



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 18, 2017 – 03:59 PM EDT

PDB ID : 4UB8
Title : Native structure of photosystem II (dataset-2) by a femtosecond X-ray laser
Authors : Suga, M.; Akita, F.; Hirata, K.; Ueno, G.; Murakami, H.; Nakajima, Y.; Shimizu, T.; Yamashita, K.; Yamamoto, M.; Ago, H.; Shen, J.R.
Deposited on : unknown
Resolution : 1.95 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

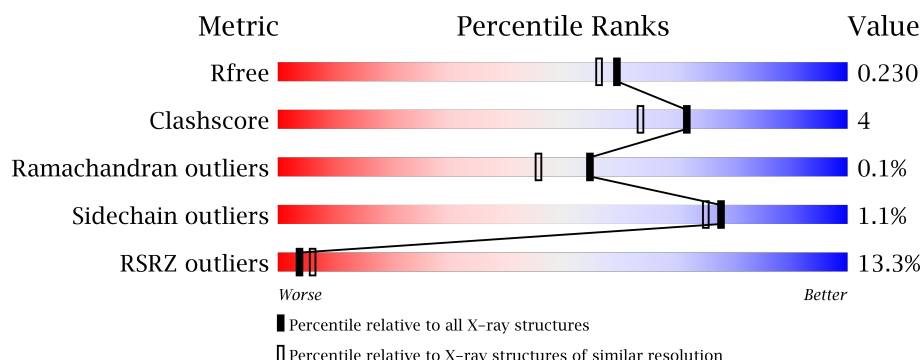
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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)) |
|-----------------------|-----------------------------|---|
| R_{free} | 100719 | 2004 (1.96-1.96) |
| Clashscore | 112137 | 2136 (1.96-1.96) |
| Ramachandran outliers | 110173 | 2117 (1.96-1.96) |
| Sidechain outliers | 110143 | 2117 (1.96-1.96) |
| RSRZ outliers | 101464 | 2018 (1.96-1.96) |

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.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | A | 344 | <div> <div>13%</div> <div> <div></div> <div>90%</div> <div>6%</div> <div>.</div> </div> </div> |
| 1 | a | 344 | <div> <div>18%</div> <div> <div></div> <div>97%</div> <div></div> <div>..</div> </div> </div> |
| 2 | B | 505 | <div> <div>8%</div> <div> <div></div> <div>90%</div> <div>10%</div> </div> </div> |
| 2 | b | 505 | <div> <div>10%</div> <div> <div></div> <div>99%</div> <div></div> <div>.</div> </div> </div> |
| 3 | C | 455 | <div> <div>6%</div> <div> <div></div> <div>90%</div> <div>9%</div> <div>.</div> </div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3 | c | 455 | |
| 4 | D | 342 | |
| 4 | d | 342 | |
| 5 | E | 84 | |
| 5 | e | 84 | |
| 6 | F | 44 | |
| 6 | f | 44 | |
| 7 | H | 65 | |
| 7 | h | 65 | |
| 8 | I | 38 | |
| 8 | i | 38 | |
| 9 | J | 39 | |
| 9 | j | 39 | |
| 10 | K | 37 | |
| 10 | k | 37 | |
| 11 | L | 37 | |
| 11 | l | 37 | |
| 12 | M | 36 | |
| 12 | m | 36 | |
| 13 | O | 244 | |
| 13 | o | 244 | |
| 14 | T | 31 | |
| 14 | t | 31 | |
| 15 | U | 104 | |
| 15 | u | 104 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 16 | V | 137 | |
| 16 | v | 137 | |
| 17 | Y | 30 | |
| 17 | y | 30 | |
| 18 | X | 40 | |
| 18 | x | 40 | |
| 19 | Z | 62 | |
| 19 | z | 62 | |
| 20 | R | 34 | |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 23 | BCT | a | 418 | - | - | - | X |
| 24 | CLA | A | 405 | X | - | - | - |
| 24 | CLA | A | 406 | X | - | - | - |
| 24 | CLA | A | 409 | X | - | - | - |
| 24 | CLA | B | 602 | X | - | - | X |
| 24 | CLA | B | 603 | X | - | - | - |
| 24 | CLA | B | 604 | X | - | - | - |
| 24 | CLA | B | 605 | X | - | - | - |
| 24 | CLA | B | 606 | X | - | - | - |
| 24 | CLA | B | 607 | X | - | - | - |
| 24 | CLA | B | 608 | X | - | - | - |
| 24 | CLA | B | 609 | X | - | - | - |
| 24 | CLA | B | 610 | X | - | - | - |
| 24 | CLA | B | 611 | X | - | - | - |
| 24 | CLA | B | 612 | X | - | - | - |
| 24 | CLA | B | 613 | X | - | - | - |
| 24 | CLA | B | 614 | X | - | - | - |
| 24 | CLA | B | 615 | X | - | - | - |
| 24 | CLA | B | 616 | X | - | - | - |
| 24 | CLA | B | 617 | X | - | - | X |
| 24 | CLA | C | 502 | X | - | - | - |
| 24 | CLA | C | 503 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 24 | CLA | C | 504 | X | - | - | - |
| 24 | CLA | C | 505 | X | - | - | - |
| 24 | CLA | C | 506 | X | - | - | - |
| 24 | CLA | C | 507 | X | - | - | - |
| 24 | CLA | C | 508 | X | - | - | - |
| 24 | CLA | C | 509 | X | - | - | - |
| 24 | CLA | C | 510 | X | - | - | - |
| 24 | CLA | C | 511 | X | - | - | - |
| 24 | CLA | C | 512 | X | - | - | - |
| 24 | CLA | C | 513 | X | - | - | - |
| 24 | CLA | C | 514 | X | - | - | - |
| 24 | CLA | D | 401 | X | - | - | - |
| 24 | CLA | D | 403 | X | - | - | - |
| 24 | CLA | D | 404 | X | - | - | - |
| 24 | CLA | a | 406 | X | - | - | - |
| 24 | CLA | a | 407 | X | - | - | - |
| 24 | CLA | a | 409 | X | - | - | - |
| 24 | CLA | b | 606 | X | - | - | X |
| 24 | CLA | b | 607 | X | - | - | - |
| 24 | CLA | b | 608 | X | - | - | - |
| 24 | CLA | b | 609 | X | - | - | - |
| 24 | CLA | b | 610 | X | - | - | - |
| 24 | CLA | b | 611 | X | - | - | - |
| 24 | CLA | b | 612 | X | - | - | - |
| 24 | CLA | b | 613 | X | - | - | - |
| 24 | CLA | b | 614 | X | - | - | - |
| 24 | CLA | b | 615 | X | - | - | - |
| 24 | CLA | b | 616 | X | - | - | - |
| 24 | CLA | b | 617 | X | - | - | - |
| 24 | CLA | b | 618 | X | - | - | - |
| 24 | CLA | b | 619 | X | - | - | - |
| 24 | CLA | b | 620 | X | - | - | - |
| 24 | CLA | b | 621 | X | - | - | - |
| 24 | CLA | c | 503 | X | - | - | - |
| 24 | CLA | c | 504 | X | - | - | - |
| 24 | CLA | c | 505 | X | - | - | - |
| 24 | CLA | c | 506 | X | - | - | - |
| 24 | CLA | c | 507 | X | - | - | - |
| 24 | CLA | c | 508 | X | - | - | - |
| 24 | CLA | c | 509 | X | - | - | - |
| 24 | CLA | c | 510 | X | - | - | - |
| 24 | CLA | c | 511 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 24 | CLA | c | 512 | X | - | - | - |
| 24 | CLA | c | 513 | X | - | - | - |
| 24 | CLA | c | 514 | X | - | - | - |
| 24 | CLA | c | 515 | X | - | - | - |
| 24 | CLA | d | 401 | X | - | - | - |
| 24 | CLA | d | 402 | X | - | - | - |
| 24 | CLA | d | 404 | X | - | - | - |
| 26 | BCR | B | 619 | - | - | - | X |
| 26 | BCR | b | 623 | - | - | - | X |
| 26 | BCR | d | 405 | - | - | - | X |
| 27 | SQD | A | 416 | - | - | - | X |
| 27 | SQD | a | 402 | - | - | - | X |
| 27 | SQD | l | 101 | - | - | - | X |
| 28 | GOL | A | 413 | - | - | - | X |
| 28 | GOL | A | 414 | - | - | - | X |
| 28 | GOL | B | 625 | - | - | - | X |
| 28 | GOL | B | 626 | - | - | - | X |
| 28 | GOL | B | 627 | - | - | - | X |
| 28 | GOL | B | 628 | - | - | - | X |
| 28 | GOL | B | 629 | - | - | - | X |
| 28 | GOL | C | 524 | - | - | - | X |
| 28 | GOL | F | 103 | - | - | - | X |
| 28 | GOL | V | 205 | - | - | - | X |
| 28 | GOL | V | 206 | - | - | - | X |
| 28 | GOL | V | 207 | - | - | - | X |
| 28 | GOL | V | 208 | - | - | - | X |
| 28 | GOL | a | 412 | - | - | - | X |
| 28 | GOL | a | 413 | - | - | - | X |
| 28 | GOL | b | 632 | - | - | - | X |
| 28 | GOL | b | 633 | - | - | - | X |
| 28 | GOL | c | 525 | - | - | - | X |
| 28 | GOL | c | 527 | - | - | - | X |
| 28 | GOL | f | 104 | - | - | - | X |
| 28 | GOL | t | 102 | - | - | - | X |
| 28 | GOL | v | 203 | - | - | - | X |
| 29 | UNL | C | 526 | - | - | - | X |
| 29 | UNL | D | 413 | - | - | - | X |
| 29 | UNL | I | 101 | - | - | - | X |
| 29 | UNL | J | 103 | - | - | - | X |
| 29 | UNL | X | 101 | - | - | - | X |
| 29 | UNL | d | 412 | - | - | - | X |
| 29 | UNL | d | 413 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 29 | UNL | i | 101 | - | - | - | X |
| 29 | UNL | j | 103 | - | - | - | X |
| 29 | UNL | k | 101 | - | - | - | X |
| 29 | UNL | k | 102 | - | - | - | X |
| 30 | LMT | A | 417 | - | - | - | X |
| 30 | LMT | B | 634 | - | - | - | X |
| 30 | LMT | E | 102 | - | - | - | X |
| 30 | LMT | I | 102 | - | - | - | X |
| 30 | LMT | M | 101 | - | - | - | X |
| 30 | LMT | a | 401 | - | - | - | X |
| 30 | LMT | a | 417 | - | - | - | X |
| 30 | LMT | b | 602 | - | - | - | X |
| 30 | LMT | f | 102 | - | - | - | X |
| 30 | LMT | m | 103 | - | - | - | X |
| 32 | PL9 | A | 419 | - | - | - | X |
| 32 | PL9 | a | 416 | - | - | - | X |
| 34 | LMG | C | 501 | - | - | - | X |
| 34 | LMG | J | 101 | - | - | - | X |
| 34 | LMG | Z | 101 | - | - | - | X |
| 34 | LMG | b | 625 | - | - | - | X |
| 34 | LMG | j | 101 | - | - | - | X |
| 34 | LMG | z | 101 | - | - | - | X |
| 35 | HTG | B | 631 | - | - | - | X |
| 35 | HTG | C | 523 | - | - | - | X |
| 35 | HTG | D | 411 | - | - | - | X |
| 35 | HTG | V | 204 | - | - | - | X |
| 35 | HTG | b | 627 | - | - | - | X |
| 35 | HTG | c | 523 | - | - | - | X |
| 36 | DGD | D | 407 | - | - | - | X |
| 36 | DGD | d | 407 | - | - | - | X |
| 39 | MG | j | 102 | - | - | - | X |

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 53958 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 Q(B) protein.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 334 | Total | C | N | O | S | 0 | 3 | 0 |
| | | | 2631 | 1725 | 431 | 460 | 15 | | | |
| 1 | a | 334 | Total | C | N | O | S | 0 | 4 | 0 |
| | | | 2634 | 1727 | 431 | 461 | 15 | | | |

- Molecule 2 is a protein called Photosystem II CP47 chlorophyll apoprotein.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2 | B | 504 | Total | C | N | O | S | 0 | 10 | 0 |
| | | | 4023 | 2642 | 667 | 701 | 13 | | | |
| 2 | b | 504 | Total | C | N | O | S | 0 | 11 | 0 |
| | | | 4028 | 2645 | 668 | 702 | 13 | | | |

- Molecule 3 is a protein called Photosystem II 44 kDa reaction center protein.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3 | C | 451 | Total | C | N | O | S | 0 | 5 | 0 |
| | | | 3506 | 2296 | 584 | 613 | 13 | | | |
| 3 | c | 455 | Total | C | N | O | S | 0 | 6 | 0 |
| | | | 3544 | 2323 | 589 | 619 | 13 | | | |

- Molecule 4 is a protein called Photosystem II D2 protein.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 4 | D | 342 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2726 | 1805 | 445 | 464 | 12 | | | |
| 4 | d | 341 | Total | C | N | O | S | 0 | 1 | 0 |
| | | | 2720 | 1802 | 444 | 462 | 12 | | | |

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 5 | E | 81 | Total | C | N | O | 0 | 2 | 0 |
| | | | 668 | 436 | 107 | 125 | | | |
| 5 | e | 81 | Total | C | N | O | 0 | 0 | 0 |
| | | | 662 | 432 | 107 | 123 | | | |

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 6 | F | 34 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 275 | 187 | 45 | 42 | 1 | | | |
| 6 | f | 32 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 257 | 175 | 43 | 38 | 1 | | | |

- Molecule 7 is a protein called Photosystem II reaction center protein H.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 7 | H | 65 | Total | C | N | O | S | 0 | 1 | 0 |
| | | | 519 | 346 | 85 | 86 | 2 | | | |
| 7 | h | 65 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 511 | 341 | 82 | 86 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 8 | I | 38 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 314 | 211 | 48 | 54 | 1 | | | |
| 8 | i | 38 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 314 | 211 | 48 | 54 | 1 | | | |

- Molecule 9 is a protein called Photosystem II reaction center protein J.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 9 | J | 38 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 272 | 182 | 42 | 47 | 1 | | | |
| 9 | j | 39 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 282 | 188 | 43 | 49 | 2 | | | |

- Molecule 10 is a protein called Photosystem II reaction center protein K.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 10 | K | 37 | Total | C | N | O | 0 | 0 | 0 |
| | | | 293 | 204 | 43 | 46 | | | |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 10 | k | 37 | Total | C | N | O | 0 | 0 | 0 |
| | | | 293 | 204 | 43 | 46 | | | |

- Molecule 11 is a protein called Photosystem II reaction center protein L.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 11 | L | 37 | Total | C | N | O | S | 0 | 1 | 0 |
| | | | 309 | 207 | 48 | 53 | 1 | | | |
| 11 | l | 37 | Total | C | N | O | S | 0 | 1 | 0 |
| | | | 309 | 207 | 48 | 53 | 1 | | | |

- Molecule 12 is a protein called Photosystem II reaction center protein M.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 12 | M | 34 | Total | C | N | O | S | 0 | 1 | 0 |
| | | | 274 | 184 | 40 | 49 | 1 | | | |
| 12 | m | 34 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 269 | 179 | 40 | 49 | 1 | | | |

- Molecule 13 is a protein called Photosystem II manganese-stabilizing polypeptide.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 13 | O | 243 | Total | C | N | O | S | 0 | 4 | 0 |
| | | | 1883 | 1178 | 315 | 385 | 5 | | | |
| 13 | o | 243 | Total | C | N | O | S | 0 | 3 | 0 |
| | | | 1879 | 1175 | 315 | 384 | 5 | | | |

- Molecule 14 is a protein called Photosystem II reaction center protein T.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 14 | T | 30 | Total | C | N | O | S | 0 | 1 | 0 |
| | | | 264 | 185 | 36 | 41 | 2 | | | |
| 14 | t | 30 | Total | C | N | O | S | 0 | 1 | 0 |
| | | | 264 | 185 | 36 | 41 | 2 | | | |

- Molecule 15 is a protein called Photosystem II 12 kDa extrinsic protein.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 15 | U | 97 | Total | C | N | O | 0 | 0 | 0 |
| | | | 774 | 491 | 129 | 154 | | | |
| 15 | u | 97 | Total | C | N | O | 0 | 0 | 0 |
| | | | 774 | 491 | 129 | 154 | | | |

- Molecule 16 is a protein called Cytochrome c-550.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16 | V | 137 | Total | C | N | O | S | 0 | 1 | 0 |
| | | | 1072 | 680 | 180 | 208 | 4 | | | |
| 16 | v | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1064 | 675 | 177 | 208 | 4 | | | |

- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 17 | Y | 29 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 215 | 142 | 37 | 33 | 3 | | | |
| 17 | y | 29 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 215 | 142 | 37 | 33 | 3 | | | |

- Molecule 18 is a protein called Photosystem II reaction center protein X.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 18 | X | 39 | Total | C | N | O | S | 0 | 1 | 0 |
| | | | 292 | 196 | 46 | 50 | | | | |
| 18 | x | 39 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 287 | 191 | 46 | 50 | | | | |

- Molecule 19 is a protein called Photosystem II reaction center protein Z.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 19 | Z | 62 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 479 | 328 | 72 | 77 | 2 | | | |
| 19 | z | 62 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 479 | 328 | 72 | 77 | 2 | | | |

- Molecule 20 is a protein called Photosystem II protein Y.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 20 | R | 34 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 273 | 186 | 47 | 40 | | | | |

- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 21 | A | 1 | Total | Fe | 0 | 0 |
| | | | 1 | 1 | | |

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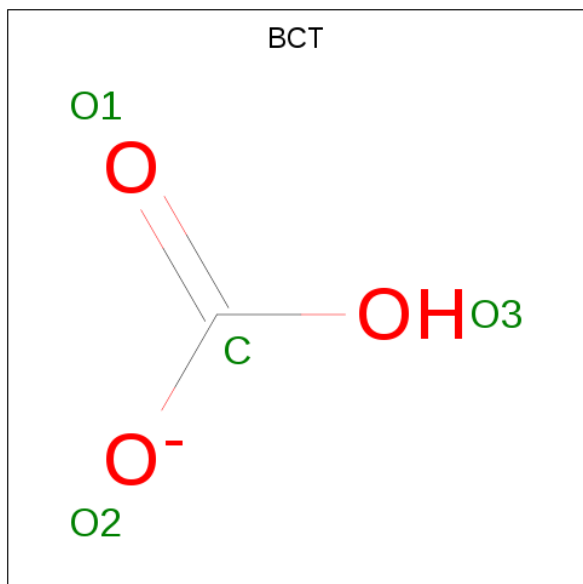
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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 21 | a | 1 | Total | Fe | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 22 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

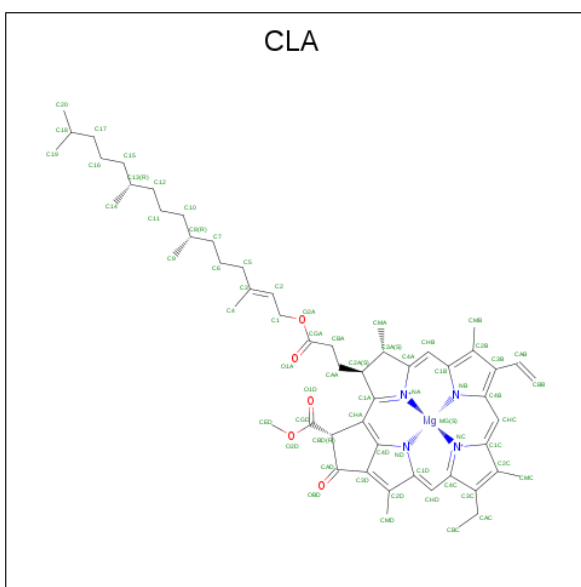
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 22 | a | 2 | Total | Cl | 0 | 0 |
| | | | 2 | 2 | | |
| 22 | A | 2 | Total | Cl | 0 | 0 |
| | | | 2 | 2 | | |
| 22 | V | 1 | Total | Cl | 0 | 0 |
| | | | 1 | 1 | | |
| 22 | u | 1 | Total | Cl | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 23 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 23 | A | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 1 | 3 | | |
| 23 | a | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 1 | 3 | | |

- Molecule 24 is CHLOROPHYLL A (three-letter code: CLA) (formula: $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_5$).

[illegible]

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 24 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | C | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | C | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | C | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | C | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | C | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | C | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | C | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | C | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | C | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | C | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | C | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | D | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | D | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | D | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |

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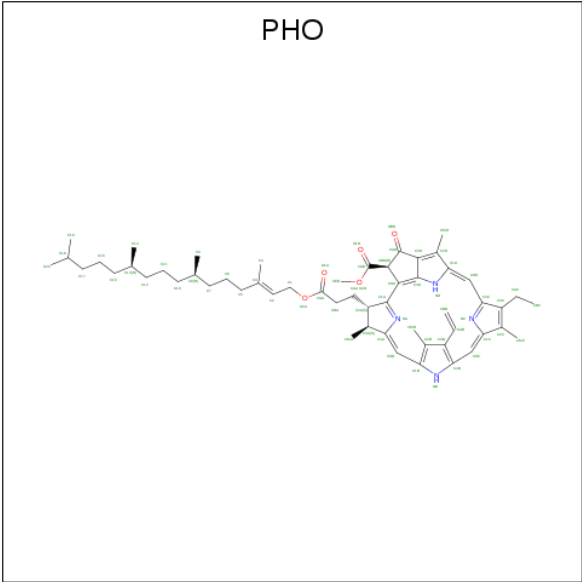
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 24 | a | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | a | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | a | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | b | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | b | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | b | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | b | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | b | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | b | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | b | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | b | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | b | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | b | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | b | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | b | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | c | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | c | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |

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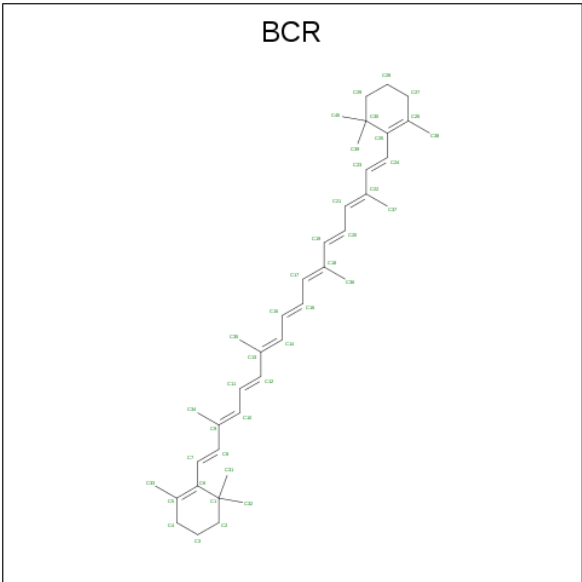
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 24 | c | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | c | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | c | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | c | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | c | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | c | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | c | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | c | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | c | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | d | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | d | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 24 | d | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |

- Molecule 25 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



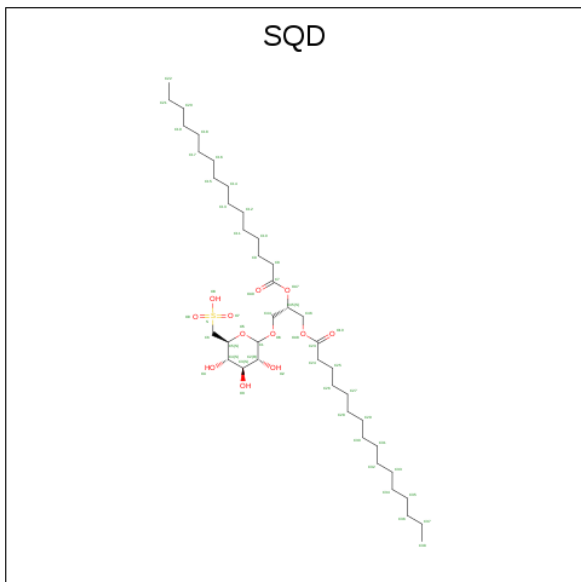
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 25 | A | 1 | Total | C | N | O | 0 | 0 |
| | | | 64 | 55 | 4 | 5 | | |
| 25 | A | 1 | Total | C | N | O | 0 | 0 |
| | | | 64 | 55 | 4 | 5 | | |
| 25 | a | 1 | Total | C | N | O | 0 | 0 |
| | | | 64 | 55 | 4 | 5 | | |
| 25 | d | 1 | Total | C | N | O | 0 | 0 |
| | | | 64 | 55 | 4 | 5 | | |

- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 26 | A | 1 | Total C 40 40 | 0 | 0 |
| 26 | B | 1 | Total C 40 40 | 0 | 0 |
| 26 | B | 1 | Total C 40 40 | 0 | 0 |
| 26 | B | 1 | Total C 40 40 | 0 | 0 |
| 26 | C | 1 | Total C 40 40 | 0 | 0 |
| 26 | C | 1 | Total C 40 40 | 0 | 0 |
| 26 | D | 1 | Total C 40 40 | 0 | 0 |
| 26 | H | 1 | Total C 40 40 | 0 | 0 |
| 26 | K | 1 | Total C 40 40 | 0 | 0 |
| 26 | T | 1 | Total C 40 40 | 0 | 0 |
| 26 | Y | 1 | Total C 40 40 | 0 | 0 |
| 26 | a | 1 | Total C 40 40 | 0 | 0 |
| 26 | b | 1 | Total C 40 40 | 0 | 0 |
| 26 | b | 1 | Total C 40 40 | 0 | 0 |
| 26 | b | 1 | Total C 40 40 | 0 | 0 |
| 26 | c | 1 | Total C 40 40 | 0 | 0 |
| 26 | c | 1 | Total C 40 40 | 0 | 0 |
| 26 | d | 1 | Total C 40 40 | 0 | 0 |
| 26 | h | 1 | Total C 40 40 | 0 | 0 |
| 26 | k | 1 | Total C 40 40 | 0 | 0 |
| 26 | t | 1 | Total C 40 40 | 0 | 0 |
| 26 | y | 1 | Total C 40 40 | 0 | 0 |

- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 27 | A | 1 | Total | C | O | S | 0 | 0 |
| | | | 54 | 41 | 12 | 1 | | |
| 27 | A | 1 | Total | C | O | S | 0 | 0 |
| | | | 54 | 41 | 12 | 1 | | |
| 27 | F | 1 | Total | C | O | S | 0 | 0 |
| | | | 43 | 30 | 12 | 1 | | |
| 27 | a | 1 | Total | C | O | S | 0 | 0 |
| | | | 54 | 41 | 12 | 1 | | |
| 27 | a | 1 | Total | C | O | S | 0 | 0 |
| | | | 54 | 41 | 12 | 1 | | |
| 27 | b | 1 | Total | C | O | S | 0 | 0 |
| | | | 54 | 41 | 12 | 1 | | |
| 27 | f | 1 | Total | C | O | S | 0 | 0 |
| | | | 43 | 30 | 12 | 1 | | |
| 27 | l | 1 | Total | C | O | S | 0 | 0 |
| | | | 54 | 41 | 12 | 1 | | |

- Molecule 28 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 28 | A | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 28 | A | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 28 | A | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 28 | B | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 28 | B | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 28 | B | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 28 | B | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 28 | B | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 28 | C | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 28 | C | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 28 | F | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 28 | O | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|--------|---------|---------|
| 28 | T | 1 | Total 6 | C 3 | O 3 | 0 | 0 |
| 28 | T | 1 | Total 6 | C 3 | O 3 | 0 | 0 |
| 28 | V | 1 | Total 6 | C 3 | O 3 | 0 | 0 |
| 28 | V | 1 | Total 6 | C 3 | O 3 | 0 | 0 |
| 28 | V | 1 | Total 6 | C 3 | O 3 | 0 | 0 |
| 28 | V | 1 | Total 6 | C 3 | O 3 | 0 | 0 |
| 28 | V | 1 | Total 6 | C 3 | O 3 | 0 | 0 |
| 28 | a | 1 | Total 6 | C 3 | O 3 | 0 | 0 |
| 28 | a | 1 | Total 6 | C 3 | O 3 | 0 | 0 |
| 28 | b | 1 | Total 6 | C 3 | O 3 | 0 | 0 |
| 28 | b | 1 | Total 6 | C 3 | O 3 | 0 | 0 |
| 28 | b | 1 | Total 6 | C 3 | O 3 | 0 | 0 |
| 28 | b | 1 | Total 6 | C 3 | O 3 | 0 | 0 |
| 28 | b | 1 | Total 6 | C 3 | O 3 | 0 | 0 |
| 28 | c | 1 | Total 6 | C 3 | O 3 | 0 | 0 |
| 28 | c | 1 | Total 6 | C 3 | O 3 | 0 | 0 |
| 28 | c | 1 | Total 6 | C 3 | O 3 | 0 | 0 |
| 28 | f | 1 | Total 6 | C 3 | O 3 | 0 | 0 |
| 28 | t | 1 | Total 6 | C 3 | O 3 | 0 | 0 |
| 28 | v | 1 | Total 6 | C 3 | O 3 | 0 | 0 |
| 28 | v | 1 | Total 6 | C 3 | O 3 | 0 | 0 |

