.41 | 1.33 |
| 18 | B | 5004 | LHG | P-O6 | 5.63 | 1.83 | 1.59 |
| 14 | B | 1235 | CLA | CHB-C4A | 5.63 | 1.41 | 1.33 |
| 14 | B | 1227 | CLA | CHB-C4A | 5.63 | 1.41 | 1.33 |
| 14 | B | 1225 | CLA | CHB-C4A | 5.64 | 1.41 | 1.33 |
| 14 | A | 1121 | CLA | CHB-C4A | 5.64 | 1.41 | 1.33 |
| 14 | A | 1107 | CLA | CHB-C4A | 5.65 | 1.41 | 1.33 |
| 14 | A | 1122 | CLA | CHB-C4A | 5.67 | 1.41 | 1.33 |
| 14 | A | 1116 | CLA | CHB-C4A | 5.67 | 1.41 | 1.33 |
| 14 | A | 1123 | CLA | CHB-C4A | 5.71 | 1.41 | 1.33 |
| 14 | B | 1012 | CLA | CHB-C4A | 5.75 | 1.41 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 14 | L | 1501 | CLA | CHB-C4A | 5.77 | 1.41 | 1.33 |
| 14 | B | 1222 | CLA | CHB-C4A | 5.77 | 1.41 | 1.33 |
| 14 | A | 1120 | CLA | CHB-C4A | 5.80 | 1.41 | 1.33 |
| 14 | A | 1104 | CLA | CHB-C4A | 5.81 | 1.41 | 1.33 |
| 14 | B | 1218 | CLA | CHB-C4A | 5.91 | 1.41 | 1.33 |
| 14 | B | 1202 | CLA | CHB-C4A | 5.96 | 1.41 | 1.33 |
| 14 | A | 1103 | CLA | CHB-C4A | 5.99 | 1.41 | 1.33 |
| 14 | A | 1110 | CLA | CHB-C4A | 6.02 | 1.41 | 1.33 |
| 14 | A | 1137 | CLA | CHB-C4A | 6.07 | 1.41 | 1.33 |
| 14 | F | 1301 | CLA | CHB-C4A | 6.07 | 1.41 | 1.33 |
| 14 | B | 1239 | CLA | CHB-C4A | 6.11 | 1.41 | 1.33 |
| 14 | B | 1204 | CLA | CHB-C4A | 6.11 | 1.41 | 1.33 |
| 14 | A | 1133 | CLA | CHB-C4A | 6.17 | 1.41 | 1.33 |
| 14 | B | 1219 | CLA | CHB-C4A | 6.18 | 1.41 | 1.33 |
| 14 | A | 1011 | CLA | CHB-C4A | 6.18 | 1.41 | 1.33 |
| 14 | B | 1021 | CLA | CHB-C4A | 6.20 | 1.41 | 1.33 |
| 14 | A | 1105 | CLA | CHB-C4A | 6.20 | 1.41 | 1.33 |
| 14 | A | 1118 | CLA | CHB-C4A | 6.22 | 1.41 | 1.33 |
| 14 | B | 1231 | CLA | CHB-C4A | 6.22 | 1.41 | 1.33 |
| 14 | A | 1125 | CLA | CHB-C4A | 6.23 | 1.41 | 1.33 |
| 14 | B | 1207 | CLA | CHB-C4A | 6.24 | 1.41 | 1.33 |
| 14 | B | 1234 | CLA | CHB-C4A | 6.32 | 1.42 | 1.33 |
| 14 | B | 1226 | CLA | CHB-C4A | 6.38 | 1.42 | 1.33 |
| 14 | A | 1134 | CLA | CHB-C4A | 6.38 | 1.42 | 1.33 |
| 14 | A | 1402 | CLA | CHB-C4A | 6.42 | 1.42 | 1.33 |
| 14 | A | 1130 | CLA | CHB-C4A | 6.57 | 1.42 | 1.33 |
| 14 | M | 1601 | CLA | CHB-C4A | 6.61 | 1.42 | 1.33 |
| 14 | J | 1302 | CLA | CHB-C4A | 6.63 | 1.42 | 1.33 |
| 14 | B | 1217 | CLA | CHB-C4A | 6.67 | 1.42 | 1.33 |
| 14 | B | 1233 | CLA | CHB-C4A | 6.68 | 1.42 | 1.33 |
| 14 | A | 1127 | CLA | CHB-C4A | 6.74 | 1.42 | 1.33 |
| 14 | A | 1113 | CLA | CHB-C4A | 6.74 | 1.42 | 1.33 |
| 14 | X | 1701 | CLA | CHB-C4A | 6.84 | 1.42 | 1.33 |
| 14 | J | 1303 | CLA | CHB-C4A | 6.90 | 1.42 | 1.33 |
| 14 | A | 1139 | CLA | CHB-C4A | 6.92 | 1.42 | 1.33 |
| 14 | B | 1230 | CLA | CHB-C4A | 6.93 | 1.42 | 1.33 |
| 14 | B | 1209 | CLA | CHB-C4A | 6.97 | 1.42 | 1.33 |
| 14 | B | 1223 | CLA | CHB-C4A | 6.99 | 1.42 | 1.33 |
| 14 | A | 1135 | CLA | CHB-C4A | 7.31 | 1.43 | 1.33 |
| 18 | A | 5003 | LHG | P-O5 | 7.34 | 1.78 | 1.51 |
| 15 | B | 2002 | PQN | C12-C13 | 7.77 | 1.52 | 1.32 |
| 15 | A | 2001 | PQN | C12-C13 | 7.77 | 1.52 | 1.32 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 18 | A | 5001 | LHG | P-O5 | 7.84 | 1.79 | 1.51 |
| 15 | B | 2002 | PQN | O1-C1 | 8.14 | 1.41 | 1.23 |
| 18 | B | 5004 | LHG | P-O5 | 8.25 | 1.81 | 1.51 |
| 15 | A | 2001 | PQN | O1-C1 | 8.63 | 1.42 | 1.23 |
| 15 | B | 2002 | PQN | O4-C4 | 8.66 | 1.42 | 1.23 |
| 15 | A | 2001 | PQN | O4-C4 | 8.97 | 1.42 | 1.23 |

All (1366) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 15 | B | 2002 | PQN | C11-C12-C13 | -7.97 | 113.14 | 126.70 |
| 15 | A | 2001 | PQN | C11-C12-C13 | -7.85 | 113.34 | 126.70 |
| 15 | A | 2001 | PQN | C15-C13-C12 | -7.82 | 106.41 | 120.98 |
| 14 | A | 1011 | CLA | O1D-CGD-CBD | -7.07 | 113.64 | 124.64 |
| 15 | B | 2002 | PQN | C15-C13-C12 | -6.64 | 108.62 | 120.98 |
| 14 | A | 1011 | CLA | C3D-CAD-CBD | -6.23 | 98.79 | 107.60 |
| 14 | A | 1104 | CLA | CAA-C2A-C3A | -4.77 | 99.84 | 112.79 |
| 14 | B | 1205 | CLA | O1D-CGD-CBD | -4.14 | 118.20 | 124.64 |
| 14 | A | 1119 | CLA | CMB-C2B-C1B | -3.95 | 121.58 | 128.31 |
| 14 | A | 1117 | CLA | CMB-C2B-C1B | -3.90 | 121.67 | 128.31 |
| 17 | A | 4008 | BCR | C38-C26-C27 | -3.89 | 105.95 | 113.47 |
| 14 | B | 1215 | CLA | CMB-C2B-C1B | -3.88 | 121.70 | 128.31 |
| 17 | B | 4004 | BCR | C38-C26-C27 | -3.79 | 106.14 | 113.47 |
| 17 | B | 4005 | BCR | C30-C25-C26 | -3.74 | 117.49 | 122.50 |
| 14 | B | 1210 | CLA | O1D-CGD-CBD | -3.68 | 118.91 | 124.64 |
| 14 | B | 1012 | CLA | OBD-CAD-CBD | -3.61 | 120.48 | 125.94 |
| 14 | A | 1022 | CLA | OBD-CAD-CBD | -3.60 | 120.50 | 125.94 |
| 14 | A | 1801 | CLA | O1D-CGD-CBD | -3.60 | 119.04 | 124.64 |
| 14 | B | 1230 | CLA | O1D-CGD-CBD | -3.60 | 119.04 | 124.64 |
| 14 | A | 1102 | CLA | O1D-CGD-CBD | -3.58 | 119.06 | 124.64 |
| 14 | B | 1226 | CLA | CMB-C2B-C1B | -3.57 | 122.23 | 128.31 |
| 14 | A | 1123 | CLA | O1D-CGD-CBD | -3.55 | 119.11 | 124.64 |
| 14 | A | 1111 | CLA | O1D-CGD-CBD | -3.55 | 119.11 | 124.64 |
| 14 | A | 1127 | CLA | CMB-C2B-C1B | -3.55 | 122.27 | 128.31 |
| 17 | B | 4014 | BCR | C33-C5-C4 | -3.55 | 106.61 | 113.47 |
| 14 | B | 1211 | CLA | O1D-CGD-CBD | -3.54 | 119.13 | 124.64 |
| 14 | B | 1227 | CLA | O1D-CGD-CBD | -3.54 | 119.13 | 124.64 |
| 17 | B | 4005 | BCR | C38-C26-C27 | -3.54 | 106.64 | 113.47 |
| 14 | A | 1106 | CLA | O1D-CGD-CBD | -3.50 | 119.19 | 124.64 |
| 14 | A | 1129 | CLA | O1D-CGD-CBD | -3.49 | 119.21 | 124.64 |
| 17 | A | 4003 | BCR | C38-C26-C27 | -3.48 | 106.74 | 113.47 |
| 14 | B | 1212 | CLA | O1D-CGD-CBD | -3.48 | 119.23 | 124.64 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | A | 4001 | BCR | C38-C26-C27 | -3.45 | 106.80 | 113.47 |
| 17 | J | 4012 | BCR | C38-C26-C27 | -3.44 | 106.81 | 113.47 |
| 14 | B | 1218 | CLA | O1D-CGD-CBD | -3.42 | 119.31 | 124.64 |
| 17 | B | 4006 | BCR | C38-C26-C27 | -3.42 | 106.86 | 113.47 |
| 14 | A | 1129 | CLA | C2C-C1C-NC | -3.41 | 107.88 | 110.22 |
| 14 | A | 1125 | CLA | O1D-CGD-CBD | -3.39 | 119.37 | 124.64 |
| 14 | J | 1303 | CLA | CAA-C2A-C3A | -3.38 | 109.01 | 116.22 |
| 14 | L | 1501 | CLA | O1D-CGD-CBD | -3.37 | 119.39 | 124.64 |
| 14 | B | 1202 | CLA | OBD-CAD-CBD | -3.35 | 120.88 | 125.94 |
| 14 | B | 1239 | CLA | OBD-CAD-CBD | -3.35 | 120.89 | 125.94 |
| 17 | I | 4020 | BCR | C33-C5-C4 | -3.35 | 107.00 | 113.47 |
| 17 | I | 4020 | BCR | C38-C26-C27 | -3.34 | 107.01 | 113.47 |
| 17 | A | 4002 | BCR | C38-C26-C27 | -3.34 | 107.02 | 113.47 |
| 14 | B | 1204 | CLA | OBD-CAD-CBD | -3.33 | 120.91 | 125.94 |
| 14 | B | 1226 | CLA | O1D-CGD-CBD | -3.32 | 119.47 | 124.64 |
| 14 | A | 1132 | CLA | O1D-CGD-CBD | -3.31 | 119.49 | 124.64 |
| 14 | A | 1113 | CLA | O1D-CGD-CBD | -3.31 | 119.50 | 124.64 |
| 17 | B | 4004 | BCR | C30-C25-C26 | -3.30 | 118.08 | 122.50 |
| 17 | L | 4019 | BCR | C33-C5-C4 | -3.30 | 107.09 | 113.47 |
| 14 | B | 1223 | CLA | CMB-C2B-C1B | -3.29 | 122.72 | 128.31 |
| 14 | B | 1201 | CLA | O1D-CGD-CBD | -3.28 | 119.53 | 124.64 |
| 14 | A | 1132 | CLA | C3B-CAB-CBB | -3.28 | 119.79 | 126.40 |
| 17 | B | 4010 | BCR | C33-C5-C4 | -3.27 | 107.16 | 113.47 |
| 17 | B | 4006 | BCR | C33-C5-C4 | -3.26 | 107.17 | 113.47 |
| 14 | A | 1103 | CLA | O1D-CGD-CBD | -3.25 | 119.58 | 124.64 |
| 14 | B | 1222 | CLA | O1D-CGD-CBD | -3.25 | 119.58 | 124.64 |
| 17 | J | 4015 | BCR | C33-C5-C4 | -3.25 | 107.19 | 113.47 |
| 14 | A | 1104 | CLA | CMB-C2B-C1B | -3.24 | 122.80 | 128.31 |
| 17 | A | 4001 | BCR | C30-C25-C26 | -3.23 | 118.17 | 122.50 |
| 14 | B | 1217 | CLA | O1D-CGD-CBD | -3.22 | 119.62 | 124.64 |
| 17 | B | 4009 | BCR | C38-C26-C27 | -3.22 | 107.24 | 113.47 |
| 14 | B | 1225 | CLA | C4-C3-C5 | -3.22 | 110.47 | 115.37 |
| 17 | I | 4018 | BCR | C38-C26-C27 | -3.22 | 107.25 | 113.47 |
| 17 | J | 4015 | BCR | C38-C26-C27 | -3.21 | 107.26 | 113.47 |
| 17 | J | 4012 | BCR | C30-C25-C26 | -3.19 | 118.23 | 122.50 |
| 17 | B | 4014 | BCR | C38-C26-C27 | -3.18 | 107.33 | 113.47 |
| 17 | A | 4008 | BCR | C30-C25-C26 | -3.16 | 118.27 | 122.50 |
| 14 | B | 1234 | CLA | O1D-CGD-CBD | -3.16 | 119.73 | 124.64 |
| 17 | B | 4004 | BCR | C33-C5-C4 | -3.14 | 107.40 | 113.47 |
| 14 | A | 1801 | CLA | C2C-C1C-NC | -3.14 | 108.07 | 110.22 |
| 17 | L | 4022 | BCR | C33-C5-C4 | -3.14 | 107.41 | 113.47 |
| 17 | A | 4007 | BCR | C38-C26-C27 | -3.12 | 107.44 | 113.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | B | 1206 | CLA | CMB-C2B-C1B | -3.12 | 123.01 | 128.31 |
| 14 | B | 1232 | CLA | CMB-C2B-C1B | -3.11 | 123.02 | 128.31 |
| 17 | F | 4016 | BCR | C33-C5-C4 | -3.10 | 107.47 | 113.47 |
| 17 | J | 4015 | BCR | C1-C6-C5 | -3.10 | 118.35 | 122.50 |
| 14 | B | 1214 | CLA | OBD-CAD-CBD | -3.09 | 121.27 | 125.94 |
| 17 | L | 4019 | BCR | C38-C26-C27 | -3.09 | 107.50 | 113.47 |
| 17 | F | 4016 | BCR | C38-C26-C27 | -3.08 | 107.51 | 113.47 |
| 14 | A | 1120 | CLA | O1D-CGD-CBD | -3.07 | 119.86 | 124.64 |
| 14 | B | 1210 | CLA | CMB-C2B-C1B | -3.07 | 123.08 | 128.31 |
| 14 | A | 1124 | CLA | CMB-C2B-C1B | -3.06 | 123.10 | 128.31 |
| 17 | A | 4003 | BCR | C33-C5-C4 | -3.06 | 107.55 | 113.47 |
| 14 | B | 1224 | CLA | O1D-CGD-CBD | -3.06 | 119.88 | 124.64 |
| 17 | A | 4011 | BCR | C33-C5-C4 | -3.06 | 107.56 | 113.47 |
| 14 | A | 1237 | CLA | O2A-CGA-O1A | -3.05 | 115.50 | 123.51 |
| 17 | A | 4001 | BCR | C33-C5-C4 | -3.05 | 107.56 | 113.47 |
| 14 | A | 1103 | CLA | CAA-C2A-C3A | -3.04 | 104.53 | 112.79 |
| 14 | B | 1221 | CLA | O1D-CGD-CBD | -3.04 | 119.91 | 124.64 |
| 14 | A | 1118 | CLA | O1D-CGD-CBD | -3.03 | 119.92 | 124.64 |
| 17 | B | 4005 | BCR | C1-C6-C5 | -3.03 | 118.45 | 122.50 |
| 17 | B | 4004 | BCR | C1-C6-C5 | -3.02 | 118.46 | 122.50 |
| 14 | A | 1112 | CLA | O1D-CGD-CBD | -3.01 | 119.95 | 124.64 |
| 14 | B | 1224 | CLA | OBD-CAD-CBD | -3.01 | 121.40 | 125.94 |
| 17 | B | 4005 | BCR | C33-C5-C4 | -3.01 | 107.66 | 113.47 |
| 18 | A | 5003 | LHG | C6-C5-C4 | -3.00 | 105.09 | 112.08 |
| 14 | A | 1103 | CLA | OBD-CAD-CBD | -3.00 | 121.41 | 125.94 |
| 14 | L | 1501 | CLA | OBD-CAD-CBD | -2.99 | 121.42 | 125.94 |
| 14 | B | 1222 | CLA | CMB-C2B-C1B | -2.99 | 123.23 | 128.31 |
| 17 | A | 4007 | BCR | C30-C25-C26 | -2.99 | 118.50 | 122.50 |
| 14 | B | 1238 | CLA | C3B-CAB-CBB | -2.98 | 120.41 | 126.40 |
| 14 | B | 1235 | CLA | OBD-CAD-CBD | -2.97 | 121.46 | 125.94 |
| 17 | B | 4010 | BCR | C38-C26-C27 | -2.97 | 107.73 | 113.47 |
| 17 | M | 4021 | BCR | C38-C26-C27 | -2.97 | 107.73 | 113.47 |
| 14 | A | 1119 | CLA | OBD-CAD-CBD | -2.96 | 121.46 | 125.94 |
| 14 | B | 1205 | CLA | CAA-C2A-C3A | -2.96 | 104.75 | 112.79 |
| 14 | B | 1229 | CLA | OBD-CAD-CBD | -2.96 | 121.48 | 125.94 |
| 14 | A | 1013 | CLA | O2A-CGA-O1A | -2.96 | 115.76 | 123.51 |
| 14 | A | 1129 | CLA | OBD-CAD-CBD | -2.95 | 121.48 | 125.94 |
| 17 | B | 4017 | BCR | C38-C26-C27 | -2.94 | 107.78 | 113.47 |
| 14 | B | 1207 | CLA | O1D-CGD-CBD | -2.94 | 120.06 | 124.64 |
| 14 | B | 1223 | CLA | O1D-CGD-CBD | -2.94 | 120.06 | 124.64 |
| 17 | A | 4002 | BCR | C33-C5-C4 | -2.94 | 107.78 | 113.47 |
| 14 | B | 1218 | CLA | C2C-C1C-NC | -2.94 | 108.21 | 110.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | M | 4021 | BCR | C1-C6-C5 | -2.93 | 118.58 | 122.50 |
| 14 | B | 1220 | CLA | OBD-CAD-CBD | -2.93 | 121.52 | 125.94 |
| 14 | A | 1113 | CLA | CMB-C2B-C1B | -2.93 | 123.33 | 128.31 |
| 17 | A | 4011 | BCR | C38-C26-C27 | -2.93 | 107.81 | 113.47 |
| 14 | B | 1202 | CLA | CMB-C2B-C1B | -2.92 | 123.34 | 128.31 |
| 14 | A | 1107 | CLA | CMB-C2B-C1B | -2.92 | 123.34 | 128.31 |
| 14 | A | 1112 | CLA | OBD-CAD-CBD | -2.92 | 121.53 | 125.94 |
| 17 | B | 4006 | BCR | C1-C6-C5 | -2.92 | 118.59 | 122.50 |
| 17 | B | 4006 | BCR | C30-C25-C26 | -2.91 | 118.60 | 122.50 |
| 14 | B | 1012 | CLA | O1D-CGD-CBD | -2.91 | 120.11 | 124.64 |
| 14 | L | 1503 | CLA | OBD-CAD-CBD | -2.91 | 121.55 | 125.94 |
| 14 | A | 1135 | CLA | O1D-CGD-CBD | -2.91 | 120.11 | 124.64 |
| 14 | A | 1106 | CLA | C2C-C1C-NC | -2.90 | 108.23 | 110.22 |
| 14 | A | 1116 | CLA | OBD-CAD-CBD | -2.89 | 121.57 | 125.94 |
| 14 | B | 1213 | CLA | OBD-CAD-CBD | -2.89 | 121.58 | 125.94 |
| 14 | B | 1219 | CLA | CMB-C2B-C1B | -2.89 | 123.40 | 128.31 |
| 14 | B | 1238 | CLA | OBD-CAD-CBD | -2.89 | 121.58 | 125.94 |
| 14 | B | 1221 | CLA | OBD-CAD-CBD | -2.88 | 121.59 | 125.94 |
| 14 | A | 1126 | CLA | OBD-CAD-CBD | -2.88 | 121.59 | 125.94 |
| 14 | J | 1302 | CLA | O1D-CGD-CBD | -2.88 | 120.16 | 124.64 |
| 17 | J | 4013 | BCR | C33-C5-C4 | -2.86 | 107.94 | 113.47 |
| 14 | B | 1023 | CLA | OBD-CAD-CBD | -2.85 | 121.63 | 125.94 |
| 17 | A | 4001 | BCR | C1-C6-C5 | -2.85 | 118.69 | 122.50 |
| 14 | B | 1235 | CLA | O1D-CGD-CBD | -2.85 | 120.20 | 124.64 |
| 14 | A | 1135 | CLA | O2A-CGA-O1A | -2.85 | 116.04 | 123.51 |
| 17 | A | 4002 | BCR | C30-C25-C26 | -2.85 | 118.69 | 122.50 |
| 17 | B | 4014 | BCR | C8-C9-C10 | -2.85 | 114.36 | 118.95 |
| 14 | A | 1108 | CLA | OBD-CAD-CBD | -2.84 | 121.65 | 125.94 |
| 14 | B | 1231 | CLA | OBD-CAD-CBD | -2.84 | 121.65 | 125.94 |
| 14 | A | 1118 | CLA | OBD-CAD-CBD | -2.84 | 121.65 | 125.94 |
| 14 | A | 1103 | CLA | CMB-C2B-C1B | -2.84 | 123.48 | 128.31 |
| 14 | B | 1215 | CLA | OBD-CAD-CBD | -2.84 | 121.65 | 125.94 |
| 14 | B | 1232 | CLA | OBD-CAD-CBD | -2.83 | 121.67 | 125.94 |
| 14 | B | 1021 | CLA | OBD-CAD-CBD | -2.83 | 121.67 | 125.94 |
| 14 | B | 1211 | CLA | OBD-CAD-CBD | -2.83 | 121.67 | 125.94 |
| 17 | A | 4007 | BCR | C33-C5-C4 | -2.82 | 108.02 | 113.47 |
| 14 | A | 1126 | CLA | CMB-C2B-C1B | -2.82 | 123.52 | 128.31 |
| 17 | A | 4003 | BCR | C1-C6-C5 | -2.81 | 118.74 | 122.50 |
| 17 | B | 4017 | BCR | C33-C5-C4 | -2.81 | 108.03 | 113.47 |
| 17 | I | 4020 | BCR | C30-C25-C26 | -2.81 | 118.74 | 122.50 |
| 17 | J | 4015 | BCR | C30-C25-C26 | -2.81 | 118.75 | 122.50 |
| 14 | A | 1136 | CLA | OBD-CAD-CBD | -2.80 | 121.71 | 125.94 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | A | 1119 | CLA | CAA-C2A-C3A | -2.79 | 105.20 | 112.79 |
| 14 | A | 1131 | CLA | CMB-C2B-C1B | -2.79 | 123.56 | 128.31 |
| 14 | A | 1102 | CLA | CMB-C2B-C1B | -2.79 | 123.56 | 128.31 |
| 17 | J | 4012 | BCR | C33-C5-C4 | -2.79 | 108.07 | 113.47 |
| 14 | A | 1132 | CLA | OBD-CAD-CBD | -2.79 | 121.72 | 125.94 |
| 14 | L | 1502 | CLA | OBD-CAD-CBD | -2.79 | 121.73 | 125.94 |
| 14 | A | 1138 | CLA | C2C-C1C-NC | -2.79 | 108.31 | 110.22 |
| 14 | B | 1021 | CLA | C7-C6-C5 | -2.79 | 104.94 | 113.16 |
| 17 | L | 4019 | BCR | C30-C25-C26 | -2.78 | 118.78 | 122.50 |
| 14 | B | 1239 | CLA | C3B-CAB-CBB | -2.78 | 120.80 | 126.40 |
| 14 | A | 1114 | CLA | CMB-C2B-C1B | -2.78 | 123.58 | 128.31 |
| 14 | B | 1236 | CLA | OBD-CAD-CBD | -2.78 | 121.74 | 125.94 |
| 14 | A | 1013 | CLA | CMB-C2B-C1B | -2.77 | 123.61 | 128.31 |
| 14 | A | 1120 | CLA | C2C-C1C-NC | -2.77 | 108.32 | 110.22 |
| 14 | A | 1131 | CLA | O1D-CGD-CBD | -2.77 | 120.34 | 124.64 |
| 14 | A | 1137 | CLA | O2A-CGA-O1A | -2.76 | 116.26 | 123.51 |
| 14 | B | 1206 | CLA | OBD-CAD-CBD | -2.76 | 121.77 | 125.94 |
| 17 | B | 4014 | BCR | C12-C13-C14 | -2.76 | 114.50 | 118.95 |
| 17 | M | 4021 | BCR | C33-C5-C4 | -2.75 | 108.15 | 113.47 |
| 14 | A | 1106 | CLA | OBD-CAD-CBD | -2.74 | 121.80 | 125.94 |
| 14 | A | 1108 | CLA | CMB-C2B-C1B | -2.74 | 123.65 | 128.31 |
| 17 | I | 4018 | BCR | C33-C5-C4 | -2.73 | 108.18 | 113.47 |
| 14 | A | 1131 | CLA | OBD-CAD-CBD | -2.73 | 121.82 | 125.94 |
| 17 | F | 4016 | BCR | C1-C6-C5 | -2.73 | 118.85 | 122.50 |
| 14 | B | 1215 | CLA | O1D-CGD-CBD | -2.72 | 120.40 | 124.64 |
| 14 | B | 1236 | CLA | C3B-CAB-CBB | -2.72 | 120.92 | 126.40 |
| 17 | A | 4003 | BCR | C30-C25-C26 | -2.72 | 118.86 | 122.50 |
| 14 | J | 1302 | CLA | OBD-CAD-CBD | -2.72 | 121.83 | 125.94 |
| 17 | B | 4010 | BCR | C30-C25-C26 | -2.72 | 118.86 | 122.50 |
| 17 | L | 4022 | BCR | C38-C26-C27 | -2.72 | 108.21 | 113.47 |
| 14 | A | 1128 | CLA | O1D-CGD-CBD | -2.72 | 120.41 | 124.64 |
| 14 | B | 1208 | CLA | CAA-C2A-C3A | -2.72 | 105.41 | 112.79 |
| 14 | A | 1118 | CLA | C2C-C1C-NC | -2.72 | 108.36 | 110.22 |
| 14 | A | 1139 | CLA | O1D-CGD-CBD | -2.71 | 120.42 | 124.64 |
| 17 | L | 4022 | BCR | C30-C25-C26 | -2.71 | 118.88 | 122.50 |
| 14 | A | 1128 | CLA | OBD-CAD-CBD | -2.70 | 121.86 | 125.94 |
| 17 | B | 4014 | BCR | C30-C25-C26 | -2.70 | 118.88 | 122.50 |
| 14 | B | 1202 | CLA | O1D-CGD-CBD | -2.70 | 120.43 | 124.64 |
| 17 | J | 4013 | BCR | C38-C26-C27 | -2.70 | 108.25 | 113.47 |
| 14 | A | 1120 | CLA | OBD-CAD-CBD | -2.70 | 121.87 | 125.94 |
| 14 | A | 1111 | CLA | OBD-CAD-CBD | -2.69 | 121.88 | 125.94 |
| 17 | F | 4016 | BCR | C30-C25-C26 | -2.69 | 118.90 | 122.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | B | 1235 | CLA | C2C-C1C-NC | -2.69 | 108.38 | 110.22 |
| 14 | A | 1101 | CLA | OBD-CAD-CBD | -2.68 | 121.89 | 125.94 |
| 14 | B | 1205 | CLA | O2A-CGA-O1A | -2.68 | 116.48 | 123.51 |
| 14 | A | 1140 | CLA | CMB-C2B-C1B | -2.67 | 123.77 | 128.31 |
| 14 | A | 1237 | CLA | CAA-C2A-C3A | -2.67 | 105.53 | 112.79 |
| 14 | A | 1119 | CLA | C2C-C1C-NC | -2.67 | 108.39 | 110.22 |
| 14 | A | 1135 | CLA | CMB-C2B-C1B | -2.67 | 123.77 | 128.31 |
| 14 | A | 1022 | CLA | C6-C5-C3 | -2.67 | 107.97 | 112.76 |
| 14 | A | 1111 | CLA | CMB-C2B-C1B | -2.67 | 123.77 | 128.31 |
| 14 | A | 1137 | CLA | O1D-CGD-CBD | -2.67 | 120.49 | 124.64 |
| 14 | B | 1228 | CLA | C2C-C1C-NC | -2.66 | 108.39 | 110.22 |
| 14 | A | 1133 | CLA | O1D-CGD-CBD | -2.66 | 120.50 | 124.64 |
| 17 | J | 4012 | BCR | C1-C6-C5 | -2.66 | 118.94 | 122.50 |
| 14 | A | 1128 | CLA | C2C-C1C-NC | -2.66 | 108.40 | 110.22 |
| 14 | A | 1237 | CLA | OBD-CAD-CBD | -2.65 | 121.94 | 125.94 |
| 17 | J | 4013 | BCR | C30-C25-C26 | -2.65 | 118.96 | 122.50 |
| 14 | B | 1224 | CLA | CMB-C2B-C1B | -2.65 | 123.81 | 128.31 |
| 14 | A | 1117 | CLA | C4-C3-C5 | -2.65 | 111.34 | 115.37 |
| 14 | X | 1701 | CLA | OBD-CAD-CBD | -2.65 | 121.95 | 125.94 |
| 14 | A | 1114 | CLA | OBD-CAD-CBD | -2.64 | 121.95 | 125.94 |
| 14 | B | 1205 | CLA | OBD-CAD-CBD | -2.64 | 121.96 | 125.94 |
| 14 | M | 1601 | CLA | O1D-CGD-CBD | -2.64 | 120.53 | 124.64 |
| 14 | B | 1208 | CLA | OBD-CAD-CBD | -2.63 | 121.97 | 125.94 |
| 17 | A | 4011 | BCR | C30-C25-C26 | -2.63 | 118.98 | 122.50 |
| 14 | A | 1125 | CLA | C2C-C1C-NC | -2.63 | 108.42 | 110.22 |
| 14 | B | 1229 | CLA | CMB-C2B-C1B | -2.63 | 123.84 | 128.31 |
| 14 | A | 1116 | CLA | C2C-C1C-NC | -2.63 | 108.42 | 110.22 |
| 14 | A | 1130 | CLA | O1D-CGD-CBD | -2.63 | 120.55 | 124.64 |
| 14 | B | 1203 | CLA | CMB-C2B-C1B | -2.63 | 123.84 | 128.31 |
| 14 | B | 1218 | CLA | OBD-CAD-CBD | -2.63 | 121.97 | 125.94 |
| 14 | B | 1216 | CLA | CMB-C2B-C1B | -2.63 | 123.85 | 128.31 |
| 14 | A | 1123 | CLA | OBD-CAD-CBD | -2.62 | 121.98 | 125.94 |
| 14 | A | 1120 | CLA | CMB-C2B-C1B | -2.62 | 123.86 | 128.31 |
| 17 | L | 4022 | BCR | C1-C6-C5 | -2.62 | 119.00 | 122.50 |
| 14 | A | 1132 | CLA | CAA-C2A-C3A | -2.62 | 105.69 | 112.79 |
| 14 | B | 1218 | CLA | CMB-C2B-C1B | -2.62 | 123.86 | 128.31 |
| 17 | M | 4021 | BCR | C30-C25-C26 | -2.61 | 119.00 | 122.50 |
| 14 | A | 1115 | CLA | CMB-C2B-C1B | -2.61 | 123.87 | 128.31 |
| 14 | A | 1127 | CLA | O1D-CGD-CBD | -2.61 | 120.58 | 124.64 |
| 14 | B | 1214 | CLA | CMB-C2B-C1B | -2.60 | 123.89 | 128.31 |
| 14 | A | 1121 | CLA | O1D-CGD-CBD | -2.60 | 120.59 | 124.64 |
| 17 | J | 4013 | BCR | C1-C6-C5 | -2.60 | 119.02 | 122.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | B | 1230 | CLA | C2C-C1C-NC | -2.60 | 108.44 | 110.22 |
| 14 | B | 1216 | CLA | CAA-C2A-C3A | -2.59 | 105.75 | 112.79 |
| 14 | A | 1022 | CLA | C2C-C1C-NC | -2.59 | 108.44 | 110.22 |
| 17 | A | 4002 | BCR | C1-C6-C5 | -2.59 | 119.03 | 122.50 |
| 14 | A | 1121 | CLA | OBD-CAD-CBD | -2.59 | 122.03 | 125.94 |
| 14 | B | 1216 | CLA | OBD-CAD-CBD | -2.59 | 122.03 | 125.94 |
| 14 | L | 1502 | CLA | CAA-C2A-C3A | -2.59 | 105.76 | 112.79 |
| 14 | A | 1124 | CLA | OBD-CAD-CBD | -2.59 | 122.03 | 125.94 |
| 14 | M | 1601 | CLA | OBD-CAD-CBD | -2.59 | 122.03 | 125.94 |
| 14 | X | 1701 | CLA | C2C-C1C-NC | -2.59 | 108.45 | 110.22 |
| 14 | A | 1129 | CLA | CAA-C2A-C3A | -2.59 | 105.77 | 112.79 |
| 14 | A | 1134 | CLA | CMB-C2B-C1B | -2.58 | 123.92 | 128.31 |
| 14 | A | 1128 | CLA | CMB-C2B-C1B | -2.58 | 123.92 | 128.31 |
| 17 | I | 4018 | BCR | C1-C6-C5 | -2.58 | 119.05 | 122.50 |
| 14 | A | 1137 | CLA | OBD-CAD-CBD | -2.57 | 122.05 | 125.94 |
| 14 | B | 1201 | CLA | CMB-C2B-C1B | -2.57 | 123.93 | 128.31 |
| 14 | A | 1101 | CLA | CMB-C2B-C1B | -2.57 | 123.94 | 128.31 |
| 14 | K | 1401 | CLA | O1D-CGD-CBD | -2.57 | 120.64 | 124.64 |
| 14 | A | 1133 | CLA | CMB-C2B-C1B | -2.57 | 123.94 | 128.31 |
| 14 | A | 1104 | CLA | O2A-CGA-O1A | -2.57 | 116.78 | 123.51 |
| 14 | B | 1212 | CLA | CMB-C2B-C1B | -2.57 | 123.95 | 128.31 |
| 14 | A | 1122 | CLA | OBD-CAD-CBD | -2.56 | 122.07 | 125.94 |
| 14 | X | 1701 | CLA | CMB-C2B-C1B | -2.56 | 123.95 | 128.31 |
| 14 | A | 1127 | CLA | OBD-CAD-CBD | -2.56 | 122.07 | 125.94 |
| 14 | A | 1128 | CLA | CAA-C2A-C3A | -2.56 | 105.84 | 112.79 |
| 14 | A | 1121 | CLA | CMB-C2B-C1B | -2.55 | 123.97 | 128.31 |
| 14 | B | 1220 | CLA | CMB-C2B-C1B | -2.55 | 123.97 | 128.31 |
| 14 | A | 1140 | CLA | OBD-CAD-CBD | -2.55 | 122.09 | 125.94 |
| 14 | A | 1101 | CLA | O1D-CGD-CBD | -2.55 | 120.67 | 124.64 |
| 14 | A | 1134 | CLA | C2C-C1C-NC | -2.55 | 108.47 | 110.22 |
| 14 | A | 1801 | CLA | CMB-C2B-C1B | -2.55 | 123.98 | 128.31 |
| 14 | B | 1213 | CLA | CMB-C2B-C1B | -2.55 | 123.98 | 128.31 |
| 14 | A | 1117 | CLA | OBD-CAD-CBD | -2.55 | 122.10 | 125.94 |
| 14 | B | 1229 | CLA | O1D-CGD-CBD | -2.55 | 120.68 | 124.64 |
| 14 | B | 1228 | CLA | OBD-CAD-CBD | -2.54 | 122.10 | 125.94 |
| 14 | A | 1122 | CLA | C3B-CAB-CBB | -2.54 | 121.28 | 126.40 |
| 14 | B | 1212 | CLA | C2C-C1C-NC | -2.54 | 108.48 | 110.22 |
| 14 | B | 1209 | CLA | CMB-C2B-C1B | -2.53 | 124.00 | 128.31 |
| 14 | J | 1302 | CLA | CMB-C2B-C1B | -2.53 | 124.01 | 128.31 |
| 14 | B | 1012 | CLA | CMB-C2B-C1B | -2.53 | 124.01 | 128.31 |
| 14 | L | 1502 | CLA | C6-C5-C3 | -2.52 | 108.23 | 112.76 |
| 14 | L | 1503 | CLA | CMB-C2B-C1B | -2.52 | 124.03 | 128.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | B | 1221 | CLA | C2C-C1C-NC | -2.52 | 108.50 | 110.22 |
| 14 | A | 1134 | CLA | O1D-CGD-CBD | -2.52 | 120.72 | 124.64 |
| 14 | B | 1239 | CLA | O1D-CGD-CBD | -2.51 | 120.73 | 124.64 |
| 14 | B | 1225 | CLA | CMB-C2B-C1B | -2.51 | 124.05 | 128.31 |
| 14 | F | 1301 | CLA | OBD-CAD-CBD | -2.51 | 122.16 | 125.94 |
| 14 | B | 1217 | CLA | CMB-C2B-C1B | -2.50 | 124.05 | 128.31 |
| 14 | B | 1216 | CLA | O1D-CGD-CBD | -2.50 | 120.75 | 124.64 |
| 14 | L | 1502 | CLA | C2C-C1C-NC | -2.50 | 108.51 | 110.22 |
| 14 | B | 1233 | CLA | OBD-CAD-CBD | -2.50 | 122.17 | 125.94 |
| 14 | A | 1126 | CLA | O1D-CGD-CBD | -2.50 | 120.75 | 124.64 |
| 14 | B | 1208 | CLA | C2C-C1C-NC | -2.50 | 108.51 | 110.22 |
| 14 | A | 1116 | CLA | CMB-C2B-C1B | -2.49 | 124.08 | 128.31 |
| 14 | A | 1116 | CLA | C3B-CAB-CBB | -2.49 | 121.39 | 126.40 |
| 17 | B | 4017 | BCR | C8-C9-C10 | -2.49 | 114.94 | 118.95 |
| 14 | B | 1234 | CLA | OBD-CAD-CBD | -2.49 | 122.19 | 125.94 |
| 14 | B | 1227 | CLA | C3B-CAB-CBB | -2.48 | 121.40 | 126.40 |
| 17 | B | 4009 | BCR | C30-C25-C26 | -2.48 | 119.18 | 122.50 |
| 14 | B | 1207 | CLA | OBD-CAD-CBD | -2.48 | 122.20 | 125.94 |
| 17 | A | 4008 | BCR | C33-C5-C4 | -2.48 | 108.68 | 113.47 |
| 14 | B | 1227 | CLA | C2C-C1C-NC | -2.48 | 108.52 | 110.22 |
| 14 | J | 1303 | CLA | CMA-C3A-C2A | -2.48 | 110.94 | 116.22 |
| 14 | B | 1236 | CLA | CMB-C2B-C1B | -2.47 | 124.11 | 128.31 |
| 14 | A | 1126 | CLA | CAA-C2A-C3A | -2.47 | 106.08 | 112.79 |
| 14 | A | 1022 | CLA | CMB-C2B-C1B | -2.47 | 124.12 | 128.31 |
| 14 | A | 1116 | CLA | O1D-CGD-CBD | -2.47 | 120.80 | 124.64 |
| 14 | A | 1135 | CLA | OBD-CAD-CBD | -2.46 | 122.22 | 125.94 |
| 14 | B | 1217 | CLA | OBD-CAD-CBD | -2.46 | 122.22 | 125.94 |
| 14 | A | 1122 | CLA | O1D-CGD-CBD | -2.46 | 120.80 | 124.64 |
| 14 | A | 1110 | CLA | OBD-CAD-CBD | -2.46 | 122.22 | 125.94 |
| 14 | B | 1239 | CLA | CMB-C2B-C1B | -2.46 | 124.12 | 128.31 |
| 14 | B | 1023 | CLA | C2C-C1C-NC | -2.46 | 108.53 | 110.22 |
| 14 | A | 1138 | CLA | O1D-CGD-CBD | -2.45 | 120.82 | 124.64 |
| 14 | B | 1224 | CLA | C2C-C1C-NC | -2.45 | 108.54 | 110.22 |
| 14 | A | 1139 | CLA | C3B-CAB-CBB | -2.45 | 121.46 | 126.40 |
| 14 | A | 1138 | CLA | CMB-C2B-C1B | -2.45 | 124.14 | 128.31 |
| 14 | B | 1231 | CLA | C2C-C1C-NC | -2.45 | 108.54 | 110.22 |
| 17 | A | 4011 | BCR | C1-C6-C5 | -2.45 | 119.22 | 122.50 |
| 14 | A | 1112 | CLA | CMB-C2B-C1B | -2.45 | 124.15 | 128.31 |
| 17 | I | 4018 | BCR | C30-C25-C26 | -2.44 | 119.23 | 122.50 |
| 17 | B | 4010 | BCR | C1-C6-C5 | -2.44 | 119.23 | 122.50 |
| 14 | K | 1401 | CLA | CMB-C2B-C1B | -2.44 | 124.16 | 128.31 |
| 14 | A | 1107 | CLA | O1D-CGD-CBD | -2.44 | 120.84 | 124.64 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | B | 1211 | CLA | CMB-C2B-C1B | -2.44 | 124.16 | 128.31 |
| 14 | J | 1302 | CLA | C2C-C1C-NC | -2.44 | 108.55 | 110.22 |
| 14 | A | 1122 | CLA | CMB-C2B-C1B | -2.44 | 124.17 | 128.31 |
| 14 | A | 1102 | CLA | C2C-C1C-NC | -2.43 | 108.55 | 110.22 |
| 14 | A | 1109 | CLA | OBD-CAD-CBD | -2.43 | 122.27 | 125.94 |
| 14 | B | 1205 | CLA | CMB-C2B-C1B | -2.43 | 124.19 | 128.31 |
| 14 | A | 1237 | CLA | CMB-C2B-C1B | -2.43 | 124.19 | 128.31 |
| 14 | A | 1133 | CLA | O2A-CGA-O1A | -2.42 | 117.16 | 123.51 |
| 14 | B | 1228 | CLA | CMB-C2B-C1B | -2.42 | 124.19 | 128.31 |
| 14 | B | 1213 | CLA | O1D-CGD-CBD | -2.42 | 120.87 | 124.64 |
| 14 | A | 1117 | CLA | O1D-CGD-CBD | -2.42 | 120.87 | 124.64 |
| 14 | B | 1209 | CLA | O1D-CGD-CBD | -2.42 | 120.88 | 124.64 |
| 14 | A | 1114 | CLA | O1D-CGD-CBD | -2.41 | 120.89 | 124.64 |
| 14 | X | 1701 | CLA | O1D-CGD-CBD | -2.41 | 120.89 | 124.64 |
| 14 | B | 1204 | CLA | O1D-CGD-CBD | -2.41 | 120.89 | 124.64 |
| 14 | B | 1225 | CLA | O1D-CGD-CBD | -2.40 | 120.90 | 124.64 |
| 17 | I | 4020 | BCR | C1-C6-C5 | -2.40 | 119.29 | 122.50 |
| 14 | B | 1230 | CLA | CMB-C2B-C1B | -2.39 | 124.24 | 128.31 |
| 14 | M | 1601 | CLA | CMB-C2B-C1B | -2.39 | 124.24 | 128.31 |