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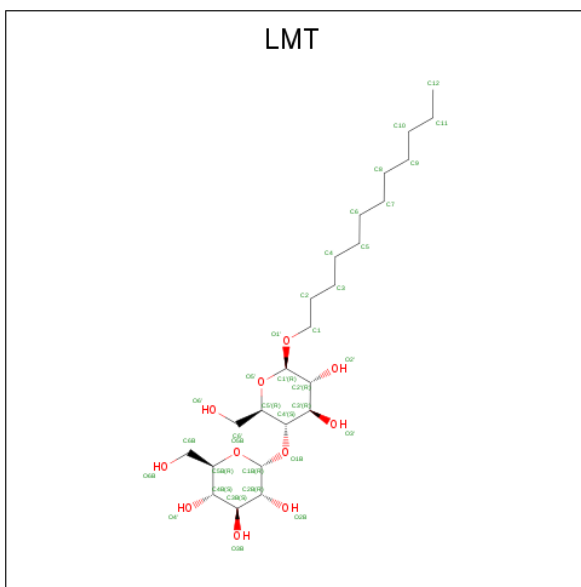
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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 28 | v | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 28 | v | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |

- Molecule 29 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

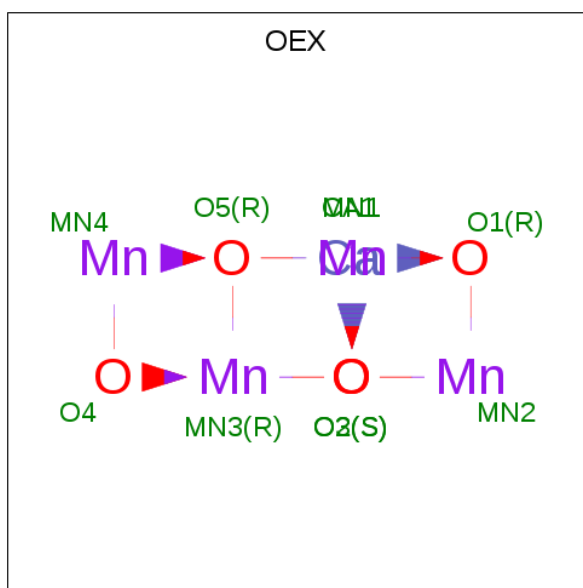
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 29 | J | 1 | Total | C | | 0 | 0 |
| | | | 10 | 10 | | | |
| 29 | i | 1 | Total | C | O | 0 | 0 |
| | | | 40 | 35 | 5 | | |
| 29 | D | 2 | Total | C | O | 0 | 0 |
| | | | 57 | 51 | 6 | | |
| 29 | k | 2 | Total | C | O | 0 | 0 |
| | | | 42 | 37 | 5 | | |
| 29 | B | 1 | Total | C | O | 0 | 0 |
| | | | 33 | 28 | 5 | | |
| 29 | I | 1 | Total | C | O | 0 | 0 |
| | | | 40 | 35 | 5 | | |
| 29 | C | 1 | Total | C | O | 0 | 0 |
| | | | 34 | 29 | 5 | | |
| 29 | a | 1 | Total | C | O | 0 | 0 |
| | | | 30 | 25 | 5 | | |
| 29 | x | 1 | Total | C | | 0 | 0 |
| | | | 10 | 10 | | | |
| 29 | A | 1 | Total | C | O | 0 | 0 |
| | | | 28 | 23 | 5 | | |
| 29 | j | 1 | Total | C | | 0 | 0 |
| | | | 10 | 10 | | | |
| 29 | X | 1 | Total | C | | 0 | 0 |
| | | | 10 | 10 | | | |
| 29 | d | 2 | Total | C | O | 0 | 0 |
| | | | 53 | 47 | 6 | | |
| 29 | m | 1 | Total | C | | 0 | 0 |
| | | | 10 | 10 | | | |
| 29 | b | 1 | Total | C | O | 0 | 0 |
| | | | 33 | 28 | 5 | | |
| 29 | M | 1 | Total | C | | 0 | 0 |
| | | | 10 | 10 | | | |

- Molecule 30 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



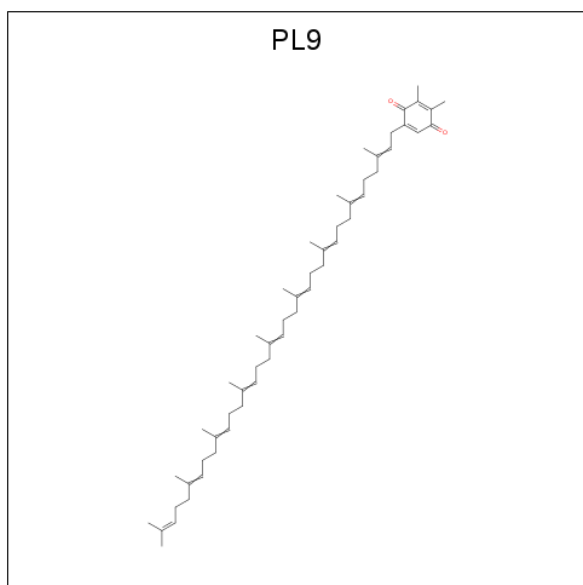
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|---------|
| 30 | A | 1 | Total 33 | C 22 | O 11 | 0 | 0 |
| 30 | B | 1 | Total 25 | C 19 | O 6 | 0 | 0 |
| 30 | D | 1 | Total 35 | C 24 | O 11 | 0 | 0 |
| 30 | E | 1 | Total 35 | C 24 | O 11 | 0 | 0 |
| 30 | I | 1 | Total 35 | C 24 | O 11 | 0 | 0 |
| 30 | M | 1 | Total 35 | C 24 | O 11 | 0 | 0 |
| 30 | M | 1 | Total 35 | C 24 | O 11 | 0 | 0 |
| 30 | a | 1 | Total 35 | C 24 | O 11 | 0 | 0 |
| 30 | a | 1 | Total 35 | C 24 | O 11 | 0 | 0 |
| 30 | b | 1 | Total 25 | C 19 | O 6 | 0 | 0 |
| 30 | b | 1 | Total 25 | C 19 | O 6 | 0 | 0 |
| 30 | f | 1 | Total 35 | C 24 | O 11 | 0 | 0 |
| 30 | m | 1 | Total 35 | C 24 | O 11 | 0 | 0 |
| 30 | m | 1 | Total 35 | C 24 | O 11 | 0 | 0 |

- Molecule 31 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 31 | A | 1 | Total | Ca | Mn | O | 0 | 0 |
| | | | 10 | 1 | 4 | 5 | | |
| 31 | a | 1 | Total | Ca | Mn | O | 0 | 0 |
| | | | 10 | 1 | 4 | 5 | | |

- Molecule 32 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $\text{C}_{53}\text{H}_{80}\text{O}_2$).

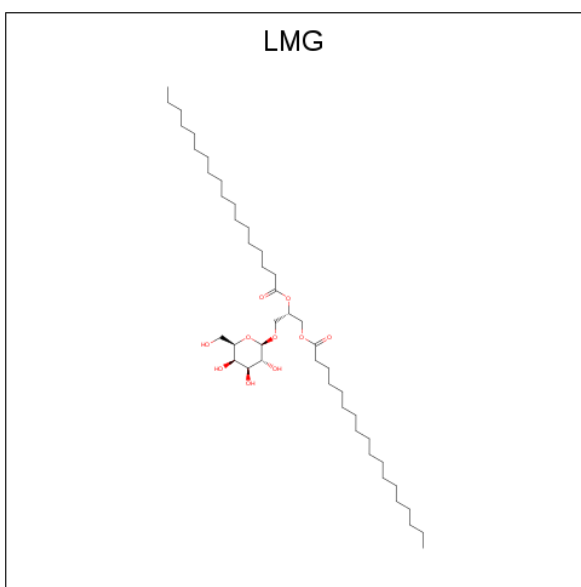


| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 32 | A | 1 | Total | C | O | 0 | 0 |
| | | | 55 | 53 | 2 | | |
| 32 | D | 1 | Total | C | O | 0 | 0 |
| | | | 55 | 53 | 2 | | |
| 32 | a | 1 | Total | C | O | 0 | 0 |
| | | | 55 | 53 | 2 | | |
| 32 | d | 1 | Total | C | O | 0 | 0 |
| | | | 55 | 53 | 2 | | |

- Molecule 33 is CALCIUM ION (three-letter code: CA) (formula: Ca).

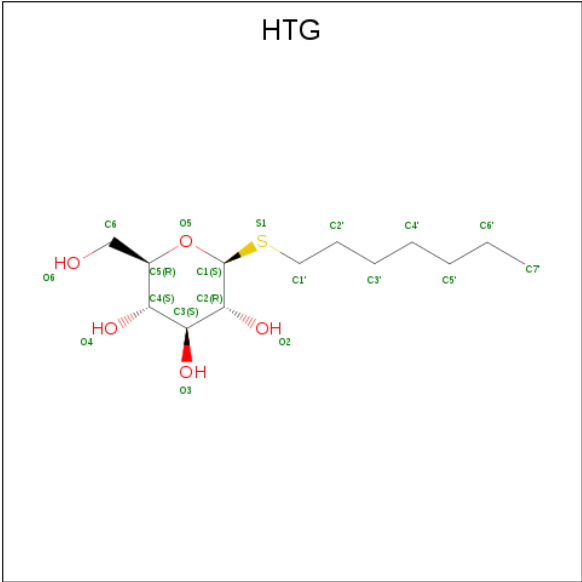
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 33 | B | 1 | Total | Ca | 0 | 0 |
| | | | 1 | 1 | | |
| 33 | c | 1 | Total | Ca | 0 | 0 |
| | | | 1 | 1 | | |
| 33 | F | 1 | Total | Ca | 0 | 0 |
| | | | 1 | 1 | | |
| 33 | o | 1 | Total | Ca | 0 | 0 |
| | | | 1 | 1 | | |
| 33 | O | 1 | Total | Ca | 0 | 0 |
| | | | 1 | 1 | | |
| 33 | b | 1 | Total | Ca | 0 | 0 |
| | | | 1 | 1 | | |
| 33 | f | 1 | Total | Ca | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 34 | B | 1 | Total | C | O | 0 | 0 |
| | | | 51 | 41 | 10 | | |
| 34 | C | 1 | Total | C | O | 0 | 0 |
| | | | 51 | 41 | 10 | | |
| 34 | C | 1 | Total | C | O | 0 | 0 |
| | | | 51 | 41 | 10 | | |
| 34 | C | 1 | Total | C | O | 0 | 0 |
| | | | 51 | 41 | 10 | | |
| 34 | J | 1 | Total | C | O | 0 | 0 |
| | | | 51 | 41 | 10 | | |
| 34 | Z | 1 | Total | C | O | 0 | 0 |
| | | | 37 | 27 | 10 | | |
| 34 | b | 1 | Total | C | O | 0 | 0 |
| | | | 51 | 41 | 10 | | |
| 34 | c | 1 | Total | C | O | 0 | 0 |
| | | | 51 | 41 | 10 | | |
| 34 | c | 1 | Total | C | O | 0 | 0 |
| | | | 51 | 41 | 10 | | |
| 34 | c | 1 | Total | C | O | 0 | 0 |
| | | | 51 | 41 | 10 | | |
| 34 | j | 1 | Total | C | O | 0 | 0 |
| | | | 51 | 41 | 10 | | |
| 34 | z | 1 | Total | C | O | 0 | 0 |
| | | | 39 | 29 | 10 | | |

- Molecule 35 is HEPTYL 1-THIOHEXOPYRANOSIDE (three-letter code: HTG) (formula: $C_{13}H_{26}O_5S$).



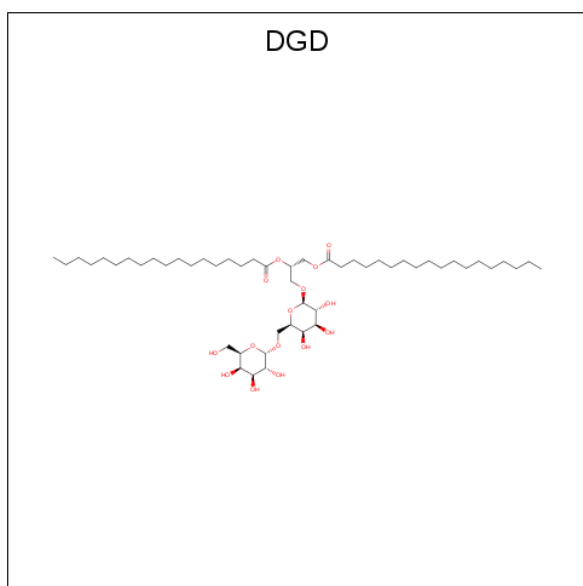
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 35 | B | 1 | Total | C | O | S | 0 | 0 |
| | | | 19 | 13 | 5 | 1 | | |
| 35 | B | 1 | Total | C | O | S | 0 | 0 |
| | | | 19 | 13 | 5 | 1 | | |
| 35 | B | 1 | Total | C | O | S | 0 | 0 |
| | | | 19 | 13 | 5 | 1 | | |
| 35 | B | 1 | Total | C | O | S | 0 | 0 |
| | | | 19 | 13 | 5 | 1 | | |
| 35 | B | 1 | Total | C | O | S | 0 | 0 |
| | | | 19 | 13 | 5 | 1 | | |
| 35 | C | 1 | Total | C | O | S | 0 | 0 |
| | | | 19 | 13 | 5 | 1 | | |
| 35 | C | 1 | Total | C | O | S | 0 | 0 |
| | | | 19 | 13 | 5 | 1 | | |
| 35 | D | 1 | Total | C | O | S | 0 | 0 |
| | | | 16 | 10 | 5 | 1 | | |
| 35 | O | 1 | Total | C | O | S | 0 | 0 |
| | | | 19 | 13 | 5 | 1 | | |
| 35 | V | 1 | Total | C | O | S | 0 | 0 |
| | | | 19 | 13 | 5 | 1 | | |
| 35 | b | 1 | Total | C | O | S | 0 | 0 |
| | | | 19 | 13 | 5 | 1 | | |
| 35 | b | 1 | Total | C | O | S | 0 | 0 |
| | | | 19 | 13 | 5 | 1 | | |
| 35 | b | 1 | Total | C | O | S | 0 | 0 |
| | | | 19 | 13 | 5 | 1 | | |
| 35 | b | 1 | Total | C | O | S | 0 | 0 |
| | | | 19 | 13 | 5 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 35 | c | 1 | Total | C | O | S | 0 | 0 |
| | | | 19 | 13 | 5 | 1 | | |
| 35 | c | 1 | Total | C | O | S | 0 | 0 |
| | | | 19 | 13 | 5 | 1 | | |
| 35 | d | 1 | Total | C | O | S | 0 | 0 |
| | | | 16 | 10 | 5 | 1 | | |

- Molecule 36 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



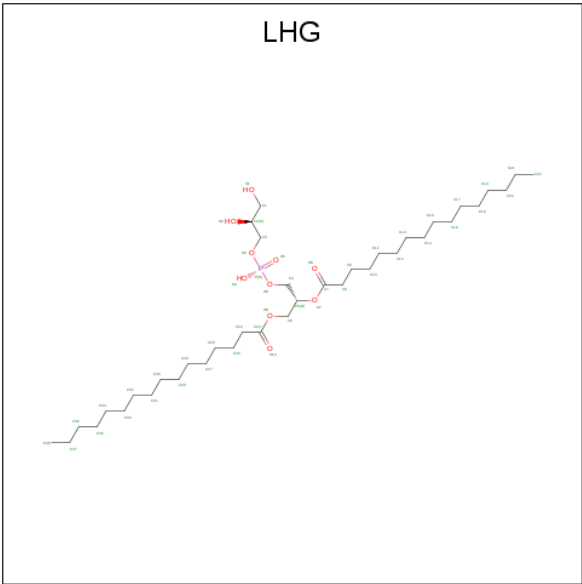
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|--|---------|---------|
| 36 | C | 1 | Total | C | O | | 0 | 0 |
| | | | 62 | 47 | 15 | | | |
| 36 | C | 1 | Total | C | O | | 0 | 0 |
| | | | 62 | 47 | 15 | | | |
| 36 | C | 1 | Total | C | O | | 0 | 0 |
| | | | 62 | 47 | 15 | | | |
| 36 | D | 1 | Total | C | O | | 0 | 0 |
| | | | 62 | 47 | 15 | | | |
| 36 | H | 1 | Total | C | O | | 0 | 0 |
| | | | 62 | 47 | 15 | | | |
| 36 | c | 1 | Total | C | O | | 0 | 0 |
| | | | 62 | 47 | 15 | | | |
| 36 | c | 1 | Total | C | O | | 0 | 0 |
| | | | 62 | 47 | 15 | | | |
| 36 | c | 1 | Total | C | O | | 0 | 0 |
| | | | 62 | 47 | 15 | | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 36 | d | 1 | Total | C | O | 0 | 0 |
| | | | 62 | 47 | 15 | | |
| 36 | h | 1 | Total | C | O | 0 | 0 |
| | | | 62 | 47 | 15 | | |

- Molecule 37 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



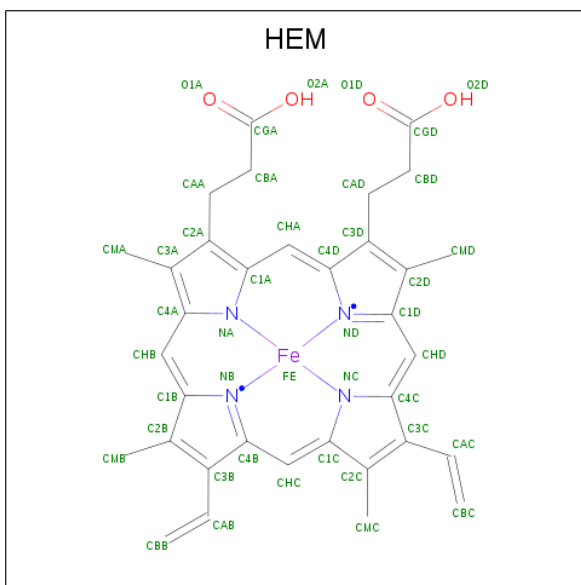
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 37 | D | 1 | Total | C | O | P | 0 | 0 |
| | | | 49 | 38 | 10 | 1 | | |
| 37 | D | 1 | Total | C | O | P | 0 | 0 |
| | | | 49 | 38 | 10 | 1 | | |
| 37 | D | 1 | Total | C | O | P | 0 | 0 |
| | | | 49 | 38 | 10 | 1 | | |
| 37 | E | 1 | Total | C | O | P | 0 | 0 |
| | | | 42 | 31 | 10 | 1 | | |
| 37 | L | 1 | Total | C | O | P | 0 | 0 |
| | | | 49 | 38 | 10 | 1 | | |
| 37 | d | 1 | Total | C | O | P | 0 | 0 |
| | | | 49 | 38 | 10 | 1 | | |
| 37 | d | 1 | Total | C | O | P | 0 | 0 |
| | | | 49 | 38 | 10 | 1 | | |
| 37 | d | 1 | Total | C | O | P | 0 | 0 |
| | | | 49 | 38 | 10 | 1 | | |
| 37 | e | 1 | Total | C | O | P | 0 | 0 |
| | | | 42 | 31 | 10 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 37 | 1 | 1 | Total | C | O | P | 0 | 0 |
| | | | 49 | 38 | 10 | 1 | | |

- Molecule 38 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 38 | E | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |
| 38 | V | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |
| 38 | e | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |
| 38 | v | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |

- Molecule 39 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 39 | J | 1 | Total Mg 1 1 | 0 | 0 |
| 39 | j | 1 | Total Mg 1 1 | 0 | 0 |

- Molecule 40 is water.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 40 | A | 146 | Total O 149 149 | 0 | 3 |
| 40 | B | 277 | Total O 280 280 | 0 | 3 |
| 40 | C | 206 | Total O 209 209 | 0 | 3 |
| 40 | D | 157 | Total O 161 161 | 0 | 4 |
| 40 | E | 28 | Total O 28 28 | 0 | 0 |
| 40 | F | 7 | Total O 7 7 | 0 | 0 |
| 40 | H | 39 | Total O 40 40 | 0 | 1 |
| 40 | I | 8 | Total O 8 8 | 0 | 0 |
| 40 | J | 12 | Total O 12 12 | 0 | 0 |
| 40 | K | 6 | Total O 6 6 | 0 | 0 |
| 40 | L | 12 | Total O 12 12 | 0 | 0 |
| 40 | M | 15 | Total O 15 15 | 0 | 0 |
| 40 | O | 164 | Total O 165 165 | 0 | 1 |
| 40 | T | 12 | Total O 13 13 | 0 | 1 |
| 40 | U | 75 | Total O 76 76 | 0 | 1 |
| 40 | V | 111 | Total O 111 111 | 0 | 0 |
| 40 | Y | 1 | Total O 1 1 | 0 | 0 |
| 40 | X | 8 | Total O 8 8 | 0 | 0 |
| 40 | a | 151 | Total O 151 151 | 0 | 0 |
| 40 | b | 247 | Total O 249 249 | 0 | 2 |
| 40 | c | 187 | Total O 189 189 | 0 | 2 |
| 40 | d | 136 | Total O 139 139 | 0 | 3 |

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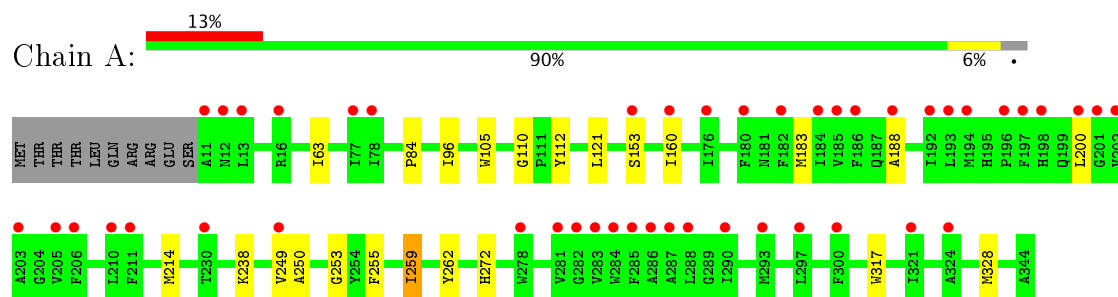
Continued from previous page...

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 40 | e | 15 | Total 15 | O 15 | 0 | 0 |
| 40 | f | 7 | Total 7 | O 7 | 0 | 0 |
| 40 | h | 36 | Total 36 | O 36 | 0 | 0 |
| 40 | i | 5 | Total 5 | O 5 | 0 | 0 |
| 40 | j | 7 | Total 7 | O 7 | 0 | 0 |
| 40 | k | 3 | Total 3 | O 3 | 0 | 0 |
| 40 | l | 10 | Total 10 | O 10 | 0 | 0 |
| 40 | m | 12 | Total 12 | O 12 | 0 | 0 |
| 40 | o | 137 | Total 137 | O 137 | 0 | 0 |
| 40 | t | 10 | Total 10 | O 10 | 0 | 0 |
| 40 | u | 89 | Total 89 | O 89 | 0 | 0 |
| 40 | v | 80 | Total 80 | O 80 | 0 | 0 |
| 40 | y | 4 | Total 4 | O 4 | 0 | 0 |
| 40 | x | 5 | Total 5 | O 5 | 0 | 0 |

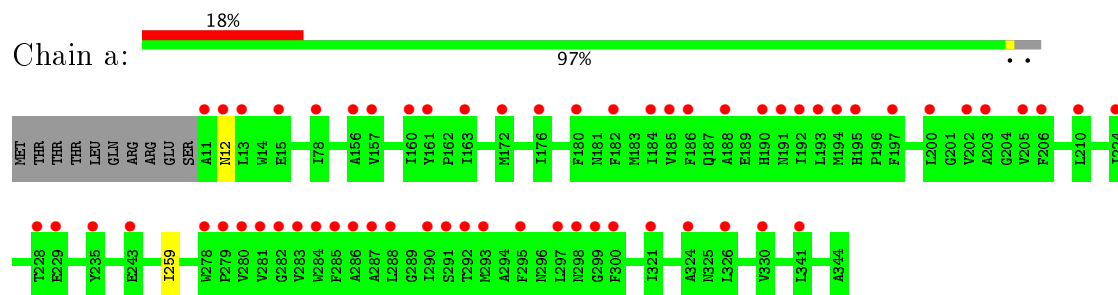
3 Residue-property plots [i](#)

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

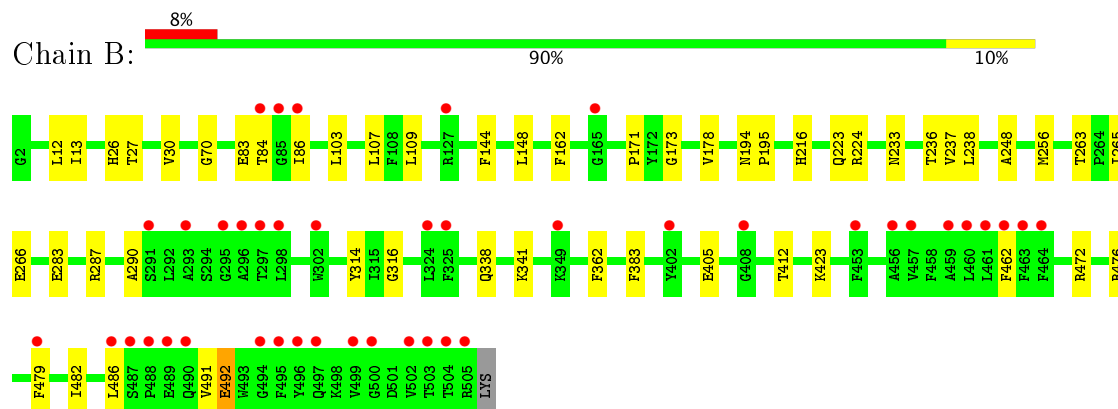
- Molecule 1: Photosystem Q(B) protein



- Molecule 1: Photosystem Q(B) protein

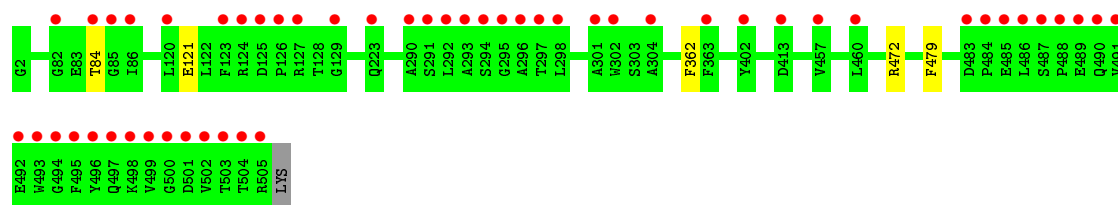


- Molecule 2: Photosystem II CP47 chlorophyll apoprotein

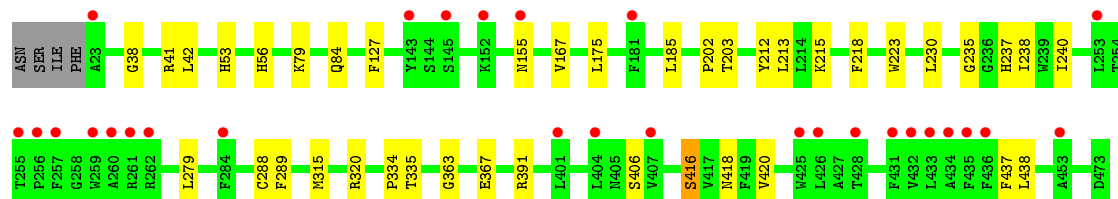
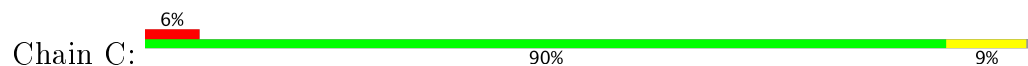


- Molecule 2: Photosystem II CP47 chlorophyll apoprotein

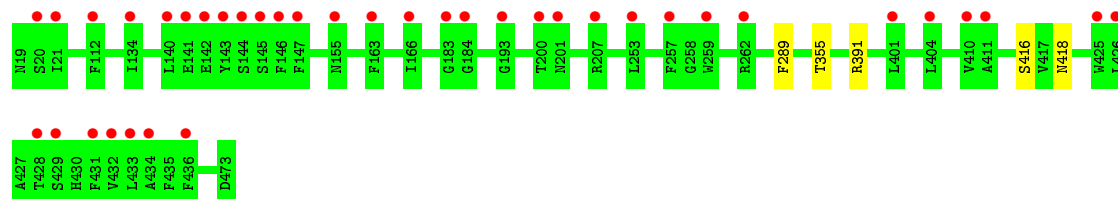




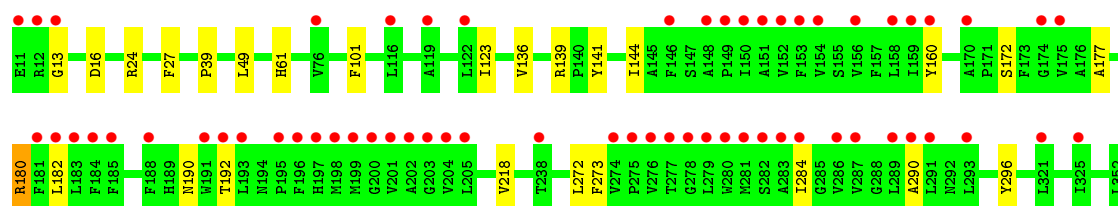
• Molecule 3: Photosystem II 44 kDa reaction center protein



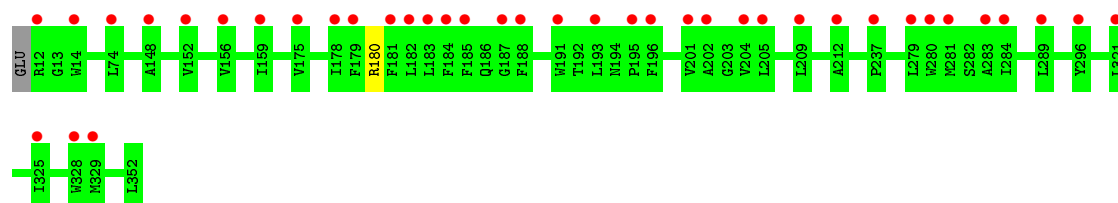
• Molecule 3: Photosystem II 44 kDa reaction center protein



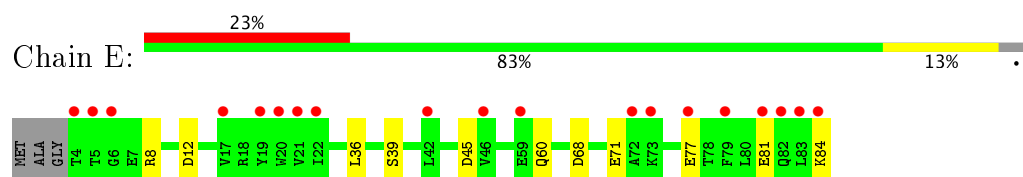
• Molecule 4: Photosystem II D2 protein



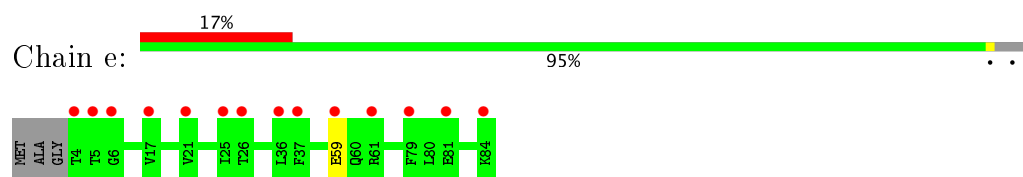
• Molecule 4: Photosystem II D2 protein



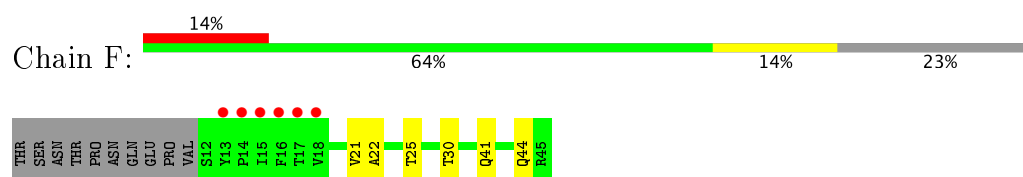
• Molecule 5: Cytochrome b559 subunit alpha



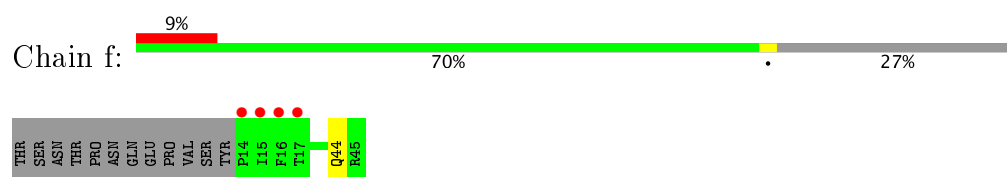
- Molecule 5: Cytochrome b559 subunit alpha



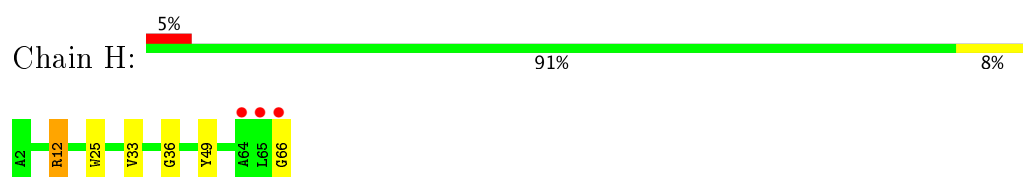
- Molecule 6: Cytochrome b559 subunit beta



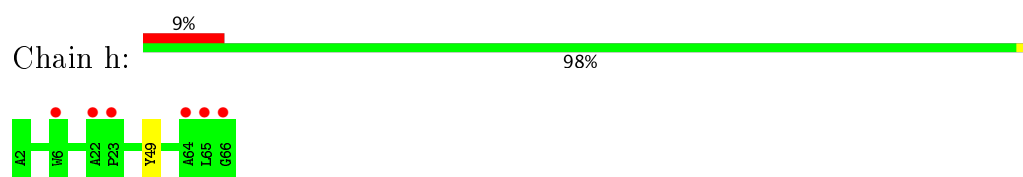
- Molecule 6: Cytochrome b559 subunit beta



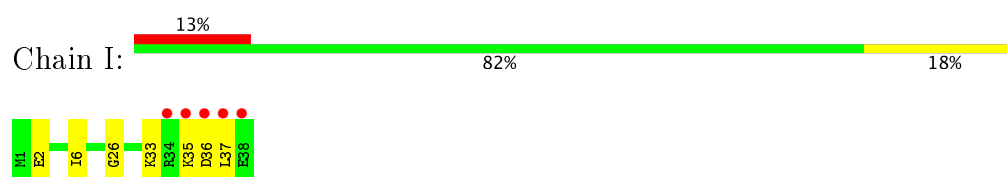
- Molecule 7: Photosystem II reaction center protein H



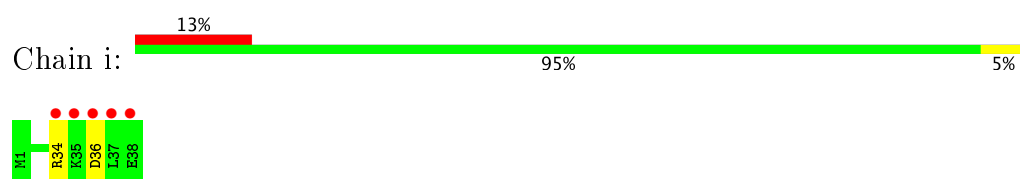
- Molecule 7: Photosystem II reaction center protein H



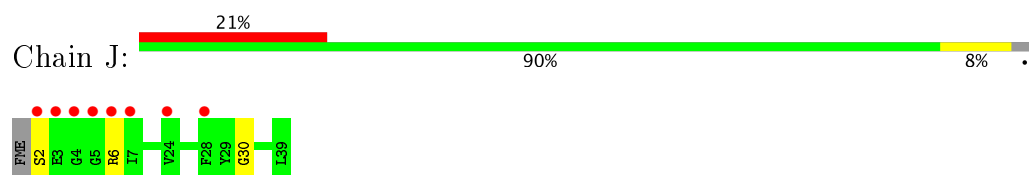
- Molecule 8: Photosystem II reaction center protein I



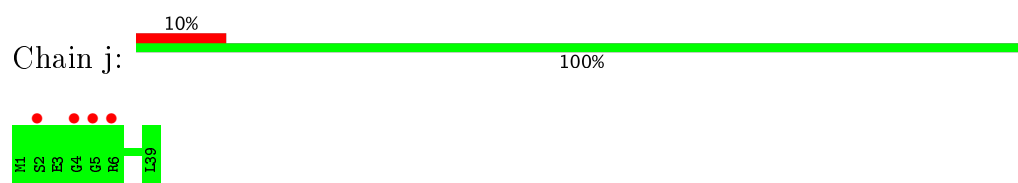
- Molecule 8: Photosystem II reaction center protein I



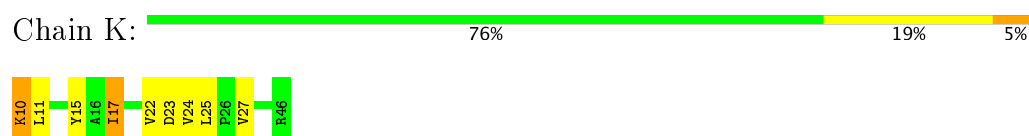
- Molecule 9: Photosystem II reaction center protein J



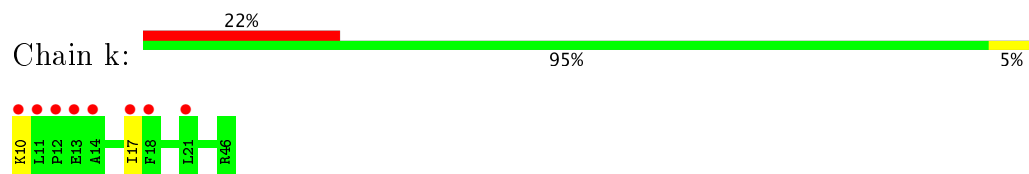
- Molecule 9: Photosystem II reaction center protein J



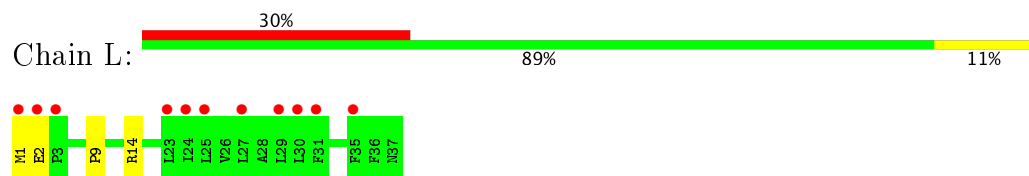
- Molecule 10: Photosystem II reaction center protein K



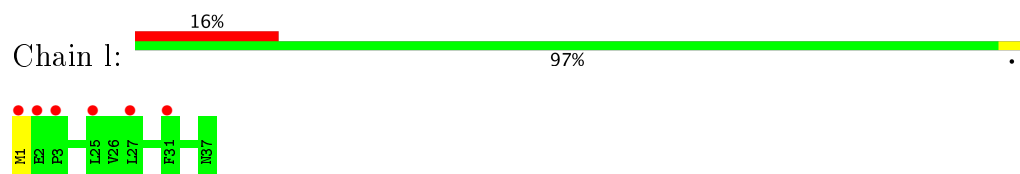
- Molecule 10: Photosystem II reaction center protein K



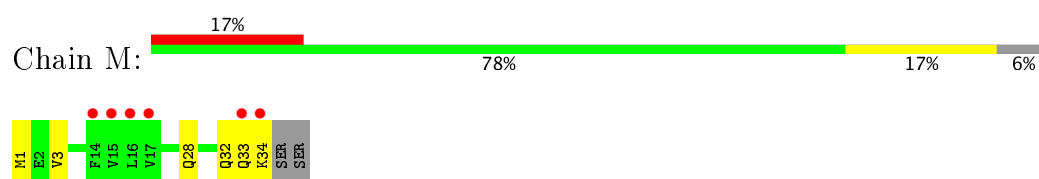
- Molecule 11: Photosystem II reaction center protein L



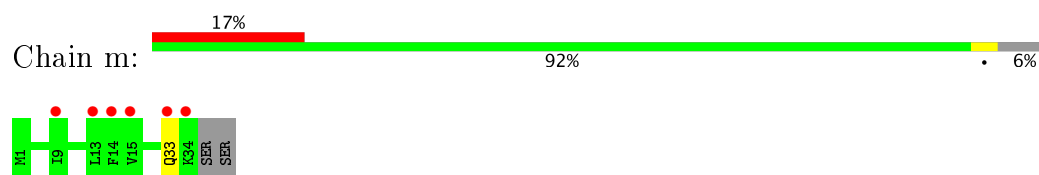
- Molecule 11: Photosystem II reaction center protein L



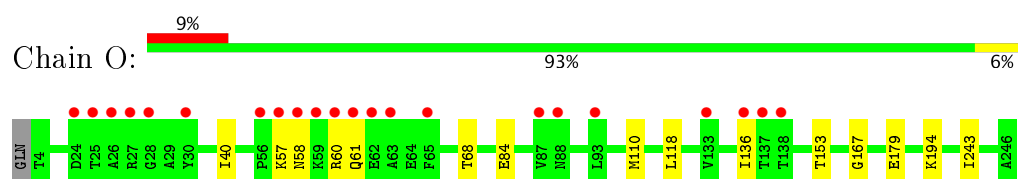
- Molecule 12: Photosystem II reaction center protein M



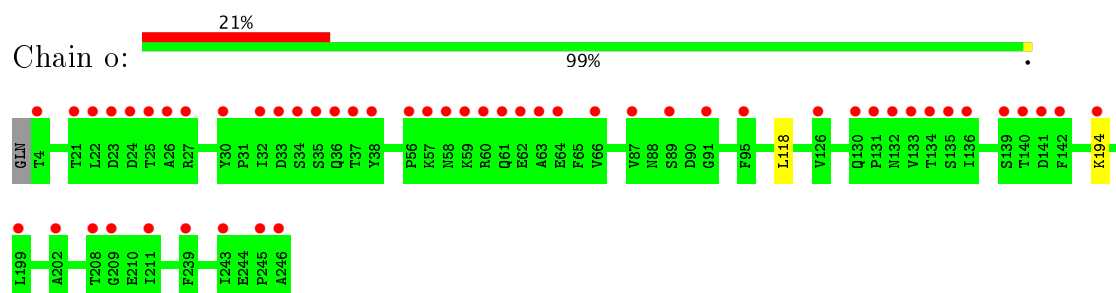
- Molecule 12: Photosystem II reaction center protein M



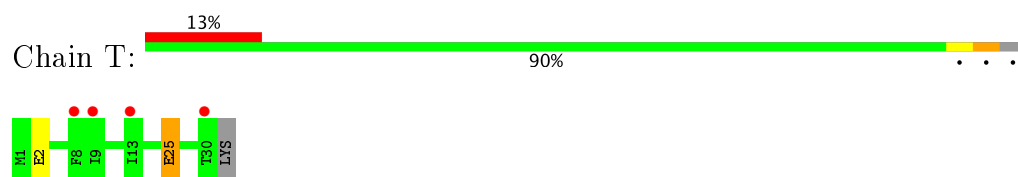
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



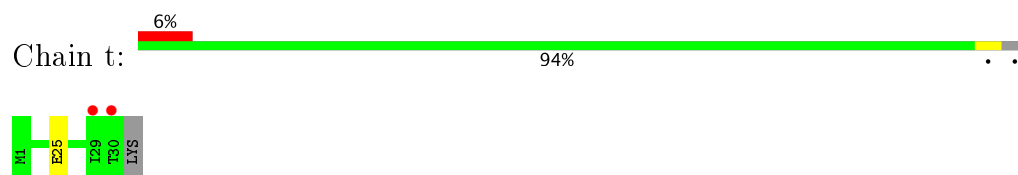
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



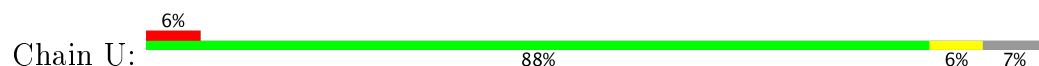
- Molecule 14: Photosystem II reaction center protein T

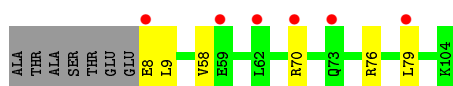


- Molecule 14: Photosystem II reaction center protein T



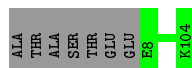
- Molecule 15: Photosystem II 12 kDa extrinsic protein





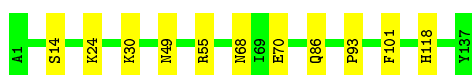
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u: 93% 7%



- Molecule 16: Cytochrome c-550

Chain V: 92% 8%



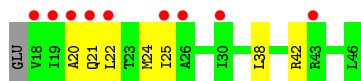
- Molecule 16: Cytochrome c-550

Chain v: 9% 99% .



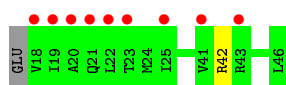
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y: 30% 73% 23% .



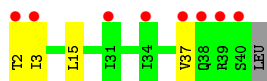
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y: 30% 93% . .



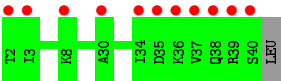
- Molecule 18: Photosystem II reaction center protein X

Chain X: 20% 88% 10% .

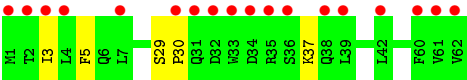


- Molecule 18: Photosystem II reaction center protein X

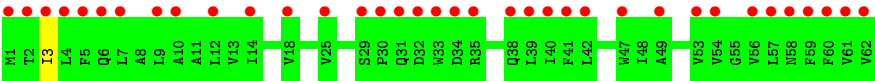
Chain x: 28% 98% .



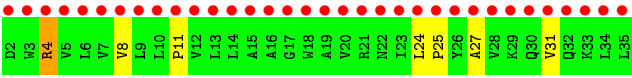
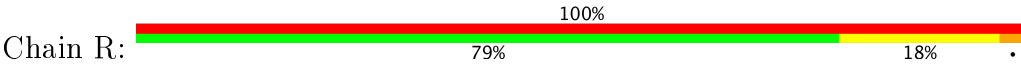
● Molecule 19: Photosystem II reaction center protein Z



● Molecule 19: Photosystem II reaction center protein Z



● Molecule 20: Photosystem II protein Y



GLOBAL-STATISTICS INFOmissingINFO

4 Model quality

4.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, GOL, MG, OEX, PHO, DGD, CL, CA, LMT, CLA, PL9, FE2, SQD, BCT, HEM, FME, UNL, HTG, 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 | 0.53 | 0/2725 | 0.59 | 0/3716 |
| 1 | a | 0.55 | 0/2731 | 0.58 | 0/3724 |
| 2 | B | 0.49 | 0/4193 | 0.56 | 0/5712 |
| 2 | b | 0.47 | 0/4201 | 0.55 | 0/5723 |
| 3 | C | 0.46 | 0/3634 | 0.54 | 0/4947 |
| 3 | c | 0.46 | 0/3676 | 0.54 | 0/5004 |
| 4 | D | 0.53 | 0/2821 | 0.56 | 0/3844 |
| 4 | d | 0.52 | 0/2818 | 0.55 | 0/3840 |
| 5 | E | 0.36 | 0/693 | 0.52 | 0/944 |
| 5 | e | 0.33 | 0/681 | 0.52 | 0/928 |
| 6 | F | 0.39 | 0/284 | 0.48 | 0/387 |
| 6 | f | 0.37 | 0/265 | 0.51 | 0/360 |
| 7 | H | 0.40 | 0/535 | 0.53 | 0/728 |
| 7 | h | 0.35 | 0/524 | 0.50 | 0/713 |
| 8 | I | 0.38 | 0/311 | 0.51 | 0/419 |
| 8 | i | 0.40 | 0/311 | 0.50 | 0/419 |
| 9 | J | 0.37 | 0/278 | 0.46 | 0/376 |
| 9 | j | 0.38 | 0/278 | 0.48 | 0/376 |
| 10 | K | 0.36 | 0/303 | 0.48 | 0/416 |
| 10 | k | 0.36 | 0/303 | 0.51 | 0/416 |
| 11 | L | 0.48 | 0/319 | 0.49 | 0/433 |
| 11 | l | 0.49 | 0/319 | 0.50 | 0/433 |
| 12 | M | 0.43 | 0/270 | 0.58 | 0/368 |
| 12 | m | 0.47 | 0/262 | 0.58 | 0/357 |
| 13 | O | 0.41 | 0/1926 | 0.56 | 0/2611 |
| 13 | o | 0.40 | 0/1919 | 0.57 | 0/2601 |
| 14 | T | 0.54 | 0/266 | 0.56 | 0/362 |
| 14 | t | 0.54 | 0/266 | 0.56 | 0/362 |
| 15 | U | 0.44 | 0/785 | 0.55 | 0/1064 |
| 15 | u | 0.42 | 0/785 | 0.56 | 0/1064 |
| 16 | V | 0.45 | 0/1096 | 0.54 | 0/1487 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|---------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 16 | v | 0.41 | 0/1085 | 0.53 | 0/1473 |
| 17 | Y | 0.29 | 0/216 | 0.46 | 0/289 |
| 17 | y | 0.28 | 0/216 | 0.46 | 0/289 |
| 18 | X | 0.34 | 0/298 | 0.44 | 0/403 |
| 18 | x | 0.34 | 0/290 | 0.48 | 0/392 |
| 19 | Z | 0.31 | 0/490 | 0.43 | 0/669 |
| 19 | z | 0.32 | 0/490 | 0.43 | 0/669 |
| 20 | R | 0.24 | 0/279 | 0.38 | 0/383 |
| All | All | 0.46 | 0/43142 | 0.55 | 0/58701 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