| 14 | B | 1221 | CLA | CMB-C2B-C1B | -2.39 | 124.24 | 128.31 |
| 14 | B | 1226 | CLA | O2A-CGA-O1A | -2.39 | 117.24 | 123.51 |
| 14 | B | 1222 | CLA | OBD-CAD-CBD | -2.39 | 122.33 | 125.94 |
| 14 | A | 1105 | CLA | OBD-CAD-CBD | -2.39 | 122.33 | 125.94 |
| 14 | A | 1115 | CLA | OBD-CAD-CBD | -2.38 | 122.34 | 125.94 |
| 14 | B | 1227 | CLA | C3C-C4C-NC | -2.38 | 107.80 | 110.21 |
| 14 | A | 1102 | CLA | OBD-CAD-CBD | -2.38 | 122.35 | 125.94 |
| 14 | B | 1219 | CLA | OBD-CAD-CBD | -2.38 | 122.35 | 125.94 |
| 14 | L | 1501 | CLA | C2C-C1C-NC | -2.38 | 108.59 | 110.22 |
| 14 | A | 1130 | CLA | CMB-C2B-C1B | -2.38 | 124.27 | 128.31 |
| 14 | A | 1134 | CLA | OBD-CAD-CBD | -2.37 | 122.35 | 125.94 |
| 14 | A | 1138 | CLA | OBD-CAD-CBD | -2.37 | 122.36 | 125.94 |
| 14 | B | 1021 | CLA | CAA-C2A-C3A | -2.37 | 106.36 | 112.79 |
| 17 | A | 4007 | BCR | C1-C6-C5 | -2.36 | 119.34 | 122.50 |
| 17 | A | 4011 | BCR | C23-C22-C21 | -2.36 | 115.15 | 118.95 |
| 14 | B | 1228 | CLA | O1D-CGD-CBD | -2.36 | 120.97 | 124.64 |
| 14 | A | 1117 | CLA | O2A-CGA-O1A | -2.35 | 117.34 | 123.51 |
| 14 | A | 1011 | CLA | CMB-C2B-C1B | -2.35 | 124.31 | 128.31 |
| 14 | A | 1104 | CLA | OBD-CAD-CBD | -2.35 | 122.40 | 125.94 |
| 14 | F | 1301 | CLA | CMB-C2B-C1B | -2.35 | 124.32 | 128.31 |
| 14 | A | 1107 | CLA | OBD-CAD-CBD | -2.35 | 122.40 | 125.94 |
| 14 | A | 1133 | CLA | OBD-CAD-CBD | -2.35 | 122.40 | 125.94 |
| 14 | A | 1140 | CLA | C2C-C1C-NC | -2.35 | 108.61 | 110.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | A | 1126 | CLA | O2A-CGA-O1A | -2.34 | 117.37 | 123.51 |
| 14 | B | 1213 | CLA | O2A-CGA-O1A | -2.34 | 117.38 | 123.51 |
| 14 | A | 1113 | CLA | OBD-CAD-CBD | -2.34 | 122.41 | 125.94 |
| 14 | J | 1303 | CLA | CMB-C2B-C1B | -2.34 | 124.34 | 128.31 |
| 14 | A | 1108 | CLA | O1D-CGD-CBD | -2.33 | 121.01 | 124.64 |
| 14 | A | 1130 | CLA | CAA-C2A-C3A | -2.33 | 106.46 | 112.79 |
| 14 | B | 1012 | CLA | O2A-CGA-O1A | -2.33 | 117.40 | 123.51 |
| 14 | A | 1106 | CLA | O2A-CGA-O1A | -2.33 | 117.40 | 123.51 |
| 14 | B | 1204 | CLA | C3C-C4C-NC | -2.33 | 107.85 | 110.21 |
| 14 | B | 1220 | CLA | O1D-CGD-CBD | -2.33 | 121.01 | 124.64 |
| 14 | A | 1109 | CLA | CMB-C2B-C1B | -2.33 | 124.35 | 128.31 |
| 14 | A | 1110 | CLA | CMB-C2B-C1B | -2.33 | 124.35 | 128.31 |
| 14 | A | 1101 | CLA | C2C-C1C-NC | -2.33 | 108.63 | 110.22 |
| 14 | A | 1801 | CLA | O2A-CGA-O1A | -2.33 | 117.41 | 123.51 |
| 17 | B | 4017 | BCR | C30-C25-C26 | -2.33 | 119.39 | 122.50 |
| 14 | A | 1107 | CLA | C2C-C1C-NC | -2.33 | 108.63 | 110.22 |
| 14 | A | 1402 | CLA | CMB-C2B-C1B | -2.32 | 124.36 | 128.31 |
| 17 | L | 4019 | BCR | C1-C6-C5 | -2.32 | 119.39 | 122.50 |
| 14 | A | 1115 | CLA | O1D-CGD-CBD | -2.32 | 121.03 | 124.64 |
| 14 | A | 1125 | CLA | CMB-C2B-C1B | -2.32 | 124.37 | 128.31 |
| 14 | A | 1105 | CLA | CMB-C2B-C1B | -2.32 | 124.37 | 128.31 |
| 14 | A | 1130 | CLA | OBD-CAD-CBD | -2.32 | 122.44 | 125.94 |
| 14 | A | 1122 | CLA | CAA-C2A-C3A | -2.32 | 106.50 | 112.79 |
| 14 | A | 1105 | CLA | O1D-CGD-CBD | -2.31 | 121.04 | 124.64 |
| 14 | L | 1503 | CLA | C2C-C1C-NC | -2.31 | 108.64 | 110.22 |
| 14 | A | 1013 | CLA | CAA-C2A-C3A | -2.30 | 106.54 | 112.79 |
| 14 | A | 1118 | CLA | O2A-CGA-O1A | -2.30 | 117.47 | 123.51 |
| 14 | A | 1139 | CLA | OBD-CAD-CBD | -2.30 | 122.47 | 125.94 |
| 14 | B | 1215 | CLA | O2A-CGA-O1A | -2.29 | 117.50 | 123.51 |
| 14 | B | 1209 | CLA | OBD-CAD-CBD | -2.29 | 122.48 | 125.94 |
| 14 | B | 1234 | CLA | C2C-C1C-NC | -2.29 | 108.65 | 110.22 |
| 14 | B | 1210 | CLA | OBD-CAD-CBD | -2.28 | 122.50 | 125.94 |
| 14 | A | 1136 | CLA | CMB-C2B-C1B | -2.28 | 124.44 | 128.31 |
| 14 | A | 1011 | CLA | CAA-C2A-C3A | -2.28 | 106.61 | 112.79 |
| 17 | A | 4008 | BCR | C1-C6-C5 | -2.28 | 119.45 | 122.50 |
| 14 | B | 1223 | CLA | OBD-CAD-CBD | -2.28 | 122.50 | 125.94 |
| 14 | B | 1238 | CLA | CMB-C2B-C1B | -2.28 | 124.44 | 128.31 |
| 14 | B | 1208 | CLA | CMB-C2B-C1B | -2.28 | 124.44 | 128.31 |
| 14 | B | 1216 | CLA | C3B-CAB-CBB | -2.27 | 121.82 | 126.40 |
| 14 | B | 1206 | CLA | O1D-CGD-CBD | -2.27 | 121.11 | 124.64 |
| 14 | B | 1211 | CLA | CAA-C2A-C3A | -2.27 | 106.63 | 112.79 |
| 14 | A | 1119 | CLA | C12-C11-C10 | -2.27 | 101.97 | 113.04 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | L | 1501 | CLA | CMB-C2B-C1B | -2.26 | 124.46 | 128.31 |
| 14 | L | 1502 | CLA | C3C-C4C-NC | -2.26 | 107.92 | 110.21 |
| 14 | B | 1220 | CLA | C2C-C1C-NC | -2.26 | 108.67 | 110.22 |
| 14 | A | 1136 | CLA | C3C-C4C-NC | -2.26 | 107.92 | 110.21 |
| 14 | B | 1023 | CLA | CMB-C2B-C1B | -2.26 | 124.47 | 128.31 |
| 17 | A | 4008 | BCR | C8-C9-C10 | -2.26 | 115.32 | 118.95 |
| 14 | A | 1139 | CLA | CMB-C2B-C1B | -2.26 | 124.48 | 128.31 |
| 14 | B | 1219 | CLA | C2C-C1C-NC | -2.26 | 108.67 | 110.22 |
| 14 | B | 1233 | CLA | CMB-C2B-C1B | -2.25 | 124.49 | 128.31 |
| 14 | K | 1401 | CLA | C3B-CAB-CBB | -2.25 | 121.88 | 126.40 |
| 14 | B | 1222 | CLA | CAA-C2A-C3A | -2.24 | 106.70 | 112.79 |
| 17 | B | 4014 | BCR | C1-C6-C5 | -2.24 | 119.50 | 122.50 |
| 14 | B | 1226 | CLA | OBD-CAD-CBD | -2.24 | 122.56 | 125.94 |
| 14 | A | 1118 | CLA | CMB-C2B-C1B | -2.24 | 124.50 | 128.31 |
| 17 | B | 4017 | BCR | C1-C6-C5 | -2.24 | 119.51 | 122.50 |
| 14 | B | 1214 | CLA | CAA-C2A-C3A | -2.23 | 106.72 | 112.79 |
| 14 | A | 1125 | CLA | OBD-CAD-CBD | -2.23 | 122.57 | 125.94 |
| 14 | A | 1123 | CLA | CMB-C2B-C1B | -2.23 | 124.51 | 128.31 |
| 14 | B | 1214 | CLA | O1D-CGD-CBD | -2.23 | 121.17 | 124.64 |
| 14 | A | 1137 | CLA | CMB-C2B-C1B | -2.22 | 124.54 | 128.31 |
| 14 | B | 1217 | CLA | C2C-C1C-NC | -2.22 | 108.70 | 110.22 |
| 14 | A | 1131 | CLA | C3B-CAB-CBB | -2.21 | 121.94 | 126.40 |
| 14 | B | 1229 | CLA | C2C-C1C-NC | -2.21 | 108.70 | 110.22 |
| 14 | B | 1203 | CLA | OBD-CAD-CBD | -2.21 | 122.60 | 125.94 |
| 14 | B | 1214 | CLA | C2C-C1C-NC | -2.21 | 108.70 | 110.22 |
| 14 | B | 1206 | CLA | C12-C11-C10 | -2.21 | 102.26 | 113.04 |
| 14 | B | 1201 | CLA | C2C-C1C-NC | -2.21 | 108.71 | 110.22 |
| 14 | B | 1225 | CLA | OBD-CAD-CBD | -2.20 | 122.61 | 125.94 |
| 17 | J | 4012 | BCR | C32-C1-C2 | -2.20 | 101.02 | 108.75 |
| 14 | A | 1110 | CLA | O2A-CGA-O1A | -2.20 | 117.73 | 123.51 |
| 14 | B | 1230 | CLA | OBD-CAD-CBD | -2.20 | 122.61 | 125.94 |
| 14 | A | 1119 | CLA | O1D-CGD-CBD | -2.20 | 121.21 | 124.64 |
| 14 | A | 1129 | CLA | O2A-CGA-O1A | -2.20 | 117.74 | 123.51 |
| 14 | L | 1502 | CLA | CMB-C2B-C1B | -2.20 | 124.57 | 128.31 |
| 14 | B | 1219 | CLA | C3C-C4C-NC | -2.20 | 107.99 | 110.21 |
| 14 | B | 1235 | CLA | C4-C3-C5 | -2.19 | 112.03 | 115.37 |
| 14 | A | 1137 | CLA | C3B-CAB-CBB | -2.19 | 121.99 | 126.40 |
| 14 | B | 1231 | CLA | C3C-C4C-NC | -2.19 | 107.99 | 110.21 |
| 14 | B | 1238 | CLA | C3C-C4C-NC | -2.19 | 108.00 | 110.21 |
| 14 | A | 1801 | CLA | OBD-CAD-CBD | -2.18 | 122.64 | 125.94 |
| 14 | A | 1130 | CLA | O2A-CGA-O1A | -2.18 | 117.78 | 123.51 |
| 14 | B | 1227 | CLA | OBD-CAD-CBD | -2.18 | 122.64 | 125.94 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | L | 1502 | CLA | O1D-CGD-CBD | -2.18 | 121.24 | 124.64 |
| 14 | M | 1601 | CLA | C2C-C1C-NC | -2.18 | 108.73 | 110.22 |
| 14 | F | 1301 | CLA | C2C-C1C-NC | -2.18 | 108.73 | 110.22 |
| 14 | B | 1235 | CLA | CMB-C2B-C1B | -2.17 | 124.61 | 128.31 |
| 14 | A | 1123 | CLA | C2C-C1C-NC | -2.17 | 108.73 | 110.22 |
| 14 | B | 1234 | CLA | CMB-C2B-C1B | -2.17 | 124.62 | 128.31 |
| 14 | A | 1103 | CLA | C3C-C4C-NC | -2.17 | 108.02 | 110.21 |
| 14 | A | 1128 | CLA | O2A-CGA-O1A | -2.16 | 117.83 | 123.51 |
| 14 | A | 1133 | CLA | C2C-C1C-NC | -2.16 | 108.74 | 110.22 |
| 14 | B | 1229 | CLA | C12-C11-C10 | -2.16 | 102.47 | 113.04 |
| 14 | B | 1227 | CLA | CMB-C2B-C1B | -2.16 | 124.63 | 128.31 |
| 14 | B | 1207 | CLA | C3B-CAB-CBB | -2.16 | 122.05 | 126.40 |
| 14 | A | 1129 | CLA | CMB-C2B-C1B | -2.16 | 124.64 | 128.31 |
| 14 | B | 1223 | CLA | C2C-C1C-NC | -2.16 | 108.74 | 110.22 |
| 17 | A | 4008 | BCR | C23-C22-C21 | -2.16 | 115.47 | 118.95 |
| 14 | B | 1205 | CLA | C3B-CAB-CBB | -2.16 | 122.06 | 126.40 |
| 14 | J | 1303 | CLA | C2C-C1C-NC | -2.15 | 108.75 | 110.22 |
| 17 | A | 4007 | BCR | C40-C30-C29 | -2.15 | 101.20 | 108.75 |
| 14 | F | 1301 | CLA | C3B-CAB-CBB | -2.15 | 122.08 | 126.40 |
| 14 | A | 1121 | CLA | O2A-CGA-O1A | -2.15 | 117.88 | 123.51 |
| 14 | A | 1125 | CLA | O2A-CGA-O1A | -2.15 | 117.88 | 123.51 |
| 14 | B | 1205 | CLA | C7-C6-C5 | -2.14 | 106.83 | 113.16 |
| 14 | B | 1235 | CLA | C3B-CAB-CBB | -2.14 | 122.09 | 126.40 |
| 14 | A | 1113 | CLA | C2C-C1C-NC | -2.14 | 108.75 | 110.22 |
| 14 | A | 1112 | CLA | C2C-C1C-NC | -2.13 | 108.76 | 110.22 |
| 14 | A | 1102 | CLA | C12-C11-C10 | -2.13 | 106.11 | 113.67 |
| 14 | A | 1122 | CLA | O2A-CGA-O1A | -2.13 | 117.92 | 123.51 |
| 17 | B | 4017 | BCR | C23-C22-C21 | -2.13 | 115.52 | 118.95 |
| 14 | L | 1502 | CLA | O2A-CGA-O1A | -2.13 | 117.93 | 123.51 |
| 17 | I | 4018 | BCR | C19-C18-C17 | -2.13 | 115.52 | 118.95 |
| 14 | A | 1106 | CLA | CMB-C2B-C1B | -2.12 | 124.70 | 128.31 |
| 14 | J | 1303 | CLA | OBD-CAD-CBD | -2.12 | 121.71 | 126.08 |
| 17 | I | 4020 | BCR | C19-C18-C17 | -2.12 | 115.54 | 118.95 |
| 14 | A | 1117 | CLA | C3C-C4C-NC | -2.12 | 108.06 | 110.21 |
| 14 | B | 1236 | CLA | O2A-CGA-O1A | -2.12 | 117.96 | 123.51 |
| 14 | A | 1120 | CLA | C3C-C4C-NC | -2.12 | 108.07 | 110.21 |
| 14 | B | 1231 | CLA | CMB-C2B-C1B | -2.12 | 124.71 | 128.31 |
| 14 | B | 1231 | CLA | CAA-C2A-C3A | -2.11 | 107.05 | 112.79 |
| 14 | A | 1107 | CLA | O2A-CGA-O1A | -2.11 | 117.97 | 123.51 |
| 14 | K | 1401 | CLA | OBD-CAD-CBD | -2.11 | 122.76 | 125.94 |
| 14 | B | 1233 | CLA | O1D-CGD-CBD | -2.11 | 121.36 | 124.64 |
| 14 | B | 1234 | CLA | O2A-CGA-O1A | -2.11 | 117.99 | 123.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | A | 1120 | CLA | O2A-CGA-O1A | -2.10 | 117.99 | 123.51 |
| 14 | A | 1110 | CLA | C3C-C4C-NC | -2.10 | 108.08 | 110.21 |
| 14 | B | 1217 | CLA | O2A-CGA-O1A | -2.10 | 118.01 | 123.51 |
| 14 | B | 1023 | CLA | C12-C11-C10 | -2.10 | 102.81 | 113.04 |
| 14 | B | 1201 | CLA | CAA-C2A-C3A | -2.10 | 107.10 | 112.79 |
| 14 | A | 1124 | CLA | O1D-CGD-CBD | -2.09 | 121.39 | 124.64 |
| 14 | A | 1104 | CLA | O1D-CGD-CBD | -2.09 | 121.39 | 124.64 |
| 14 | X | 1701 | CLA | C3B-CAB-CBB | -2.09 | 122.20 | 126.40 |
| 14 | B | 1235 | CLA | C3C-C4C-NC | -2.08 | 108.10 | 110.21 |
| 17 | A | 4011 | BCR | C32-C1-C2 | -2.08 | 101.44 | 108.75 |
| 14 | B | 1213 | CLA | C2C-C1C-NC | -2.08 | 108.80 | 110.22 |
| 14 | A | 1139 | CLA | O2A-CGA-O1A | -2.08 | 118.06 | 123.51 |
| 14 | L | 1501 | CLA | O2A-CGA-O1A | -2.08 | 118.07 | 123.51 |
| 14 | B | 1206 | CLA | CAA-C2A-C3A | -2.07 | 107.16 | 112.79 |
| 14 | A | 1104 | CLA | C3C-C4C-NC | -2.07 | 108.11 | 110.21 |
| 14 | B | 1217 | CLA | C3B-CAB-CBB | -2.07 | 122.23 | 126.40 |
| 14 | L | 1501 | CLA | C4-C3-C5 | -2.07 | 112.22 | 115.37 |
| 14 | A | 1237 | CLA | CMA-C3A-C2A | -2.07 | 104.92 | 113.99 |
| 14 | A | 1133 | CLA | C3C-C4C-NC | -2.06 | 108.12 | 110.21 |
| 14 | B | 1235 | CLA | CAA-C2A-C3A | -2.06 | 107.20 | 112.79 |
| 17 | J | 4013 | BCR | C40-C30-C29 | -2.06 | 101.53 | 108.75 |
| 14 | A | 1402 | CLA | C3B-CAB-CBB | -2.06 | 122.26 | 126.40 |
| 14 | A | 1013 | CLA | OBD-CAD-CBD | -2.06 | 122.83 | 125.94 |
| 14 | A | 1102 | CLA | O2A-CGA-O1A | -2.05 | 118.13 | 123.51 |
| 14 | A | 1109 | CLA | O2A-CGA-O1A | -2.05 | 118.13 | 123.51 |
| 14 | B | 1209 | CLA | C2C-C1C-NC | -2.05 | 108.82 | 110.22 |
| 17 | B | 4010 | BCR | C40-C30-C29 | -2.05 | 101.55 | 108.75 |
| 14 | A | 1113 | CLA | CAA-C2A-C3A | -2.05 | 107.23 | 112.79 |
| 14 | L | 1503 | CLA | O1D-CGD-CBD | -2.05 | 121.45 | 124.64 |
| 14 | A | 1109 | CLA | O1D-CGD-CBD | -2.04 | 121.47 | 124.64 |
| 14 | B | 1232 | CLA | C2C-C1C-NC | -2.04 | 108.82 | 110.22 |
| 14 | K | 1401 | CLA | C2C-C1C-NC | -2.04 | 108.83 | 110.22 |
| 14 | A | 1131 | CLA | O2A-CGA-O1A | -2.04 | 118.17 | 123.51 |
| 14 | A | 1138 | CLA | CAA-C2A-C3A | -2.04 | 107.26 | 112.79 |
| 14 | B | 1219 | CLA | O1D-CGD-CBD | -2.03 | 121.47 | 124.64 |
| 14 | B | 1234 | CLA | C3B-CAB-CBB | -2.03 | 122.31 | 126.40 |
| 14 | F | 1301 | CLA | O1D-CGD-CBD | -2.03 | 121.48 | 124.64 |
| 14 | A | 1110 | CLA | O1D-CGD-CBD | -2.03 | 121.48 | 124.64 |
| 14 | A | 1107 | CLA | C3B-CAB-CBB | -2.03 | 122.32 | 126.40 |
| 14 | B | 1224 | CLA | O1A-CGA-CBA | -2.03 | 116.00 | 123.76 |
| 14 | B | 1212 | CLA | OBD-CAD-CBD | -2.02 | 122.88 | 125.94 |
| 14 | J | 1303 | CLA | C3C-C4C-NC | -2.02 | 108.16 | 110.21 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | B | 1214 | CLA | O2A-CGA-O1A | -2.02 | 118.21 | 123.51 |
| 14 | B | 1204 | CLA | CMB-C2B-C1B | -2.02 | 124.88 | 128.31 |
| 14 | B | 1012 | CLA | C2C-C1C-NC | -2.02 | 108.84 | 110.22 |
| 14 | A | 1140 | CLA | O1D-CGD-CBD | -2.02 | 121.50 | 124.64 |
| 14 | B | 1232 | CLA | O1D-CGD-CBD | -2.02 | 121.50 | 124.64 |
| 17 | J | 4013 | BCR | C19-C18-C17 | -2.02 | 115.70 | 118.95 |
| 14 | A | 1116 | CLA | O2A-CGA-O1A | -2.02 | 118.22 | 123.51 |