4.2 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 | 2631 | 0 | 2538 | 24 | 0 |
| 1 | a | 2634 | 0 | 2543 | 0 | 0 |
| 2 | B | 4023 | 0 | 3904 | 52 | 0 |
| 2 | b | 4028 | 0 | 3910 | 0 | 0 |
| 3 | C | 3506 | 0 | 3439 | 33 | 0 |
| 3 | c | 3544 | 0 | 3480 | 0 | 0 |
| 4 | D | 2726 | 0 | 2627 | 27 | 0 |
| 4 | d | 2720 | 0 | 2626 | 0 | 0 |
| 5 | E | 668 | 0 | 658 | 8 | 0 |
| 5 | e | 662 | 0 | 648 | 0 | 0 |
| 6 | F | 275 | 0 | 282 | 4 | 0 |
| 6 | f | 257 | 0 | 269 | 0 | 0 |
| 7 | H | 519 | 0 | 545 | 8 | 0 |
| 7 | h | 511 | 0 | 532 | 0 | 0 |
| 8 | I | 314 | 0 | 328 | 5 | 0 |
| 8 | i | 314 | 0 | 328 | 0 | 0 |
| 9 | J | 272 | 0 | 279 | 3 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 9 | j | 282 | 0 | 290 | 0 | 0 |
| 10 | K | 293 | 0 | 305 | 8 | 0 |
| 10 | k | 293 | 0 | 305 | 0 | 0 |
| 11 | L | 309 | 0 | 327 | 3 | 0 |
| 11 | l | 309 | 0 | 327 | 0 | 0 |
| 12 | M | 274 | 0 | 299 | 8 | 0 |
| 12 | m | 269 | 0 | 288 | 0 | 0 |
| 13 | O | 1883 | 0 | 1865 | 10 | 0 |
| 13 | o | 1879 | 0 | 1858 | 0 | 0 |
| 14 | T | 264 | 0 | 267 | 3 | 0 |
| 14 | t | 264 | 0 | 267 | 0 | 0 |
| 15 | U | 774 | 0 | 773 | 3 | 0 |
| 15 | u | 774 | 0 | 773 | 0 | 0 |
| 16 | V | 1072 | 0 | 1086 | 9 | 0 |
| 16 | v | 1064 | 0 | 1073 | 0 | 0 |
| 17 | Y | 215 | 0 | 246 | 5 | 0 |
| 17 | y | 215 | 0 | 246 | 0 | 0 |
| 18 | X | 292 | 0 | 328 | 3 | 0 |
| 18 | x | 287 | 0 | 317 | 0 | 0 |
| 19 | Z | 479 | 0 | 516 | 4 | 0 |
| 19 | z | 479 | 0 | 516 | 0 | 0 |
| 20 | R | 273 | 0 | 305 | 4 | 0 |
| 21 | A | 1 | 0 | 0 | 0 | 0 |
| 21 | a | 1 | 0 | 0 | 0 | 0 |
| 22 | A | 2 | 0 | 0 | 0 | 0 |
| 22 | V | 1 | 0 | 0 | 1 | 0 |
| 22 | a | 2 | 0 | 0 | 0 | 0 |
| 22 | u | 1 | 0 | 0 | 0 | 0 |
| 23 | A | 4 | 0 | 0 | 0 | 0 |
| 23 | a | 4 | 0 | 0 | 0 | 0 |
| 24 | A | 195 | 0 | 216 | 13 | 0 |
| 24 | B | 1040 | 0 | 1152 | 50 | 0 |
| 24 | C | 845 | 0 | 936 | 53 | 0 |
| 24 | D | 195 | 0 | 216 | 11 | 0 |
| 24 | a | 195 | 0 | 216 | 0 | 0 |
| 24 | b | 1040 | 0 | 1152 | 0 | 0 |
| 24 | c | 845 | 0 | 936 | 0 | 0 |
| 24 | d | 195 | 0 | 216 | 0 | 0 |
| 25 | A | 128 | 0 | 148 | 2 | 0 |
| 25 | a | 64 | 0 | 74 | 0 | 0 |
| 25 | d | 64 | 0 | 74 | 0 | 0 |
| 26 | A | 40 | 0 | 56 | 3 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 26 | B | 120 | 0 | 168 | 6 | 0 |
| 26 | C | 80 | 0 | 112 | 7 | 0 |
| 26 | D | 40 | 0 | 56 | 4 | 0 |
| 26 | H | 40 | 0 | 56 | 6 | 0 |
| 26 | K | 40 | 0 | 56 | 2 | 0 |
| 26 | T | 40 | 0 | 56 | 5 | 0 |
| 26 | Y | 40 | 0 | 56 | 2 | 0 |
| 26 | a | 40 | 0 | 56 | 0 | 0 |
| 26 | b | 120 | 0 | 168 | 0 | 0 |
| 26 | c | 80 | 0 | 112 | 0 | 0 |
| 26 | d | 40 | 0 | 56 | 0 | 0 |
| 26 | h | 40 | 0 | 56 | 0 | 0 |
| 26 | k | 40 | 0 | 56 | 0 | 0 |
| 26 | t | 40 | 0 | 56 | 0 | 0 |
| 26 | y | 40 | 0 | 56 | 0 | 0 |
| 27 | A | 108 | 0 | 156 | 8 | 0 |
| 27 | F | 43 | 0 | 53 | 5 | 0 |
| 27 | a | 108 | 0 | 155 | 0 | 0 |
| 27 | b | 54 | 0 | 78 | 0 | 0 |
| 27 | f | 43 | 0 | 53 | 0 | 0 |
| 27 | l | 54 | 0 | 78 | 0 | 0 |
| 28 | A | 18 | 0 | 24 | 4 | 0 |
| 28 | B | 42 | 0 | 56 | 4 | 0 |
| 28 | C | 12 | 0 | 16 | 3 | 0 |
| 28 | F | 6 | 0 | 8 | 0 | 0 |
| 28 | O | 6 | 0 | 8 | 0 | 0 |
| 28 | T | 12 | 0 | 16 | 1 | 0 |
| 28 | V | 30 | 0 | 40 | 4 | 0 |
| 28 | a | 12 | 0 | 16 | 0 | 0 |
| 28 | b | 30 | 0 | 40 | 0 | 0 |
| 28 | c | 18 | 0 | 24 | 0 | 0 |
| 28 | f | 6 | 0 | 7 | 0 | 0 |
| 28 | t | 6 | 0 | 8 | 0 | 0 |
| 28 | v | 24 | 0 | 32 | 0 | 0 |
| 29 | A | 28 | 0 | 0 | 0 | 0 |
| 29 | B | 33 | 0 | 0 | 0 | 0 |
| 29 | C | 34 | 0 | 0 | 0 | 0 |
| 29 | D | 57 | 0 | 0 | 0 | 0 |
| 29 | I | 40 | 0 | 0 | 0 | 0 |
| 29 | J | 10 | 0 | 0 | 0 | 0 |
| 29 | M | 10 | 0 | 0 | 0 | 0 |
| 29 | X | 10 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 29 | a | 30 | 0 | 0 | 0 | 0 |
| 29 | b | 33 | 0 | 0 | 0 | 0 |
| 29 | d | 53 | 0 | 0 | 0 | 0 |
| 29 | i | 40 | 0 | 0 | 0 | 0 |
| 29 | j | 10 | 0 | 0 | 0 | 0 |
| 29 | k | 42 | 0 | 0 | 0 | 0 |
| 29 | m | 10 | 0 | 0 | 0 | 0 |
| 29 | x | 10 | 0 | 0 | 0 | 0 |
| 30 | A | 33 | 0 | 39 | 0 | 0 |
| 30 | B | 25 | 0 | 35 | 1 | 0 |
| 30 | D | 35 | 0 | 46 | 1 | 0 |
| 30 | E | 35 | 0 | 46 | 0 | 0 |
| 30 | I | 35 | 0 | 46 | 2 | 0 |
| 30 | M | 70 | 0 | 92 | 3 | 0 |
| 30 | a | 70 | 0 | 92 | 0 | 0 |
| 30 | b | 50 | 0 | 70 | 0 | 0 |
| 30 | f | 35 | 0 | 46 | 0 | 0 |
| 30 | m | 70 | 0 | 92 | 0 | 0 |
| 31 | A | 10 | 0 | 0 | 0 | 0 |
| 31 | a | 10 | 0 | 0 | 0 | 0 |
| 32 | A | 55 | 0 | 80 | 4 | 0 |
| 32 | D | 55 | 0 | 80 | 0 | 0 |
| 32 | a | 55 | 0 | 80 | 0 | 0 |
| 32 | d | 55 | 0 | 80 | 0 | 0 |
| 33 | B | 1 | 0 | 0 | 0 | 0 |
| 33 | F | 1 | 0 | 0 | 0 | 0 |
| 33 | O | 1 | 0 | 0 | 0 | 0 |
| 33 | b | 1 | 0 | 0 | 0 | 0 |
| 33 | c | 1 | 0 | 0 | 0 | 0 |
| 33 | f | 1 | 0 | 0 | 0 | 0 |
| 33 | o | 1 | 0 | 0 | 0 | 0 |
| 34 | B | 51 | 0 | 72 | 2 | 0 |
| 34 | C | 153 | 0 | 216 | 11 | 0 |
| 34 | J | 51 | 0 | 72 | 3 | 0 |
| 34 | Z | 37 | 0 | 44 | 6 | 0 |
| 34 | b | 51 | 0 | 72 | 0 | 0 |
| 34 | c | 153 | 0 | 216 | 0 | 0 |
| 34 | j | 51 | 0 | 72 | 0 | 0 |
| 34 | z | 39 | 0 | 48 | 0 | 0 |
| 35 | B | 95 | 0 | 130 | 1 | 0 |
| 35 | C | 38 | 0 | 52 | 3 | 0 |
| 35 | D | 16 | 0 | 17 | 3 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 35 | O | 19 | 0 | 26 | 0 | 0 |
| 35 | V | 19 | 0 | 26 | 1 | 0 |
| 35 | b | 76 | 0 | 104 | 0 | 0 |
| 35 | c | 38 | 0 | 52 | 0 | 0 |
| 35 | d | 16 | 0 | 17 | 0 | 0 |
| 36 | C | 186 | 0 | 246 | 10 | 0 |
| 36 | D | 62 | 0 | 82 | 6 | 0 |
| 36 | H | 62 | 0 | 82 | 2 | 0 |
| 36 | c | 186 | 0 | 246 | 0 | 0 |
| 36 | d | 62 | 0 | 82 | 0 | 0 |
| 36 | h | 62 | 0 | 82 | 0 | 0 |
| 37 | D | 147 | 0 | 222 | 12 | 0 |
| 37 | E | 42 | 0 | 57 | 6 | 0 |
| 37 | L | 49 | 0 | 74 | 1 | 0 |
| 37 | d | 147 | 0 | 222 | 0 | 0 |
| 37 | e | 42 | 0 | 57 | 0 | 0 |
| 37 | l | 49 | 0 | 74 | 0 | 0 |
| 38 | E | 43 | 0 | 30 | 0 | 0 |
| 38 | V | 43 | 0 | 30 | 0 | 0 |
| 38 | e | 43 | 0 | 30 | 0 | 0 |
| 38 | v | 43 | 0 | 30 | 0 | 0 |
| 39 | J | 1 | 0 | 0 | 0 | 0 |
| 39 | j | 1 | 0 | 0 | 0 | 0 |
| 40 | A | 149 | 0 | 0 | 2 | 0 |
| 40 | B | 280 | 0 | 0 | 6 | 0 |
| 40 | C | 209 | 0 | 0 | 4 | 0 |
| 40 | D | 161 | 0 | 0 | 2 | 0 |
| 40 | E | 28 | 0 | 0 | 1 | 0 |
| 40 | F | 7 | 0 | 0 | 0 | 0 |
| 40 | H | 40 | 0 | 0 | 0 | 0 |
| 40 | I | 8 | 0 | 0 | 0 | 0 |
| 40 | J | 12 | 0 | 0 | 1 | 0 |
| 40 | K | 6 | 0 | 0 | 1 | 0 |
| 40 | L | 12 | 0 | 0 | 1 | 0 |
| 40 | M | 15 | 0 | 0 | 0 | 0 |
| 40 | O | 165 | 0 | 0 | 2 | 0 |
| 40 | T | 13 | 0 | 0 | 0 | 0 |
| 40 | U | 76 | 0 | 0 | 2 | 0 |
| 40 | V | 111 | 0 | 0 | 1 | 0 |
| 40 | X | 8 | 0 | 0 | 0 | 0 |
| 40 | Y | 1 | 0 | 0 | 0 | 0 |
| 40 | a | 151 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 40 | b | 249 | 0 | 0 | 0 | 0 |
| 40 | c | 189 | 0 | 0 | 0 | 0 |
| 40 | d | 139 | 0 | 0 | 0 | 0 |
| 40 | e | 15 | 0 | 0 | 0 | 0 |
| 40 | f | 7 | 0 | 0 | 0 | 0 |
| 40 | h | 36 | 0 | 0 | 0 | 0 |
| 40 | i | 5 | 0 | 0 | 0 | 0 |
| 40 | j | 7 | 0 | 0 | 0 | 0 |
| 40 | k | 3 | 0 | 0 | 0 | 0 |
| 40 | l | 10 | 0 | 0 | 0 | 0 |
| 40 | m | 12 | 0 | 0 | 0 | 0 |
| 40 | o | 137 | 0 | 0 | 0 | 0 |
| 40 | t | 10 | 0 | 0 | 0 | 0 |
| 40 | u | 89 | 0 | 0 | 0 | 0 |
| 40 | v | 80 | 0 | 0 | 0 | 0 |
| 40 | x | 5 | 0 | 0 | 0 | 0 |
| 40 | y | 4 | 0 | 0 | 0 | 0 |
| All | All | 53958 | 0 | 52755 | 346 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (346) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:214:MET:HG2 | 32:A:419:PL9:H102 | 1.51 | 0.93 |
| 1:A:250:ALA:HA | 2:B:491:VAL:HG11 | 2.30 | 0.92 |
| 24:B:616:CLA:H71 | 24:B:617:CLA:H192 | 1.64 | 0.78 |
| 24:C:503:CLA:H193 | 35:C:522:HTG:H3'1 | 1.67 | 0.74 |
| 24:C:504:CLA:H61 | 24:C:514:CLA:H42 | 27.00 | 0.74 |
| 24:C:507:CLA:HMC2 | 24:C:508:CLA:H102 | 1.68 | 0.73 |
| 8:I:26:GLY:HA3 | 30:I:102:LMT:H6'1 | 1.70 | 0.73 |
| 1:A:253:GLY:HA3 | 2:B:491:VAL:HG12 | 3.53 | 0.73 |
| 24:C:503:CLA:H202 | 24:C:509:CLA:HBB1 | 29.02 | 0.72 |
| 26:B:620:BCR:H331 | 26:B:620:BCR:HC8 | 1.73 | 0.71 |
| 32:A:419:PL9:H471 | 27:F:101:SQD:H302 | 1.71 | 0.71 |
| 36:D:407:DGD:HD4 | 5:E:45:ASP:HB3 | 1.73 | 0.70 |
| 24:C:508:CLA:HMC2 | 24:C:509:CLA:H102 | 29.18 | 0.68 |
| 24:C:510:CLA:HBB1 | 24:C:510:CLA:HMB1 | 1.77 | 0.66 |
| 13:O:58:ASN:HD21 | 13:O:61:GLN:HB2 | 1.60 | 0.66 |
| 27:A:411:SQD:H251 | 37:D:410:LHG:H131 | 1.78 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 4:D:101:PHE:HB3 | 36:D:407:DGD:HG2 | 2.07 | 0.66 |
| 24:A:406:CLA:HBB1 | 24:A:406:CLA:HMB1 | 1.92 | 0.65 |
| 18:X:2:THR:HG22 | 18:X:3:ILE:HG12 | 4.88 | 0.65 |
| 24:B:615:CLA:H18 | 34:B:621:LMG:H421 | 1.78 | 0.64 |
| 24:C:511:CLA:HBC3 | 24:C:511:CLA:H192 | 1.80 | 0.62 |
| 3:C:213[B]:LEU:HD11 | 26:C:516:BCR:H373 | 4.79 | 0.62 |
| 2:B:341:LYS:HA | 2:B:405[A]:GLU:HG2 | 1.82 | 0.62 |
| 2:B:248:ALA:HA | 24:B:604:CLA:H42 | 1.81 | 0.62 |
| 1:A:238:LYS:NZ | 40:A:628:HOH:O | 65.39 | 0.61 |
| 24:B:614:CLA:HBB1 | 24:B:614:CLA:HMB1 | 1.82 | 0.61 |
| 2:B:266:GLU:HB3 | 28:B:628:GOL:H11 | 1.82 | 0.61 |
| 1:A:183:MET:HA | 24:A:405:CLA:HMD2 | 1.83 | 0.61 |
| 2:B:171:PRO:HD3 | 7:H:66:GLY:HA2 | 1.81 | 0.61 |
| 24:B:606:CLA:HBB1 | 24:B:606:CLA:HHC | 1.81 | 0.60 |
| 24:C:511:CLA:HBB1 | 24:C:511:CLA:HMB1 | 1.94 | 0.60 |
| 13:O:68:THR:HG22 | 13:O:110[B]:MET:HG2 | 1.82 | 0.60 |
| 3:C:213[A]:LEU:HG | 24:C:508:CLA:H202 | 14.70 | 0.60 |
| 32:A:419:PL9:H502 | 4:D:39:PRO:HG3 | 1.83 | 0.60 |
| 27:A:416:SQD:H271 | 2:B:109:LEU:HD13 | 60.04 | 0.59 |
| 3:C:167:VAL:HG13 | 24:C:514:CLA:H71 | 13.26 | 0.59 |
| 24:D:401:CLA:HMB1 | 24:D:401:CLA:HBB1 | 1.87 | 0.59 |
| 2:B:12:LEU:HB2 | 24:B:617:CLA:HMC2 | 13.30 | 0.58 |
| 36:D:407:DGD:HAW1 | 27:F:101:SQD:H383 | 4.37 | 0.58 |
| 2:B:266:GLU:HB3 | 28:B:633:GOL:H11 | 25.83 | 0.57 |
| 40:B:953:HOH:O | 7:H:12[A]:ARG:NH2 | 2.38 | 0.57 |
| 24:C:505:CLA:HBB1 | 24:C:505:CLA:HHC | 4.33 | 0.57 |
| 5:E:45:ASP:OD2 | 20:R:4:ARG:NH2 | 2.38 | 0.57 |
| 1:A:183:MET:HA | 24:A:406:CLA:HMD2 | 12.21 | 0.57 |
| 24:B:602:CLA:H91 | 26:H:101:BCR:H21C | 1.86 | 0.56 |
| 24:C:513:CLA:HMB1 | 24:C:513:CLA:HBB1 | 2.34 | 0.56 |
| 24:C:513:CLA:H101 | 24:C:514:CLA:H141 | 1.87 | 0.56 |
| 24:C:503:CLA:C4D | 24:C:505:CLA:H2 | 17.62 | 0.56 |
| 1:A:262:TYR:HB3 | 37:E:101:LHG:HC62 | 4.53 | 0.56 |
| 2:B:103:LEU:HD21 | 24:B:606:CLA:HMC3 | 1.87 | 0.55 |
| 3:C:438:LEU:HD11 | 24:C:507:CLA:HBB1 | 17.25 | 0.55 |
| 2:B:462:PHE:CE1 | 24:B:614:CLA:HMB3 | 2.41 | 0.55 |
| 6:F:30:THR:HG21 | 34:J:101:LMG:H412 | 1.88 | 0.55 |
| 28:A:413:GOL:H11 | 12:M:1:FME:HG2 | 1.88 | 0.55 |
| 2:B:216:HIS:HE1 | 24:B:610:CLA:C1A | 2.19 | 0.55 |
| 34:B:621:LMG:H242 | 4:D:284:ILE:HD13 | 1.86 | 0.55 |
| 26:Y:101:BCR:H321 | 26:Y:101:BCR:HC8 | 1.88 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 35:D:411:HTG:H1 | 7:H:25:TRP:CG | 2.75 | 0.55 |
| 24:C:514:CLA:HAB | 26:C:515:BCR:H24C | 1.88 | 0.55 |
| 2:B:70:GLY:HA2 | 2:B:178:VAL:HG21 | 1.88 | 0.55 |
| 37:D:410:LHG:H112 | 37:D:410:LHG:H382 | 1.88 | 0.55 |
| 2:B:224:ARG:HD3 | 7:H:25:TRP:CE2 | 2.41 | 0.55 |
| 10:K:23:ASP:OD2 | 17:Y:21:GLN:NE2 | 2.64 | 0.55 |
| 24:A:405:CLA:HBB1 | 24:A:405:CLA:HMB1 | 1.89 | 0.54 |
| 28:A:412:GOL:H11 | 12:M:1:FME:HG2 | 19.33 | 0.54 |
| 24:A:406:CLA:H91 | 34:J:101:LMG:H221 | 1.88 | 0.54 |
| 30:B:634:LMT:H2' | 28:B:635:GOL:H2 | 1.88 | 0.54 |
| 4:D:24:ARG:HD3 | 18:X:37:VAL:HG22 | 2.00 | 0.54 |
| 4:D:13:GLY:HA3 | 35:D:411:HTG:H62 | 1.89 | 0.54 |
| 2:B:216:HIS:HE1 | 24:B:614:CLA:C1A | 26.58 | 0.54 |
| 2:B:482:ILE:HD12 | 2:B:486:LEU:HD13 | 2.11 | 0.54 |
| 2:B:103:LEU:HD21 | 24:B:610:CLA:HMC3 | 26.26 | 0.54 |
| 3:C:215:LYS:HG3 | 3:C:223:TRP:HA | 4.36 | 0.54 |
| 24:C:507:CLA:HMB1 | 24:C:507:CLA:HBB1 | 1.88 | 0.54 |
| 26:D:405:BCR:H313 | 36:D:407:DGD:HA91 | 2.48 | 0.53 |
| 24:D:404:CLA:H162 | 7:H:33:VAL:HG13 | 11.14 | 0.53 |
| 34:C:501:LMG:H242 | 24:C:507:CLA:H92 | 14.83 | 0.53 |
| 6:F:21:VAL:O | 6:F:25:THR:HG23 | 2.08 | 0.53 |
| 10:K:17:ILE:H | 10:K:17:ILE:HD13 | 1.73 | 0.53 |
| 11:L:2:GLU:O | 40:L:207:HOH:O | 3.23 | 0.53 |
| 12:M:28:GLN:O | 12:M:32:GLN:HG3 | 2.10 | 0.53 |
| 16:V:70:GLU:HB2 | 28:V:205:GOL:H12 | 1.90 | 0.52 |
| 32:A:419:PL9:H13 | 32:A:419:PL9:H101 | 1.90 | 0.52 |
| 36:D:407:DGD:O1B | 36:D:407:DGD:O2D | 2.32 | 0.52 |
| 37:D:410:LHG:H132 | 37:D:410:LHG:H372 | 1.91 | 0.52 |
| 26:B:620:BCR:C8 | 26:B:620:BCR:H331 | 2.35 | 0.52 |
| 24:B:617:CLA:HMB1 | 24:B:617:CLA:HBB1 | 1.92 | 0.52 |
| 2:B:86[B]:ILE:HD12 | 2:B:86[B]:ILE:H | 1.74 | 0.52 |
| 3:C:437:PHE:CE1 | 24:C:511:CLA:HMB3 | 2.45 | 0.52 |
| 12:M:33:GLN:HB2 | 12:M:33:GLN:HB2 | 0.00 | 0.52 |
| 24:B:617:CLA:HED2 | 24:B:617:CLA:H43 | 1.91 | 0.51 |
| 4:D:61:HIS:HD2 | 40:D:599:HOH:O | 1.92 | 0.51 |
| 10:K:11:LEU:HD11 | 10:K:22:VAL:HG21 | 1.91 | 0.51 |
| 3:C:41:ARG:NH1 | 24:C:513:CLA:HMD1 | 19.82 | 0.51 |
| 4:D:192:THR:HG23 | 24:D:403:CLA:HBC2 | 1.91 | 0.51 |
| 8:I:36:ASP:OD1 | 8:I:36:ASP:N | 2.43 | 0.51 |
| 3:C:391:ARG:NH2 | 40:C:776:HOH:O | 2.44 | 0.51 |
| 1:A:121[A]:LEU:HD21 | 24:A:409:CLA:HMB3 | 5.50 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:C:508:CLA:H71 | 26:C:516:BCR:H10C | 12.63 | 0.50 |
| 28:C:525:GOL:H2 | 40:C:708:HOH:O | 12.32 | 0.50 |
| 6:F:41:GLN:OE1 | 9:J:30:GLY:HA3 | 2.15 | 0.50 |
| 1:A:188:ALA:HB2 | 1:A:328:MET:HB2 | 2.01 | 0.50 |
| 3:C:155:ASN:OD1 | 40:C:757:HOH:O | 2.19 | 0.50 |
| 24:C:503:CLA:H42 | 24:C:504:CLA:HMD1 | 7.41 | 0.50 |
| 40:U:230[A]:HOH:O | 22:V:202:CL:CL | 2.56 | 0.50 |
| 26:H:101:BCR:H331 | 26:H:101:BCR:C8 | 2.42 | 0.50 |
| 3:C:212:TYR:O | 3:C:215:LYS:HG2 | 4.56 | 0.50 |
| 2:B:412:THR:O | 40:B:758:HOH:O | 76.24 | 0.49 |
| 24:C:512:CLA:HMB1 | 24:C:512:CLA:HBB1 | 2.29 | 0.49 |
| 5:E:77:GLU:O | 5:E:81:GLU:HG2 | 2.77 | 0.49 |
| 24:C:509:CLA:HBC3 | 24:C:511:CLA:H71 | 1.92 | 0.49 |
| 19:Z:37:LYS:NZ | 34:Z:101:LMG:HC5 | 3.64 | 0.49 |
| 11:L:14:ARG:HB3 | 14:T:25[A]:GLU:HG2 | 1.93 | 0.49 |
| 2:B:103:LEU:HB2 | 24:B:611:CLA:H62 | 13.82 | 0.49 |
| 27:A:411:SQD:H302 | 24:C:510:CLA:H71 | 25.60 | 0.49 |
| 3:C:185:LEU:HB2 | 3:C:230:LEU:HD13 | 1.92 | 0.49 |
| 34:C:501:LMG:H152 | 36:C:517:DGD:HA82 | 1.94 | 0.49 |
| 10:K:15:TYR:CZ | 19:Z:5:PHE:HZ | 2.51 | 0.49 |
| 1:A:153:SER:HB2 | 24:A:406:CLA:H43 | 18.78 | 0.49 |
| 1:A:317:TRP:CZ3 | 4:D:180:ARG:HD2 | 2.48 | 0.49 |
| 15:U:58:VAL:HG12 | 15:U:79:LEU:HD22 | 2.18 | 0.49 |
| 4:D:24:ARG:NH2 | 27:F:101:SQD:O4 | 2.46 | 0.49 |
| 3:C:38:GLY:HA3 | 24:C:513:CLA:HMD3 | 17.43 | 0.48 |
| 10:K:24:VAL:HG13 | 17:Y:25:ILE:HD13 | 2.08 | 0.48 |
| 3:C:320:ARG:HB2 | 28:C:525:GOL:H32 | 17.15 | 0.48 |
| 24:B:610:CLA:HHC | 24:B:610:CLA:HBB1 | 2.18 | 0.48 |
| 27:A:411:SQD:H142 | 37:D:410:LHG:H152 | 4.52 | 0.48 |
| 8:I:2:GLU:O | 8:I:6:ILE:HG12 | 2.14 | 0.48 |
| 24:B:611:CLA:HBB1 | 24:B:611:CLA:HHC | 1.96 | 0.48 |
| 24:A:405:CLA:CBF | 24:D:401:CLA:HAC2 | 2.43 | 0.48 |
| 3:C:79:LYS:HB3 | 3:C:84:GLN:NE2 | 2.46 | 0.48 |
| 2:B:383:PHE:CZ | 13:O:167:GLY:HA2 | 2.53 | 0.48 |
| 3:C:363:GLY:O | 3:C:367:GLU:HG2 | 2.42 | 0.48 |
| 24:D:404:CLA:H142 | 7:H:36:GLY:HA3 | 7.21 | 0.48 |
| 26:H:101:BCR:H331 | 26:H:101:BCR:HC8 | 1.95 | 0.48 |
| 26:T:102:BCR:H311 | 26:T:102:BCR:HC8 | 1.95 | 0.48 |
| 24:B:608:CLA:HBB1 | 24:B:608:CLA:HMB1 | 2.59 | 0.47 |
| 26:T:102:BCR:H331 | 26:T:102:BCR:HC7 | 1.56 | 0.47 |
| 24:C:514:CLA:HBC1 | 34:Z:101:LMG:H171 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:C:203:THR:O | 3:C:235:GLY:HA3 | 2.14 | 0.47 |
| 37:E:101:LHG:H241 | 37:E:101:LHG:HC61 | 1.70 | 0.47 |
| 24:C:508:CLA:C3D | 24:C:509:CLA:H193 | 28.27 | 0.47 |
| 4:D:160:TYR:HA | 4:D:290:ALA:HB2 | 1.96 | 0.47 |
| 16:V:30:LYS:HD3 | 16:V:118:HIS:NE2 | 3.39 | 0.47 |
| 14:T:25[A]:GLU:HG3 | 28:T:101:GOL:H2 | 1.96 | 0.47 |
| 34:C:501:LMG:H211 | 36:C:517:DGD:HA61 | 1.96 | 0.47 |
| 2:B:224:ARG:HD3 | 7:H:25:TRP:CD2 | 2.50 | 0.47 |
| 28:B:635:GOL:H31 | 30:M:101:LMT:H6D | 1.96 | 0.47 |
| 16:V:14:SER:HA | 28:V:208:GOL:H12 | 1.97 | 0.47 |
| 9:J:2:SER:N | 40:J:208:HOH:O | 2.48 | 0.47 |
| 13:O:84:GLU:OE2 | 40:O:543:HOH:O | 2.20 | 0.47 |
| 24:B:606:CLA:H91 | 26:H:101:BCR:H21C | 22.23 | 0.47 |
| 2:B:248:ALA:HA | 24:B:608:CLA:H42 | 25.01 | 0.46 |
| 27:A:411:SQD:H251 | 37:D:410:LHG:H121 | 3.64 | 0.46 |
| 34:J:101:LMG:H221 | 34:J:101:LMG:H192 | 4.75 | 0.46 |
| 1:A:84:PRO:HA | 1:A:112:TYR:CG | 2.50 | 0.46 |
| 24:B:609:CLA:H43 | 24:B:610:CLA:H2 | 8.05 | 0.46 |
| 10:K:10:LYS:N | 10:K:10:LYS:HD2 | 2.34 | 0.46 |
| 16:V:24:LYS:HD3 | 28:V:207:GOL:H2 | 1.98 | 0.46 |
| 4:D:49:LEU:HD13 | 26:D:405:BCR:C15 | 2.45 | 0.46 |
| 1:A:160:ILE:HD11 | 36:C:517:DGD:HBT2 | 1.98 | 0.46 |
| 24:C:502:CLA:H192 | 24:C:507:CLA:C1B | 2.45 | 0.46 |
| 2:B:476:ARG:NH1 | 40:B:951:HOH:O | 2.46 | 0.46 |
| 24:B:612:CLA:H161 | 24:B:612:CLA:H192 | 1.81 | 0.46 |
| 3:C:437:PHE:CE1 | 24:C:512:CLA:HMB3 | 14.46 | 0.46 |
| 35:D:411:HTG:H1 | 7:H:25:TRP:CD1 | 2.53 | 0.46 |
| 24:C:509:CLA:H122 | 24:C:509:CLA:H162 | 1.75 | 0.46 |
| 26:C:516:BCR:H15C | 26:C:516:BCR:H351 | 1.90 | 0.46 |
| 24:C:502:CLA:C4D | 24:C:504:CLA:H2 | 2.46 | 0.46 |
| 36:C:518:DGD:HA81 | 36:C:518:DGD:HAE2 | 1.68 | 0.46 |
| 4:D:141:TYR:OH | 37:D:408:LHG:O4 | 2.29 | 0.45 |
| 37:D:410:LHG:H331 | 37:D:410:LHG:H302 | 1.57 | 0.45 |
| 2:B:162:PHE:O | 24:B:611:CLA:HHD | 30.81 | 0.45 |
| 3:C:38:GLY:HA3 | 24:C:512:CLA:HMD3 | 1.98 | 0.45 |
| 4:D:123:ILE:HD11 | 36:H:102:DGD:HAE1 | 1.97 | 0.45 |
| 24:B:609:CLA:HMD2 | 24:B:617:CLA:H203 | 29.77 | 0.45 |
| 37:D:410:LHG:H141 | 37:D:410:LHG:H322 | 1.99 | 0.45 |
| 25:A:408:PHO:NC | 25:A:408:PHO:ND | 2.67 | 0.45 |
| 2:B:83:GLU:C | 2:B:86[B]:ILE:HD11 | 2.37 | 0.45 |
| 26:K:101:BCR:H371 | 26:K:101:BCR:H24C | 1.73 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 36:C:519:DGD:HBF1 | 37:D:410:LHG:H211 | 1.98 | 0.45 |
| 4:D:123:ILE:HD11 | 36:H:102:DGD:HAH2 | 1.97 | 0.45 |
| 2:B:223:GLN:NE2 | 40:B:937:HOH:O | 2.30 | 0.45 |
| 24:D:404:CLA:H171 | 18:X:15[A]:LEU:HD13 | 1.99 | 0.45 |
| 24:D:404:CLA:HBA1 | 24:D:404:CLA:H3A | 2.00 | 0.45 |
| 4:D:141:TYR:HA | 4:D:144:ILE:HD12 | 1.99 | 0.45 |
| 20:R:8:VAL:O | 20:R:11:PRO:HD2 | 2.17 | 0.45 |
| 3:C:218:PHE:HE2 | 34:C:501:LMG:H111 | 1.80 | 0.45 |
| 34:Z:101:LMG:H142 | 34:Z:101:LMG:H111 | 2.52 | 0.45 |
| 2:B:256:MET:HA | 2:B:263:THR:HG21 | 2.26 | 0.44 |
| 17:Y:22:LEU:HA | 17:Y:25:ILE:HG22 | 2.07 | 0.44 |
| 24:C:504:CLA:HAB | 34:C:521:LMG:H241 | 1.99 | 0.44 |
| 2:B:338:GLN:HA | 13:O:57:LYS:HE3 | 40.65 | 0.44 |
| 3:C:288:CYS:SG | 36:C:517:DGD:HB32 | 2.58 | 0.44 |
| 28:A:412:GOL:C1 | 12:M:1:FME:HG2 | 18.81 | 0.44 |
| 26:A:410:BCR:H371 | 26:A:410:BCR:H24C | 1.76 | 0.44 |
| 1:A:200:LEU:HG | 36:C:519:DGD:HAT2 | 1.98 | 0.44 |
| 1:A:272:HIS:CD2 | 4:D:218:VAL:HG21 | 2.71 | 0.44 |
| 4:D:16:ASP:OD2 | 30:D:402:LMT:O6' | 2.34 | 0.44 |
| 26:T:102:BCR:H321 | 26:T:102:BCR:HC8 | 1.99 | 0.44 |
| 1:A:214:MET:HE2 | 1:A:255:PHE:CE1 | 2.53 | 0.44 |
| 2:B:233:ASN:O | 2:B:236:THR:HG22 | 2.18 | 0.44 |
| 2:B:314:TYR:CE2 | 2:B:316:GLY:HA3 | 2.53 | 0.44 |
| 24:C:514:CLA:HMD1 | 34:Z:101:LMG:HC8 | 1.99 | 0.44 |
| 36:C:519:DGD:HAE2 | 36:C:519:DGD:HA81 | 2.01 | 0.44 |
| 26:H:101:BCR:H24C | 26:H:101:BCR:H371 | 1.76 | 0.44 |
| 40:A:615[B]:HOH:O | 16:V:30:LYS:HE2 | 2.17 | 0.44 |
| 1:A:96:ILE:HG12 | 1:A:105:TRP:CE2 | 2.64 | 0.44 |
| 26:B:619:BCR:H371 | 26:B:619:BCR:H24C | 1.81 | 0.44 |
| 11:L:9:PRO:HA | 30:M:102:LMT:H6D | 16.81 | 0.44 |
| 28:A:413:GOL:C1 | 12:M:1:FME:HG2 | 2.48 | 0.44 |
| 34:C:520:LMG:H182 | 34:C:520:LMG:H301 | 5.59 | 0.44 |
| 5:E:60:GLN:NE2 | 40:E:228:HOH:O | 2.51 | 0.44 |
| 8:I:35:LYS:O | 8:I:37:LEU:N | 2.61 | 0.44 |
| 1:A:96:ILE:HD12 | 24:A:409:CLA:HMD1 | 2.00 | 0.44 |
| 2:B:491:VAL:HG12 | 4:D:136:VAL:HG13 | 2.00 | 0.44 |
| 5:E:68:ASP:OD1 | 5:E:71:GLU:N | 2.42 | 0.44 |
| 16:V:55[B]:ARG:NH1 | 40:V:388:HOH:O | 2.51 | 0.44 |
| 27:F:101:SQD:H342 | 27:F:101:SQD:H311 | 1.65 | 0.43 |
| 26:Y:101:BCR:H351 | 26:Y:101:BCR:H15C | 1.89 | 0.43 |
| 2:B:290:ALA:O | 40:B:730:HOH:O | 40.60 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:423:LYS:HD3 | 2:B:423:LYS:HA | 1.79 | 0.43 |
| 24:C:502:CLA:HMD2 | 24:C:503:CLA:H101 | 2.00 | 0.43 |
| 13:O:136:ILE:HD12 | 13:O:243:ILE:HD13 | 4.75 | 0.43 |
| 13:O:40:ILE:HG12 | 13:O:243:ILE:HD13 | 1.99 | 0.43 |
| 35:V:204:HTG:H4'1 | 35:V:204:HTG:H1'1 | 1.78 | 0.43 |
| 24:B:607:CLA:H102 | 24:B:607:CLA:H61 | 1.72 | 0.43 |
| 4:D:190:ASN:HB2 | 4:D:296:TYR:CD1 | 2.57 | 0.43 |
| 4:D:272:LEU:HD23 | 4:D:272:LEU:C | 2.40 | 0.43 |
| 4:D:273:PHE:CE2 | 37:L:101:LHG:H112 | 2.52 | 0.43 |
| 17:Y:20:ALA:O | 17:Y:24:MET:HG2 | 2.18 | 0.43 |
| 2:B:13:ILE:HG12 | 24:B:613:CLA:HAC2 | 2.01 | 0.43 |
| 24:B:615:CLA:H71 | 24:B:615:CLA:H112 | 1.62 | 0.43 |
| 3:C:175:LEU:HD23 | 3:C:237:HIS:CG | 2.53 | 0.43 |
| 27:A:411:SQD:H361 | 27:A:411:SQD:H332 | 4.73 | 0.43 |
| 24:B:614:CLA:H43 | 37:D:408:LHG:H372 | 2.01 | 0.43 |
| 3:C:279:LEU:HD22 | 24:C:510:CLA:HED2 | 2.00 | 0.43 |
| 1:A:63:ILE:HB | 3:C:335:THR:HG21 | 2.01 | 0.43 |
| 5:E:8:ARG:HH21 | 5:E:12:ASP:HB3 | 2.97 | 0.43 |
| 2:B:30:VAL:HG12 | 24:B:610:CLA:HHD | 31.15 | 0.43 |
| 24:B:615:CLA:H62 | 24:B:615:CLA:H41 | 1.88 | 0.43 |
| 24:A:406:CLA:HMD3 | 4:D:182:LEU:HD11 | 2.00 | 0.43 |
| 2:B:144:PHE:CE2 | 2:B:148:LEU:HD11 | 2.53 | 0.43 |
| 2:B:216:HIS:CE1 | 24:B:610:CLA:NA | 2.86 | 0.43 |
| 24:D:401:CLA:H203 | 24:D:401:CLA:H162 | 1.80 | 0.43 |
| 27:A:411:SQD:H131 | 37:D:410:LHG:H142 | 1.99 | 0.43 |
| 26:T:102:BCR:H371 | 26:T:102:BCR:H24C | 1.84 | 0.43 |
| 1:A:105:TRP:NE1 | 1:A:110:GLY:HA3 | 2.34 | 0.43 |
| 3:C:406:SER:HA | 3:C:420:VAL:HG23 | 2.16 | 0.43 |
| 24:C:511:CLA:H191 | 24:C:514:CLA:HAC1 | 20.96 | 0.43 |
| 24:C:505:CLA:HBB1 | 34:C:521:LMG:H231 | 17.70 | 0.43 |
| 12:M:34:LYS:HG2 | 30:M:102:LMT:O3B | 2.18 | 0.43 |
| 24:B:604:CLA:CGA | 24:B:604:CLA:H3A | 2.48 | 0.43 |
| 24:C:510:CLA:H203 | 36:C:518:DGD:HA92 | 33.55 | 0.43 |
| 34:C:520:LMG:H242 | 34:C:520:LMG:H211 | 1.81 | 0.43 |
| 4:D:139:ARG:NH2 | 40:D:635:HOH:O | 51.45 | 0.43 |
| 9:J:6:ARG:H | 9:J:6:ARG:HG2 | 1.69 | 0.43 |
| 2:B:283:GLU:OE2 | 2:B:287[B]:ARG:NE | 2.51 | 0.42 |
| 2:B:26:HIS:HB2 | 24:B:613:CLA:HMB2 | 2.00 | 0.42 |
| 24:C:507:CLA:HAA1 | 24:C:507:CLA:HBD | 2.30 | 0.42 |
| 15:U:76:ARG:NH2 | 40:U:201:HOH:O | 2.51 | 0.42 |
| 24:B:606:CLA:H143 | 24:B:606:CLA:C1B | 16.82 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:C:514:CLA:HAB | 26:C:515:BCR:H371 | 2.00 | 0.42 |
| 3:C:202:PRO:HD2 | 35:C:523:HTG:H62 | 2.01 | 0.42 |
| 37:E:101:LHG:H152 | 6:F:22:ALA:HB1 | 2.71 | 0.42 |
| 2:B:238:LEU:N | 24:B:617:CLA:HMD3 | 22.30 | 0.42 |
| 2:B:492:GLU:HG3 | 40:B:915:HOH:O | 2.19 | 0.42 |
| 24:B:611:CLA:H152 | 24:B:611:CLA:H111 | 4.37 | 0.42 |
| 26:B:618:BCR:H371 | 26:B:618:BCR:H24C | 1.77 | 0.42 |
| 34:C:520:LMG:H192 | 10:K:27:VAL:HG11 | 2.02 | 0.42 |
| 5:E:84:LYS:HA | 5:E:84:LYS:HD3 | 1.91 | 0.42 |
| 19:Z:29:SER:HA | 19:Z:30:PRO:HD3 | 1.85 | 0.42 |
| 24:B:607:CLA:H142 | 24:B:607:CLA:H111 | 1.83 | 0.42 |
| 36:C:518:DGD:HB61 | 36:C:518:DGD:HB32 | 3.36 | 0.42 |
| 12:M:3:VAL:HG11 | 14:T:2:GLU:HG2 | 2.01 | 0.42 |
| 3:C:127:PHE:CE1 | 34:Z:101:LMG:H152 | 5.34 | 0.42 |
| 24:B:615:CLA:HBD | 24:B:615:CLA:HAA1 | 2.00 | 0.42 |
| 26:C:515:BCR:H15C | 26:C:515:BCR:H351 | 1.92 | 0.42 |
| 26:C:516:BCR:H371 | 26:C:516:BCR:H24C | 1.73 | 0.42 |
| 25:A:408:PHO:H161 | 24:D:401:CLA:HMB3 | 32.73 | 0.42 |
| 1:A:259:ILE:HA | 37:E:101:LHG:H202 | 5.02 | 0.42 |
| 13:O:179:GLU:HG2 | 40:O:499:HOH:O | 2.19 | 0.42 |
| 3:C:218:PHE:CE2 | 34:C:501:LMG:H111 | 2.54 | 0.42 |
| 1:A:249:VAL:HG12 | 2:B:491:VAL:HG21 | 2.02 | 0.42 |
| 26:B:618:BCR:H11C | 26:B:618:BCR:H341 | 1.86 | 0.42 |
| 17:Y:38:LEU:O | 17:Y:42:ARG:HD3 | 2.20 | 0.42 |
| 24:A:405:CLA:HBD | 24:D:401:CLA:HAC2 | 2.00 | 0.41 |
| 24:A:409:CLA:H102 | 24:A:409:CLA:H61 | 1.76 | 0.41 |
| 2:B:27:THR:HG22 | 2:B:107:LEU:HD13 | 2.08 | 0.41 |
| 19:Z:37:LYS:HZ3 | 34:Z:101:LMG:HC5 | 4.07 | 0.41 |
| 24:B:617:CLA:H62 | 24:B:617:CLA:H41 | 1.52 | 0.41 |
| 24:C:512:CLA:HMB2 | 26:K:101:BCR:H382 | 2.02 | 0.41 |
| 15:U:8:GLU:HG2 | 15:U:9:LEU:H | 1.84 | 0.41 |
| 16:V:68:ASN:OD1 | 28:V:205:GOL:H2 | 2.19 | 0.41 |
| 1:A:253:GLY:HA3 | 2:B:491:VAL:HB | 2.02 | 0.41 |
| 35:B:623:HTG:H1 | 35:B:623:HTG:H2'2 | 1.86 | 0.41 |
| 13:O:58:ASN:C | 13:O:60:ARG:H | 2.49 | 0.41 |
| 2:B:491:VAL:HG13 | 4:D:136:VAL:HG13 | 3.29 | 0.41 |
| 5:E:36:LEU:HA | 5:E:39:SER:OG | 2.20 | 0.41 |
| 3:C:240:ILE:HD13 | 3:C:240:ILE:HA | 1.84 | 0.41 |
| 24:C:503:CLA:C3D | 24:C:505:CLA:H2 | 18.64 | 0.41 |
| 3:C:334:PRO:HA | 13:O:153:THR:OG1 | 2.20 | 0.41 |
| 26:B:620:BCR:H24C | 26:B:620:BCR:H371 | 1.82 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:R:24:LEU:N | 20:R:25:PRO:HD2 | 2.36 | 0.41 |
| 26:T:102:BCR:H11C | 26:T:102:BCR:H341 | 1.97 | 0.41 |
| 2:B:194:ASN:HA | 2:B:195:PRO:HD3 | 1.90 | 0.41 |
| 24:C:502:CLA:H42 | 24:C:503:CLA:HMD1 | 2.02 | 0.41 |
| 28:C:524:GOL:O1 | 16:V:49:ASN:ND2 | 2.48 | 0.41 |
| 27:F:101:SQD:H45 | 27:F:101:SQD:H81 | 4.74 | 0.41 |
| 24:C:507:CLA:H52 | 30:I:102:LMT:H71 | 2.02 | 0.41 |
| 2:B:173:GLY:HA3 | 2:B:265:ILE:HD11 | 2.03 | 0.41 |
| 24:B:617:CLA:H93 | 24:B:617:CLA:H61 | 1.95 | 0.41 |
| 24:C:509:CLA:HBB1 | 24:C:509:CLA:HMB1 | 2.03 | 0.41 |
| 3:C:42:LEU:HD21 | 24:C:513:CLA:H2A | 18.64 | 0.41 |
| 4:D:172:SER:HB2 | 4:D:177:ALA:HB1 | 2.02 | 0.41 |
| 16:V:93:PRO:HA | 16:V:101:PHE:CD2 | 2.66 | 0.41 |
| 2:B:216:HIS:CE1 | 24:B:614:CLA:NA | 25.95 | 0.41 |
| 26:D:405:BCR:HC22 | 36:D:407:DGD:HA72 | 2.89 | 0.41 |
| 24:B:605:CLA:HMB1 | 24:B:605:CLA:HBB1 | 2.03 | 0.41 |
| 24:B:606:CLA:H72 | 24:B:606:CLA:H2 | 4.80 | 0.41 |
| 2:B:237:VAL:HG12 | 24:B:617:CLA:HMD1 | 21.39 | 0.41 |
| 24:C:514:CLA:O1A | 40:C:782:HOH:O | 49.22 | 0.41 |
| 24:D:401:CLA:H43 | 24:D:401:CLA:O1A | 2.20 | 0.41 |
| 10:K:25:LEU:HB2 | 40:K:201:HOH:O | 2.21 | 0.41 |
| 20:R:27:ALA:O | 20:R:31:VAL:HG23 | 2.21 | 0.41 |
| 26:A:410:BCR:H11C | 26:A:410:BCR:H341 | 1.95 | 0.40 |
| 27:A:416:SQD:H301 | 27:A:416:SQD:H272 | 1.85 | 0.40 |
| 2:B:237:VAL:HG12 | 24:B:613:CLA:HMD1 | 2.03 | 0.40 |
| 2:B:238:LEU:N | 24:B:613:CLA:HMD3 | 2.36 | 0.40 |
| 24:C:508:CLA:H92 | 24:C:508:CLA:H61 | 1.75 | 0.40 |
| 3:C:56:HIS:HB2 | 24:C:511:CLA:HMB2 | 8.48 | 0.40 |
| 26:D:405:BCR:H15C | 26:D:405:BCR:H351 | 1.97 | 0.40 |
| 3:C:53:HIS:CB | 24:C:513:CLA:HMD1 | 2.52 | 0.40 |
| 8:I:33:LYS:HA | 8:I:33:LYS:HD3 | 1.89 | 0.40 |
| 37:D:410:LHG:H272 | 37:D:410:LHG:H242 | 1.95 | 0.40 |
| 1:A:153:SER:CB | 24:A:406:CLA:H43 | 18.49 | 0.40 |
| 24:B:604:CLA:HAB | 24:B:606:CLA:H171 | 2.03 | 0.40 |
| 24:B:610:CLA:H62 | 24:B:610:CLA:H41 | 4.32 | 0.40 |
| 24:B:613:CLA:HAB | 4:D:123:ILE:HG12 | 28.02 | 0.40 |
| 24:B:617:CLA:H152 | 24:B:617:CLA:H111 | 1.93 | 0.40 |
| 4:D:27:PHE:CD1 | 37:E:101:LHG:HC12 | 2.57 | 0.40 |
| 26:H:101:BCR:H312 | 26:H:101:BCR:HC32 | 2.05 | 0.40 |
| 26:A:410:BCR:H15C | 26:A:410:BCR:H351 | 1.84 | 0.40 |
| 3:C:238:ILE:HD13 | 35:C:523:HTG:H2'1 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:C:506:CLA:HMD2 | 34:C:520:LMG:H291 | 39.46 | 0.40 |
| 37:E:101:LHG:H282 | 37:E:101:LHG:H251 | 3.79 | 0.40 |