| 17 | B | 4010 | BCR | C19-C18-C17 | -2.01 | 115.71 | 118.95 |
| 14 | A | 1133 | CLA | C3B-CAB-CBB | -2.01 | 122.35 | 126.40 |
| 14 | A | 1402 | CLA | OBD-CAD-CBD | -2.00 | 121.96 | 126.08 |
| 14 | A | 1138 | CLA | O2A-CGA-O1A | -2.00 | 118.26 | 123.51 |
| 14 | B | 1201 | CLA | O2A-CGA-O1A | -2.00 | 118.27 | 123.51 |
| 14 | B | 1204 | CLA | OBD-CAD-C3D | 2.00 | 131.63 | 128.09 |
| 17 | M | 4021 | BCR | C37-C22-C23 | 2.00 | 121.36 | 118.08 |
| 17 | B | 4004 | BCR | C37-C22-C23 | 2.01 | 121.36 | 118.08 |
| 17 | F | 4016 | BCR | C36-C18-C19 | 2.01 | 121.36 | 118.08 |
| 14 | A | 1122 | CLA | CED-O2D-CGD | 2.01 | 120.75 | 115.97 |
| 14 | A | 1138 | CLA | C2A-C1A-CHA | 2.01 | 127.04 | 123.80 |
| 17 | B | 4010 | BCR | C20-C21-C22 | 2.02 | 130.16 | 127.22 |
| 17 | A | 4003 | BCR | C32-C1-C6 | 2.02 | 113.42 | 110.33 |
| 14 | B | 1224 | CLA | CED-O2D-CGD | 2.02 | 120.77 | 115.97 |
| 14 | A | 1129 | CLA | C2A-C1A-CHA | 2.02 | 127.05 | 123.80 |
| 14 | B | 1202 | CLA | CBA-CAA-C2A | 2.02 | 119.17 | 113.96 |
| 17 | F | 4016 | BCR | C1-C6-C7 | 2.02 | 121.74 | 115.96 |
| 17 | B | 4004 | BCR | C34-C9-C8 | 2.03 | 121.39 | 118.08 |
| 17 | A | 4003 | BCR | C15-C14-C13 | 2.03 | 130.17 | 127.22 |
| 14 | A | 1131 | CLA | CED-O2D-CGD | 2.03 | 120.80 | 115.97 |
| 17 | A | 4003 | BCR | C28-C27-C26 | 2.03 | 117.24 | 113.87 |
| 17 | A | 4008 | BCR | C8-C7-C6 | 2.04 | 133.15 | 127.24 |
| 14 | A | 1110 | CLA | C2A-C1A-CHA | 2.04 | 127.08 | 123.80 |
| 17 | B | 4004 | BCR | C40-C30-C25 | 2.04 | 113.45 | 110.33 |
| 17 | B | 4010 | BCR | C34-C9-C8 | 2.04 | 121.42 | 118.08 |
| 14 | A | 1022 | CLA | C2A-C1A-CHA | 2.04 | 127.08 | 123.80 |
| 14 | B | 1239 | CLA | CMB-C2B-C3B | 2.04 | 129.08 | 125.09 |
| 17 | B | 4014 | BCR | C11-C10-C9 | 2.05 | 130.19 | 127.22 |
| 14 | A | 1106 | CLA | CED-O2D-CGD | 2.05 | 120.83 | 115.97 |
| 14 | B | 1208 | CLA | C2A-C1A-CHA | 2.05 | 127.10 | 123.80 |
| 14 | B | 1217 | CLA | CBA-CAA-C2A | 2.05 | 119.24 | 113.96 |
| 14 | A | 1022 | CLA | CED-O2D-CGD | 2.05 | 120.84 | 115.97 |
| 14 | A | 1102 | CLA | CMB-C2B-C3B | 2.05 | 129.10 | 125.09 |
| 17 | B | 4006 | BCR | C1-C6-C7 | 2.05 | 121.83 | 115.96 |
| 14 | B | 1239 | CLA | CED-O2D-CGD | 2.06 | 120.87 | 115.97 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 14 | B | 1225 | CLA | C2A-C1A-CHA | 2.06 | 127.12 | 123.80 |
| 17 | B | 4010 | BCR | C1-C6-C7 | 2.07 | 121.86 | 115.96 |
| 14 | B | 1216 | CLA | C2A-C1A-CHA | 2.07 | 127.12 | 123.80 |
| 17 | M | 4021 | BCR | C35-C13-C12 | 2.07 | 121.46 | 118.08 |
| 14 | B | 1205 | CLA | CED-O2D-CGD | 2.07 | 120.89 | 115.97 |
| 14 | B | 1223 | CLA | CED-O2D-CGD | 2.07 | 120.89 | 115.97 |
| 17 | B | 4005 | BCR | C15-C14-C13 | 2.07 | 130.23 | 127.22 |
| 17 | A | 4003 | BCR | C35-C13-C12 | 2.07 | 121.47 | 118.08 |
| 14 | A | 1125 | CLA | C2A-C1A-CHA | 2.08 | 127.14 | 123.80 |
| 17 | A | 4011 | BCR | C37-C22-C23 | 2.08 | 121.47 | 118.08 |
| 14 | B | 1239 | CLA | OBD-CAD-C3D | 2.08 | 131.77 | 128.09 |
| 17 | B | 4006 | BCR | C20-C21-C22 | 2.08 | 130.24 | 127.22 |
| 17 | J | 4015 | BCR | C16-C17-C18 | 2.08 | 130.25 | 127.22 |
| 17 | A | 4002 | BCR | C15-C14-C13 | 2.09 | 130.25 | 127.22 |
| 17 | B | 4004 | BCR | C20-C21-C22 | 2.09 | 130.25 | 127.22 |
| 17 | L | 4019 | BCR | C37-C22-C23 | 2.09 | 121.49 | 118.08 |
| 14 | B | 1220 | CLA | C2A-C1A-CHA | 2.09 | 127.16 | 123.80 |
| 17 | I | 4018 | BCR | C1-C6-C7 | 2.09 | 121.92 | 115.96 |
| 17 | L | 4019 | BCR | C23-C24-C25 | 2.09 | 133.31 | 127.24 |
| 14 | L | 1501 | CLA | C2A-C1A-CHA | 2.09 | 127.17 | 123.80 |
| 14 | A | 1111 | CLA | CMB-C2B-C3B | 2.09 | 129.18 | 125.09 |
| 14 | A | 1126 | CLA | C2A-C3A-C4A | 2.10 | 103.99 | 101.84 |
| 17 | J | 4013 | BCR | C1-C6-C7 | 2.10 | 121.95 | 115.96 |
| 17 | J | 4013 | BCR | C15-C14-C13 | 2.10 | 130.27 | 127.22 |
| 14 | A | 1110 | CLA | CED-O2D-CGD | 2.10 | 120.96 | 115.97 |
| 17 | B | 4006 | BCR | C32-C1-C6 | 2.10 | 113.55 | 110.33 |
| 14 | A | 1130 | CLA | C2A-C1A-CHA | 2.10 | 127.19 | 123.80 |
| 17 | B | 4006 | BCR | C30-C25-C24 | 2.11 | 121.98 | 115.96 |
| 14 | A | 1108 | CLA | CBA-CAA-C2A | 2.11 | 119.50 | 113.78 |
| 17 | J | 4013 | BCR | C34-C9-C8 | 2.11 | 121.53 | 118.08 |
| 17 | J | 4013 | BCR | C35-C13-C12 | 2.11 | 121.53 | 118.08 |
| 14 | A | 1121 | CLA | C2A-C1A-CHA | 2.11 | 127.20 | 123.80 |
| 14 | A | 1126 | CLA | C2A-C1A-CHA | 2.11 | 127.20 | 123.80 |
| 17 | A | 4003 | BCR | C8-C7-C6 | 2.11 | 133.38 | 127.24 |
| 17 | B | 4017 | BCR | C11-C10-C9 | 2.12 | 130.30 | 127.22 |
| 17 | B | 4009 | BCR | C30-C25-C24 | 2.12 | 122.01 | 115.96 |
| 14 | B | 1223 | CLA | C2A-C1A-CHA | 2.12 | 127.21 | 123.80 |
| 17 | B | 4004 | BCR | C1-C6-C7 | 2.12 | 122.02 | 115.96 |
| 17 | F | 4016 | BCR | C40-C30-C25 | 2.12 | 113.58 | 110.33 |
| 17 | M | 4021 | BCR | C32-C1-C6 | 2.12 | 113.58 | 110.33 |
| 17 | J | 4015 | BCR | C40-C30-C25 | 2.12 | 113.58 | 110.33 |
| 14 | L | 1501 | CLA | CBA-CAA-C2A | 2.13 | 119.44 | 113.96 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 17 | A | 4002 | BCR | C32-C1-C6 | 2.13 | 113.58 | 110.33 |
| 17 | J | 4012 | BCR | C37-C22-C23 | 2.13 | 121.56 | 118.08 |
| 17 | F | 4016 | BCR | C30-C25-C24 | 2.13 | 122.04 | 115.96 |
| 14 | A | 1102 | CLA | CED-O2D-CGD | 2.13 | 121.03 | 115.97 |
| 17 | B | 4017 | BCR | C15-C14-C13 | 2.13 | 130.32 | 127.22 |
| 17 | J | 4013 | BCR | C28-C27-C26 | 2.13 | 117.40 | 113.87 |
| 17 | B | 4009 | BCR | C36-C18-C19 | 2.14 | 121.57 | 118.08 |
| 17 | A | 4011 | BCR | C34-C9-C8 | 2.14 | 121.57 | 118.08 |
| 14 | A | 1402 | CLA | C2A-C1A-CHA | 2.14 | 127.24 | 123.80 |
| 17 | B | 4006 | BCR | C36-C18-C19 | 2.14 | 121.58 | 118.08 |
| 17 | L | 4022 | BCR | C30-C25-C24 | 2.14 | 122.07 | 115.96 |
| 14 | B | 1215 | CLA | CBA-CAA-C2A | 2.14 | 119.47 | 113.96 |
| 17 | B | 4006 | BCR | C34-C9-C8 | 2.14 | 121.58 | 118.08 |
| 14 | X | 1701 | CLA | CED-O2D-CGD | 2.14 | 121.06 | 115.97 |
| 14 | B | 1226 | CLA | CED-O2D-CGD | 2.14 | 121.06 | 115.97 |
| 14 | A | 1139 | CLA | CED-O2D-CGD | 2.15 | 121.07 | 115.97 |
| 14 | A | 1108 | CLA | C2A-C1A-CHA | 2.15 | 127.25 | 123.80 |
| 14 | A | 1135 | CLA | CMB-C2B-C3B | 2.15 | 129.29 | 125.09 |
| 17 | A | 4001 | BCR | C35-C13-C12 | 2.15 | 121.59 | 118.08 |
| 14 | B | 1228 | CLA | C2A-C3A-C4A | 2.15 | 104.04 | 101.84 |
| 17 | A | 4001 | BCR | C37-C22-C23 | 2.15 | 121.59 | 118.08 |
| 14 | A | 1117 | CLA | C5-C3-C2 | 2.15 | 124.98 | 120.98 |
| 14 | B | 1023 | CLA | OBD-CAD-C3D | 2.15 | 131.89 | 128.09 |
| 14 | B | 1225 | CLA | C2A-C3A-C4A | 2.15 | 104.04 | 101.84 |
| 17 | I | 4018 | BCR | C34-C9-C8 | 2.15 | 121.60 | 118.08 |
| 14 | B | 1213 | CLA | CBA-CAA-C2A | 2.15 | 119.51 | 113.96 |
| 17 | I | 4020 | BCR | C1-C6-C7 | 2.16 | 122.12 | 115.96 |
| 17 | I | 4018 | BCR | C32-C1-C6 | 2.16 | 113.64 | 110.33 |
| 17 | B | 4005 | BCR | C36-C18-C19 | 2.17 | 121.62 | 118.08 |
| 17 | B | 4017 | BCR | C23-C24-C25 | 2.17 | 133.53 | 127.24 |
| 14 | A | 1130 | CLA | CMB-C2B-C3B | 2.17 | 129.33 | 125.09 |
| 14 | J | 1303 | CLA | C2A-C1A-CHA | 2.17 | 127.29 | 123.80 |
| 14 | A | 1132 | CLA | C5-C3-C2 | 2.17 | 125.02 | 120.98 |
| 14 | B | 1224 | CLA | CAA-CBA-CGA | 2.17 | 119.55 | 113.28 |
| 17 | L | 4022 | BCR | C32-C1-C6 | 2.17 | 113.65 | 110.33 |
| 17 | B | 4005 | BCR | C34-C9-C8 | 2.17 | 121.64 | 118.08 |
| 17 | B | 4014 | BCR | C40-C30-C25 | 2.18 | 113.66 | 110.33 |
| 14 | A | 1106 | CLA | CBA-CAA-C2A | 2.18 | 119.58 | 113.96 |
| 14 | A | 1105 | CLA | C2A-C1A-CHA | 2.18 | 127.31 | 123.80 |
| 17 | B | 4004 | BCR | C8-C7-C6 | 2.18 | 133.57 | 127.24 |
| 14 | A | 1118 | CLA | CED-O2D-CGD | 2.18 | 121.15 | 115.97 |
| 17 | B | 4014 | BCR | C24-C23-C22 | 2.18 | 129.50 | 126.21 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 14 | L | 1503 | CLA | CBA-CAA-C2A | 2.18 | 119.58 | 113.96 |
| 14 | A | 1237 | CLA | CBA-CAA-C2A | 2.19 | 119.59 | 113.96 |
| 14 | A | 1140 | CLA | C2A-C3A-C4A | 2.19 | 104.08 | 101.84 |
| 14 | A | 1103 | CLA | CBA-CAA-C2A | 2.19 | 119.60 | 113.96 |
| 17 | A | 4008 | BCR | C7-C8-C9 | 2.19 | 129.52 | 126.21 |
| 17 | B | 4005 | BCR | C35-C13-C12 | 2.19 | 121.67 | 118.08 |
| 17 | A | 4002 | BCR | C1-C6-C7 | 2.19 | 122.23 | 115.96 |
| 14 | B | 1222 | CLA | CED-O2D-CGD | 2.20 | 121.19 | 115.97 |
| 14 | B | 1224 | CLA | OBD-CAD-C3D | 2.20 | 131.99 | 128.09 |
| 14 | A | 1129 | CLA | C1-C2-C3 | 2.20 | 130.40 | 126.64 |
| 17 | B | 4006 | BCR | C40-C30-C25 | 2.21 | 113.70 | 110.33 |
| 14 | B | 1222 | CLA | C2A-C1A-CHA | 2.21 | 127.35 | 123.80 |
| 14 | B | 1234 | CLA | CED-O2D-CGD | 2.21 | 121.22 | 115.97 |
| 17 | A | 4007 | BCR | C23-C24-C25 | 2.21 | 133.67 | 127.24 |
| 14 | A | 1136 | CLA | CED-O2D-CGD | 2.23 | 121.26 | 115.97 |
| 17 | A | 4002 | BCR | C23-C24-C25 | 2.23 | 133.72 | 127.24 |
| 17 | J | 4015 | BCR | C30-C25-C24 | 2.23 | 122.34 | 115.96 |
| 14 | A | 1116 | CLA | C2A-C1A-CHA | 2.23 | 127.40 | 123.80 |
| 14 | B | 1219 | CLA | CBA-CAA-C2A | 2.24 | 119.72 | 113.96 |
| 17 | J | 4013 | BCR | C24-C23-C22 | 2.24 | 129.59 | 126.21 |
| 14 | B | 1235 | CLA | CBA-CAA-C2A | 2.24 | 119.73 | 113.96 |
| 17 | A | 4001 | BCR | C1-C6-C7 | 2.24 | 122.37 | 115.96 |
| 14 | A | 1101 | CLA | C2A-C1A-CHA | 2.24 | 127.41 | 123.80 |
| 14 | A | 1139 | CLA | C2A-C1A-CHA | 2.25 | 127.41 | 123.80 |
| 14 | B | 1227 | CLA | CED-O2D-CGD | 2.25 | 121.31 | 115.97 |
| 17 | A | 4002 | BCR | C40-C30-C25 | 2.25 | 113.77 | 110.33 |
| 14 | B | 1214 | CLA | C2A-C1A-CHA | 2.25 | 127.42 | 123.80 |
| 14 | A | 1113 | CLA | C2A-C1A-CHA | 2.25 | 127.42 | 123.80 |
| 14 | B | 1219 | CLA | CMB-C2B-C3B | 2.25 | 129.49 | 125.09 |
| 14 | A | 1107 | CLA | C2A-C3A-C4A | 2.25 | 104.15 | 101.84 |
| 17 | A | 4007 | BCR | C1-C6-C7 | 2.26 | 122.40 | 115.96 |
| 14 | A | 1114 | CLA | C2A-C1A-CHA | 2.26 | 127.44 | 123.80 |
| 14 | A | 1126 | CLA | CMB-C2B-C3B | 2.26 | 129.51 | 125.09 |
| 14 | A | 1104 | CLA | CAA-CBA-CGA | 2.26 | 119.81 | 113.28 |
| 14 | A | 1117 | CLA | C2A-C1A-CHA | 2.27 | 127.45 | 123.80 |
| 14 | X | 1701 | CLA | C2A-C1A-CHA | 2.27 | 127.45 | 123.80 |
| 14 | B | 1203 | CLA | CED-O2D-CGD | 2.27 | 121.36 | 115.97 |
| 17 | A | 4008 | BCR | C34-C9-C8 | 2.27 | 121.79 | 118.08 |
| 14 | A | 1117 | CLA | C2A-C3A-C4A | 2.27 | 104.17 | 101.84 |
| 14 | B | 1212 | CLA | C2A-C1A-CHA | 2.28 | 127.46 | 123.80 |
| 14 | A | 1237 | CLA | CED-O2D-CGD | 2.28 | 121.38 | 115.97 |
| 14 | B | 1203 | CLA | CMB-C2B-C3B | 2.28 | 129.54 | 125.09 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 14 | A | 1128 | CLA | CED-O2D-CGD | 2.28 | 121.38 | 115.97 |
| 14 | A | 1127 | CLA | CED-O2D-CGD | 2.28 | 121.39 | 115.97 |
| 14 | B | 1233 | CLA | CED-O2D-CGD | 2.29 | 121.40 | 115.97 |
| 17 | A | 4001 | BCR | C32-C1-C6 | 2.29 | 113.83 | 110.33 |
| 14 | B | 1202 | CLA | CMB-C2B-C3B | 2.29 | 129.57 | 125.09 |
| 14 | A | 1120 | CLA | C2A-C1A-CHA | 2.30 | 127.50 | 123.80 |
| 14 | B | 1204 | CLA | CED-O2D-CGD | 2.30 | 121.44 | 115.97 |
| 14 | A | 1103 | CLA | CMB-C2B-C3B | 2.30 | 129.59 | 125.09 |
| 17 | B | 4014 | BCR | C36-C18-C19 | 2.31 | 121.85 | 118.08 |
| 17 | B | 4017 | BCR | C24-C23-C22 | 2.31 | 129.69 | 126.21 |
| 14 | A | 1123 | CLA | C2A-C1A-CHA | 2.31 | 127.52 | 123.80 |
| 14 | A | 1102 | CLA | C2A-C1A-CHA | 2.31 | 127.53 | 123.80 |
| 14 | B | 1229 | CLA | C2A-C3A-C4A | 2.32 | 104.22 | 101.84 |
| 14 | F | 1301 | CLA | CED-O2D-CGD | 2.32 | 121.48 | 115.97 |
| 14 | A | 1126 | CLA | CED-O2D-CGD | 2.32 | 121.49 | 115.97 |
| 14 | A | 1123 | CLA | CED-O2D-CGD | 2.32 | 121.49 | 115.97 |
| 14 | A | 1013 | CLA | CMB-C2B-C3B | 2.32 | 129.63 | 125.09 |
| 17 | L | 4019 | BCR | C36-C18-C19 | 2.33 | 121.89 | 118.08 |
| 14 | B | 1210 | CLA | C2A-C1A-CHA | 2.33 | 127.55 | 123.80 |
| 14 | B | 1222 | CLA | O2A-CGA-CBA | 2.33 | 120.97 | 112.34 |
| 14 | A | 1112 | CLA | C2A-C1A-CHA | 2.33 | 127.56 | 123.80 |
| 14 | A | 1111 | CLA | C2A-C1A-CHA | 2.34 | 127.56 | 123.80 |
| 17 | A | 4008 | BCR | C37-C22-C23 | 2.34 | 121.91 | 118.08 |
| 14 | K | 1401 | CLA | CED-O2D-CGD | 2.34 | 121.54 | 115.97 |
| 14 | B | 1235 | CLA | C2A-C3A-C4A | 2.35 | 104.24 | 101.84 |
| 14 | B | 1236 | CLA | CED-O2D-CGD | 2.35 | 121.54 | 115.97 |
| 14 | A | 1107 | CLA | CBA-CAA-C2A | 2.35 | 120.00 | 113.96 |
| 14 | A | 1140 | CLA | CBA-CAA-C2A | 2.35 | 120.01 | 113.96 |
| 14 | A | 1134 | CLA | C2A-C1A-CHA | 2.35 | 127.58 | 123.80 |
| 17 | A | 4003 | BCR | C30-C25-C24 | 2.35 | 122.68 | 115.96 |
| 14 | B | 1211 | CLA | CED-O2D-CGD | 2.35 | 121.56 | 115.97 |
| 14 | A | 1135 | CLA | C2A-C1A-CHA | 2.35 | 127.59 | 123.80 |
| 17 | I | 4020 | BCR | C30-C25-C24 | 2.36 | 122.69 | 115.96 |
| 14 | B | 1202 | CLA | CED-O2D-CGD | 2.36 | 121.57 | 115.97 |
| 17 | J | 4012 | BCR | C35-C13-C12 | 2.36 | 121.94 | 118.08 |
| 17 | A | 4002 | BCR | C30-C25-C24 | 2.36 | 122.69 | 115.96 |
| 14 | M | 1601 | CLA | C2A-C1A-CHA | 2.36 | 127.60 | 123.80 |
| 14 | B | 1213 | CLA | CED-O2D-CGD | 2.36 | 121.58 | 115.97 |
| 14 | A | 1131 | CLA | CMB-C2B-C3B | 2.37 | 129.72 | 125.09 |
| 14 | B | 1230 | CLA | CBA-CAA-C2A | 2.37 | 120.06 | 113.96 |