There are no symmetry-related clashes.

4.3 Torsion angles [i](#)

4.3.1 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 | 335/344 (97%) | 330 (98%) | 4 (1%) | 1 (0%) | 44 | 33 |
| 1 | a | 336/344 (98%) | 331 (98%) | 4 (1%) | 1 (0%) | 44 | 33 |
| 2 | B | 512/505 (101%) | 507 (99%) | 5 (1%) | 0 | 100 | 100 |
| 2 | b | 513/505 (102%) | 504 (98%) | 9 (2%) | 0 | 100 | 100 |
| 3 | C | 454/455 (100%) | 445 (98%) | 7 (2%) | 2 (0%) | 38 | 25 |
| 3 | c | 459/455 (101%) | 447 (97%) | 10 (2%) | 2 (0%) | 38 | 25 |
| 4 | D | 340/342 (99%) | 331 (97%) | 9 (3%) | 0 | 100 | 100 |
| 4 | d | 340/342 (99%) | 332 (98%) | 8 (2%) | 0 | 100 | 100 |
| 5 | E | 81/84 (96%) | 80 (99%) | 1 (1%) | 0 | 100 | 100 |
| 5 | e | 79/84 (94%) | 77 (98%) | 2 (2%) | 0 | 100 | 100 |
| 6 | F | 32/44 (73%) | 32 (100%) | 0 | 0 | 100 | 100 |
| 6 | f | 30/44 (68%) | 30 (100%) | 0 | 0 | 100 | 100 |
| 7 | H | 64/65 (98%) | 61 (95%) | 3 (5%) | 0 | 100 | 100 |
| 7 | h | 63/65 (97%) | 59 (94%) | 4 (6%) | 0 | 100 | 100 |
| 8 | I | 36/38 (95%) | 33 (92%) | 3 (8%) | 0 | 100 | 100 |
| 8 | i | 36/38 (95%) | 33 (92%) | 2 (6%) | 1 (3%) | 6 | 1 |
| 9 | J | 36/39 (92%) | 35 (97%) | 1 (3%) | 0 | 100 | 100 |
| 9 | j | 37/39 (95%) | 36 (97%) | 1 (3%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 10 | K | 35/37 (95%) | 35 (100%) | 0 | 0 | 100 | 100 |
| 10 | k | 35/37 (95%) | 35 (100%) | 0 | 0 | 100 | 100 |
| 11 | L | 36/37 (97%) | 36 (100%) | 0 | 0 | 100 | 100 |
| 11 | l | 36/37 (97%) | 36 (100%) | 0 | 0 | 100 | 100 |
| 12 | M | 33/36 (92%) | 33 (100%) | 0 | 0 | 100 | 100 |
| 12 | m | 32/36 (89%) | 32 (100%) | 0 | 0 | 100 | 100 |
| 13 | O | 245/244 (100%) | 242 (99%) | 3 (1%) | 0 | 100 | 100 |
| 13 | o | 244/244 (100%) | 238 (98%) | 6 (2%) | 0 | 100 | 100 |
| 14 | T | 29/31 (94%) | 29 (100%) | 0 | 0 | 100 | 100 |
| 14 | t | 29/31 (94%) | 29 (100%) | 0 | 0 | 100 | 100 |
| 15 | U | 95/104 (91%) | 92 (97%) | 3 (3%) | 0 | 100 | 100 |
| 15 | u | 95/104 (91%) | 92 (97%) | 3 (3%) | 0 | 100 | 100 |
| 16 | V | 136/137 (99%) | 130 (96%) | 6 (4%) | 0 | 100 | 100 |
| 16 | v | 135/137 (98%) | 130 (96%) | 5 (4%) | 0 | 100 | 100 |
| 17 | Y | 27/30 (90%) | 27 (100%) | 0 | 0 | 100 | 100 |
| 17 | y | 27/30 (90%) | 27 (100%) | 0 | 0 | 100 | 100 |
| 18 | X | 38/40 (95%) | 37 (97%) | 1 (3%) | 0 | 100 | 100 |
| 18 | x | 37/40 (92%) | 36 (97%) | 1 (3%) | 0 | 100 | 100 |
| 19 | Z | 60/62 (97%) | 59 (98%) | 1 (2%) | 0 | 100 | 100 |
| 19 | z | 60/62 (97%) | 59 (98%) | 1 (2%) | 0 | 100 | 100 |
| 20 | R | 32/34 (94%) | 31 (97%) | 1 (3%) | 0 | 100 | 100 |
| All | All | 5279/5382 (98%) | 5168 (98%) | 104 (2%) | 7 (0%) | 55 | 46 |

All (7) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 3 | C | 416[A] | SER |
| 3 | C | 416[B] | SER |
| 3 | c | 416[A] | SER |
| 3 | c | 416[B] | SER |
| 8 | i | 36 | ASP |
| 1 | a | 259 | ILE |
| 1 | A | 259 | ILE |

4.3.2 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 | 272/279 (98%) | 272 (100%) | 0 | 100 | 100 |
| 1 | a | 273/279 (98%) | 272 (100%) | 1 (0%) | 93 | 92 |
| 2 | B | 412/403 (102%) | 407 (99%) | 5 (1%) | 75 | 72 |
| 2 | b | 413/403 (102%) | 408 (99%) | 5 (1%) | 75 | 72 |
| 3 | C | 357/356 (100%) | 352 (99%) | 5 (1%) | 71 | 67 |
| 3 | c | 362/356 (102%) | 358 (99%) | 4 (1%) | 78 | 75 |
| 4 | D | 277/277 (100%) | 276 (100%) | 1 (0%) | 93 | 92 |
| 4 | d | 277/277 (100%) | 276 (100%) | 1 (0%) | 93 | 92 |
| 5 | E | 74/73 (101%) | 74 (100%) | 0 | 100 | 100 |
| 5 | e | 72/73 (99%) | 71 (99%) | 1 (1%) | 71 | 67 |
| 6 | F | 28/38 (74%) | 27 (96%) | 1 (4%) | 40 | 26 |
| 6 | f | 26/38 (68%) | 25 (96%) | 1 (4%) | 38 | 24 |
| 7 | H | 55/54 (102%) | 52 (94%) | 3 (6%) | 25 | 11 |
| 7 | h | 54/54 (100%) | 53 (98%) | 1 (2%) | 62 | 55 |
| 8 | I | 34/34 (100%) | 34 (100%) | 0 | 100 | 100 |
| 8 | i | 34/34 (100%) | 33 (97%) | 1 (3%) | 48 | 35 |
| 9 | J | 26/26 (100%) | 26 (100%) | 0 | 100 | 100 |
| 9 | j | 26/26 (100%) | 26 (100%) | 0 | 100 | 100 |
| 10 | K | 30/30 (100%) | 28 (93%) | 2 (7%) | 19 | 7 |
| 10 | k | 30/30 (100%) | 28 (93%) | 2 (7%) | 19 | 7 |
| 11 | L | 36/35 (103%) | 35 (97%) | 1 (3%) | 49 | 37 |
| 11 | l | 36/35 (103%) | 35 (97%) | 1 (3%) | 49 | 37 |
| 12 | M | 31/32 (97%) | 31 (100%) | 0 | 100 | 100 |
| 12 | m | 30/32 (94%) | 29 (97%) | 1 (3%) | 43 | 30 |
| 13 | O | 210/207 (101%) | 208 (99%) | 2 (1%) | 80 | 78 |
| 13 | o | 209/207 (101%) | 207 (99%) | 2 (1%) | 80 | 78 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|----------|-------------|-----|
| 14 | T | 27/27 (100%) | 25 (93%) | 2 (7%) | 16 | 5 |
| 14 | t | 27/27 (100%) | 25 (93%) | 2 (7%) | 16 | 5 |
| 15 | U | 84/89 (94%) | 83 (99%) | 1 (1%) | 75 | 72 |
| 15 | u | 84/89 (94%) | 84 (100%) | 0 | 100 | 100 |
| 16 | V | 118/117 (101%) | 117 (99%) | 1 (1%) | 85 | 83 |
| 16 | v | 117/117 (100%) | 116 (99%) | 1 (1%) | 82 | 81 |
| 17 | Y | 22/23 (96%) | 22 (100%) | 0 | 100 | 100 |
| 17 | y | 22/23 (96%) | 21 (96%) | 1 (4%) | 32 | 17 |
| 18 | X | 33/33 (100%) | 33 (100%) | 0 | 100 | 100 |
| 18 | x | 32/33 (97%) | 32 (100%) | 0 | 100 | 100 |
| 19 | Z | 52/52 (100%) | 51 (98%) | 1 (2%) | 62 | 55 |
| 19 | z | 52/52 (100%) | 51 (98%) | 1 (2%) | 62 | 55 |
| 20 | R | 29/29 (100%) | 28 (97%) | 1 (3%) | 42 | 29 |
| All | All | 4383/4399 (100%) | 4331 (99%) | 52 (1%) | 78 | 72 |

All (52) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 2 | B | 84 | THR |
| 2 | B | 362 | PHE |
| 2 | B | 472 | ARG |
| 2 | B | 479 | PHE |
| 2 | B | 492 | GLU |
| 3 | C | 289 | PHE |
| 3 | C | 315 | MET |
| 3 | C | 416[A] | SER |
| 3 | C | 416[B] | SER |
| 3 | C | 418 | ASN |
| 4 | D | 180 | ARG |
| 6 | F | 44 | GLN |
| 7 | H | 12[A] | ARG |
| 7 | H | 12[B] | ARG |
| 7 | H | 49 | TYR |
| 10 | K | 10 | LYS |
| 10 | K | 17 | ILE |
| 11 | L | 1 | MET |
| 13 | O | 118 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-------|------|
| 13 | O | 194 | LYS |
| 14 | T | 25[A] | GLU |
| 14 | T | 25[B] | GLU |
| 15 | U | 70 | ARG |
| 16 | V | 86 | GLN |
| 19 | Z | 3 | ILE |
| 20 | R | 4 | ARG |
| 1 | a | 12 | ASN |
| 2 | b | 84 | THR |
| 2 | b | 121 | GLU |
| 2 | b | 362 | PHE |
| 2 | b | 472 | ARG |
| 2 | b | 479 | PHE |
| 3 | c | 289 | PHE |
| 3 | c | 355 | THR |
| 3 | c | 391 | ARG |
| 3 | c | 418 | ASN |
| 4 | d | 180 | ARG |
| 5 | e | 59 | GLU |
| 6 | f | 44 | GLN |
| 7 | h | 49 | TYR |
| 8 | i | 34 | ARG |
| 10 | k | 10 | LYS |
| 10 | k | 17 | ILE |
| 11 | l | 1 | MET |
| 12 | m | 33 | GLN |
| 13 | o | 118 | LEU |
| 13 | o | 194 | LYS |
| 14 | t | 25[A] | GLU |
| 14 | t | 25[B] | GLU |
| 16 | v | 86 | GLN |
| 17 | y | 42 | ARG |
| 19 | z | 3 | ILE |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | D | 61 | HIS |
| 4 | D | 142 | ASN |
| 19 | Z | 31 | GLN |
| 2 | b | 497 | GLN |
| 13 | o | 109 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15 | u | 81 | HIS |
| 19 | z | 6 | GLN |

4.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 8 | FME | I | 1 | 8 | 9,9,10 | 0.61 | 0 | 7,9,11 | 1.44 | 2 (28%) |
| 12 | FME | M | 1 | 12 | 9,9,10 | 0.60 | 0 | 7,9,11 | 1.44 | 1 (14%) |
| 14 | FME | T | 1 | 14 | 9,9,10 | 0.69 | 0 | 7,9,11 | 1.62 | 2 (28%) |
| 8 | FME | i | 1 | 8 | 9,9,10 | 0.57 | 0 | 7,9,11 | 1.36 | 1 (14%) |
| 9 | FME | j | 1 | 9 | 9,9,10 | 0.59 | 0 | 7,9,11 | 1.39 | 2 (28%) |
| 12 | FME | m | 1 | 12 | 9,9,10 | 0.64 | 0 | 7,9,11 | 1.29 | 1 (14%) |
| 14 | FME | t | 1 | 14 | 9,9,10 | 0.86 | 0 | 7,9,11 | 1.98 | 2 (28%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|---------|
| 8 | FME | I | 1 | 8 | - | 0/6/9/11 | 0/0/0/0 |
| 12 | FME | M | 1 | 12 | - | 0/6/9/11 | 0/0/0/0 |
| 14 | FME | T | 1 | 14 | - | 0/6/9/11 | 0/0/0/0 |
| 8 | FME | i | 1 | 8 | - | 0/6/9/11 | 0/0/0/0 |
| 9 | FME | j | 1 | 9 | - | 0/6/9/11 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|---------|
| 12 | FME | m | 1 | 12 | - | 0/6/9/11 | 0/0/0/0 |
| 14 | FME | t | 1 | 14 | - | 0/6/9/11 | 0/0/0/0 |

There are no bond length outliers.