| 14 | B | 1023 | CLA | O2D-CGD-CBD | 2.37 | 114.64 | 111.22 |
| 17 | A | 4003 | BCR | C1-C6-C7 | 2.37 | 122.73 | 115.96 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 14 | A | 1132 | CLA | CED-O2D-CGD | 2.37 | 121.60 | 115.97 |
| 14 | B | 1204 | CLA | C2A-C3A-C4A | 2.37 | 104.27 | 101.84 |
| 14 | A | 1113 | CLA | CMB-C2B-C3B | 2.37 | 129.73 | 125.09 |
| 17 | J | 4012 | BCR | C24-C23-C22 | 2.38 | 129.80 | 126.21 |
| 14 | A | 1137 | CLA | CED-O2D-CGD | 2.38 | 121.62 | 115.97 |
| 17 | F | 4016 | BCR | C7-C8-C9 | 2.38 | 129.81 | 126.21 |
| 17 | A | 4008 | BCR | C1-C6-C7 | 2.38 | 122.76 | 115.96 |
| 17 | I | 4020 | BCR | C36-C18-C19 | 2.38 | 121.98 | 118.08 |
| 17 | J | 4013 | BCR | C40-C30-C25 | 2.38 | 113.98 | 110.33 |
| 14 | A | 1132 | CLA | C2A-C3A-C4A | 2.39 | 104.28 | 101.84 |
| 14 | B | 1205 | CLA | C2A-C3A-C4A | 2.39 | 104.29 | 101.84 |
| 14 | A | 1117 | CLA | CBA-CAA-C2A | 2.39 | 120.13 | 113.96 |
| 14 | B | 1215 | CLA | CED-O2D-CGD | 2.39 | 121.66 | 115.97 |
| 14 | B | 1233 | CLA | C2A-C1A-CHA | 2.40 | 127.66 | 123.80 |
| 14 | A | 1113 | CLA | CED-O2D-CGD | 2.40 | 121.67 | 115.97 |
| 14 | A | 1118 | CLA | C2A-C1A-CHA | 2.40 | 127.67 | 123.80 |
| 14 | B | 1239 | CLA | C2A-C3A-C4A | 2.40 | 104.30 | 101.84 |
| 17 | A | 4011 | BCR | C1-C6-C7 | 2.41 | 122.83 | 115.96 |
| 17 | B | 4014 | BCR | C35-C13-C12 | 2.41 | 122.01 | 118.08 |
| 17 | B | 4017 | BCR | C34-C9-C8 | 2.41 | 122.01 | 118.08 |
| 14 | B | 1215 | CLA | C6-C5-C3 | 2.42 | 117.10 | 112.76 |
| 17 | B | 4014 | BCR | C23-C24-C25 | 2.42 | 134.26 | 127.24 |
| 17 | B | 4006 | BCR | C23-C24-C25 | 2.42 | 134.27 | 127.24 |
| 14 | A | 1123 | CLA | C2A-C3A-C4A | 2.42 | 104.32 | 101.84 |
| 14 | A | 1120 | CLA | CED-O2D-CGD | 2.42 | 121.73 | 115.97 |
| 17 | J | 4013 | BCR | C36-C18-C19 | 2.43 | 122.05 | 118.08 |
| 14 | B | 1228 | CLA | CED-O2D-CGD | 2.44 | 121.76 | 115.97 |
| 17 | M | 4021 | BCR | C8-C7-C6 | 2.44 | 134.33 | 127.24 |
| 17 | A | 4007 | BCR | C40-C30-C25 | 2.44 | 114.06 | 110.33 |
| 14 | A | 1111 | CLA | CED-O2D-CGD | 2.45 | 121.79 | 115.97 |
| 17 | A | 4002 | BCR | C24-C23-C22 | 2.45 | 129.91 | 126.21 |
| 17 | B | 4006 | BCR | C35-C13-C12 | 2.45 | 122.09 | 118.08 |
| 14 | B | 1209 | CLA | CED-O2D-CGD | 2.45 | 121.80 | 115.97 |
| 14 | B | 1239 | CLA | CBA-CAA-C2A | 2.46 | 120.29 | 113.96 |
| 17 | I | 4020 | BCR | C29-C30-C25 | 2.46 | 114.14 | 110.48 |
| 14 | A | 1124 | CLA | C2A-C3A-C4A | 2.46 | 104.36 | 101.84 |
| 14 | B | 1219 | CLA | C2A-C3A-C4A | 2.46 | 104.36 | 101.84 |
| 14 | A | 1105 | CLA | CED-O2D-CGD | 2.46 | 121.82 | 115.97 |
| 14 | B | 1207 | CLA | CED-O2D-CGD | 2.47 | 121.84 | 115.97 |
| 17 | A | 4002 | BCR | C7-C8-C9 | 2.47 | 129.94 | 126.21 |
| 14 | B | 1232 | CLA | C2A-C1A-CHA | 2.48 | 127.79 | 123.80 |
| 14 | A | 1129 | CLA | CED-O2D-CGD | 2.48 | 121.86 | 115.97 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 14 | A | 1116 | CLA | CBA-CAA-C2A | 2.48 | 120.36 | 113.96 |
| 14 | B | 1021 | CLA | O2D-CGD-CBD | 2.49 | 114.81 | 111.22 |
| 14 | B | 1210 | CLA | CED-O2D-CGD | 2.49 | 121.89 | 115.97 |
| 14 | B | 1218 | CLA | C2A-C1A-CHA | 2.50 | 127.83 | 123.80 |
| 14 | B | 1210 | CLA | CMB-C2B-C3B | 2.50 | 129.98 | 125.09 |
| 17 | B | 4014 | BCR | C34-C9-C8 | 2.51 | 122.18 | 118.08 |
| 17 | B | 4009 | BCR | C35-C13-C12 | 2.51 | 120.71 | 114.61 |
| 14 | B | 1021 | CLA | C6-C5-C3 | 2.51 | 117.27 | 112.76 |
| 14 | B | 1225 | CLA | CED-O2D-CGD | 2.51 | 121.94 | 115.97 |
| 17 | B | 4010 | BCR | C30-C25-C24 | 2.52 | 123.15 | 115.96 |
| 14 | A | 1119 | CLA | O2A-CGA-CBA | 2.52 | 119.61 | 111.85 |
| 14 | A | 1134 | CLA | CED-O2D-CGD | 2.52 | 121.96 | 115.97 |
| 14 | B | 1217 | CLA | C2A-C1A-CHA | 2.52 | 127.86 | 123.80 |
| 14 | A | 1801 | CLA | CED-O2D-CGD | 2.52 | 121.97 | 115.97 |
| 14 | B | 1223 | CLA | CMB-C2B-C3B | 2.52 | 130.03 | 125.09 |
| 17 | J | 4013 | BCR | C23-C24-C25 | 2.53 | 134.57 | 127.24 |
| 14 | A | 1133 | CLA | C6-C5-C3 | 2.53 | 117.30 | 112.76 |
| 14 | B | 1213 | CLA | C2A-C3A-C4A | 2.53 | 104.43 | 101.84 |
| 14 | B | 1222 | CLA | CMB-C2B-C3B | 2.53 | 130.03 | 125.09 |
| 14 | B | 1216 | CLA | CED-O2D-CGD | 2.53 | 121.99 | 115.97 |
| 17 | A | 4007 | BCR | C32-C1-C6 | 2.53 | 114.20 | 110.33 |
| 14 | B | 1206 | CLA | CED-O2D-CGD | 2.54 | 122.00 | 115.97 |
| 14 | B | 1238 | CLA | C2A-C3A-C4A | 2.54 | 104.44 | 101.84 |
| 14 | A | 1022 | CLA | O2A-CGA-CBA | 2.54 | 119.66 | 111.85 |
| 14 | A | 1115 | CLA | CED-O2D-CGD | 2.54 | 122.00 | 115.97 |
| 14 | J | 1302 | CLA | C2A-C1A-CHA | 2.54 | 127.89 | 123.80 |
| 14 | A | 1115 | CLA | C2A-C3A-C4A | 2.54 | 104.45 | 101.84 |
| 14 | B | 1201 | CLA | C2A-C3A-C4A | 2.55 | 104.45 | 101.84 |
| 17 | J | 4012 | BCR | C1-C6-C7 | 2.55 | 123.24 | 115.96 |
| 14 | F | 1301 | CLA | C2A-C1A-CHA | 2.55 | 127.90 | 123.80 |
| 19 | B | 5002 | LMG | C7-O1-C1 | 2.56 | 119.15 | 113.81 |
| 14 | A | 1104 | CLA | O2D-CGD-CBD | 2.56 | 114.91 | 111.22 |
| 17 | I | 4020 | BCR | C37-C22-C23 | 2.56 | 122.27 | 118.08 |
| 17 | A | 4011 | BCR | C15-C14-C13 | 2.56 | 130.95 | 127.22 |
| 17 | I | 4020 | BCR | C3-C4-C5 | 2.57 | 118.13 | 113.87 |
| 17 | B | 4010 | BCR | C36-C18-C19 | 2.57 | 122.28 | 118.08 |
| 14 | B | 1214 | CLA | CED-O2D-CGD | 2.57 | 122.08 | 115.97 |
| 14 | A | 1801 | CLA | C2A-C1A-CHA | 2.57 | 127.94 | 123.80 |
| 14 | A | 1108 | CLA | CED-O2D-CGD | 2.57 | 122.08 | 115.97 |
| 14 | A | 1110 | CLA | C2A-C3A-C4A | 2.57 | 104.48 | 101.84 |
| 14 | A | 1117 | CLA | CMB-C2B-C3B | 2.58 | 130.12 | 125.09 |
| 14 | A | 1124 | CLA | CMB-C2B-C3B | 2.58 | 130.13 | 125.09 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 14 | A | 1133 | CLA | CED-O2D-CGD | 2.58 | 122.10 | 115.97 |
| 14 | A | 1119 | CLA | CAA-CBA-CGA | 2.58 | 120.74 | 113.28 |
| 17 | B | 4010 | BCR | C16-C17-C18 | 2.59 | 130.98 | 127.22 |
| 17 | I | 4018 | BCR | C23-C24-C25 | 2.60 | 134.79 | 127.24 |
| 14 | A | 1104 | CLA | CMB-C2B-C3B | 2.60 | 130.18 | 125.09 |
| 14 | B | 1221 | CLA | C2A-C1A-CHA | 2.61 | 128.00 | 123.80 |
| 14 | M | 1601 | CLA | C2A-C3A-C4A | 2.61 | 104.51 | 101.84 |
| 17 | A | 4011 | BCR | C30-C25-C24 | 2.61 | 123.42 | 115.96 |
| 14 | A | 1114 | CLA | C2A-C3A-C4A | 2.61 | 104.52 | 101.84 |
| 17 | L | 4019 | BCR | C8-C7-C6 | 2.61 | 134.83 | 127.24 |
| 14 | A | 1112 | CLA | CED-O2D-CGD | 2.61 | 122.18 | 115.97 |
| 14 | A | 1116 | CLA | CED-O2D-CGD | 2.62 | 122.19 | 115.97 |
| 17 | A | 4001 | BCR | C8-C7-C6 | 2.62 | 134.85 | 127.24 |
| 14 | A | 1109 | CLA | CED-O2D-CGD | 2.63 | 122.21 | 115.97 |
| 14 | B | 1225 | CLA | CBA-CAA-C2A | 2.63 | 120.73 | 113.96 |
| 17 | A | 4008 | BCR | C23-C24-C25 | 2.63 | 134.87 | 127.24 |
| 14 | A | 1140 | CLA | CED-O2D-CGD | 2.63 | 122.21 | 115.97 |
| 17 | B | 4005 | BCR | C32-C1-C6 | 2.63 | 114.35 | 110.33 |
| 14 | A | 1108 | CLA | C2A-C3A-C4A | 2.63 | 104.54 | 101.84 |
| 17 | B | 4010 | BCR | C32-C1-C6 | 2.64 | 114.36 | 110.33 |
| 14 | A | 1103 | CLA | CED-O2D-CGD | 2.64 | 122.23 | 115.97 |
| 17 | A | 4008 | BCR | C11-C10-C9 | 2.64 | 131.05 | 127.22 |
| 14 | A | 1101 | CLA | C2A-C3A-C4A | 2.64 | 104.54 | 101.84 |
| 17 | I | 4018 | BCR | C36-C18-C19 | 2.64 | 122.40 | 118.08 |
| 14 | A | 1134 | CLA | C2A-C3A-C4A | 2.64 | 104.55 | 101.84 |
| 14 | A | 1130 | CLA | CED-O2D-CGD | 2.64 | 122.25 | 115.97 |
| 14 | A | 1140 | CLA | C6-C5-C3 | 2.65 | 117.52 | 112.76 |
| 14 | B | 1221 | CLA | C6-C5-C3 | 2.65 | 117.52 | 112.76 |
| 14 | B | 1238 | CLA | O2A-CGA-CBA | 2.65 | 120.02 | 111.85 |
| 14 | B | 1232 | CLA | CED-O2D-CGD | 2.66 | 122.28 | 115.97 |
| 14 | B | 1021 | CLA | CED-O2D-CGD | 2.66 | 122.28 | 115.97 |
| 17 | L | 4022 | BCR | C8-C7-C6 | 2.66 | 134.97 | 127.24 |
| 17 | B | 4006 | BCR | C28-C27-C26 | 2.67 | 118.29 | 113.87 |
| 17 | B | 4005 | BCR | C1-C6-C7 | 2.68 | 123.60 | 115.96 |
| 14 | A | 1117 | CLA | CED-O2D-CGD | 2.68 | 122.33 | 115.97 |
| 14 | B | 1230 | CLA | C2A-C3A-C4A | 2.68 | 104.59 | 101.84 |
| 14 | J | 1302 | CLA | CED-O2D-CGD | 2.68 | 122.34 | 115.97 |
| 17 | L | 4019 | BCR | C29-C30-C25 | 2.68 | 114.47 | 110.48 |
| 14 | B | 1218 | CLA | CED-O2D-CGD | 2.68 | 122.35 | 115.97 |
| 14 | A | 1106 | CLA | C2A-C3A-C4A | 2.69 | 104.59 | 101.84 |
| 14 | B | 1210 | CLA | C2A-C3A-C4A | 2.69 | 104.59 | 101.84 |
| 14 | A | 1127 | CLA | CMB-C2B-C3B | 2.69 | 130.36 | 125.09 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 14 | B | 1219 | CLA | CED-O2D-CGD | 2.70 | 122.38 | 115.97 |
| 14 | B | 1215 | CLA | C2A-C3A-C4A | 2.70 | 104.61 | 101.84 |
| 17 | A | 4007 | BCR | C30-C25-C24 | 2.71 | 123.70 | 115.96 |
| 14 | B | 1231 | CLA | CED-O2D-CGD | 2.71 | 122.41 | 115.97 |
| 14 | A | 1104 | CLA | C2A-C1A-CHA | 2.72 | 128.18 | 123.80 |
| 14 | B | 1230 | CLA | CED-O2D-CGD | 2.72 | 122.44 | 115.97 |
| 14 | B | 1218 | CLA | C2A-C3A-C4A | 2.72 | 104.63 | 101.84 |
| 14 | A | 1128 | CLA | O2A-CGA-CBA | 2.72 | 120.23 | 111.85 |
| 14 | K | 1401 | CLA | C2A-C3A-C4A | 2.73 | 104.63 | 101.84 |
| 14 | B | 1236 | CLA | C2A-C3A-C4A | 2.74 | 104.64 | 101.84 |
| 14 | B | 1212 | CLA | C2A-C3A-C4A | 2.74 | 104.64 | 101.84 |
| 14 | B | 1012 | CLA | C2A-C3A-C4A | 2.74 | 104.65 | 101.84 |
| 14 | B | 1217 | CLA | CED-O2D-CGD | 2.74 | 122.48 | 115.97 |
| 17 | I | 4018 | BCR | C29-C30-C25 | 2.74 | 114.56 | 110.48 |
| 17 | B | 4005 | BCR | C20-C21-C22 | 2.75 | 131.22 | 127.22 |
| 17 | J | 4012 | BCR | C36-C18-C19 | 2.75 | 122.58 | 118.08 |
| 14 | B | 1221 | CLA | CED-O2D-CGD | 2.75 | 122.51 | 115.97 |
| 14 | A | 1129 | CLA | C2A-C3A-C4A | 2.75 | 104.66 | 101.84 |
| 14 | B | 1012 | CLA | C2A-C1A-CHA | 2.76 | 128.24 | 123.80 |
| 17 | J | 4013 | BCR | C30-C25-C24 | 2.76 | 123.85 | 115.96 |
| 17 | A | 4001 | BCR | C23-C24-C25 | 2.76 | 135.26 | 127.24 |
| 14 | B | 1234 | CLA | O2A-CGA-CBA | 2.77 | 120.36 | 111.85 |
| 14 | B | 1234 | CLA | C2A-C3A-C4A | 2.77 | 104.67 | 101.84 |
| 17 | M | 4021 | BCR | C1-C6-C7 | 2.77 | 123.89 | 115.96 |
| 14 | A | 1138 | CLA | C2A-C3A-C4A | 2.78 | 104.68 | 101.84 |
| 14 | B | 1208 | CLA | CED-O2D-CGD | 2.78 | 122.57 | 115.97 |
| 14 | A | 1013 | CLA | O2D-CGD-CBD | 2.78 | 115.23 | 111.22 |
| 17 | J | 4012 | BCR | C8-C7-C6 | 2.78 | 135.31 | 127.24 |
| 14 | B | 1023 | CLA | CED-O2D-CGD | 2.78 | 122.58 | 115.97 |
| 14 | F | 1301 | CLA | C2A-C3A-C4A | 2.79 | 104.70 | 101.84 |
| 14 | A | 1105 | CLA | C2A-C3A-C4A | 2.79 | 104.70 | 101.84 |
| 14 | B | 1227 | CLA | C2A-C3A-C4A | 2.80 | 104.70 | 101.84 |
| 17 | I | 4020 | BCR | C7-C8-C9 | 2.80 | 130.44 | 126.21 |
| 14 | B | 1203 | CLA | O2A-CGA-CBA | 2.80 | 120.47 | 111.85 |
| 17 | B | 4014 | BCR | C15-C14-C13 | 2.81 | 131.30 | 127.22 |
| 17 | B | 4005 | BCR | C23-C24-C25 | 2.81 | 135.40 | 127.24 |
| 17 | B | 4014 | BCR | C32-C1-C6 | 2.81 | 114.63 | 110.33 |
| 17 | B | 4010 | BCR | C29-C30-C25 | 2.82 | 114.67 | 110.48 |
| 14 | B | 1235 | CLA | CED-O2D-CGD | 2.82 | 122.66 | 115.97 |
| 14 | A | 1133 | CLA | C2A-C3A-C4A | 2.82 | 104.73 | 101.84 |
| 14 | A | 1132 | CLA | O2A-CGA-CBA | 2.82 | 120.54 | 111.85 |
| 14 | A | 1104 | CLA | CED-O2D-CGD | 2.83 | 122.69 | 115.97 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 14 | L | 1503 | CLA | C2A-C3A-C4A | 2.83 | 104.74 | 101.84 |
| 17 | L | 4019 | BCR | C30-C25-C24 | 2.83 | 124.05 | 115.96 |
| 17 | L | 4019 | BCR | C40-C30-C25 | 2.83 | 114.66 | 110.33 |
| 14 | B | 1216 | CLA | C2A-C3A-C4A | 2.83 | 104.74 | 101.84 |
| 14 | B | 1217 | CLA | C2A-C3A-C4A | 2.84 | 104.75 | 101.84 |
| 14 | B | 1206 | CLA | C2A-C3A-C4A | 2.84 | 104.75 | 101.84 |
| 14 | A | 1112 | CLA | C2A-C3A-C4A | 2.84 | 104.75 | 101.84 |
| 17 | A | 4001 | BCR | C24-C23-C22 | 2.84 | 130.51 | 126.21 |
| 14 | M | 1601 | CLA | CED-O2D-CGD | 2.84 | 122.73 | 115.97 |
| 17 | L | 4022 | BCR | C29-C30-C25 | 2.85 | 114.72 | 110.48 |
| 14 | A | 1121 | CLA | C2A-C3A-C4A | 2.85 | 104.76 | 101.84 |
| 14 | A | 1109 | CLA | C2A-C3A-C4A | 2.85 | 104.76 | 101.84 |
| 14 | A | 1114 | CLA | CED-O2D-CGD | 2.86 | 122.77 | 115.97 |
| 14 | B | 1220 | CLA | C2A-C3A-C4A | 2.87 | 104.78 | 101.84 |
| 14 | A | 1102 | CLA | C2A-C3A-C4A | 2.88 | 104.79 | 101.84 |
| 17 | F | 4016 | BCR | C24-C23-C22 | 2.88 | 130.56 | 126.21 |
| 14 | B | 1215 | CLA | CMB-C2B-C3B | 2.88 | 130.72 | 125.09 |
| 17 | A | 4003 | BCR | C7-C8-C9 | 2.88 | 130.56 | 126.21 |
| 14 | B | 1203 | CLA | C2A-C3A-C4A | 2.89 | 104.80 | 101.84 |
| 14 | A | 1013 | CLA | CED-O2D-CGD | 2.90 | 122.85 | 115.97 |
| 14 | A | 1022 | CLA | C2A-C3A-C4A | 2.90 | 104.81 | 101.84 |
| 14 | A | 1801 | CLA | C2A-C3A-C4A | 2.90 | 104.81 | 101.84 |
| 14 | J | 1302 | CLA | C2A-C3A-C4A | 2.90 | 104.81 | 101.84 |
| 14 | A | 1131 | CLA | O2A-CGA-CBA | 2.91 | 120.80 | 111.85 |
| 14 | A | 1139 | CLA | C2A-C3A-C4A | 2.91 | 104.82 | 101.84 |
| 17 | A | 4011 | BCR | C32-C1-C6 | 2.91 | 114.78 | 110.33 |
| 14 | A | 1402 | CLA | OBD-CAD-C3D | 2.92 | 130.35 | 127.44 |
| 14 | A | 1107 | CLA | C2A-C1A-CHA | 2.92 | 128.50 | 123.80 |
| 17 | I | 4020 | BCR | C32-C1-C6 | 2.92 | 114.80 | 110.33 |
| 14 | A | 1116 | CLA | C2A-C3A-C4A | 2.92 | 104.83 | 101.84 |
| 18 | A | 5003 | LHG | O7-C7-C8 | 2.93 | 117.69 | 111.53 |