All (11) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 14 | t | 1 | FME | O-C-CA | -3.53 | 116.92 | 125.15 |
| 14 | T | 1 | FME | O-C-CA | -3.29 | 117.48 | 125.15 |
| 8 | I | 1 | FME | O-C-CA | -2.54 | 119.23 | 125.15 |
| 8 | i | 1 | FME | O-C-CA | -2.48 | 119.36 | 125.15 |
| 12 | m | 1 | FME | O-C-CA | -2.45 | 119.43 | 125.15 |
| 9 | j | 1 | FME | O-C-CA | -2.33 | 119.71 | 125.15 |
| 12 | M | 1 | FME | O-C-CA | -2.29 | 119.80 | 125.15 |
| 14 | T | 1 | FME | CA-N-CN | -2.29 | 119.31 | 122.82 |
| 8 | I | 1 | FME | CA-N-CN | -2.11 | 119.58 | 122.82 |
| 14 | t | 1 | FME | CE-SD-CG | -2.09 | 92.84 | 100.35 |
| 9 | j | 1 | FME | CB-CA-C | -2.01 | 108.33 | 111.65 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 12 | M | 1 | FME | 4 | 0 |

4.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

4.6 Ligand geometry [i](#)

Of 252 ligands modelled in this entry, 19 are unknown and 17 are monoatomic - leaving 216 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$ |
| 23 | BCT | A | 404 | 21 | 0,3,3 | 0.00 | - | 0,3,3 | 0.00 | - |
| 24 | CLA | A | 405 | - | 56,73,73 | 2.00 | 12 (21%) | 65,113,113 | 2.46 | 23 (35%) |
| 24 | CLA | A | 406 | 40 | 56,73,73 | 1.96 | 12 (21%) | 65,113,113 | 2.20 | 24 (36%) |
| 25 | PHO | A | 407 | - | 67,69,69 | 2.14 | 16 (23%) | 87,99,99 | 1.85 | 20 (22%) |
| 25 | PHO | A | 408 | - | 67,69,69 | 2.07 | 15 (22%) | 87,99,99 | 1.96 | 23 (26%) |
| 24 | CLA | A | 409 | - | 56,73,73 | 1.98 | 12 (21%) | 65,113,113 | 2.19 | 22 (33%) |
| 26 | BCR | A | 410 | - | 41,41,41 | 1.00 | 1 (2%) | 56,56,56 | 1.32 | 7 (12%) |
| 27 | SQD | A | 411 | - | 53,54,54 | 0.95 | 3 (5%) | 63,65,65 | 1.74 | 12 (19%) |
| 28 | GOL | A | 412 | - | 5,5,5 | 0.21 | 0 | 5,5,5 | 0.64 | 0 |
| 28 | GOL | A | 413 | - | 5,5,5 | 0.42 | 0 | 5,5,5 | 0.57 | 0 |
| 28 | GOL | A | 414 | - | 5,5,5 | 0.39 | 0 | 5,5,5 | 0.19 | 0 |
| 27 | SQD | A | 416 | - | 53,54,54 | 1.03 | 3 (5%) | 63,65,65 | 1.29 | 9 (14%) |
| 30 | LMT | A | 417 | - | 34,34,36 | 0.39 | 0 | 45,45,47 | 1.09 | 3 (6%) |
| 31 | OEX | A | 418 | 1,3,40 | 0,15,15 | 0.00 | - | 0,32,32 | 0.00 | - |
| 32 | PL9 | A | 419 | - | 55,55,55 | 0.61 | 1 (1%) | 69,69,69 | 1.80 | 19 (27%) |
| 24 | CLA | B | 602 | 40 | 56,73,73 | 1.97 | 12 (21%) | 65,113,113 | 2.22 | 22 (33%) |
| 24 | CLA | B | 603 | - | 56,73,73 | 1.95 | 12 (21%) | 65,113,113 | 2.32 | 24 (36%) |
| 24 | CLA | B | 604 | - | 56,73,73 | 2.00 | 12 (21%) | 65,113,113 | 2.43 | 25 (38%) |
| 24 | CLA | B | 605 | - | 56,73,73 | 1.82 | 11 (19%) | 65,113,113 | 2.47 | 19 (29%) |
| 24 | CLA | B | 606 | - | 56,73,73 | 1.88 | 12 (21%) | 65,113,113 | 2.42 | 21 (32%) |
| 24 | CLA | B | 607 | - | 56,73,73 | 1.92 | 12 (21%) | 65,113,113 | 2.44 | 22 (33%) |
| 24 | CLA | B | 608 | 40 | 56,73,73 | 1.97 | 12 (21%) | 65,113,113 | 2.33 | 23 (35%) |
| 24 | CLA | B | 609 | - | 56,73,73 | 1.99 | 12 (21%) | 65,113,113 | 2.31 | 20 (30%) |
| 24 | CLA | B | 610 | - | 56,73,73 | 1.91 | 11 (19%) | 65,113,113 | 2.25 | 21 (32%) |
| 24 | CLA | B | 611 | 40 | 56,73,73 | 1.94 | 12 (21%) | 65,113,113 | 2.33 | 22 (33%) |
| 24 | CLA | B | 612 | - | 56,73,73 | 1.96 | 12 (21%) | 65,113,113 | 2.28 | 20 (30%) |
| 24 | CLA | B | 613 | - | 56,73,73 | 1.95 | 12 (21%) | 65,113,113 | 2.26 | 20 (30%) |
| 24 | CLA | B | 614 | - | 56,73,73 | 1.96 | 12 (21%) | 65,113,113 | 2.29 | 23 (35%) |
| 24 | CLA | B | 615 | - | 56,73,73 | 1.87 | 12 (21%) | 65,113,113 | 2.29 | 20 (30%) |
| 24 | CLA | B | 616 | - | 56,73,73 | 1.90 | 12 (21%) | 65,113,113 | 2.21 | 22 (33%) |
| 24 | CLA | B | 617 | - | 56,73,73 | 1.98 | 12 (21%) | 65,113,113 | 2.31 | 18 (27%) |
| 26 | BCR | B | 618 | - | 41,41,41 | 1.02 | 1 (2%) | 56,56,56 | 1.24 | 5 (8%) |
| 26 | BCR | B | 619 | - | 41,41,41 | 1.05 | 1 (2%) | 56,56,56 | 0.99 | 3 (5%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 26 | BCR | B | 620 | - | 41,41,41 | 1.02 | 1 (2%) | 56,56,56 | 1.45 | 12 (21%) |
| 34 | LMG | B | 621 | - | 51,51,55 | 0.90 | 2 (3%) | 59,59,63 | 1.06 | 4 (6%) |
| 35 | HTG | B | 622 | - | 19,19,19 | 1.18 | 1 (5%) | 23,24,24 | 1.57 | 3 (13%) |
| 35 | HTG | B | 623 | - | 19,19,19 | 0.87 | 1 (5%) | 23,24,24 | 1.35 | 2 (8%) |
| 35 | HTG | B | 624 | - | 19,19,19 | 1.04 | 2 (10%) | 23,24,24 | 2.04 | 3 (13%) |
| 28 | GOL | B | 625 | - | 5,5,5 | 0.29 | 0 | 5,5,5 | 0.55 | 0 |
| 28 | GOL | B | 626 | - | 5,5,5 | 0.28 | 0 | 5,5,5 | 0.45 | 0 |
| 28 | GOL | B | 627 | - | 5,5,5 | 0.30 | 0 | 5,5,5 | 0.67 | 0 |
| 28 | GOL | B | 628 | - | 5,5,5 | 0.39 | 0 | 5,5,5 | 0.26 | 0 |
| 28 | GOL | B | 629 | - | 5,5,5 | 0.29 | 0 | 5,5,5 | 0.37 | 0 |
| 35 | HTG | B | 630 | - | 19,19,19 | 0.96 | 2 (10%) | 23,24,24 | 1.50 | 1 (4%) |
| 35 | HTG | B | 631 | - | 19,19,19 | 1.01 | 2 (10%) | 23,24,24 | 1.64 | 2 (8%) |
| 28 | GOL | B | 633 | - | 5,5,5 | 0.26 | 0 | 5,5,5 | 0.64 | 0 |
| 30 | LMT | B | 634 | - | 25,25,36 | 0.48 | 0 | 30,30,47 | 0.73 | 0 |
| 28 | GOL | B | 635 | - | 5,5,5 | 0.37 | 0 | 5,5,5 | 0.27 | 0 |
| 34 | LMG | C | 501 | - | 51,51,55 | 0.95 | 2 (3%) | 59,59,63 | 1.13 | 2 (3%) |
| 24 | CLA | C | 502 | - | 56,73,73 | 1.92 | 12 (21%) | 65,113,113 | 2.26 | 19 (29%) |
| 24 | CLA | C | 503 | - | 56,73,73 | 1.96 | 12 (21%) | 65,113,113 | 2.30 | 21 (32%) |
| 24 | CLA | C | 504 | - | 56,73,73 | 1.98 | 12 (21%) | 65,113,113 | 2.23 | 20 (30%) |
| 24 | CLA | C | 505 | 40 | 56,73,73 | 1.94 | 12 (21%) | 65,113,113 | 2.25 | 18 (27%) |
| 24 | CLA | C | 506 | - | 56,73,73 | 1.97 | 12 (21%) | 65,113,113 | 2.28 | 16 (24%) |
| 24 | CLA | C | 507 | - | 56,73,73 | 1.93 | 12 (21%) | 65,113,113 | 2.32 | 23 (35%) |
| 24 | CLA | C | 508 | 40 | 56,73,73 | 1.95 | 12 (21%) | 65,113,113 | 2.28 | 20 (30%) |
| 24 | CLA | C | 509 | - | 56,73,73 | 1.98 | 12 (21%) | 65,113,113 | 2.32 | 21 (32%) |
| 24 | CLA | C | 510 | - | 56,73,73 | 2.00 | 12 (21%) | 65,113,113 | 2.33 | 19 (29%) |
| 24 | CLA | C | 511 | - | 56,73,73 | 1.98 | 12 (21%) | 65,113,113 | 2.28 | 20 (30%) |
| 24 | CLA | C | 512 | 3 | 56,73,73 | 1.90 | 12 (21%) | 65,113,113 | 2.16 | 15 (23%) |
| 24 | CLA | C | 513 | - | 56,73,73 | 1.94 | 12 (21%) | 65,113,113 | 2.31 | 24 (36%) |
| 24 | CLA | C | 514 | - | 56,73,73 | 1.94 | 12 (21%) | 65,113,113 | 2.25 | 21 (32%) |
| 26 | BCR | C | 515 | - | 41,41,41 | 1.03 | 1 (2%) | 56,56,56 | 1.36 | 5 (8%) |
| 26 | BCR | C | 516 | - | 41,41,41 | 1.00 | 1 (2%) | 56,56,56 | 1.39 | 7 (12%) |
| 36 | DGD | C | 517 | - | 63,63,67 | 0.83 | 2 (3%) | 77,77,81 | 1.09 | 5 (6%) |
| 36 | DGD | C | 518 | - | 63,63,67 | 0.88 | 2 (3%) | 77,77,81 | 1.05 | 5 (6%) |
| 36 | DGD | C | 519 | - | 63,63,67 | 0.81 | 2 (3%) | 77,77,81 | 0.92 | 3 (3%) |
| 34 | LMG | C | 520 | - | 51,51,55 | 0.95 | 2 (3%) | 59,59,63 | 1.14 | 5 (8%) |
| 34 | LMG | C | 521 | - | 51,51,55 | 0.95 | 2 (3%) | 59,59,63 | 1.17 | 5 (8%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 35 | HTG | C | 522 | - | 19,19,19 | 0.99 | 2 (10%) | 23,24,24 | 1.46 | 2 (8%) |
| 35 | HTG | C | 523 | - | 19,19,19 | 1.00 | 2 (10%) | 23,24,24 | 1.87 | 3 (13%) |
| 28 | GOL | C | 524 | - | 5,5,5 | 0.30 | 0 | 5,5,5 | 0.86 | 0 |
| 28 | GOL | C | 525 | - | 5,5,5 | 0.28 | 0 | 5,5,5 | 0.70 | 0 |
| 24 | CLA | D | 401 | 40 | 56,73,73 | 1.99 | 12 (21%) | 65,113,113 | 2.31 | 24 (36%) |
| 30 | LMT | D | 402 | - | 36,36,36 | 0.48 | 0 | 47,47,47 | 1.06 | 4 (8%) |
| 24 | CLA | D | 403 | - | 56,73,73 | 1.95 | 12 (21%) | 65,113,113 | 2.40 | 21 (32%) |
| 24 | CLA | D | 404 | - | 56,73,73 | 1.93 | 12 (21%) | 65,113,113 | 2.21 | 21 (32%) |
| 26 | BCR | D | 405 | - | 41,41,41 | 1.03 | 1 (2%) | 56,56,56 | 1.70 | 12 (21%) |
| 32 | PL9 | D | 406 | - | 55,55,55 | 0.74 | 2 (3%) | 69,69,69 | 1.47 | 14 (20%) |
| 36 | DGD | D | 407 | - | 63,63,67 | 0.95 | 4 (6%) | 77,77,81 | 1.34 | 9 (11%) |
| 37 | LHG | D | 408 | - | 48,48,48 | 0.84 | 2 (4%) | 49,54,54 | 1.13 | 5 (10%) |
| 37 | LHG | D | 409 | - | 48,48,48 | 0.84 | 2 (4%) | 49,54,54 | 1.12 | 5 (10%) |
| 37 | LHG | D | 410 | - | 48,48,48 | 0.92 | 2 (4%) | 49,54,54 | 0.99 | 3 (6%) |
| 35 | HTG | D | 411 | - | 16,16,19 | 1.14 | 2 (12%) | 20,21,24 | 1.08 | 1 (5%) |
| 37 | LHG | E | 101 | - | 41,41,48 | 1.00 | 2 (4%) | 42,47,54 | 1.14 | 3 (7%) |
| 30 | LMT | E | 102 | - | 36,36,36 | 0.46 | 0 | 47,47,47 | 0.80 | 0 |
| 38 | HEM | E | 103 | 5,6 | 28,50,50 | 0.87 | 3 (10%) | 17,82,82 | 2.37 | 4 (23%) |
| 27 | SQD | F | 101 | - | 42,43,54 | 1.10 | 3 (7%) | 52,54,65 | 1.69 | 9 (17%) |
| 28 | GOL | F | 103 | 33 | 5,5,5 | 0.35 | 0 | 5,5,5 | 0.33 | 0 |
| 26 | BCR | H | 101 | - | 41,41,41 | 1.03 | 1 (2%) | 56,56,56 | 1.25 | 5 (8%) |
| 36 | DGD | H | 102 | - | 63,63,67 | 0.92 | 3 (4%) | 77,77,81 | 0.93 | 4 (5%) |
| 30 | LMT | I | 102 | - | 36,36,36 | 0.45 | 0 | 47,47,47 | 1.27 | 5 (10%) |
| 34 | LMG | J | 101 | 39 | 51,51,55 | 0.83 | 2 (3%) | 59,59,63 | 1.03 | 5 (8%) |
| 26 | BCR | K | 101 | - | 41,41,41 | 1.01 | 1 (2%) | 56,56,56 | 1.45 | 12 (21%) |
| 37 | LHG | L | 101 | - | 48,48,48 | 0.87 | 2 (4%) | 49,54,54 | 1.19 | 5 (10%) |
| 30 | LMT | M | 101 | - | 36,36,36 | 0.57 | 1 (2%) | 47,47,47 | 0.90 | 2 (4%) |
| 30 | LMT | M | 102 | - | 36,36,36 | 0.40 | 0 | 47,47,47 | 0.92 | 1 (2%) |
| 28 | GOL | O | 302 | - | 5,5,5 | 0.33 | 0 | 5,5,5 | 0.33 | 0 |
| 35 | HTG | O | 303 | - | 19,19,19 | 1.05 | 1 (5%) | 23,24,24 | 1.03 | 1 (4%) |
| 28 | GOL | T | 101 | - | 5,5,5 | 0.44 | 0 | 5,5,5 | 0.27 | 0 |
| 26 | BCR | T | 102 | - | 41,41,41 | 1.02 | 1 (2%) | 56,56,56 | 1.38 | 10 (17%) |
| 28 | GOL | T | 103 | - | 5,5,5 | 0.38 | 0 | 5,5,5 | 0.23 | 0 |
| 28 | GOL | V | 201 | - | 5,5,5 | 0.34 | 0 | 5,5,5 | 0.42 | 0 |
| 38 | HEM | V | 203 | 16 | 28,50,50 | 0.88 | 1 (3%) | 17,82,82 | 1.58 | 5 (29%) |
| 35 | HTG | V | 204 | - | 19,19,19 | 0.98 | 2 (10%) | 23,24,24 | 1.40 | 3 (13%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|--------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 28 | GOL | V | 205 | - | 5,5,5 | 0.34 | 0 | 5,5,5 | 0.30 | 0 |
| 28 | GOL | V | 206 | - | 5,5,5 | 0.33 | 0 | 5,5,5 | 0.45 | 0 |
| 28 | GOL | V | 207 | - | 5,5,5 | 0.34 | 0 | 5,5,5 | 0.47 | 0 |
| 28 | GOL | V | 208 | - | 5,5,5 | 0.34 | 0 | 5,5,5 | 0.26 | 0 |
| 26 | BCR | Y | 101 | - | 41,41,41 | 1.00 | 1 (2%) | 56,56,56 | 1.47 | 8 (14%) |
| 34 | LMG | Z | 101 | - | 37,37,55 | 0.95 | 2 (5%) | 45,45,63 | 1.49 | 6 (13%) |
| 30 | LMT | a | 401 | - | 36,36,36 | 0.45 | 0 | 47,47,47 | 1.02 | 3 (6%) |
| 27 | SQD | a | 402 | - | 53,54,54 | 1.01 | 3 (5%) | 63,65,65 | 1.30 | 7 (11%) |
| 24 | CLA | a | 406 | - | 56,73,73 | 1.93 | 12 (21%) | 65,113,113 | 2.36 | 22 (33%) |
| 24 | CLA | a | 407 | 40 | 56,73,73 | 1.92 | 12 (21%) | 65,113,113 | 2.22 | 21 (32%) |
| 25 | PHO | a | 408 | - | 67,69,69 | 2.14 | 15 (22%) | 87,99,99 | 1.86 | 18 (20%) |
| 24 | CLA | a | 409 | - | 56,73,73 | 1.91 | 13 (23%) | 65,113,113 | 2.33 | 22 (33%) |
| 26 | BCR | a | 410 | - | 41,41,41 | 1.12 | 1 (2%) | 56,56,56 | 1.34 | 8 (14%) |
| 27 | SQD | a | 411 | - | 53,54,54 | 0.93 | 3 (5%) | 63,65,65 | 1.74 | 13 (20%) |
| 28 | GOL | a | 412 | - | 5,5,5 | 0.33 | 0 | 5,5,5 | 0.52 | 0 |
| 28 | GOL | a | 413 | - | 5,5,5 | 0.40 | 0 | 5,5,5 | 0.28 | 0 |
| 31 | OEX | a | 415 | 1,3,40 | 0,15,15 | 0.00 | - | 0,32,32 | 0.00 | - |
| 32 | PL9 | a | 416 | - | 55,55,55 | 0.61 | 2 (3%) | 69,69,69 | 1.79 | 18 (26%) |
| 30 | LMT | a | 417 | - | 36,36,36 | 0.44 | 0 | 47,47,47 | 0.87 | 2 (4%) |
| 23 | BCT | a | 418 | 21 | 0,3,3 | 0.00 | - | 0,3,3 | 0.00 | - |
| 27 | SQD | b | 601 | - | 53,54,54 | 1.00 | 3 (5%) | 63,65,65 | 1.75 | 11 (17%) |
| 30 | LMT | b | 602 | - | 25,25,36 | 0.46 | 0 | 30,30,47 | 1.31 | 3 (10%) |
| 35 | HTG | b | 603 | - | 19,19,19 | 1.05 | 2 (10%) | 23,24,24 | 1.48 | 1 (4%) |
| 35 | HTG | b | 604 | - | 19,19,19 | 1.00 | 2 (10%) | 23,24,24 | 1.22 | 1 (4%) |
| 24 | CLA | b | 606 | 40 | 56,73,73 | 1.97 | 12 (21%) | 65,113,113 | 2.16 | 17 (26%) |
| 24 | CLA | b | 607 | - | 56,73,73 | 1.99 | 12 (21%) | 65,113,113 | 2.37 | 25 (38%) |
| 24 | CLA | b | 608 | - | 56,73,73 | 1.97 | 12 (21%) | 65,113,113 | 2.43 | 25 (38%) |
| 24 | CLA | b | 609 | - | 56,73,73 | 1.97 | 11 (19%) | 65,113,113 | 2.42 | 18 (27%) |
| 24 | CLA | b | 610 | - | 56,73,73 | 1.87 | 12 (21%) | 65,113,113 | 2.33 | 20 (30%) |
| 24 | CLA | b | 611 | - | 56,73,73 | 1.92 | 12 (21%) | 65,113,113 | 2.27 | 22 (33%) |
| 24 | CLA | b | 612 | 40 | 56,73,73 | 1.89 | 10 (17%) | 65,113,113 | 2.45 | 22 (33%) |
| 24 | CLA | b | 613 | - | 56,73,73 | 1.95 | 12 (21%) | 65,113,113 | 2.26 | 24 (36%) |
| 24 | CLA | b | 614 | - | 56,73,73 | 1.96 | 12 (21%) | 65,113,113 | 2.31 | 22 (33%) |
| 24 | CLA | b | 615 | 40 | 56,73,73 | 1.99 | 12 (21%) | 65,113,113 | 2.25 | 20 (30%) |
| 24 | CLA | b | 616 | - | 56,73,73 | 1.93 | 12 (21%) | 65,113,113 | 2.38 | 19 (29%) |
| 24 | CLA | b | 617 | - | 56,73,73 | 1.95 | 11 (19%) | 65,113,113 | 2.24 | 19 (29%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 24 | CLA | b | 618 | - | 56,73,73 | 1.98 | 12 (21%) | 65,113,113 | 2.42 | 18 (27%) |
| 24 | CLA | b | 619 | - | 56,73,73 | 1.93 | 12 (21%) | 65,113,113 | 2.41 | 23 (35%) |
| 24 | CLA | b | 620 | - | 56,73,73 | 1.96 | 12 (21%) | 65,113,113 | 2.22 | 18 (27%) |
| 24 | CLA | b | 621 | - | 56,73,73 | 1.97 | 12 (21%) | 65,113,113 | 2.31 | 20 (30%) |
| 26 | BCR | b | 622 | - | 41,41,41 | 1.12 | 2 (4%) | 56,56,56 | 1.36 | 4 (7%) |
| 26 | BCR | b | 623 | - | 41,41,41 | 1.05 | 1 (2%) | 56,56,56 | 1.12 | 4 (7%) |
| 26 | BCR | b | 624 | - | 41,41,41 | 0.97 | 1 (2%) | 56,56,56 | 1.24 | 8 (14%) |
| 34 | LMG | b | 625 | - | 51,51,55 | 0.89 | 2 (3%) | 59,59,63 | 1.05 | 4 (6%) |
| 30 | LMT | b | 626 | - | 25,25,36 | 0.49 | 0 | 30,30,47 | 0.67 | 0 |
| 35 | HTG | b | 627 | - | 19,19,19 | 0.85 | 1 (5%) | 23,24,24 | 1.43 | 3 (13%) |
| 35 | HTG | b | 628 | - | 19,19,19 | 1.08 | 2 (10%) | 23,24,24 | 2.05 | 3 (13%) |
| 28 | GOL | b | 629 | - | 5,5,5 | 0.36 | 0 | 5,5,5 | 0.27 | 0 |
| 28 | GOL | b | 630 | - | 5,5,5 | 0.30 | 0 | 5,5,5 | 0.16 | 0 |
| 28 | GOL | b | 631 | - | 5,5,5 | 0.31 | 0 | 5,5,5 | 0.45 | 0 |
| 28 | GOL | b | 632 | - | 5,5,5 | 0.41 | 0 | 5,5,5 | 0.53 | 0 |
| 28 | GOL | b | 633 | - | 5,5,5 | 0.35 | 0 | 5,5,5 | 0.37 | 0 |
| 34 | LMG | c | 501 | - | 51,51,55 | 0.87 | 2 (3%) | 59,59,63 | 1.27 | 6 (10%) |
| 24 | CLA | c | 503 | - | 56,73,73 | 1.95 | 12 (21%) | 65,113,113 | 2.30 | 20 (30%) |
| 24 | CLA | c | 504 | - | 56,73,73 | 1.89 | 12 (21%) | 65,113,113 | 2.22 | 18 (27%) |
| 24 | CLA | c | 505 | - | 56,73,73 | 1.89 | 12 (21%) | 65,113,113 | 2.27 | 20 (30%) |
| 24 | CLA | c | 506 | 40 | 56,73,73 | 1.96 | 12 (21%) | 65,113,113 | 2.26 | 22 (33%) |
| 24 | CLA | c | 507 | - | 56,73,73 | 1.87 | 12 (21%) | 65,113,113 | 2.28 | 15 (23%) |
| 24 | CLA | c | 508 | - | 56,73,73 | 1.89 | 12 (21%) | 65,113,113 | 2.25 | 25 (38%) |
| 24 | CLA | c | 509 | 40 | 56,73,73 | 1.93 | 12 (21%) | 65,113,113 | 2.37 | 18 (27%) |
| 24 | CLA | c | 510 | - | 56,73,73 | 2.02 | 12 (21%) | 65,113,113 | 2.34 | 23 (35%) |
| 24 | CLA | c | 511 | - | 56,73,73 | 2.02 | 12 (21%) | 65,113,113 | 2.32 | 20 (30%) |
| 24 | CLA | c | 512 | - | 56,73,73 | 1.95 | 12 (21%) | 65,113,113 | 2.22 | 22 (33%) |
| 24 | CLA | c | 513 | 3 | 56,73,73 | 1.92 | 11 (19%) | 65,113,113 | 2.18 | 19 (29%) |
| 24 | CLA | c | 514 | - | 56,73,73 | 1.95 | 12 (21%) | 65,113,113 | 2.19 | 24 (36%) |
| 24 | CLA | c | 515 | - | 56,73,73 | 1.95 | 12 (21%) | 65,113,113 | 2.18 | 21 (32%) |
| 26 | BCR | c | 516 | - | 41,41,41 | 1.06 | 2 (4%) | 56,56,56 | 1.40 | 9 (16%) |
| 36 | DGD | c | 517 | - | 63,63,67 | 0.83 | 2 (3%) | 77,77,81 | 1.12 | 6 (7%) |
| 36 | DGD | c | 518 | - | 63,63,67 | 0.89 | 2 (3%) | 77,77,81 | 1.01 | 3 (3%) |
| 36 | DGD | c | 519 | - | 63,63,67 | 0.87 | 2 (3%) | 77,77,81 | 1.00 | 3 (3%) |
| 34 | LMG | c | 520 | - | 51,51,55 | 0.93 | 2 (3%) | 59,59,63 | 0.94 | 2 (3%) |
| 34 | LMG | c | 521 | - | 51,51,55 | 0.94 | 2 (3%) | 59,59,63 | 1.10 | 5 (8%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 35 | HTG | c | 522 | - | 19,19,19 | 0.98 | 2 (10%) | 23,24,24 | 1.73 | 2 (8%) |
| 35 | HTG | c | 523 | - | 19,19,19 | 1.02 | 2 (10%) | 23,24,24 | 1.59 | 2 (8%) |
| 28 | GOL | c | 524 | - | 5,5,5 | 0.28 | 0 | 5,5,5 | 0.36 | 0 |
| 28 | GOL | c | 525 | - | 5,5,5 | 0.34 | 0 | 5,5,5 | 0.56 | 0 |
| 26 | BCR | c | 526 | - | 41,41,41 | 1.04 | 1 (2%) | 56,56,56 | 1.49 | 10 (17%) |
| 28 | GOL | c | 527 | - | 5,5,5 | 0.39 | 0 | 5,5,5 | 0.29 | 0 |
| 24 | CLA | d | 401 | 40 | 56,73,73 | 1.97 | 11 (19%) | 65,113,113 | 2.30 | 20 (30%) |
| 24 | CLA | d | 402 | - | 56,73,73 | 1.92 | 12 (21%) | 65,113,113 | 2.43 | 22 (33%) |
| 25 | PHO | d | 403 | - | 67,69,69 | 2.14 | 16 (23%) | 87,99,99 | 1.94 | 22 (25%) |
| 24 | CLA | d | 404 | - | 56,73,73 | 1.90 | 12 (21%) | 65,113,113 | 2.18 | 21 (32%) |
| 26 | BCR | d | 405 | - | 41,41,41 | 1.03 | 1 (2%) | 56,56,56 | 1.77 | 13 (23%) |
| 32 | PL9 | d | 406 | - | 55,55,55 | 0.69 | 1 (1%) | 69,69,69 | 1.51 | 14 (20%) |
| 36 | DGD | d | 407 | - | 63,63,67 | 0.93 | 2 (3%) | 77,77,81 | 1.07 | 6 (7%) |
| 37 | LHG | d | 408 | - | 48,48,48 | 0.86 | 2 (4%) | 49,54,54 | 1.04 | 5 (10%) |
| 37 | LHG | d | 409 | - | 48,48,48 | 0.88 | 2 (4%) | 49,54,54 | 1.13 | 5 (10%) |
| 37 | LHG | d | 410 | - | 48,48,48 | 0.92 | 2 (4%) | 49,54,54 | 1.01 | 3 (6%) |
| 35 | HTG | d | 411 | - | 16,16,19 | 1.19 | 2 (12%) | 20,21,24 | 1.84 | 1 (5%) |
| 37 | LHG | e | 101 | - | 41,41,48 | 1.02 | 2 (4%) | 42,47,54 | 1.10 | 3 (7%) |
| 38 | HEM | e | 102 | 5,6 | 28,50,50 | 0.93 | 2 (7%) | 17,82,82 | 2.32 | 3 (17%) |
| 27 | SQD | f | 101 | - | 42,43,54 | 1.15 | 3 (7%) | 52,54,65 | 1.65 | 9 (17%) |
| 30 | LMT | f | 102 | - | 36,36,36 | 0.47 | 0 | 47,47,47 | 0.81 | 0 |
| 28 | GOL | f | 104 | 33 | 5,5,5 | 0.32 | 0 | 5,5,5 | 0.23 | 0 |
| 26 | BCR | h | 101 | - | 41,41,41 | 1.02 | 1 (2%) | 56,56,56 | 1.32 | 8 (14%) |
| 36 | DGD | h | 102 | - | 63,63,67 | 0.88 | 3 (4%) | 77,77,81 | 1.02 | 7 (9%) |
| 34 | LMG | j | 101 | 39 | 51,51,55 | 0.92 | 2 (3%) | 59,59,63 | 1.00 | 3 (5%) |
| 26 | BCR | k | 103 | - | 41,41,41 | 1.03 | 1 (2%) | 56,56,56 | 1.32 | 5 (8%) |
| 27 | SQD | l | 101 | - | 53,54,54 | 0.97 | 3 (5%) | 63,65,65 | 1.56 | 10 (15%) |
| 37 | LHG | l | 102 | - | 48,48,48 | 0.94 | 2 (4%) | 49,54,54 | 1.05 | 3 (6%) |
| 30 | LMT | m | 102 | - | 36,36,36 | 0.49 | 0 | 47,47,47 | 1.05 | 2 (4%) |
| 30 | LMT | m | 103 | - | 36,36,36 | 0.56 | 1 (2%) | 47,47,47 | 1.07 | 4 (8%) |
| 26 | BCR | t | 101 | - | 41,41,41 | 1.04 | 1 (2%) | 56,56,56 | 1.31 | 8 (14%) |
| 28 | GOL | t | 102 | - | 5,5,5 | 0.31 | 0 | 5,5,5 | 0.29 | 0 |
| 28 | GOL | v | 201 | - | 5,5,5 | 0.32 | 0 | 5,5,5 | 0.36 | 0 |
| 38 | HEM | v | 202 | 16 | 28,50,50 | 0.82 | 1 (3%) | 17,82,82 | 1.26 | 1 (5%) |
| 28 | GOL | v | 203 | - | 5,5,5 | 0.23 | 0 | 5,5,5 | 0.47 | 0 |
| 28 | GOL | v | 204 | - | 5,5,5 | 0.30 | 0 | 5,5,5 | 0.35 | 0 |
| 28 | GOL | v | 205 | - | 5,5,5 | 0.32 | 0 | 5,5,5 | 0.43 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 26 | BCR | y | 101 | - | 41,41,41 | 1.01 | 1 (2%) | 56,56,56 | 1.54 | 10 (17%) |
| 34 | LMG | z | 101 | - | 39,39,55 | 1.10 | 2 (5%) | 47,47,63 | 1.20 | 4 (8%) |

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 |
|-----|------|-------|-----|--------|-----------|--------------|---------|
| 23 | BCT | A | 404 | 21 | - | 0/0/0/0 | 0/0/0/0 |
| 24 | CLA | A | 405 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | A | 406 | 40 | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 25 | PHO | A | 407 | - | - | 0/53/103/103 | 0/1/6/6 |
| 25 | PHO | A | 408 | - | - | 0/53/103/103 | 0/1/6/6 |
| 24 | CLA | A | 409 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 26 | BCR | A | 410 | - | - | 0/29/63/63 | 0/2/2/2 |
| 27 | SQD | A | 411 | - | - | 0/49/69/69 | 0/1/1/1 |
| 28 | GOL | A | 412 | - | - | 0/4/4/4 | 0/0/0/0 |
| 28 | GOL | A | 413 | - | - | 0/4/4/4 | 0/0/0/0 |
| 28 | GOL | A | 414 | - | - | 0/4/4/4 | 0/0/0/0 |
| 27 | SQD | A | 416 | - | - | 0/49/69/69 | 0/1/1/1 |
| 30 | LMT | A | 417 | - | - | 0/19/59/61 | 0/2/2/2 |
| 31 | OEX | A | 418 | 1,3,40 | - | 0/0/68/68 | 0/0/6/6 |
| 32 | PL9 | A | 419 | - | - | 0/53/73/73 | 0/1/1/1 |
| 24 | CLA | B | 602 | 40 | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | B | 603 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | B | 604 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | B | 605 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | B | 606 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | B | 607 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | B | 608 | 40 | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | B | 609 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | B | 610 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | B | 611 | 40 | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | B | 612 | - | 1/1/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | B | 613 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | B | 614 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | B | 615 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|--------------|---------|
| 24 | CLA | B | 616 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | B | 617 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 26 | BCR | B | 618 | - | - | 0/29/63/63 | 0/2/2/2 |
| 26 | BCR | B | 619 | - | - | 0/29/63/63 | 0/2/2/2 |
| 26 | BCR | B | 620 | - | - | 0/29/63/63 | 0/2/2/2 |
| 34 | LMG | B | 621 | - | - | 0/46/66/70 | 0/1/1/1 |
| 35 | HTG | B | 622 | - | - | 0/10/30/30 | 0/1/1/1 |
| 35 | HTG | B | 623 | - | - | 0/10/30/30 | 0/1/1/1 |
| 35 | HTG | B | 624 | - | - | 0/10/30/30 | 0/1/1/1 |
| 28 | GOL | B | 625 | - | - | 0/4/4/4 | 0/0/0/0 |
| 28 | GOL | B | 626 | - | - | 0/4/4/4 | 0/0/0/0 |
| 28 | GOL | B | 627 | - | - | 0/4/4/4 | 0/0/0/0 |
| 28 | GOL | B | 628 | - | - | 0/4/4/4 | 0/0/0/0 |
| 28 | GOL | B | 629 | - | - | 0/4/4/4 | 0/0/0/0 |
| 35 | HTG | B | 630 | - | - | 0/10/30/30 | 0/1/1/1 |
| 35 | HTG | B | 631 | - | - | 0/10/30/30 | 0/1/1/1 |
| 28 | GOL | B | 633 | - | - | 0/4/4/4 | 0/0/0/0 |
| 30 | LMT | B | 634 | - | - | 0/17/37/61 | 0/1/1/2 |
| 28 | GOL | B | 635 | - | - | 0/4/4/4 | 0/0/0/0 |
| 34 | LMG | C | 501 | - | - | 0/46/66/70 | 0/1/1/1 |
| 24 | CLA | C | 502 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | C | 503 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | C | 504 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | C | 505 | 40 | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | C | 506 | - | 1/1/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | C | 507 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | C | 508 | 40 | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | C | 509 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | C | 510 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | C | 511 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | C | 512 | 3 | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | C | 513 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | C | 514 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 26 | BCR | C | 515 | - | - | 0/29/63/63 | 0/2/2/2 |
| 26 | BCR | C | 516 | - | - | 0/29/63/63 | 0/2/2/2 |
| 36 | DGD | C | 517 | - | - | 0/51/91/95 | 0/2/2/2 |
| 36 | DGD | C | 518 | - | - | 0/51/91/95 | 0/2/2/2 |
| 36 | DGD | C | 519 | - | - | 0/51/91/95 | 0/2/2/2 |
| 34 | LMG | C | 520 | - | - | 0/46/66/70 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|--------------|---------|
| 34 | LMG | C | 521 | - | - | 0/46/66/70 | 0/1/1/1 |
| 35 | HTG | C | 522 | - | - | 0/10/30/30 | 0/1/1/1 |
| 35 | HTG | C | 523 | - | - | 0/10/30/30 | 0/1/1/1 |
| 28 | GOL | C | 524 | - | - | 0/4/4/4 | 0/0/0/0 |
| 28 | GOL | C | 525 | - | - | 0/4/4/4 | 0/0/0/0 |
| 24 | CLA | D | 401 | 40 | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 30 | LMT | D | 402 | - | - | 0/21/61/61 | 0/2/2/2 |
| 24 | CLA | D | 403 | - | 1/1/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | D | 404 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 26 | BCR | D | 405 | - | - | 0/29/63/63 | 0/2/2/2 |
| 32 | PL9 | D | 406 | - | - | 0/53/73/73 | 0/1/1/1 |
| 36 | DGD | D | 407 | - | - | 1/51/91/95 | 0/2/2/2 |
| 37 | LHG | D | 408 | - | - | 0/53/53/53 | 0/0/0/0 |
| 37 | LHG | D | 409 | - | - | 0/53/53/53 | 0/0/0/0 |
| 37 | LHG | D | 410 | - | - | 0/53/53/53 | 0/0/0/0 |
| 35 | HTG | D | 411 | - | - | 0/7/27/30 | 0/1/1/1 |
| 37 | LHG | E | 101 | - | - | 0/46/46/53 | 0/0/0/0 |
| 30 | LMT | E | 102 | - | - | 0/21/61/61 | 0/2/2/2 |
| 38 | HEM | E | 103 | 5,6 | - | 0/6/54/54 | 0/0/8/8 |
| 27 | SQD | F | 101 | - | - | 0/38/58/69 | 0/1/1/1 |
| 28 | GOL | F | 103 | 33 | - | 0/4/4/4 | 0/0/0/0 |
| 26 | BCR | H | 101 | - | - | 0/29/63/63 | 0/2/2/2 |
| 36 | DGD | H | 102 | - | - | 0/51/91/95 | 0/2/2/2 |
| 30 | LMT | I | 102 | - | - | 0/21/61/61 | 0/2/2/2 |
| 34 | LMG | J | 101 | 39 | - | 0/46/66/70 | 0/1/1/1 |
| 26 | BCR | K | 101 | - | - | 0/29/63/63 | 0/2/2/2 |
| 37 | LHG | L | 101 | - | - | 0/53/53/53 | 0/0/0/0 |
| 30 | LMT | M | 101 | - | - | 0/21/61/61 | 0/2/2/2 |
| 30 | LMT | M | 102 | - | - | 0/21/61/61 | 0/2/2/2 |
| 28 | GOL | O | 302 | - | - | 0/4/4/4 | 0/0/0/0 |
| 35 | HTG | O | 303 | - | - | 0/10/30/30 | 0/1/1/1 |
| 28 | GOL | T | 101 | - | - | 0/4/4/4 | 0/0/0/0 |
| 26 | BCR | T | 102 | - | - | 0/29/63/63 | 0/2/2/2 |
| 28 | GOL | T | 103 | - | - | 0/4/4/4 | 0/0/0/0 |
| 28 | GOL | V | 201 | - | - | 0/4/4/4 | 0/0/0/0 |
| 38 | HEM | V | 203 | 16 | - | 0/6/54/54 | 0/0/8/8 |
| 35 | HTG | V | 204 | - | - | 0/10/30/30 | 0/1/1/1 |
| 28 | GOL | V | 205 | - | - | 0/4/4/4 | 0/0/0/0 |
| 28 | GOL | V | 206 | - | - | 0/4/4/4 | 0/0/0/0 |
| 28 | GOL | V | 207 | - | - | 0/4/4/4 | 0/0/0/0 |
| 28 | GOL | V | 208 | - | - | 0/4/4/4 | 0/0/0/0 |
| 26 | BCR | Y | 101 | - | - | 0/29/63/63 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|--------|-----------|--------------|---------|
| 34 | LMG | Z | 101 | - | - | 1/31/51/70 | 0/1/1/1 |
| 30 | LMT | a | 401 | - | - | 0/21/61/61 | 0/2/2/2 |
| 27 | SQD | a | 402 | - | - | 0/49/69/69 | 0/1/1/1 |
| 24 | CLA | a | 406 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | a | 407 | 40 | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 25 | PHO | a | 408 | - | - | 0/53/103/103 | 0/1/6/6 |
| 24 | CLA | a | 409 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 26 | BCR | a | 410 | - | - | 0/29/63/63 | 0/2/2/2 |
| 27 | SQD | a | 411 | - | - | 0/49/69/69 | 0/1/1/1 |
| 28 | GOL | a | 412 | - | - | 0/4/4/4 | 0/0/0/0 |
| 28 | GOL | a | 413 | - | - | 0/4/4/4 | 0/0/0/0 |
| 31 | OEX | a | 415 | 1,3,40 | - | 0/0/68/68 | 0/0/6/6 |
| 32 | PL9 | a | 416 | - | - | 0/53/73/73 | 0/1/1/1 |
| 30 | LMT | a | 417 | - | - | 0/21/61/61 | 0/2/2/2 |
| 23 | BCT | a | 418 | 21 | - | 0/0/0/0 | 0/0/0/0 |
| 27 | SQD | b | 601 | - | - | 1/49/69/69 | 0/1/1/1 |
| 30 | LMT | b | 602 | - | - | 0/17/37/61 | 0/1/1/2 |
| 35 | HTG | b | 603 | - | - | 0/10/30/30 | 0/1/1/1 |
| 35 | HTG | b | 604 | - | - | 0/10/30/30 | 0/1/1/1 |
| 24 | CLA | b | 606 | 40 | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | b | 607 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | b | 608 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | b | 609 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | b | 610 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | b | 611 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | b | 612 | 40 | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | b | 613 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | b | 614 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | b | 615 | 40 | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | b | 616 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | b | 617 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | b | 618 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | b | 619 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | b | 620 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | b | 621 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 26 | BCR | b | 622 | - | - | 0/29/63/63 | 0/2/2/2 |
| 26 | BCR | b | 623 | - | - | 0/29/63/63 | 0/2/2/2 |
| 26 | BCR | b | 624 | - | - | 0/29/63/63 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|--------------|---------|
| 34 | LMG | b | 625 | - | - | 0/46/66/70 | 0/1/1/1 |
| 30 | LMT | b | 626 | - | - | 0/17/37/61 | 0/1/1/2 |
| 35 | HTG | b | 627 | - | - | 0/10/30/30 | 0/1/1/1 |
| 35 | HTG | b | 628 | - | - | 0/10/30/30 | 0/1/1/1 |
| 28 | GOL | b | 629 | - | - | 0/4/4/4 | 0/0/0/0 |
| 28 | GOL | b | 630 | - | - | 0/4/4/4 | 0/0/0/0 |
| 28 | GOL | b | 631 | - | - | 0/4/4/4 | 0/0/0/0 |
| 28 | GOL | b | 632 | - | - | 0/4/4/4 | 0/0/0/0 |
| 28 | GOL | b | 633 | - | - | 0/4/4/4 | 0/0/0/0 |
| 34 | LMG | c | 501 | - | - | 0/46/66/70 | 0/1/1/1 |
| 24 | CLA | c | 503 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | c | 504 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | c | 505 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | c | 506 | 40 | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | c | 507 | - | 1/1/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | c | 508 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | c | 509 | 40 | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | c | 510 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | c | 511 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | c | 512 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | c | 513 | 3 | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | c | 514 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | c | 515 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 26 | BCR | c | 516 | - | - | 0/29/63/63 | 0/2/2/2 |
| 36 | DGD | c | 517 | - | - | 0/51/91/95 | 0/2/2/2 |
| 36 | DGD | c | 518 | - | - | 0/51/91/95 | 0/2/2/2 |
| 36 | DGD | c | 519 | - | - | 0/51/91/95 | 0/2/2/2 |
| 34 | LMG | c | 520 | - | - | 0/46/66/70 | 0/1/1/1 |
| 34 | LMG | c | 521 | - | - | 0/46/66/70 | 0/1/1/1 |
| 35 | HTG | c | 522 | - | - | 0/10/30/30 | 0/1/1/1 |
| 35 | HTG | c | 523 | - | - | 0/10/30/30 | 0/1/1/1 |
| 28 | GOL | c | 524 | - | - | 0/4/4/4 | 0/0/0/0 |
| 28 | GOL | c | 525 | - | - | 0/4/4/4 | 0/0/0/0 |
| 26 | BCR | c | 526 | - | - | 0/29/63/63 | 0/2/2/2 |
| 28 | GOL | c | 527 | - | - | 0/4/4/4 | 0/0/0/0 |
| 24 | CLA | d | 401 | 40 | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | CLA | d | 402 | - | 1/1/20/25 | 0/37/135/135 | 0/0/9/9 |
| 25 | PHO | d | 403 | - | - | 0/53/103/103 | 0/1/6/6 |
| 24 | CLA | d | 404 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 26 | BCR | d | 405 | - | - | 0/29/63/63 | 0/2/2/2 |
| 32 | PL9 | d | 406 | - | - | 0/53/73/73 | 0/1/1/1 |
| 36 | DGD | d | 407 | - | - | 0/51/91/95 | 0/2/2/2 |
| 37 | LHG | d | 408 | - | - | 0/53/53/53 | 0/0/0/0 |
| 37 | LHG | d | 409 | - | - | 0/53/53/53 | 0/0/0/0 |
| 37 | LHG | d | 410 | - | - | 0/53/53/53 | 0/0/0/0 |
| 35 | HTG | d | 411 | - | - | 0/7/27/30 | 0/1/1/1 |
| 37 | LHG | e | 101 | - | - | 0/46/46/53 | 0/0/0/0 |
| 38 | HEM | e | 102 | 5,6 | - | 0/6/54/54 | 0/0/8/8 |
| 27 | SQD | f | 101 | - | - | 2/38/58/69 | 0/1/1/1 |
| 30 | LMT | f | 102 | - | - | 0/21/61/61 | 0/2/2/2 |
| 28 | GOL | f | 104 | 33 | - | 0/4/4/4 | 0/0/0/0 |
| 26 | BCR | h | 101 | - | - | 0/29/63/63 | 0/2/2/2 |
| 36 | DGD | h | 102 | - | - | 0/51/91/95 | 0/2/2/2 |
| 34 | LMG | j | 101 | 39 | - | 0/46/66/70 | 0/1/1/1 |
| 26 | BCR | k | 103 | - | - | 0/29/63/63 | 0/2/2/2 |
| 27 | SQD | l | 101 | - | - | 0/49/69/69 | 0/1/1/1 |
| 37 | LHG | l | 102 | - | - | 0/53/53/53 | 0/0/0/0 |
| 30 | LMT | m | 102 | - | - | 0/21/61/61 | 0/2/2/2 |
| 30 | LMT | m | 103 | - | - | 0/21/61/61 | 0/2/2/2 |
| 26 | BCR | t | 101 | - | - | 0/29/63/63 | 0/2/2/2 |
| 28 | GOL | t | 102 | - | - | 0/4/4/4 | 0/0/0/0 |
| 28 | GOL | v | 201 | - | - | 0/4/4/4 | 0/0/0/0 |
| 38 | HEM | v | 202 | 16 | - | 0/6/54/54 | 0/0/8/8 |
| 28 | GOL | v | 203 | - | - | 0/4/4/4 | 0/0/0/0 |
| 28 | GOL | v | 204 | - | - | 0/4/4/4 | 0/0/0/0 |
| 28 | GOL | v | 205 | - | - | 0/4/4/4 | 0/0/0/0 |
| 26 | BCR | y | 101 | - | - | 0/29/63/63 | 0/2/2/2 |
| 34 | LMG | z | 101 | - | - | 0/34/54/70 | 0/1/1/1 |