| 14 | B | 1221 | CLA | C2A-C3A-C4A | 2.93 | 104.84 | 101.84 |
| 14 | A | 1124 | CLA | O2A-CGA-CBA | 2.93 | 120.87 | 111.85 |
| 17 | B | 4009 | BCR | C40-C30-C25 | 2.93 | 114.81 | 110.33 |
| 17 | I | 4018 | BCR | C7-C8-C9 | 2.93 | 130.64 | 126.21 |
| 14 | A | 1136 | CLA | O2D-CGD-CBD | 2.94 | 115.46 | 111.22 |
| 14 | B | 1209 | CLA | C2A-C3A-C4A | 2.94 | 104.85 | 101.84 |
| 17 | A | 4008 | BCR | C2-C1-C6 | 2.94 | 114.86 | 110.48 |
| 14 | A | 1137 | CLA | C2A-C3A-C4A | 2.95 | 104.86 | 101.84 |
| 14 | B | 1211 | CLA | O2A-CGA-CBA | 2.95 | 120.93 | 111.85 |
| 17 | A | 4011 | BCR | C16-C17-C18 | 2.95 | 131.51 | 127.22 |
| 17 | B | 4006 | BCR | C24-C23-C22 | 2.96 | 130.67 | 126.21 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 14 | B | 1208 | CLA | C2A-C3A-C4A | 2.96 | 104.87 | 101.84 |
| 17 | B | 4010 | BCR | C24-C23-C22 | 2.97 | 130.70 | 126.21 |
| 14 | A | 1138 | CLA | CED-O2D-CGD | 2.97 | 123.03 | 115.97 |
| 14 | A | 1128 | CLA | C2A-C3A-C4A | 2.98 | 104.89 | 101.84 |
| 14 | B | 1207 | CLA | C2A-C1A-CHA | 2.98 | 128.60 | 123.80 |
| 14 | A | 1113 | CLA | C2A-C3A-C4A | 2.98 | 104.89 | 101.84 |
| 14 | L | 1503 | CLA | O2A-CGA-CBA | 2.99 | 121.04 | 111.85 |
| 14 | B | 1226 | CLA | CMB-C2B-C3B | 2.99 | 130.94 | 125.09 |
| 17 | B | 4009 | BCR | C24-C23-C22 | 2.99 | 130.73 | 126.21 |
| 14 | L | 1502 | CLA | O2A-CGA-CBA | 3.00 | 121.08 | 111.85 |
| 14 | A | 1119 | CLA | CED-O2D-CGD | 3.00 | 123.09 | 115.97 |
| 14 | A | 1115 | CLA | O2A-CGA-CBA | 3.00 | 121.09 | 111.85 |
| 18 | A | 5001 | LHG | O7-C7-C8 | 3.00 | 117.86 | 111.53 |
| 17 | A | 4002 | BCR | C29-C30-C25 | 3.01 | 114.95 | 110.48 |
| 17 | B | 4017 | BCR | C29-C30-C25 | 3.01 | 114.95 | 110.48 |
| 14 | B | 1238 | CLA | CED-O2D-CGD | 3.02 | 123.13 | 115.97 |
| 14 | A | 1135 | CLA | C2A-C3A-C4A | 3.02 | 104.93 | 101.84 |
| 14 | A | 1127 | CLA | C2A-C3A-C4A | 3.02 | 104.93 | 101.84 |
| 14 | B | 1230 | CLA | O2A-CGA-CBA | 3.02 | 121.14 | 111.85 |
| 14 | B | 1206 | CLA | O2A-CGA-CBA | 3.02 | 121.15 | 111.85 |
| 14 | A | 1122 | CLA | C2A-C3A-C4A | 3.02 | 104.94 | 101.84 |
| 14 | A | 1122 | CLA | O2A-CGA-CBA | 3.03 | 121.17 | 111.85 |
| 14 | B | 1228 | CLA | O2A-CGA-CBA | 3.03 | 121.18 | 111.85 |
| 17 | B | 4004 | BCR | C7-C8-C9 | 3.04 | 130.80 | 126.21 |
| 17 | B | 4017 | BCR | C7-C8-C9 | 3.04 | 130.80 | 126.21 |
| 14 | B | 1239 | CLA | O2A-CGA-CBA | 3.05 | 121.23 | 111.85 |
| 17 | L | 4019 | BCR | C2-C1-C6 | 3.05 | 115.02 | 110.48 |
| 18 | B | 5004 | LHG | O7-C7-C8 | 3.06 | 117.98 | 111.53 |
| 17 | L | 4019 | BCR | C24-C23-C22 | 3.07 | 130.84 | 126.21 |
| 14 | B | 1232 | CLA | O2D-CGD-CBD | 3.07 | 115.64 | 111.22 |
| 14 | B | 1219 | CLA | O2A-CGA-CBA | 3.07 | 121.31 | 111.85 |
| 14 | B | 1216 | CLA | O2A-CGA-CBA | 3.07 | 121.31 | 111.85 |
| 14 | A | 1237 | CLA | C2A-C3A-C4A | 3.08 | 104.99 | 101.84 |
| 17 | A | 4003 | BCR | C40-C30-C25 | 3.08 | 115.04 | 110.33 |
| 14 | B | 1223 | CLA | C2A-C3A-C4A | 3.09 | 105.00 | 101.84 |
| 17 | B | 4009 | BCR | C29-C30-C25 | 3.09 | 115.08 | 110.48 |
| 14 | B | 1221 | CLA | O2A-CGA-CBA | 3.10 | 121.38 | 111.85 |
| 14 | B | 1021 | CLA | O2A-CGA-CBA | 3.10 | 121.40 | 111.85 |
| 14 | A | 1118 | CLA | C2A-C3A-C4A | 3.11 | 105.02 | 101.84 |
| 14 | A | 1123 | CLA | O2A-CGA-CBA | 3.11 | 121.43 | 111.85 |
| 14 | A | 1119 | CLA | C2A-C3A-C4A | 3.11 | 105.03 | 101.84 |
| 14 | A | 1138 | CLA | O2D-CGD-CBD | 3.12 | 115.72 | 111.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 14 | B | 1226 | CLA | O2A-CGA-CBA | 3.12 | 121.45 | 111.85 |
| 14 | A | 1119 | CLA | CMB-C2B-C3B | 3.12 | 131.20 | 125.09 |
| 14 | B | 1225 | CLA | C5-C3-C2 | 3.13 | 126.81 | 120.98 |
| 17 | B | 4005 | BCR | C2-C1-C6 | 3.13 | 115.14 | 110.48 |
| 14 | B | 1023 | CLA | C2A-C3A-C4A | 3.13 | 105.05 | 101.84 |
| 14 | L | 1502 | CLA | C2A-C3A-C4A | 3.14 | 105.06 | 101.84 |
| 17 | A | 4001 | BCR | C2-C1-C6 | 3.14 | 115.16 | 110.48 |
| 14 | B | 1233 | CLA | C2A-C3A-C4A | 3.14 | 105.06 | 101.84 |
| 14 | B | 1023 | CLA | O2A-CGA-CBA | 3.15 | 121.53 | 111.85 |
| 14 | B | 1211 | CLA | C2A-C3A-C4A | 3.15 | 105.07 | 101.84 |
| 14 | B | 1021 | CLA | C2A-C3A-C4A | 3.16 | 105.08 | 101.84 |
| 18 | A | 5003 | LHG | O8-C23-C24 | 3.16 | 120.59 | 111.16 |
| 19 | B | 5002 | LMG | O8-C28-C29 | 3.17 | 121.60 | 111.85 |
| 14 | B | 1236 | CLA | O2A-CGA-CBA | 3.17 | 121.61 | 111.85 |
| 17 | B | 4004 | BCR | C23-C24-C25 | 3.18 | 136.49 | 127.24 |
| 14 | A | 1111 | CLA | C2A-C3A-C4A | 3.18 | 105.10 | 101.84 |
| 17 | J | 4013 | BCR | C7-C8-C9 | 3.18 | 131.02 | 126.21 |
| 14 | B | 1226 | CLA | C2A-C3A-C4A | 3.18 | 105.10 | 101.84 |
| 14 | B | 1232 | CLA | C2A-C3A-C4A | 3.20 | 105.12 | 101.84 |
| 17 | A | 4007 | BCR | C2-C1-C6 | 3.20 | 115.24 | 110.48 |
| 14 | A | 1119 | CLA | O2D-CGD-CBD | 3.20 | 115.84 | 111.22 |
| 14 | B | 1012 | CLA | O2A-CGA-CBA | 3.20 | 121.70 | 111.85 |
| 14 | X | 1701 | CLA | C2A-C3A-C4A | 3.21 | 105.13 | 101.84 |
| 14 | B | 1214 | CLA | C2A-C3A-C4A | 3.21 | 105.13 | 101.84 |
| 17 | A | 4003 | BCR | C2-C1-C6 | 3.22 | 115.27 | 110.48 |
| 14 | A | 1104 | CLA | CBA-CAA-C2A | 3.22 | 122.26 | 113.96 |
| 17 | J | 4012 | BCR | C23-C24-C25 | 3.22 | 136.60 | 127.24 |
| 14 | B | 1210 | CLA | O2A-CGA-CBA | 3.22 | 121.77 | 111.85 |
| 14 | B | 1202 | CLA | O2A-CGA-CBA | 3.22 | 121.77 | 111.85 |
| 14 | B | 1229 | CLA | O2A-CGA-CBA | 3.23 | 121.78 | 111.85 |
| 14 | A | 1136 | CLA | O2A-CGA-CBA | 3.24 | 121.82 | 111.85 |
| 14 | A | 1103 | CLA | O2A-CGA-CBA | 3.24 | 121.84 | 111.85 |
| 14 | A | 1111 | CLA | O2A-CGA-CBA | 3.25 | 121.86 | 111.85 |
| 14 | A | 1125 | CLA | C2A-C3A-C4A | 3.25 | 105.17 | 101.84 |
| 17 | B | 4004 | BCR | C24-C23-C22 | 3.26 | 131.13 | 126.21 |
| 17 | B | 4004 | BCR | C29-C30-C25 | 3.26 | 115.33 | 110.48 |
| 14 | B | 1223 | CLA | O2A-CGA-CBA | 3.26 | 121.88 | 111.85 |
| 17 | A | 4007 | BCR | C29-C30-C25 | 3.26 | 115.33 | 110.48 |
| 14 | A | 1133 | CLA | O2A-CGA-CBA | 3.27 | 121.92 | 111.85 |
| 14 | A | 1131 | CLA | C2A-C3A-C4A | 3.29 | 105.21 | 101.84 |
| 17 | J | 4013 | BCR | C38-C26-C25 | 3.29 | 128.13 | 124.62 |
| 14 | A | 1130 | CLA | O2A-CGA-CBA | 3.30 | 121.99 | 111.85 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 14 | B | 1238 | CLA | O2D-CGD-CBD | 3.30 | 115.98 | 111.22 |
| 14 | A | 1109 | CLA | O2D-CGD-CBD | 3.30 | 115.98 | 111.22 |
| 14 | A | 1011 | CLA | O2A-CGA-CBA | 3.31 | 122.02 | 111.85 |
| 17 | F | 4016 | BCR | C29-C30-C25 | 3.31 | 115.40 | 110.48 |
| 14 | A | 1013 | CLA | C2A-C3A-C4A | 3.31 | 105.23 | 101.84 |
| 14 | A | 1138 | CLA | O2A-CGA-CBA | 3.31 | 122.04 | 111.85 |
| 14 | J | 1303 | CLA | OBD-CAD-C3D | 3.31 | 130.75 | 127.44 |
| 18 | A | 5001 | LHG | O8-C23-C24 | 3.31 | 122.04 | 111.85 |
| 17 | M | 4021 | BCR | C29-C30-C25 | 3.31 | 115.41 | 110.48 |
| 14 | B | 1204 | CLA | O2A-CGA-CBA | 3.31 | 122.05 | 111.85 |
| 14 | B | 1207 | CLA | O2A-CGA-CBA | 3.32 | 122.06 | 111.85 |
| 14 | A | 1126 | CLA | O2A-CGA-CBA | 3.33 | 122.11 | 111.85 |
| 14 | A | 1402 | CLA | C2A-C3A-C4A | 3.34 | 105.26 | 101.84 |
| 14 | A | 1129 | CLA | O2A-CGA-CBA | 3.34 | 122.12 | 111.85 |
| 14 | A | 1114 | CLA | O2A-CGA-CBA | 3.34 | 122.14 | 111.85 |
| 14 | A | 1101 | CLA | O2A-CGA-CBA | 3.35 | 122.14 | 111.85 |
| 17 | A | 4008 | BCR | C29-C30-C25 | 3.35 | 115.46 | 110.48 |
| 14 | A | 1120 | CLA | C2A-C3A-C4A | 3.36 | 105.28 | 101.84 |
| 14 | B | 1205 | CLA | C4A-NA-C1A | 3.37 | 110.65 | 106.38 |
| 17 | F | 4016 | BCR | C2-C1-C6 | 3.38 | 115.51 | 110.48 |
| 14 | B | 1235 | CLA | O2A-CGA-CBA | 3.38 | 122.26 | 111.85 |
| 17 | L | 4022 | BCR | C2-C1-C6 | 3.39 | 115.52 | 110.48 |
| 14 | L | 1501 | CLA | O2A-CGA-CBA | 3.39 | 122.30 | 111.85 |
| 17 | A | 4008 | BCR | C24-C23-C22 | 3.39 | 131.34 | 126.21 |
| 14 | B | 1225 | CLA | C4A-NA-C1A | 3.40 | 110.69 | 106.38 |
| 14 | A | 1102 | CLA | O2A-CGA-CBA | 3.40 | 122.31 | 111.85 |
| 17 | B | 4009 | BCR | C20-C21-C22 | 3.40 | 132.17 | 127.22 |
| 14 | A | 1237 | CLA | O2D-CGD-CBD | 3.40 | 116.13 | 111.22 |
| 14 | A | 1130 | CLA | C2A-C3A-C4A | 3.41 | 105.33 | 101.84 |
| 17 | F | 4016 | BCR | C15-C14-C13 | 3.41 | 132.18 | 127.22 |
| 17 | J | 4015 | BCR | C29-C30-C25 | 3.41 | 115.56 | 110.48 |
| 14 | B | 1202 | CLA | C2A-C3A-C4A | 3.42 | 105.34 | 101.84 |
| 17 | B | 4010 | BCR | C2-C1-C6 | 3.42 | 115.57 | 110.48 |
| 17 | B | 4006 | BCR | C2-C1-C6 | 3.43 | 115.58 | 110.48 |
| 17 | M | 4021 | BCR | C2-C1-C6 | 3.43 | 115.59 | 110.48 |
| 17 | B | 4017 | BCR | C2-C1-C6 | 3.43 | 115.59 | 110.48 |
| 17 | A | 4001 | BCR | C29-C30-C25 | 3.46 | 115.62 | 110.48 |
| 14 | A | 1109 | CLA | O2A-CGA-CBA | 3.46 | 122.50 | 111.85 |
| 17 | B | 4014 | BCR | C29-C30-C25 | 3.46 | 115.64 | 110.48 |
| 14 | A | 1022 | CLA | C4A-NA-C1A | 3.47 | 110.78 | 106.38 |
| 17 | B | 4014 | BCR | C2-C1-C6 | 3.47 | 115.64 | 110.48 |
| 14 | B | 1225 | CLA | O2D-CGD-CBD | 3.48 | 116.24 | 111.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 17 | A | 4002 | BCR | C2-C1-C6 | 3.48 | 115.66 | 110.48 |
| 14 | A | 1011 | CLA | C4A-NA-C1A | 3.49 | 110.81 | 106.38 |
| 17 | A | 4011 | BCR | C29-C30-C25 | 3.50 | 115.69 | 110.48 |
| 14 | A | 1125 | CLA | O2A-CGA-CBA | 3.50 | 122.62 | 111.85 |
| 14 | A | 1126 | CLA | O2D-CGD-CBD | 3.50 | 116.27 | 111.22 |
| 14 | B | 1202 | CLA | C4A-NA-C1A | 3.52 | 110.84 | 106.38 |
| 17 | J | 4015 | BCR | C24-C23-C22 | 3.54 | 131.56 | 126.21 |
| 17 | J | 4012 | BCR | C2-C1-C6 | 3.54 | 115.75 | 110.48 |
| 14 | B | 1213 | CLA | O2A-CGA-CBA | 3.55 | 122.79 | 111.85 |
| 17 | A | 4003 | BCR | C24-C23-C22 | 3.57 | 131.60 | 126.21 |
| 14 | A | 1117 | CLA | O2D-CGD-CBD | 3.57 | 116.37 | 111.22 |
| 17 | B | 4005 | BCR | C29-C30-C25 | 3.58 | 115.81 | 110.48 |
| 14 | B | 1214 | CLA | O2D-CGD-CBD | 3.58 | 116.38 | 111.22 |
| 14 | B | 1210 | CLA | C4A-NA-C1A | 3.59 | 110.93 | 106.38 |
| 14 | B | 1208 | CLA | O2D-CGD-CBD | 3.60 | 116.41 | 111.22 |
| 14 | B | 1201 | CLA | O2A-CGA-CBA | 3.60 | 122.92 | 111.85 |
| 17 | A | 4007 | BCR | C24-C23-C22 | 3.61 | 131.66 | 126.21 |
| 14 | A | 1106 | CLA | O2A-CGA-CBA | 3.61 | 122.95 | 111.85 |
| 14 | A | 1105 | CLA | O2A-CGA-CBA | 3.61 | 122.95 | 111.85 |
| 14 | A | 1237 | CLA | C4A-NA-C1A | 3.61 | 110.96 | 106.38 |
| 14 | B | 1203 | CLA | O2D-CGD-CBD | 3.61 | 116.43 | 111.22 |
| 14 | A | 1140 | CLA | O2D-CGD-CBD | 3.62 | 116.44 | 111.22 |
| 14 | A | 1126 | CLA | C4A-NA-C1A | 3.63 | 110.98 | 106.38 |
| 14 | A | 1137 | CLA | C4A-NA-C1A | 3.64 | 110.99 | 106.38 |
| 14 | B | 1012 | CLA | C4A-NA-C1A | 3.64 | 111.00 | 106.38 |
| 17 | B | 4010 | BCR | C7-C8-C9 | 3.64 | 131.71 | 126.21 |
| 14 | B | 1203 | CLA | C4A-NA-C1A | 3.64 | 111.00 | 106.38 |
| 14 | A | 1013 | CLA | C4A-NA-C1A | 3.65 | 111.00 | 106.38 |
| 14 | A | 1132 | CLA | C4A-NA-C1A | 3.65 | 111.01 | 106.38 |
| 14 | B | 1236 | CLA | C4A-NA-C1A | 3.66 | 111.02 | 106.38 |
| 14 | A | 1110 | CLA | O2A-CGA-CBA | 3.66 | 123.12 | 111.85 |
| 17 | A | 4008 | BCR | C33-C5-C6 | 3.66 | 128.53 | 124.62 |
| 14 | B | 1236 | CLA | O2D-CGD-CBD | 3.67 | 116.51 | 111.22 |
| 14 | A | 1116 | CLA | O2A-CGA-CBA | 3.67 | 123.13 | 111.85 |
| 17 | B | 4005 | BCR | C24-C23-C22 | 3.68 | 131.77 | 126.21 |
| 17 | J | 4013 | BCR | C29-C30-C25 | 3.68 | 115.95 | 110.48 |
| 14 | B | 1214 | CLA | O2A-CGA-CBA | 3.69 | 123.21 | 111.85 |
| 17 | I | 4020 | BCR | C33-C5-C6 | 3.69 | 128.56 | 124.62 |
| 17 | J | 4013 | BCR | C2-C1-C6 | 3.70 | 115.98 | 110.48 |
| 14 | A | 1128 | CLA | C4A-NA-C1A | 3.71 | 111.09 | 106.38 |
| 14 | A | 1108 | CLA | O2D-CGD-CBD | 3.72 | 116.58 | 111.22 |
| 14 | B | 1023 | CLA | C4A-NA-C1A | 3.72 | 111.10 | 106.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 14 | A | 1011 | CLA | OBD-CAD-C3D | 3.73 | 134.69 | 128.09 |
| 14 | A | 1103 | CLA | C4A-NA-C1A | 3.73 | 111.11 | 106.38 |
| 14 | B | 1217 | CLA | O2A-CGA-CBA | 3.73 | 123.34 | 111.85 |
| 14 | B | 1238 | CLA | C4A-NA-C1A | 3.73 | 111.12 | 106.38 |
| 14 | A | 1011 | CLA | C2A-C3A-C4A | 3.74 | 105.67 | 101.84 |
| 14 | A | 1115 | CLA | C4A-NA-C1A | 3.74 | 111.12 | 106.38 |
| 14 | A | 1131 | CLA | C4A-NA-C1A | 3.74 | 111.13 | 106.38 |
| 17 | J | 4013 | BCR | C33-C5-C6 | 3.74 | 128.61 | 124.62 |
| 14 | A | 1127 | CLA | O2A-CGA-CBA | 3.74 | 123.37 | 111.85 |
| 14 | A | 1116 | CLA | O2D-CGD-CBD | 3.75 | 116.63 | 111.22 |
| 17 | M | 4021 | BCR | C33-C5-C6 | 3.75 | 128.62 | 124.62 |
| 14 | B | 1226 | CLA | C4A-NA-C1A | 3.76 | 111.15 | 106.38 |
| 14 | B | 1219 | CLA | O2D-CGD-CBD | 3.76 | 116.64 | 111.22 |
| 14 | A | 1121 | CLA | O2A-CGA-CBA | 3.76 | 123.42 | 111.85 |
| 14 | B | 1231 | CLA | C2A-C3A-C4A | 3.76 | 105.69 | 101.84 |
| 14 | A | 1103 | CLA | C2A-C3A-C4A | 3.77 | 105.70 | 101.84 |
| 14 | L | 1503 | CLA | C4A-NA-C1A | 3.78 | 111.17 | 106.38 |
| 17 | M | 4021 | BCR | C24-C23-C22 | 3.79 | 131.93 | 126.21 |
| 14 | B | 1234 | CLA | C4A-NA-C1A | 3.79 | 111.19 | 106.38 |
| 14 | B | 1216 | CLA | O2D-CGD-CBD | 3.81 | 116.71 | 111.22 |
| 17 | B | 4014 | BCR | C7-C8-C9 | 3.81 | 131.96 | 126.21 |
| 14 | A | 1139 | CLA | O2A-CGA-CBA | 3.81 | 123.57 | 111.85 |
| 14 | A | 1121 | CLA | C4A-NA-C1A | 3.81 | 111.22 | 106.38 |
| 14 | A | 1104 | CLA | C4A-NA-C1A | 3.82 | 111.22 | 106.38 |
| 14 | A | 1122 | CLA | O2D-CGD-CBD | 3.82 | 116.73 | 111.22 |
| 17 | A | 4003 | BCR | C29-C30-C25 | 3.82 | 116.17 | 110.48 |
| 14 | B | 1207 | CLA | O2D-CGD-CBD | 3.83 | 116.74 | 111.22 |
| 14 | B | 1213 | CLA | C4A-NA-C1A | 3.83 | 111.25 | 106.38 |
| 17 | A | 4011 | BCR | C24-C23-C22 | 3.84 | 132.01 | 126.21 |
| 14 | B | 1224 | CLA | C4A-NA-C1A | 3.85 | 111.26 | 106.38 |
| 14 | K | 1401 | CLA | C4A-NA-C1A | 3.85 | 111.26 | 106.38 |
| 14 | A | 1801 | CLA | O2A-CGA-CBA | 3.85 | 123.71 | 111.85 |
| 14 | A | 1118 | CLA | O2A-CGA-CBA | 3.85 | 123.71 | 111.85 |
| 14 | F | 1301 | CLA | O2D-CGD-CBD | 3.86 | 116.78 | 111.22 |
| 14 | A | 1123 | CLA | C4A-NA-C1A | 3.86 | 111.28 | 106.38 |
| 14 | A | 1108 | CLA | C4A-NA-C1A | 3.86 | 111.28 | 106.38 |
| 17 | B | 4004 | BCR | C2-C1-C6 | 3.87 | 116.23 | 110.48 |
| 17 | J | 4012 | BCR | C29-C30-C25 | 3.87 | 116.24 | 110.48 |
| 14 | A | 1237 | CLA | O2A-CGA-CBA | 3.87 | 123.76 | 111.85 |
| 14 | A | 1136 | CLA | C4A-NA-C1A | 3.87 | 111.30 | 106.38 |
| 17 | J | 4015 | BCR | C8-C7-C6 | 3.88 | 138.50 | 127.24 |
| 14 | L | 1501 | CLA | C4A-NA-C1A | 3.88 | 111.30 | 106.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 14 | B | 1215 | CLA | O2A-CGA-CBA | 3.88 | 123.78 | 111.85 |
| 14 | A | 1117 | CLA | O2A-CGA-CBA | 3.88 | 123.80 | 111.85 |
| 14 | A | 1120 | CLA | O2A-CGA-CBA | 3.88 | 123.81 | 111.85 |
| 17 | A | 4011 | BCR | C2-C1-C6 | 3.88 | 116.26 | 110.48 |
| 14 | B | 1206 | CLA | C4A-NA-C1A | 3.89 | 111.32 | 106.38 |
| 14 | B | 1206 | CLA | O2D-CGD-CBD | 3.90 | 116.85 | 111.22 |
| 14 | A | 1127 | CLA | C4A-NA-C1A | 3.90 | 111.33 | 106.38 |
| 14 | B | 1205 | CLA | O2A-CGA-CBA | 3.90 | 123.86 | 111.85 |
| 14 | B | 1208 | CLA | C4A-NA-C1A | 3.90 | 111.33 | 106.38 |
| 14 | A | 1107 | CLA | O2D-CGD-CBD | 3.90 | 116.85 | 111.22 |
| 17 | B | 4005 | BCR | C7-C8-C9 | 3.91 | 132.12 | 126.21 |
| 14 | B | 1232 | CLA | C4A-NA-C1A | 3.92 | 111.35 | 106.38 |
| 17 | J | 4015 | BCR | C2-C1-C6 | 3.92 | 116.31 | 110.48 |
| 14 | B | 1233 | CLA | O2D-CGD-CBD | 3.92 | 116.87 | 111.22 |
| 14 | A | 1107 | CLA | O2A-CGA-CBA | 3.92 | 123.91 | 111.85 |
| 14 | B | 1221 | CLA | C4A-NA-C1A | 3.92 | 111.36 | 106.38 |
| 14 | A | 1140 | CLA | O2A-CGA-CBA | 3.92 | 123.93 | 111.85 |
| 14 | A | 1139 | CLA | C4A-NA-C1A | 3.93 | 111.36 | 106.38 |
| 14 | A | 1140 | CLA | C4A-NA-C1A | 3.93 | 111.37 | 106.38 |
| 14 | A | 1119 | CLA | C4A-NA-C1A | 3.93 | 111.37 | 106.38 |
| 14 | L | 1502 | CLA | C4A-NA-C1A | 3.94 | 111.38 | 106.38 |
| 14 | A | 1112 | CLA | C4A-NA-C1A | 3.94 | 111.38 | 106.38 |
| 14 | B | 1222 | CLA | C2A-C3A-C4A | 3.95 | 105.89 | 101.84 |
| 14 | A | 1122 | CLA | C4A-NA-C1A | 3.95 | 111.39 | 106.38 |
| 14 | B | 1229 | CLA | C4A-NA-C1A | 3.95 | 111.40 | 106.38 |
| 14 | B | 1220 | CLA | C4A-NA-C1A | 3.96 | 111.40 | 106.38 |
| 17 | A | 4011 | BCR | C40-C30-C25 | 3.96 | 116.39 | 110.33 |
| 17 | A | 4007 | BCR | C33-C5-C6 | 3.98 | 128.86 | 124.62 |
| 14 | A | 1101 | CLA | C4A-NA-C1A | 3.99 | 111.44 | 106.38 |
| 14 | B | 1021 | CLA | C4A-NA-C1A | 4.00 | 111.45 | 106.38 |
| 17 | I | 4020 | BCR | C24-C23-C22 | 4.00 | 132.26 | 126.21 |
| 17 | B | 4017 | BCR | C38-C26-C25 | 4.01 | 128.89 | 124.62 |
| 14 | B | 1211 | CLA | C4A-NA-C1A | 4.01 | 111.47 | 106.38 |
| 17 | B | 4017 | BCR | C33-C5-C6 | 4.01 | 128.89 | 124.62 |
| 14 | B | 1214 | CLA | C4A-NA-C1A | 4.01 | 111.47 | 106.38 |
| 14 | A | 1124 | CLA | C4A-NA-C1A | 4.03 | 111.50 | 106.38 |
| 14 | A | 1133 | CLA | O2D-CGD-CBD | 4.04 | 117.04 | 111.22 |
| 14 | B | 1231 | CLA | C4A-NA-C1A | 4.04 | 111.50 | 106.38 |
| 14 | B | 1212 | CLA | C4A-NA-C1A | 4.04 | 111.50 | 106.38 |
| 14 | A | 1116 | CLA | C4A-NA-C1A | 4.04 | 111.51 | 106.38 |
| 14 | B | 1228 | CLA | C4A-NA-C1A | 4.05 | 111.52 | 106.38 |
| 14 | B | 1225 | CLA | O2A-CGA-CBA | 4.05 | 124.32 | 111.85 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 17 | B | 4010 | BCR | C38-C26-C25 | 4.06 | 128.94 | 124.62 |
| 17 | A | 4002 | BCR | C33-C5-C6 | 4.06 | 128.95 | 124.62 |
| 17 | A | 4011 | BCR | C38-C26-C25 | 4.06 | 128.95 | 124.62 |
| 14 | B | 1216 | CLA | C4A-NA-C1A | 4.06 | 111.53 | 106.38 |
| 14 | B | 1239 | CLA | C4A-NA-C1A | 4.08 | 111.55 | 106.38 |
| 14 | A | 1105 | CLA | O2D-CGD-CBD | 4.08 | 117.11 | 111.22 |
| 14 | A | 1138 | CLA | C4A-NA-C1A | 4.09 | 111.56 | 106.38 |
| 17 | F | 4016 | BCR | C33-C5-C6 | 4.09 | 128.98 | 124.62 |
| 14 | A | 1115 | CLA | O2D-CGD-CBD | 4.09 | 117.12 | 111.22 |
| 14 | A | 1134 | CLA | O2D-CGD-CBD | 4.09 | 117.12 | 111.22 |
| 14 | A | 1110 | CLA | O2D-CGD-CBD | 4.10 | 117.13 | 111.22 |
| 14 | A | 1125 | CLA | C4A-NA-C1A | 4.10 | 111.58 | 106.38 |
| 14 | A | 1102 | CLA | C4A-NA-C1A | 4.11 | 111.59 | 106.38 |
| 14 | A | 1137 | CLA | O2A-CGA-CBA | 4.12 | 124.53 | 111.85 |
| 14 | A | 1402 | CLA | C4A-NA-C1A | 4.12 | 111.61 | 106.38 |
| 14 | A | 1106 | CLA | C4A-NA-C1A | 4.12 | 111.61 | 106.38 |
| 14 | A | 1013 | CLA | O2A-CGA-CBA | 4.13 | 124.56 | 111.85 |
| 14 | B | 1235 | CLA | C4A-NA-C1A | 4.14 | 111.63 | 106.38 |
| 14 | A | 1105 | CLA | C4A-NA-C1A | 4.14 | 111.63 | 106.38 |
| 14 | B | 1223 | CLA | C4A-NA-C1A | 4.14 | 111.63 | 106.38 |
| 14 | A | 1135 | CLA | C4A-NA-C1A | 4.14 | 111.63 | 106.38 |
| 14 | A | 1135 | CLA | O2A-CGA-CBA | 4.15 | 124.62 | 111.85 |
| 14 | B | 1201 | CLA | C4A-NA-C1A | 4.17 | 111.67 | 106.38 |
| 14 | B | 1222 | CLA | C4A-NA-C1A | 4.17 | 111.67 | 106.38 |
| 14 | B | 1207 | CLA | C4A-NA-C1A | 4.18 | 111.68 | 106.38 |
| 17 | J | 4012 | BCR | C33-C5-C6 | 4.18 | 129.08 | 124.62 |
| 14 | A | 1111 | CLA | C4A-NA-C1A | 4.18 | 111.69 | 106.38 |
| 17 | I | 4020 | BCR | C38-C26-C25 | 4.18 | 129.08 | 124.62 |
| 14 | A | 1022 | CLA | O2D-CGD-CBD | 4.19 | 117.26 | 111.22 |
| 14 | A | 1117 | CLA | C4A-NA-C1A | 4.19 | 111.70 | 106.38 |
| 14 | A | 1129 | CLA | C4A-NA-C1A | 4.19 | 111.70 | 106.38 |
| 14 | B | 1204 | CLA | C4A-NA-C1A | 4.20 | 111.72 | 106.38 |
| 14 | B | 1215 | CLA | O2D-CGD-CBD | 4.21 | 117.29 | 111.22 |
| 14 | A | 1133 | CLA | C4A-NA-C1A | 4.21 | 111.72 | 106.38 |
| 14 | A | 1107 | CLA | C4A-NA-C1A | 4.22 | 111.73 | 106.38 |
| 14 | A | 1135 | CLA | O2D-CGD-CBD | 4.22 | 117.31 | 111.22 |
| 14 | B | 1220 | CLA | O2D-CGD-CBD | 4.22 | 117.31 | 111.22 |
| 14 | B | 1219 | CLA | C4A-NA-C1A | 4.23 | 111.74 | 106.38 |
| 17 | A | 4011 | BCR | C33-C5-C6 | 4.23 | 129.13 | 124.62 |
| 14 | A | 1139 | CLA | O2D-CGD-CBD | 4.25 | 117.34 | 111.22 |
| 17 | I | 4018 | BCR | C2-C1-C6 | 4.25 | 116.81 | 110.48 |
| 14 | A | 1120 | CLA | C4A-NA-C1A | 4.25 | 111.77 | 106.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 14 | B | 1215 | CLA | C4A-NA-C1A | 4.25 | 111.78 | 106.38 |
| 14 | B | 1235 | CLA | O2D-CGD-CBD | 4.26 | 117.36 | 111.22 |
| 17 | B | 4005 | BCR | C33-C5-C6 | 4.26 | 129.16 | 124.62 |
| 14 | B | 1230 | CLA | C4A-NA-C1A | 4.27 | 111.79 | 106.38 |
| 14 | B | 1239 | CLA | O2D-CGD-CBD | 4.27 | 117.38 | 111.22 |
| 14 | J | 1303 | CLA | C4A-NA-C1A | 4.27 | 111.80 | 106.38 |
| 17 | B | 4009 | BCR | C38-C26-C25 | 4.28 | 129.18 | 124.62 |
| 17 | A | 4011 | BCR | C7-C8-C9 | 4.28 | 132.68 | 126.21 |
| 14 | A | 1124 | CLA | O2D-CGD-CBD | 4.28 | 117.39 | 111.22 |
| 14 | A | 1109 | CLA | C4A-NA-C1A | 4.29 | 111.82 | 106.38 |
| 14 | A | 1114 | CLA | C4A-NA-C1A | 4.29 | 111.82 | 106.38 |
| 18 | A | 5003 | LHG | C25-C24-C23 | 4.29 | 137.56 | 113.94 |
| 14 | L | 1502 | CLA | O2D-CGD-CBD | 4.30 | 117.42 | 111.22 |
| 14 | A | 1112 | CLA | O2D-CGD-CBD | 4.30 | 117.42 | 111.22 |
| 14 | B | 1224 | CLA | O2D-CGD-CBD | 4.31 | 117.44 | 111.22 |
| 14 | F | 1301 | CLA | C4A-NA-C1A | 4.31 | 111.85 | 106.38 |
| 14 | A | 1131 | CLA | O2D-CGD-CBD | 4.33 | 117.46 | 111.22 |
| 14 | B | 1224 | CLA | CBA-CAA-C2A | 4.33 | 125.12 | 113.96 |
| 14 | B | 1227 | CLA | C4A-NA-C1A | 4.33 | 111.88 | 106.38 |
| 17 | L | 4019 | BCR | C38-C26-C25 | 4.34 | 129.25 | 124.62 |
| 14 | A | 1118 | CLA | O2D-CGD-CBD | 4.36 | 117.51 | 111.22 |
| 14 | B | 1213 | CLA | O2D-CGD-CBD | 4.37 | 117.52 | 111.22 |
| 14 | X | 1701 | CLA | O2D-CGD-CBD | 4.37 | 117.52 | 111.22 |
| 14 | A | 1134 | CLA | C4A-NA-C1A | 4.38 | 111.94 | 106.38 |
| 14 | L | 1503 | CLA | O2D-CGD-CBD | 4.39 | 117.55 | 111.22 |
| 17 | B | 4006 | BCR | C38-C26-C25 | 4.39 | 129.30 | 124.62 |
| 14 | B | 1233 | CLA | C4A-NA-C1A | 4.39 | 111.96 | 106.38 |
| 14 | X | 1701 | CLA | C4A-NA-C1A | 4.40 | 111.96 | 106.38 |
| 14 | A | 1801 | CLA | C4A-NA-C1A | 4.40 | 111.96 | 106.38 |
| 14 | B | 1209 | CLA | O2D-CGD-CBD | 4.41 | 117.58 | 111.22 |
| 14 | A | 1130 | CLA | O2D-CGD-CBD | 4.42 | 117.60 | 111.22 |
| 14 | J | 1302 | CLA | C4A-NA-C1A | 4.43 | 112.00 | 106.38 |
| 17 | A | 4007 | BCR | C38-C26-C25 | 4.43 | 129.34 | 124.62 |
| 14 | A | 1137 | CLA | O2D-CGD-CBD | 4.44 | 117.62 | 111.22 |
| 17 | A | 4003 | BCR | C33-C5-C6 | 4.44 | 129.35 | 124.62 |
| 17 | B | 4006 | BCR | C7-C8-C9 | 4.45 | 132.93 | 126.21 |
| 17 | A | 4001 | BCR | C33-C5-C6 | 4.45 | 129.36 | 124.62 |
| 14 | B | 1218 | CLA | C4A-NA-C1A | 4.45 | 112.03 | 106.38 |
| 14 | A | 1114 | CLA | O2D-CGD-CBD | 4.45 | 117.64 | 111.22 |
| 17 | B | 4006 | BCR | C29-C30-C25 | 4.46 | 117.11 | 110.48 |
| 14 | A | 1110 | CLA | C4A-NA-C1A | 4.46 | 112.04 | 106.38 |
| 14 | B | 1209 | CLA | C4A-NA-C1A | 4.46 | 112.04 | 106.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 14 | A | 1118 | CLA | C4A-NA-C1A | 4.48 | 112.06 | 106.38 |
| 14 | B | 1204 | CLA | O2D-CGD-CBD | 4.48 | 117.68 | 111.22 |
| 14 | A | 1127 | CLA | O2D-CGD-CBD | 4.48 | 117.68 | 111.22 |
| 14 | B | 1224 | CLA | O2A-CGA-CBA | 4.49 | 125.66 | 111.85 |
| 14 | A | 1113 | CLA | C4A-NA-C1A | 4.51 | 112.10 | 106.38 |
| 17 | M | 4021 | BCR | C38-C26-C25 | 4.52 | 129.43 | 124.62 |
| 17 | B | 4014 | BCR | C38-C26-C25 | 4.54 | 129.46 | 124.62 |
| 17 | I | 4018 | BCR | C38-C26-C25 | 4.57 | 129.49 | 124.62 |
| 14 | M | 1601 | CLA | C4A-NA-C1A | 4.57 | 112.18 | 106.38 |
| 17 | A | 4002 | BCR | C38-C26-C25 | 4.59 | 129.51 | 124.62 |
| 14 | A | 1130 | CLA | C4A-NA-C1A | 4.59 | 112.21 | 106.38 |
| 14 | B | 1217 | CLA | C4A-NA-C1A | 4.62 | 112.24 | 106.38 |
| 17 | F | 4016 | BCR | C38-C26-C25 | 4.62 | 129.55 | 124.62 |
| 14 | A | 1011 | CLA | CGD-CBD-CHA | 4.63 | 126.77 | 110.88 |
| 14 | B | 1231 | CLA | O2D-CGD-CBD | 4.64 | 117.91 | 111.22 |
| 17 | L | 4022 | BCR | C38-C26-C25 | 4.65 | 129.57 | 124.62 |
| 14 | A | 1111 | CLA | O2D-CGD-CBD | 4.66 | 117.94 | 111.22 |
| 14 | A | 1104 | CLA | C2A-C3A-C4A | 4.68 | 106.64 | 101.84 |
| 14 | B | 1228 | CLA | O2D-CGD-CBD | 4.70 | 118.00 | 111.22 |
| 17 | A | 4003 | BCR | C38-C26-C25 | 4.72 | 129.65 | 124.62 |
| 14 | B | 1221 | CLA | O2D-CGD-CBD | 4.73 | 118.05 | 111.22 |
| 14 | A | 1104 | CLA | O2A-CGA-CBA | 4.75 | 126.48 | 111.85 |
| 17 | J | 4015 | BCR | C38-C26-C25 | 4.75 | 129.69 | 124.62 |
| 14 | A | 1120 | CLA | O2D-CGD-CBD | 4.76 | 118.08 | 111.22 |
| 14 | A | 1103 | CLA | O2D-CGD-CBD | 4.77 | 118.11 | 111.22 |
| 14 | K | 1401 | CLA | O2D-CGD-CBD | 4.78 | 118.11 | 111.22 |
| 14 | B | 1223 | CLA | O2D-CGD-CBD | 4.80 | 118.14 | 111.22 |
| 17 | B | 4004 | BCR | C33-C5-C6 | 4.81 | 129.74 | 124.62 |
| 17 | I | 4018 | BCR | C33-C5-C6 | 4.81 | 129.75 | 124.62 |
| 17 | B | 4010 | BCR | C33-C5-C6 | 4.84 | 129.78 | 124.62 |
| 14 | B | 1202 | CLA | O2D-CGD-CBD | 4.84 | 118.20 | 111.22 |
| 14 | B | 1210 | CLA | O2D-CGD-CBD | 4.84 | 118.21 | 111.22 |
| 14 | J | 1302 | CLA | O2D-CGD-CBD | 4.90 | 118.29 | 111.22 |
| 17 | B | 4006 | BCR | C33-C5-C6 | 4.91 | 129.85 | 124.62 |
| 14 | A | 1121 | CLA | O2D-CGD-CBD | 4.91 | 118.30 | 111.22 |
| 14 | B | 1218 | CLA | O2D-CGD-CBD | 4.92 | 118.31 | 111.22 |
| 17 | J | 4015 | BCR | C33-C5-C6 | 4.93 | 129.88 | 124.62 |
| 14 | B | 1234 | CLA | O2D-CGD-CBD | 4.94 | 118.35 | 111.22 |
| 14 | B | 1227 | CLA | O2D-CGD-CBD | 5.00 | 118.43 | 111.22 |
| 14 | B | 1229 | CLA | O2D-CGD-CBD | 5.01 | 118.44 | 111.22 |
| 14 | A | 1129 | CLA | O2D-CGD-CBD | 5.03 | 118.48 | 111.22 |
| 14 | B | 1217 | CLA | O2D-CGD-CBD | 5.04 | 118.50 | 111.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | L | 4019 | BCR | C33-C5-C6 | 5.07 | 130.02 | 124.62 |
| 14 | M | 1601 | CLA | O2D-CGD-CBD | 5.07 | 118.54 | 111.22 |
| 14 | A | 1128 | CLA | O2D-CGD-CBD | 5.09 | 118.57 | 111.22 |
| 14 | A | 1106 | CLA | O2D-CGD-CBD | 5.15 | 118.64 | 111.22 |
| 14 | A | 1101 | CLA | O2D-CGD-CBD | 5.18 | 118.69 | 111.22 |
| 14 | B | 1222 | CLA | O2D-CGD-CBD | 5.23 | 118.77 | 111.22 |
| 17 | J | 4012 | BCR | C38-C26-C25 | 5.23 | 130.20 | 124.62 |
| 14 | A | 1125 | CLA | O2D-CGD-CBD | 5.24 | 118.78 | 111.22 |
| 17 | B | 4014 | BCR | C33-C5-C6 | 5.26 | 130.22 | 124.62 |
| 14 | A | 1113 | CLA | O2D-CGD-CBD | 5.26 | 118.81 | 111.22 |
| 14 | A | 1123 | CLA | O2D-CGD-CBD | 5.27 | 118.82 | 111.22 |
| 17 | A | 4001 | BCR | C38-C26-C25 | 5.31 | 130.28 | 124.62 |
| 17 | L | 4022 | BCR | C33-C5-C6 | 5.33 | 130.31 | 124.62 |
| 14 | B | 1212 | CLA | O2D-CGD-CBD | 5.37 | 118.96 | 111.22 |
| 14 | B | 1211 | CLA | O2D-CGD-CBD | 5.53 | 119.20 | 111.22 |
| 14 | A | 1801 | CLA | O2D-CGD-CBD | 5.55 | 119.22 | 111.22 |
| 14 | B | 1230 | CLA | O2D-CGD-CBD | 5.59 | 119.29 | 111.22 |
| 14 | B | 1205 | CLA | O2D-CGD-CBD | 5.61 | 119.31 | 111.22 |
| 14 | A | 1102 | CLA | O2D-CGD-CBD | 5.66 | 119.38 | 111.22 |
| 17 | A | 4008 | BCR | C38-C26-C25 | 5.68 | 130.68 | 124.62 |
| 19 | B | 5002 | LMG | C30-C29-C28 | 5.74 | 135.97 | 113.57 |
| 14 | L | 1501 | CLA | O2D-CGD-CBD | 5.78 | 119.55 | 111.22 |
| 18 | A | 5001 | LHG | C25-C24-C23 | 5.80 | 136.18 | 113.57 |
| 14 | B | 1201 | CLA | O2D-CGD-CBD | 5.88 | 119.70 | 111.22 |
| 17 | B | 4005 | BCR | C38-C26-C25 | 5.97 | 130.99 | 124.62 |
| 14 | B | 1226 | CLA | O2D-CGD-CBD | 6.01 | 119.90 | 111.22 |
| 14 | A | 1132 | CLA | O2D-CGD-CBD | 6.02 | 119.91 | 111.22 |
| 14 | B | 1012 | CLA | O2D-CGD-CBD | 6.04 | 119.94 | 111.22 |
| 17 | B | 4004 | BCR | C38-C26-C25 | 6.19 | 131.22 | 124.62 |
| 15 | B | 2002 | PQN | C14-C13-C15 | 6.98 | 126.01 | 115.37 |
| 15 | A | 2001 | PQN | C14-C13-C15 | 8.13 | 127.76 | 115.37 |
| 14 | A | 1011 | CLA | O2D-CGD-CBD | 10.56 | 126.47 | 111.22 |

All (249) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|------|
| 14 | F | 1301 | CLA | NC |
| 14 | F | 1301 | CLA | ND |
| 14 | F | 1301 | CLA | NA |
| 14 | A | 1115 | CLA | NA |
| 14 | B | 1206 | CLA | ND |
| 14 | B | 1227 | CLA | NC |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|------|
| 14 | B | 1227 | CLA | ND |
| 14 | B | 1227 | CLA | NA |
| 14 | B | 1023 | CLA | NA |
| 14 | B | 1204 | CLA | NC |
| 14 | B | 1204 | CLA | ND |
| 14 | B | 1204 | CLA | NA |
| 14 | B | 1208 | CLA | ND |
| 14 | B | 1208 | CLA | NA |
| 14 | A | 1137 | CLA | ND |
| 14 | A | 1237 | CLA | NC |
| 14 | A | 1237 | CLA | ND |
| 14 | A | 1237 | CLA | NA |
| 14 | B | 1230 | CLA | NC |
| 14 | B | 1230 | CLA | ND |
| 14 | B | 1230 | CLA | NA |
| 14 | B | 1203 | CLA | NA |
| 14 | B | 1203 | CLA | NC |
| 14 | B | 1203 | CLA | ND |
| 14 | A | 1011 | CLA | NC |
| 14 | A | 1011 | CLA | ND |
| 14 | A | 1011 | CLA | NA |
| 14 | A | 1134 | CLA | NC |
| 14 | A | 1134 | CLA | ND |
| 14 | A | 1134 | CLA | NA |
| 14 | A | 1139 | CLA | NC |
| 14 | A | 1139 | CLA | ND |
| 14 | A | 1139 | CLA | NA |
| 14 | B | 1219 | CLA | NC |
| 14 | B | 1219 | CLA | ND |
| 14 | B | 1219 | CLA | NA |
| 14 | B | 1229 | CLA | NC |
| 14 | B | 1229 | CLA | ND |
| 14 | B | 1229 | CLA | NA |
| 14 | B | 1228 | CLA | NC |
| 14 | B | 1228 | CLA | ND |
| 14 | B | 1228 | CLA | NA |
| 14 | A | 1124 | CLA | NC |
| 14 | A | 1124 | CLA | ND |
| 14 | A | 1124 | CLA | NA |
| 14 | B | 1233 | CLA | NC |
| 14 | B | 1233 | CLA | ND |
| 14 | B | 1233 | CLA | NA |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|------|
| 14 | B | 1232 | CLA | NC |
| 14 | B | 1232 | CLA | ND |
| 14 | B | 1232 | CLA | NA |
| 14 | A | 1117 | CLA | NC |
| 14 | A | 1117 | CLA | ND |
| 14 | A | 1117 | CLA | NA |
| 14 | A | 1402 | CLA | NA |
| 14 | A | 1402 | CLA | NC |
| 14 | A | 1402 | CLA | ND |
| 14 | A | 1111 | CLA | NC |
| 14 | A | 1111 | CLA | ND |
| 14 | A | 1111 | CLA | NA |
| 14 | A | 1135 | CLA | NC |
| 14 | A | 1135 | CLA | ND |
| 14 | A | 1135 | CLA | NA |
| 14 | B | 1207 | CLA | NC |
| 14 | B | 1207 | CLA | ND |
| 14 | B | 1207 | CLA | NA |
| 14 | A | 1138 | CLA | NC |
| 14 | A | 1138 | CLA | ND |
| 14 | A | 1138 | CLA | NA |
| 14 | L | 1501 | CLA | NC |
| 14 | L | 1501 | CLA | ND |
| 14 | L | 1501 | CLA | NA |
| 14 | A | 1113 | CLA | NC |
| 14 | A | 1113 | CLA | ND |
| 14 | A | 1113 | CLA | NA |
| 14 | B | 1012 | CLA | ND |
| 14 | B | 1012 | CLA | NA |
| 14 | B | 1222 | CLA | NC |
| 14 | B | 1222 | CLA | ND |
| 14 | B | 1222 | CLA | NA |
| 14 | B | 1213 | CLA | NC |
| 14 | B | 1213 | CLA | ND |
| 14 | B | 1213 | CLA | NA |
| 14 | A | 1133 | CLA | NC |
| 14 | A | 1133 | CLA | ND |
| 14 | A | 1133 | CLA | NA |
| 14 | A | 1114 | CLA | NC |
| 14 | A | 1114 | CLA | ND |
| 14 | A | 1114 | CLA | NA |
| 14 | X | 1701 | CLA | NC |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|------|
| 14 | X | 1701 | CLA | ND |
| 14 | X | 1701 | CLA | NA |
| 14 | B | 1239 | CLA | NC |
| 14 | B | 1239 | CLA | NA |
| 14 | A | 1129 | CLA | NC |
| 14 | A | 1129 | CLA | ND |
| 14 | A | 1129 | CLA | NA |
| 14 | J | 1303 | CLA | NC |
| 14 | J | 1303 | CLA | ND |
| 14 | J | 1303 | CLA | NA |
| 14 | B | 1021 | CLA | ND |
| 14 | A | 1126 | CLA | ND |
| 14 | B | 1238 | CLA | NC |
| 14 | B | 1238 | CLA | ND |
| 14 | B | 1226 | CLA | NC |
| 14 | B | 1226 | CLA | ND |
| 14 | B | 1226 | CLA | NA |
| 14 | A | 1125 | CLA | NC |
| 14 | A | 1125 | CLA | ND |
| 14 | A | 1125 | CLA | NA |
| 14 | A | 1120 | CLA | NC |
| 14 | A | 1120 | CLA | ND |
| 14 | A | 1120 | CLA | NA |
| 14 | B | 1205 | CLA | ND |
| 14 | B | 1205 | CLA | NA |
| 14 | A | 1013 | CLA | ND |
| 14 | A | 1013 | CLA | NA |
| 14 | A | 1022 | CLA | ND |
| 14 | A | 1022 | CLA | NA |
| 14 | A | 1118 | CLA | NC |
| 14 | A | 1118 | CLA | ND |
| 14 | A | 1118 | CLA | NA |
| 14 | B | 1224 | CLA | ND |
| 14 | A | 1130 | CLA | NC |
| 14 | A | 1130 | CLA | ND |
| 14 | A | 1130 | CLA | NA |
| 14 | A | 1140 | CLA | NC |
| 14 | A | 1140 | CLA | ND |
| 14 | A | 1140 | CLA | NA |
| 14 | A | 1110 | CLA | NC |
| 14 | A | 1110 | CLA | ND |
| 14 | A | 1110 | CLA | NA |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|------|
| 14 | L | 1503 | CLA | NC |
| 14 | L | 1503 | CLA | ND |
| 14 | L | 1503 | CLA | NA |
| 14 | B | 1201 | CLA | ND |
| 14 | B | 1201 | CLA | NA |
| 14 | B | 1235 | CLA | NC |
| 14 | B | 1235 | CLA | ND |
| 14 | B | 1235 | CLA | NA |
| 14 | A | 1109 | CLA | NC |
| 14 | A | 1109 | CLA | ND |
| 14 | A | 1109 | CLA | NA |
| 14 | B | 1220 | CLA | NC |
| 14 | B | 1220 | CLA | ND |
| 14 | B | 1220 | CLA | NA |
| 14 | B | 1221 | CLA | NC |
| 14 | B | 1221 | CLA | ND |
| 14 | B | 1221 | CLA | NA |
| 14 | B | 1210 | CLA | NA |
| 14 | B | 1210 | CLA | NC |
| 14 | B | 1210 | CLA | ND |
| 14 | A | 1123 | CLA | NC |
| 14 | A | 1123 | CLA | ND |
| 14 | A | 1123 | CLA | NA |
| 14 | A | 1102 | CLA | NC |
| 14 | A | 1102 | CLA | ND |
| 14 | A | 1102 | CLA | NA |
| 14 | L | 1502 | CLA | NC |
| 14 | L | 1502 | CLA | NA |
| 14 | A | 1107 | CLA | NC |
| 14 | A | 1107 | CLA | ND |
| 14 | A | 1107 | CLA | NA |
| 14 | A | 1122 | CLA | NC |
| 14 | A | 1122 | CLA | ND |
| 14 | A | 1122 | CLA | NA |
| 14 | B | 1217 | CLA | NC |
| 14 | B | 1217 | CLA | ND |
| 14 | B | 1217 | CLA | NA |
| 14 | A | 1112 | CLA | NC |
| 14 | A | 1112 | CLA | ND |
| 14 | A | 1112 | CLA | NA |
| 14 | B | 1209 | CLA | NC |
| 14 | B | 1209 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|------|
| 14 | B | 1209 | CLA | NA |
| 14 | J | 1302 | CLA | NC |
| 14 | J | 1302 | CLA | ND |
| 14 | J | 1302 | CLA | NA |
| 14 | A | 1119 | CLA | NC |
| 14 | A | 1119 | CLA | ND |
| 14 | A | 1119 | CLA | NA |
| 14 | B | 1225 | CLA | NA |
| 14 | A | 1801 | CLA | NC |
| 14 | A | 1801 | CLA | ND |
| 14 | A | 1801 | CLA | NA |
| 14 | B | 1202 | CLA | NA |
| 14 | B | 1202 | CLA | NC |
| 14 | B | 1202 | CLA | ND |
| 14 | A | 1127 | CLA | NC |
| 14 | A | 1127 | CLA | ND |
| 18 | A | 5003 | LHG | C2 |
| 14 | A | 1116 | CLA | NC |
| 14 | A | 1116 | CLA | ND |
| 14 | A | 1116 | CLA | NA |
| 14 | A | 1136 | CLA | ND |
| 14 | A | 1136 | CLA | NA |
| 14 | A | 1105 | CLA | ND |
| 14 | A | 1105 | CLA | NA |
| 14 | A | 1132 | CLA | NC |
| 14 | A | 1132 | CLA | ND |
| 14 | A | 1132 | CLA | NA |
| 14 | B | 1216 | CLA | NC |
| 14 | B | 1216 | CLA | ND |
| 14 | B | 1216 | CLA | NA |
| 14 | B | 1211 | CLA | NC |
| 14 | B | 1211 | CLA | ND |
| 14 | B | 1211 | CLA | NA |
| 14 | A | 1128 | CLA | NC |
| 14 | A | 1128 | CLA | ND |
| 14 | A | 1128 | CLA | NA |
| 14 | A | 1106 | CLA | NC |
| 14 | A | 1106 | CLA | ND |
| 14 | A | 1106 | CLA | NA |
| 14 | B | 1212 | CLA | NC |
| 14 | B | 1212 | CLA | NA |
| 14 | B | 1218 | CLA | NC |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|------|
| 14 | B | 1218 | CLA | ND |
| 14 | B | 1218 | CLA | NA |
| 14 | A | 1104 | CLA | NC |
| 14 | A | 1104 | CLA | ND |
| 14 | A | 1104 | CLA | NA |
| 14 | B | 1231 | CLA | NC |
| 14 | B | 1231 | CLA | ND |
| 14 | B | 1231 | CLA | NA |
| 14 | A | 1101 | CLA | NC |
| 14 | A | 1101 | CLA | ND |
| 14 | A | 1101 | CLA | NA |
| 14 | A | 1121 | CLA | ND |
| 14 | A | 1121 | CLA | NA |
| 14 | M | 1601 | CLA | NC |
| 14 | M | 1601 | CLA | ND |
| 14 | M | 1601 | CLA | NA |
| 14 | B | 1223 | CLA | NC |
| 14 | B | 1223 | CLA | ND |
| 14 | B | 1223 | CLA | NA |
| 14 | A | 1103 | CLA | NA |
| 14 | A | 1103 | CLA | NC |
| 14 | A | 1103 | CLA | ND |
| 14 | B | 1215 | CLA | NC |
| 14 | B | 1215 | CLA | ND |
| 14 | B | 1215 | CLA | NA |
| 14 | K | 1401 | CLA | NC |
| 14 | K | 1401 | CLA | NA |
| 14 | B | 1214 | CLA | NC |
| 14 | B | 1214 | CLA | ND |
| 14 | B | 1214 | CLA | NA |
| 14 | B | 1234 | CLA | NC |
| 14 | B | 1234 | CLA | ND |
| 14 | B | 1234 | CLA | NA |

All (1) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | A | 1114 | CLA | CED-O2D-CGD-CBD |

There are no ring outliers.

114 monomers are involved in 339 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 14 | A | 1011 | CLA | 9 | 0 |
| 14 | A | 1013 | CLA | 10 | 0 |
| 14 | A | 1022 | CLA | 3 | 0 |
| 14 | A | 1101 | CLA | 2 | 0 |
| 14 | A | 1102 | CLA | 1 | 0 |
| 14 | A | 1103 | CLA | 6 | 0 |
| 14 | A | 1104 | CLA | 4 | 0 |
| 14 | A | 1105 | CLA | 2 | 0 |
| 14 | A | 1106 | CLA | 6 | 0 |
| 14 | A | 1107 | CLA | 4 | 0 |
| 14 | A | 1108 | CLA | 4 | 0 |
| 14 | A | 1109 | CLA | 1 | 0 |
| 14 | A | 1111 | CLA | 1 | 0 |
| 14 | A | 1112 | CLA | 5 | 0 |
| 14 | A | 1114 | CLA | 2 | 0 |
| 14 | A | 1116 | CLA | 5 | 0 |
| 14 | A | 1117 | CLA | 6 | 0 |
| 14 | A | 1118 | CLA | 5 | 0 |
| 14 | A | 1119 | CLA | 4 | 0 |
| 14 | A | 1120 | CLA | 2 | 0 |
| 14 | A | 1121 | CLA | 1 | 0 |
| 14 | A | 1122 | CLA | 2 | 0 |
| 14 | A | 1123 | CLA | 4 | 0 |
| 14 | A | 1124 | CLA | 5 | 0 |
| 14 | A | 1125 | CLA | 3 | 0 |
| 14 | A | 1126 | CLA | 14 | 0 |
| 14 | A | 1127 | CLA | 1 | 0 |
| 14 | A | 1128 | CLA | 7 | 0 |
| 14 | A | 1129 | CLA | 1 | 0 |
| 14 | A | 1130 | CLA | 2 | 0 |
| 14 | A | 1132 | CLA | 4 | 0 |
| 14 | A | 1133 | CLA | 4 | 0 |
| 14 | A | 1134 | CLA | 2 | 0 |
| 14 | A | 1135 | CLA | 2 | 0 |
| 14 | A | 1136 | CLA | 7 | 0 |
| 14 | A | 1137 | CLA | 3 | 0 |
| 14 | A | 1138 | CLA | 2 | 0 |
| 14 | A | 1140 | CLA | 8 | 0 |
| 14 | A | 1237 | CLA | 5 | 0 |
| 14 | A | 1402 | CLA | 1 | 0 |
| 14 | A | 1801 | CLA | 5 | 0 |
| 15 | A | 2001 | PQN | 1 | 0 |
| 17 | A | 4001 | BCR | 2 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 17 | A | 4002 | BCR | 2 | 0 |
| 17 | A | 4003 | BCR | 1 | 0 |
| 17 | A | 4007 | BCR | 4 | 0 |
| 17 | A | 4008 | BCR | 1 | 0 |
| 17 | A | 4011 | BCR | 13 | 0 |
| 18 | A | 5001 | LHG | 4 | 0 |
| 18 | A | 5003 | LHG | 2 | 0 |
| 14 | B | 1012 | CLA | 17 | 0 |
| 14 | B | 1021 | CLA | 8 | 0 |
| 14 | B | 1023 | CLA | 4 | 0 |
| 14 | B | 1201 | CLA | 2 | 0 |
| 14 | B | 1202 | CLA | 3 | 0 |
| 14 | B | 1203 | CLA | 6 | 0 |
| 14 | B | 1204 | CLA | 1 | 0 |
| 14 | B | 1205 | CLA | 3 | 0 |
| 14 | B | 1206 | CLA | 2 | 0 |
| 14 | B | 1207 | CLA | 5 | 0 |
| 14 | B | 1208 | CLA | 1 | 0 |
| 14 | B | 1209 | CLA | 1 | 0 |
| 14 | B | 1210 | CLA | 6 | 0 |
| 14 | B | 1211 | CLA | 6 | 0 |
| 14 | B | 1212 | CLA | 2 | 0 |
| 14 | B | 1213 | CLA | 3 | 0 |
| 14 | B | 1214 | CLA | 8 | 0 |
| 14 | B | 1215 | CLA | 6 | 0 |
| 14 | B | 1216 | CLA | 5 | 0 |
| 14 | B | 1217 | CLA | 2 | 0 |
| 14 | B | 1218 | CLA | 1 | 0 |
| 14 | B | 1219 | CLA | 4 | 0 |
| 14 | B | 1220 | CLA | 3 | 0 |
| 14 | B | 1221 | CLA | 10 | 0 |
| 14 | B | 1222 | CLA | 2 | 0 |
| 14 | B | 1223 | CLA | 3 | 0 |
| 14 | B | 1224 | CLA | 5 | 0 |
| 14 | B | 1225 | CLA | 8 | 0 |
| 14 | B | 1226 | CLA | 7 | 0 |
| 14 | B | 1227 | CLA | 5 | 0 |
| 14 | B | 1228 | CLA | 2 | 0 |
| 14 | B | 1229 | CLA | 6 | 0 |
| 14 | B | 1230 | CLA | 7 | 0 |
| 14 | B | 1232 | CLA | 3 | 0 |
| 14 | B | 1233 | CLA | 2 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 14 | B | 1234 | CLA | 3 | 0 |
| 14 | B | 1235 | CLA | 2 | 0 |
| 14 | B | 1236 | CLA | 4 | 0 |
| 14 | B | 1238 | CLA | 3 | 0 |
| 15 | B | 2002 | PQN | 1 | 0 |
| 17 | B | 4004 | BCR | 1 | 0 |
| 17 | B | 4005 | BCR | 1 | 0 |
| 17 | B | 4006 | BCR | 5 | 0 |
| 17 | B | 4009 | BCR | 5 | 0 |
| 17 | B | 4010 | BCR | 3 | 0 |
| 17 | B | 4014 | BCR | 1 | 0 |
| 17 | B | 4017 | BCR | 1 | 0 |
| 19 | B | 5002 | LMG | 5 | 0 |
| 18 | B | 5004 | LHG | 1 | 0 |
| 14 | F | 1301 | CLA | 1 | 0 |
| 17 | F | 4016 | BCR | 2 | 0 |
| 17 | I | 4018 | BCR | 3 | 0 |
| 14 | J | 1302 | CLA | 1 | 0 |
| 17 | J | 4012 | BCR | 4 | 0 |
| 17 | J | 4013 | BCR | 7 | 0 |
| 17 | J | 4015 | BCR | 5 | 0 |
| 14 | K | 1401 | CLA | 1 | 0 |
| 14 | L | 1501 | CLA | 2 | 0 |
| 14 | L | 1502 | CLA | 8 | 0 |
| 14 | L | 1503 | CLA | 2 | 0 |
| 17 | L | 4022 | BCR | 1 | 0 |
| 14 | M | 1601 | CLA | 1 | 0 |
| 17 | M | 4021 | BCR | 2 | 0 |
| 14 | X | 1701 | 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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.