All (1056) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 26 | c | 526 | BCR | C23-C22 | -4.97 | 1.35 | 1.45 |
| 26 | C | 515 | BCR | C23-C22 | -4.77 | 1.35 | 1.45 |
| 26 | d | 405 | BCR | C23-C22 | -4.75 | 1.35 | 1.45 |
| 26 | y | 101 | BCR | C23-C22 | -4.75 | 1.35 | 1.45 |
| 26 | C | 516 | BCR | C23-C22 | -4.72 | 1.35 | 1.45 |
| 26 | B | 620 | BCR | C23-C22 | -4.65 | 1.35 | 1.45 |
| 26 | b | 624 | BCR | C23-C22 | -4.62 | 1.35 | 1.45 |
| 26 | k | 103 | BCR | C23-C22 | -4.59 | 1.35 | 1.45 |
| 26 | D | 405 | BCR | C23-C22 | -4.59 | 1.35 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 26 | a | 410 | BCR | C23-C22 | -4.57 | 1.36 | 1.45 |
| 26 | h | 101 | BCR | C23-C22 | -4.55 | 1.36 | 1.45 |
| 35 | B | 622 | HTG | C1'-S1 | -4.53 | 1.75 | 1.81 |
| 26 | T | 102 | BCR | C23-C22 | -4.51 | 1.36 | 1.45 |
| 26 | c | 516 | BCR | C23-C22 | -4.45 | 1.36 | 1.45 |
| 26 | b | 623 | BCR | C23-C22 | -4.43 | 1.36 | 1.45 |
| 26 | t | 101 | BCR | C23-C22 | -4.43 | 1.36 | 1.45 |
| 26 | H | 101 | BCR | C23-C22 | -4.42 | 1.36 | 1.45 |
| 26 | Y | 101 | BCR | C23-C22 | -4.41 | 1.36 | 1.45 |
| 26 | b | 622 | BCR | C23-C22 | -4.36 | 1.36 | 1.45 |
| 26 | B | 618 | BCR | C23-C22 | -4.32 | 1.36 | 1.45 |
| 26 | K | 101 | BCR | C23-C22 | -4.30 | 1.36 | 1.45 |
| 26 | A | 410 | BCR | C23-C22 | -4.28 | 1.36 | 1.45 |
| 26 | B | 619 | BCR | C23-C22 | -4.26 | 1.36 | 1.45 |
| 35 | d | 411 | HTG | C1'-S1 | -3.98 | 1.76 | 1.81 |
| 35 | b | 603 | HTG | C1'-S1 | -3.96 | 1.76 | 1.81 |
| 35 | O | 303 | HTG | C1'-S1 | -3.86 | 1.76 | 1.81 |
| 35 | b | 628 | HTG | C1'-S1 | -3.78 | 1.76 | 1.81 |
| 35 | B | 624 | HTG | C1'-S1 | -3.64 | 1.76 | 1.81 |
| 35 | c | 523 | HTG | C1'-S1 | -3.60 | 1.76 | 1.81 |
| 35 | B | 631 | HTG | C1'-S1 | -3.53 | 1.76 | 1.81 |
| 35 | D | 411 | HTG | C1'-S1 | -3.52 | 1.76 | 1.81 |
| 25 | A | 407 | PHO | C4A-NA | -3.47 | 1.26 | 1.35 |
| 35 | C | 523 | HTG | C1'-S1 | -3.46 | 1.76 | 1.81 |
| 35 | b | 604 | HTG | C1'-S1 | -3.45 | 1.76 | 1.81 |
| 25 | d | 403 | PHO | C4A-NA | -3.44 | 1.26 | 1.35 |
| 35 | B | 630 | HTG | C1'-S1 | -3.44 | 1.77 | 1.81 |
| 25 | A | 408 | PHO | C4A-NA | -3.39 | 1.27 | 1.35 |
| 35 | C | 522 | HTG | C1'-S1 | -3.35 | 1.77 | 1.81 |
| 35 | V | 204 | HTG | C1'-S1 | -3.31 | 1.77 | 1.81 |
| 35 | c | 522 | HTG | C1'-S1 | -3.28 | 1.77 | 1.81 |
| 35 | B | 623 | HTG | C1'-S1 | -3.26 | 1.77 | 1.81 |
| 35 | b | 627 | HTG | C1'-S1 | -3.14 | 1.77 | 1.81 |
| 25 | a | 408 | PHO | C4A-NA | -2.97 | 1.28 | 1.35 |
| 27 | A | 416 | SQD | C6-S | -2.68 | 1.66 | 1.77 |
| 27 | a | 402 | SQD | C6-S | -2.66 | 1.66 | 1.77 |
| 27 | A | 411 | SQD | C6-S | -2.66 | 1.66 | 1.77 |
| 27 | f | 101 | SQD | C6-S | -2.66 | 1.66 | 1.77 |
| 38 | e | 102 | HEM | C3B-C2B | -2.61 | 1.36 | 1.40 |
| 35 | D | 411 | HTG | C1-S1 | -2.53 | 1.76 | 1.80 |
| 27 | a | 411 | SQD | C6-S | -2.49 | 1.67 | 1.77 |
| 35 | C | 522 | HTG | C1-S1 | -2.42 | 1.76 | 1.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 38 | e | 102 | HEM | C4D-ND | -2.41 | 1.33 | 1.36 |
| 35 | c | 522 | HTG | C1-S1 | -2.40 | 1.77 | 1.80 |
| 27 | b | 601 | SQD | C6-S | -2.38 | 1.67 | 1.77 |
| 38 | v | 202 | HEM | C3B-C2B | -2.37 | 1.37 | 1.40 |
| 35 | b | 628 | HTG | C1-S1 | -2.35 | 1.77 | 1.80 |
| 35 | c | 523 | HTG | C1-S1 | -2.32 | 1.77 | 1.80 |
| 35 | B | 631 | HTG | C1-S1 | -2.30 | 1.77 | 1.80 |
| 38 | E | 103 | HEM | C4D-ND | -2.30 | 1.34 | 1.36 |
| 35 | d | 411 | HTG | C1-S1 | -2.29 | 1.77 | 1.80 |
| 35 | V | 204 | HTG | C1-S1 | -2.28 | 1.77 | 1.80 |
| 38 | E | 103 | HEM | C3B-C2B | -2.27 | 1.37 | 1.40 |
| 27 | l | 101 | SQD | C6-S | -2.27 | 1.68 | 1.77 |
| 27 | F | 101 | SQD | C6-S | -2.19 | 1.68 | 1.77 |
| 24 | a | 409 | CLA | C1C-NC | -2.18 | 1.34 | 1.37 |
| 35 | b | 604 | HTG | C1-S1 | -2.16 | 1.77 | 1.80 |
| 25 | A | 407 | PHO | C1A-NA | -2.11 | 1.33 | 1.37 |
| 38 | E | 103 | HEM | C1B-NB | -2.07 | 1.34 | 1.36 |
| 35 | C | 523 | HTG | C1-S1 | -2.06 | 1.77 | 1.80 |
| 35 | b | 603 | HTG | C1-S1 | -2.04 | 1.77 | 1.80 |
| 35 | B | 624 | HTG | C1-S1 | -2.04 | 1.77 | 1.80 |
| 38 | V | 203 | HEM | C1B-NB | -2.04 | 1.34 | 1.36 |
| 25 | A | 408 | PHO | C1A-NA | -2.03 | 1.33 | 1.37 |
| 35 | B | 630 | HTG | C1-S1 | -2.01 | 1.77 | 1.80 |
| 26 | c | 516 | BCR | C1-C6 | -2.00 | 1.51 | 1.53 |
| 24 | b | 606 | CLA | C4C-C3C | 2.00 | 1.48 | 1.45 |
| 25 | d | 403 | PHO | C4C-C3C | 2.01 | 1.49 | 1.45 |
| 36 | D | 407 | DGD | O5D-C1E | 2.01 | 1.43 | 1.40 |
| 24 | C | 502 | CLA | CHD-C4C | 2.01 | 1.47 | 1.41 |
| 25 | a | 408 | PHO | C1C-C2C | 2.03 | 1.50 | 1.45 |
| 26 | b | 622 | BCR | C19-C18 | 2.03 | 1.50 | 1.45 |
| 24 | D | 404 | CLA | CHD-C4C | 2.03 | 1.47 | 1.41 |
| 24 | c | 506 | CLA | CHD-C4C | 2.03 | 1.47 | 1.41 |
| 24 | A | 406 | CLA | C1C-C2C | 2.04 | 1.48 | 1.44 |
| 24 | B | 615 | CLA | C4C-C3C | 2.04 | 1.48 | 1.45 |
| 24 | A | 405 | CLA | CHD-C4C | 2.04 | 1.47 | 1.41 |
| 24 | d | 401 | CLA | CHD-C4C | 2.06 | 1.47 | 1.41 |
| 32 | D | 406 | PL9 | C2-C3 | 2.08 | 1.40 | 1.34 |
| 24 | B | 613 | CLA | CHD-C4C | 2.08 | 1.47 | 1.41 |
| 25 | A | 407 | PHO | C4C-C3C | 2.08 | 1.49 | 1.45 |
| 24 | c | 512 | CLA | C4C-C3C | 2.09 | 1.48 | 1.45 |
| 24 | b | 618 | CLA | CHD-C4C | 2.09 | 1.47 | 1.41 |
| 24 | B | 607 | CLA | CHD-C4C | 2.11 | 1.47 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 24 | B | 617 | CLA | C1C-C2C | 2.12 | 1.48 | 1.44 |
| 24 | B | 617 | CLA | CHD-C4C | 2.12 | 1.47 | 1.41 |
| 24 | b | 619 | CLA | C1C-C2C | 2.12 | 1.48 | 1.44 |
| 24 | c | 509 | CLA | CHD-C4C | 2.12 | 1.47 | 1.41 |
| 24 | c | 503 | CLA | CHD-C4C | 2.13 | 1.47 | 1.41 |
| 24 | B | 604 | CLA | CHD-C4C | 2.13 | 1.47 | 1.41 |
| 32 | a | 416 | PL9 | C2-C3 | 2.14 | 1.40 | 1.34 |
| 24 | B | 603 | CLA | CHD-C4C | 2.14 | 1.47 | 1.41 |
| 24 | B | 616 | CLA | CHD-C4C | 2.16 | 1.47 | 1.41 |
| 24 | b | 620 | CLA | C1C-C2C | 2.16 | 1.48 | 1.44 |
| 24 | c | 505 | CLA | CHD-C4C | 2.16 | 1.47 | 1.41 |
| 24 | B | 608 | CLA | CHD-C4C | 2.16 | 1.47 | 1.41 |
| 24 | b | 611 | CLA | C4C-C3C | 2.16 | 1.48 | 1.45 |
| 24 | B | 610 | CLA | CHD-C4C | 2.17 | 1.47 | 1.41 |
| 24 | c | 510 | CLA | CHD-C4C | 2.17 | 1.47 | 1.41 |
| 24 | b | 607 | CLA | CHD-C4C | 2.17 | 1.47 | 1.41 |
| 24 | c | 508 | CLA | C1C-C2C | 2.18 | 1.48 | 1.44 |
| 24 | B | 606 | CLA | CHD-C4C | 2.18 | 1.47 | 1.41 |
| 24 | C | 514 | CLA | C4C-C3C | 2.18 | 1.48 | 1.45 |
| 24 | C | 504 | CLA | CHD-C4C | 2.19 | 1.47 | 1.41 |
| 24 | C | 513 | CLA | CHD-C4C | 2.19 | 1.47 | 1.41 |
| 25 | d | 403 | PHO | C4D-CHA | 2.19 | 1.50 | 1.44 |
| 24 | B | 604 | CLA | C4C-C3C | 2.19 | 1.48 | 1.45 |
| 36 | D | 407 | DGD | O3G-C1D | 2.19 | 1.44 | 1.40 |
| 24 | D | 401 | CLA | CHD-C4C | 2.21 | 1.47 | 1.41 |
| 24 | b | 617 | CLA | C4C-C3C | 2.21 | 1.48 | 1.45 |
| 24 | b | 611 | CLA | CHD-C4C | 2.21 | 1.47 | 1.41 |
| 24 | B | 610 | CLA | C1C-C2C | 2.21 | 1.48 | 1.44 |
| 24 | D | 404 | CLA | C4C-C3C | 2.21 | 1.48 | 1.45 |
| 24 | C | 514 | CLA | CHD-C4C | 2.21 | 1.47 | 1.41 |
| 24 | B | 609 | CLA | CHD-C4C | 2.21 | 1.47 | 1.41 |
| 24 | B | 602 | CLA | CHD-C4C | 2.22 | 1.47 | 1.41 |
| 24 | B | 606 | CLA | C4C-C3C | 2.22 | 1.49 | 1.45 |
| 24 | B | 615 | CLA | CHD-C4C | 2.22 | 1.47 | 1.41 |
| 24 | b | 616 | CLA | C4C-C3C | 2.22 | 1.49 | 1.45 |
| 24 | b | 620 | CLA | CHD-C4C | 2.22 | 1.47 | 1.41 |
| 24 | A | 406 | CLA | C4C-C3C | 2.23 | 1.49 | 1.45 |
| 24 | B | 612 | CLA | CHD-C4C | 2.24 | 1.47 | 1.41 |
| 24 | A | 409 | CLA | CHD-C4C | 2.24 | 1.47 | 1.41 |
| 24 | B | 607 | CLA | C4C-C3C | 2.24 | 1.49 | 1.45 |
| 30 | m | 103 | LMT | O1'-C1' | 2.24 | 1.44 | 1.40 |
| 24 | C | 506 | CLA | CHD-C4C | 2.25 | 1.47 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 24 | C | 507 | CLA | CHD-C4C | 2.25 | 1.47 | 1.41 |
| 24 | B | 614 | CLA | CHD-C4C | 2.25 | 1.47 | 1.41 |
| 24 | b | 613 | CLA | CHD-C4C | 2.26 | 1.47 | 1.41 |
| 24 | C | 514 | CLA | C1C-C2C | 2.26 | 1.48 | 1.44 |
| 24 | b | 621 | CLA | C1C-C2C | 2.26 | 1.48 | 1.44 |
| 24 | C | 508 | CLA | C4C-C3C | 2.27 | 1.49 | 1.45 |
| 24 | c | 504 | CLA | C4C-C3C | 2.27 | 1.49 | 1.45 |
| 24 | b | 610 | CLA | CHD-C4C | 2.27 | 1.48 | 1.41 |
| 24 | C | 508 | CLA | CHD-C4C | 2.27 | 1.48 | 1.41 |
| 24 | B | 602 | CLA | C4C-C3C | 2.27 | 1.49 | 1.45 |
| 24 | b | 616 | CLA | CHD-C4C | 2.27 | 1.48 | 1.41 |
| 24 | B | 617 | CLA | C4B-CHC | 2.29 | 1.46 | 1.40 |
| 24 | C | 511 | CLA | C4C-C3C | 2.29 | 1.49 | 1.45 |
| 24 | D | 403 | CLA | CHD-C4C | 2.29 | 1.48 | 1.41 |
| 24 | A | 409 | CLA | C4C-C3C | 2.29 | 1.49 | 1.45 |
| 24 | d | 401 | CLA | C4C-C3C | 2.30 | 1.49 | 1.45 |
| 24 | B | 617 | CLA | C4C-C3C | 2.30 | 1.49 | 1.45 |
| 24 | c | 512 | CLA | CHD-C4C | 2.31 | 1.48 | 1.41 |
| 24 | c | 505 | CLA | C4C-C3C | 2.31 | 1.49 | 1.45 |
| 24 | B | 611 | CLA | CHD-C4C | 2.31 | 1.48 | 1.41 |
| 24 | b | 615 | CLA | CHD-C4C | 2.31 | 1.48 | 1.41 |
| 24 | b | 608 | CLA | C4C-C3C | 2.31 | 1.49 | 1.45 |
| 24 | B | 605 | CLA | C4C-C3C | 2.31 | 1.49 | 1.45 |
| 24 | c | 504 | CLA | C1C-C2C | 2.31 | 1.49 | 1.44 |
| 24 | b | 616 | CLA | C1C-C2C | 2.31 | 1.49 | 1.44 |
| 24 | a | 409 | CLA | CHD-C4C | 2.32 | 1.48 | 1.41 |
| 24 | b | 614 | CLA | CHD-C4C | 2.32 | 1.48 | 1.41 |
| 24 | A | 406 | CLA | C4B-CHC | 2.33 | 1.46 | 1.40 |
| 24 | b | 614 | CLA | C1C-C2C | 2.33 | 1.49 | 1.44 |
| 24 | B | 616 | CLA | C1C-C2C | 2.33 | 1.49 | 1.44 |
| 30 | M | 101 | LMT | O1'-C1' | 2.34 | 1.44 | 1.40 |
| 24 | d | 404 | CLA | CHD-C4C | 2.34 | 1.48 | 1.41 |
| 24 | a | 406 | CLA | C1C-C2C | 2.35 | 1.49 | 1.44 |
| 24 | a | 406 | CLA | CHD-C4C | 2.35 | 1.48 | 1.41 |
| 24 | C | 510 | CLA | CHD-C4C | 2.35 | 1.48 | 1.41 |
| 24 | C | 511 | CLA | CHD-C4C | 2.35 | 1.48 | 1.41 |
| 24 | c | 504 | CLA | CHD-C4C | 2.36 | 1.48 | 1.41 |
| 24 | c | 508 | CLA | C4C-C3C | 2.36 | 1.49 | 1.45 |
| 24 | d | 401 | CLA | C4B-CHC | 2.37 | 1.46 | 1.40 |
| 24 | C | 512 | CLA | C1C-C2C | 2.37 | 1.49 | 1.44 |
| 24 | B | 611 | CLA | C1C-C2C | 2.37 | 1.49 | 1.44 |
| 24 | C | 503 | CLA | CHD-C4C | 2.37 | 1.48 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 24 | C | 509 | CLA | CHD-C4C | 2.37 | 1.48 | 1.41 |
| 24 | b | 610 | CLA | C4C-C3C | 2.37 | 1.49 | 1.45 |
| 24 | C | 512 | CLA | C4C-C3C | 2.38 | 1.49 | 1.45 |
| 24 | c | 503 | CLA | C1C-C2C | 2.39 | 1.49 | 1.44 |
| 24 | b | 608 | CLA | CHD-C4C | 2.39 | 1.48 | 1.41 |
| 24 | b | 620 | CLA | C4C-C3C | 2.39 | 1.49 | 1.45 |
| 24 | a | 407 | CLA | C4C-C3C | 2.39 | 1.49 | 1.45 |
| 24 | C | 507 | CLA | C4C-C3C | 2.39 | 1.49 | 1.45 |
| 24 | a | 409 | CLA | C1C-C2C | 2.40 | 1.49 | 1.44 |
| 24 | d | 404 | CLA | C4C-C3C | 2.40 | 1.49 | 1.45 |
| 24 | C | 507 | CLA | C1C-C2C | 2.40 | 1.49 | 1.44 |
| 24 | c | 514 | CLA | CHD-C4C | 2.41 | 1.48 | 1.41 |
| 36 | h | 102 | DGD | O5D-C1E | 2.41 | 1.44 | 1.40 |
| 24 | c | 509 | CLA | C4C-C3C | 2.41 | 1.49 | 1.45 |
| 24 | c | 513 | CLA | C4C-C3C | 2.42 | 1.49 | 1.45 |
| 24 | B | 609 | CLA | C4C-C3C | 2.42 | 1.49 | 1.45 |
| 24 | b | 606 | CLA | CHD-C4C | 2.43 | 1.48 | 1.41 |
| 24 | d | 402 | CLA | C4C-C3C | 2.43 | 1.49 | 1.45 |
| 24 | a | 409 | CLA | C4B-CHC | 2.44 | 1.46 | 1.40 |
| 24 | C | 507 | CLA | C4B-CHC | 2.44 | 1.46 | 1.40 |
| 24 | B | 609 | CLA | C4B-CHC | 2.44 | 1.46 | 1.40 |
| 36 | H | 102 | DGD | O5D-C1E | 2.45 | 1.44 | 1.40 |
| 24 | C | 512 | CLA | CHD-C4C | 2.45 | 1.48 | 1.41 |
| 24 | B | 615 | CLA | C1C-C2C | 2.45 | 1.49 | 1.44 |
| 24 | c | 507 | CLA | CHD-C4C | 2.45 | 1.48 | 1.41 |
| 24 | b | 613 | CLA | C4C-C3C | 2.45 | 1.49 | 1.45 |
| 24 | b | 621 | CLA | CHD-C4C | 2.46 | 1.48 | 1.41 |
| 24 | b | 621 | CLA | C4B-CHC | 2.46 | 1.46 | 1.40 |
| 24 | d | 402 | CLA | CHD-C4C | 2.47 | 1.48 | 1.41 |
| 24 | c | 508 | CLA | CHD-C4C | 2.47 | 1.48 | 1.41 |
| 24 | B | 616 | CLA | C4C-C3C | 2.47 | 1.49 | 1.45 |
| 24 | C | 512 | CLA | C4B-CHC | 2.47 | 1.46 | 1.40 |
| 24 | b | 607 | CLA | C4C-C3C | 2.47 | 1.49 | 1.45 |
| 24 | B | 612 | CLA | C4C-C3C | 2.48 | 1.49 | 1.45 |
| 24 | C | 513 | CLA | C4C-C3C | 2.48 | 1.49 | 1.45 |
| 24 | c | 511 | CLA | C4C-C3C | 2.48 | 1.49 | 1.45 |
| 24 | a | 407 | CLA | CHD-C4C | 2.49 | 1.48 | 1.41 |
| 24 | c | 515 | CLA | C1C-C2C | 2.49 | 1.49 | 1.44 |
| 32 | D | 406 | PL9 | C6-C5 | 2.49 | 1.48 | 1.35 |
| 24 | C | 505 | CLA | C1C-C2C | 2.49 | 1.49 | 1.44 |
| 24 | a | 406 | CLA | C4B-CHC | 2.49 | 1.46 | 1.40 |
| 24 | c | 515 | CLA | CHD-C4C | 2.50 | 1.48 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 24 | C | 505 | CLA | CHD-C4C | 2.50 | 1.48 | 1.41 |
| 24 | b | 612 | CLA | C1C-C2C | 2.50 | 1.49 | 1.44 |
| 24 | B | 608 | CLA | C1C-C2C | 2.50 | 1.49 | 1.44 |
| 24 | c | 508 | CLA | C4B-CHC | 2.50 | 1.46 | 1.40 |
| 24 | c | 513 | CLA | CHD-C4C | 2.50 | 1.48 | 1.41 |
| 24 | c | 506 | CLA | C4C-C3C | 2.51 | 1.49 | 1.45 |
| 24 | c | 511 | CLA | CHD-C4C | 2.51 | 1.48 | 1.41 |
| 24 | a | 409 | CLA | C4C-C3C | 2.52 | 1.49 | 1.45 |
| 24 | c | 504 | CLA | C4B-CHC | 2.52 | 1.46 | 1.40 |
| 24 | C | 506 | CLA | C1C-C2C | 2.52 | 1.49 | 1.44 |
| 24 | b | 606 | CLA | C1C-C2C | 2.52 | 1.49 | 1.44 |
| 24 | b | 618 | CLA | C4C-C3C | 2.52 | 1.49 | 1.45 |
| 24 | B | 608 | CLA | C4C-C3C | 2.52 | 1.49 | 1.45 |
| 24 | b | 614 | CLA | C4C-C3C | 2.52 | 1.49 | 1.45 |
| 24 | D | 401 | CLA | C1C-C2C | 2.53 | 1.49 | 1.44 |
| 24 | b | 619 | CLA | C4B-CHC | 2.53 | 1.46 | 1.40 |
| 24 | c | 513 | CLA | C4B-CHC | 2.53 | 1.46 | 1.40 |
| 24 | c | 503 | CLA | C4B-CHC | 2.53 | 1.46 | 1.40 |
| 24 | B | 605 | CLA | C1C-C2C | 2.53 | 1.49 | 1.44 |
| 32 | d | 406 | PL9 | C6-C5 | 2.54 | 1.48 | 1.35 |
| 24 | b | 613 | CLA | C1C-C2C | 2.54 | 1.49 | 1.44 |
| 24 | c | 515 | CLA | C1B-CHB | 2.54 | 1.46 | 1.40 |
| 24 | C | 502 | CLA | C4C-C3C | 2.54 | 1.49 | 1.45 |
| 24 | c | 514 | CLA | C4C-C3C | 2.54 | 1.49 | 1.45 |
| 24 | B | 615 | CLA | C4B-CHC | 2.55 | 1.46 | 1.40 |
| 32 | A | 419 | PL9 | C6-C5 | 2.55 | 1.48 | 1.35 |
| 24 | B | 602 | CLA | C1C-C2C | 2.55 | 1.49 | 1.44 |
| 24 | B | 609 | CLA | C1C-C2C | 2.55 | 1.49 | 1.44 |
| 24 | C | 504 | CLA | C4C-C3C | 2.57 | 1.49 | 1.45 |
| 24 | b | 619 | CLA | CHD-C4C | 2.57 | 1.48 | 1.41 |
| 24 | C | 505 | CLA | C4B-CHC | 2.58 | 1.47 | 1.40 |
| 24 | D | 401 | CLA | C4B-CHC | 2.59 | 1.47 | 1.40 |
| 24 | D | 401 | CLA | C1B-CHB | 2.59 | 1.47 | 1.40 |
| 24 | a | 407 | CLA | C1C-C2C | 2.60 | 1.49 | 1.44 |
| 24 | A | 406 | CLA | CHD-C4C | 2.60 | 1.48 | 1.41 |
| 24 | b | 607 | CLA | C1C-C2C | 2.60 | 1.49 | 1.44 |
| 34 | Z | 101 | LMG | O8-C28 | 2.60 | 1.46 | 1.33 |
| 24 | c | 510 | CLA | C4C-C3C | 2.60 | 1.49 | 1.45 |
| 24 | C | 509 | CLA | C1C-C2C | 2.60 | 1.49 | 1.44 |
| 24 | B | 613 | CLA | C1C-C2C | 2.60 | 1.49 | 1.44 |
| 24 | B | 611 | CLA | C4C-C3C | 2.60 | 1.49 | 1.45 |
| 24 | c | 506 | CLA | C4B-CHC | 2.61 | 1.47 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 24 | B | 612 | CLA | C1B-CHB | 2.61 | 1.47 | 1.40 |
| 25 | a | 408 | PHO | CHB-C4A | 2.61 | 1.46 | 1.40 |
| 32 | a | 416 | PL9 | C6-C5 | 2.61 | 1.49 | 1.35 |
| 24 | c | 514 | CLA | C1C-C2C | 2.61 | 1.49 | 1.44 |
| 24 | c | 515 | CLA | C4C-C3C | 2.62 | 1.49 | 1.45 |
| 24 | B | 609 | CLA | C1B-CHB | 2.62 | 1.47 | 1.40 |
| 24 | C | 511 | CLA | C1C-C2C | 2.62 | 1.49 | 1.44 |
| 24 | b | 619 | CLA | C1B-CHB | 2.62 | 1.47 | 1.40 |
| 24 | c | 511 | CLA | C1C-C2C | 2.63 | 1.49 | 1.44 |
| 24 | B | 603 | CLA | C4C-C3C | 2.63 | 1.49 | 1.45 |
| 24 | c | 509 | CLA | C1C-C2C | 2.63 | 1.49 | 1.44 |
| 24 | b | 618 | CLA | C4B-CHC | 2.63 | 1.47 | 1.40 |
| 24 | C | 504 | CLA | C1C-C2C | 2.64 | 1.49 | 1.44 |
| 24 | c | 503 | CLA | C4C-C3C | 2.64 | 1.49 | 1.45 |
| 24 | B | 603 | CLA | C1C-C2C | 2.64 | 1.49 | 1.44 |
| 24 | B | 602 | CLA | C1B-CHB | 2.65 | 1.47 | 1.40 |
| 24 | B | 606 | CLA | C1C-C2C | 2.65 | 1.49 | 1.44 |
| 24 | b | 614 | CLA | C4B-CHC | 2.66 | 1.47 | 1.40 |
| 24 | c | 506 | CLA | C1B-CHB | 2.66 | 1.47 | 1.40 |
| 24 | C | 502 | CLA | C4B-CHC | 2.66 | 1.47 | 1.40 |
| 24 | B | 614 | CLA | C1C-C2C | 2.66 | 1.49 | 1.44 |
| 24 | B | 603 | CLA | C4B-CHC | 2.66 | 1.47 | 1.40 |
| 24 | b | 620 | CLA | C1B-CHB | 2.66 | 1.47 | 1.40 |
| 24 | d | 402 | CLA | C1C-C2C | 2.67 | 1.49 | 1.44 |
| 24 | A | 409 | CLA | C1C-C2C | 2.67 | 1.49 | 1.44 |
| 24 | D | 404 | CLA | C1B-CHB | 2.67 | 1.47 | 1.40 |
| 24 | b | 617 | CLA | C1C-C2C | 2.67 | 1.49 | 1.44 |
| 24 | C | 513 | CLA | C4B-CHC | 2.67 | 1.47 | 1.40 |
| 24 | C | 514 | CLA | C4B-CHC | 2.67 | 1.47 | 1.40 |
| 24 | b | 610 | CLA | C1C-C2C | 2.68 | 1.49 | 1.44 |
| 24 | B | 613 | CLA | C4B-CHC | 2.68 | 1.47 | 1.40 |
| 24 | a | 409 | CLA | C1B-CHB | 2.68 | 1.47 | 1.40 |
| 24 | c | 514 | CLA | C1B-CHB | 2.68 | 1.47 | 1.40 |
| 24 | C | 510 | CLA | C1C-C2C | 2.69 | 1.49 | 1.44 |
| 24 | b | 610 | CLA | C1B-CHB | 2.69 | 1.47 | 1.40 |
| 24 | C | 513 | CLA | C1B-CHB | 2.69 | 1.47 | 1.40 |
| 24 | C | 509 | CLA | C4B-CHC | 2.70 | 1.47 | 1.40 |
| 24 | c | 508 | CLA | C1B-CHB | 2.70 | 1.47 | 1.40 |
| 24 | a | 407 | CLA | C1B-CHB | 2.70 | 1.47 | 1.40 |
| 24 | b | 619 | CLA | C4C-C3C | 2.70 | 1.49 | 1.45 |
| 24 | B | 603 | CLA | C1B-CHB | 2.70 | 1.47 | 1.40 |
| 24 | B | 616 | CLA | C4B-CHC | 2.71 | 1.47 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 24 | c | 509 | CLA | C4B-CHC | 2.71 | 1.47 | 1.40 |
| 24 | b | 620 | CLA | C4B-CHC | 2.71 | 1.47 | 1.40 |
| 24 | C | 505 | CLA | C4C-C3C | 2.72 | 1.49 | 1.45 |
| 24 | d | 402 | CLA | C4B-CHC | 2.72 | 1.47 | 1.40 |
| 24 | b | 611 | CLA | C1B-CHB | 2.72 | 1.47 | 1.40 |
| 24 | A | 405 | CLA | C4B-CHC | 2.72 | 1.47 | 1.40 |
| 24 | C | 508 | CLA | C1B-CHB | 2.73 | 1.47 | 1.40 |
| 24 | C | 502 | CLA | C1C-C2C | 2.73 | 1.49 | 1.44 |
| 24 | b | 612 | CLA | C1B-CHB | 2.73 | 1.47 | 1.40 |
| 24 | B | 615 | CLA | C1B-CHB | 2.74 | 1.47 | 1.40 |
| 24 | d | 404 | CLA | C1B-CHB | 2.75 | 1.47 | 1.40 |
| 24 | c | 507 | CLA | C1C-C2C | 2.76 | 1.49 | 1.44 |
| 24 | b | 609 | CLA | C4C-C3C | 2.76 | 1.49 | 1.45 |
| 24 | C | 503 | CLA | C4C-C3C | 2.76 | 1.49 | 1.45 |
| 24 | C | 502 | CLA | C1B-CHB | 2.76 | 1.47 | 1.40 |
| 24 | b | 613 | CLA | C1B-CHB | 2.76 | 1.47 | 1.40 |
| 25 | A | 408 | PHO | CHB-C4A | 2.76 | 1.47 | 1.40 |
| 24 | B | 612 | CLA | C1C-C2C | 2.77 | 1.49 | 1.44 |
| 24 | c | 512 | CLA | C1C-C2C | 2.77 | 1.49 | 1.44 |
| 24 | b | 612 | CLA | C4B-CHC | 2.78 | 1.47 | 1.40 |
| 24 | C | 513 | CLA | C1C-C2C | 2.78 | 1.49 | 1.44 |
| 24 | D | 401 | CLA | C4C-C3C | 2.78 | 1.49 | 1.45 |
| 24 | C | 504 | CLA | C1B-CHB | 2.78 | 1.47 | 1.40 |
| 24 | B | 604 | CLA | C4B-CHC | 2.79 | 1.47 | 1.40 |
| 24 | C | 506 | CLA | C4B-CHC | 2.79 | 1.47 | 1.40 |
| 24 | B | 610 | CLA | C4B-CHC | 2.79 | 1.47 | 1.40 |
| 24 | B | 614 | CLA | C4B-CHC | 2.80 | 1.47 | 1.40 |
| 24 | B | 607 | CLA | C1B-CHB | 2.80 | 1.47 | 1.40 |
| 24 | C | 503 | CLA | C1C-C2C | 2.80 | 1.49 | 1.44 |
| 24 | B | 607 | CLA | C4B-CHC | 2.81 | 1.47 | 1.40 |
| 24 | b | 615 | CLA | C4C-C3C | 2.81 | 1.50 | 1.45 |
| 24 | c | 510 | CLA | C1B-CHB | 2.81 | 1.47 | 1.40 |
| 24 | B | 605 | CLA | C4B-CHC | 2.82 | 1.47 | 1.40 |
| 24 | D | 403 | CLA | C4B-CHC | 2.82 | 1.47 | 1.40 |
| 24 | c | 515 | CLA | C4B-CHC | 2.82 | 1.47 | 1.40 |
| 24 | D | 403 | CLA | C4C-C3C | 2.82 | 1.50 | 1.45 |
| 24 | A | 409 | CLA | C1B-CHB | 2.82 | 1.47 | 1.40 |
| 24 | C | 508 | CLA | C1C-C2C | 2.82 | 1.50 | 1.44 |
| 24 | D | 404 | CLA | C4B-CHC | 2.82 | 1.47 | 1.40 |
| 24 | C | 504 | CLA | C4B-CHC | 2.83 | 1.47 | 1.40 |
| 24 | c | 507 | CLA | C4B-CHC | 2.83 | 1.47 | 1.40 |
| 24 | B | 616 | CLA | C1B-CHB | 2.84 | 1.47 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 24 | c | 507 | CLA | C1B-CHB | 2.84 | 1.47 | 1.40 |
| 24 | c | 511 | CLA | C4B-CHC | 2.84 | 1.47 | 1.40 |
| 24 | A | 405 | CLA | C1C-C2C | 2.84 | 1.50 | 1.44 |
| 24 | c | 512 | CLA | C4B-CHC | 2.85 | 1.47 | 1.40 |
| 24 | b | 611 | CLA | C1C-C2C | 2.85 | 1.50 | 1.44 |
| 24 | b | 607 | CLA | C1B-CHB | 2.86 | 1.47 | 1.40 |
| 24 | b | 608 | CLA | C1B-CHB | 2.87 | 1.47 | 1.40 |
| 24 | d | 404 | CLA | C1C-C2C | 2.87 | 1.50 | 1.44 |
| 24 | b | 606 | CLA | C1B-CHB | 2.87 | 1.47 | 1.40 |
| 24 | b | 618 | CLA | C1C-C2C | 2.87 | 1.50 | 1.44 |
| 24 | b | 621 | CLA | C4C-C3C | 2.88 | 1.50 | 1.45 |
| 24 | D | 404 | CLA | C1C-C2C | 2.88 | 1.50 | 1.44 |
| 24 | a | 406 | CLA | C4C-C3C | 2.88 | 1.50 | 1.45 |
| 24 | c | 505 | CLA | C1C-C2C | 2.89 | 1.50 | 1.44 |
| 24 | c | 505 | CLA | C1B-CHB | 2.89 | 1.47 | 1.40 |
| 24 | C | 510 | CLA | C4B-CHC | 2.89 | 1.47 | 1.40 |
| 24 | B | 606 | CLA | C4B-CHC | 2.89 | 1.47 | 1.40 |
| 24 | B | 606 | CLA | C1B-CHB | 2.89 | 1.47 | 1.40 |
| 24 | b | 607 | CLA | C4B-CHC | 2.89 | 1.47 | 1.40 |
| 24 | C | 506 | CLA | C4C-C3C | 2.89 | 1.50 | 1.45 |
| 25 | A | 407 | PHO | CHB-C4A | 2.90 | 1.47 | 1.40 |
| 24 | c | 511 | CLA | C1B-CHB | 2.91 | 1.47 | 1.40 |
| 24 | C | 510 | CLA | C4C-C3C | 2.91 | 1.50 | 1.45 |
| 24 | C | 511 | CLA | C4B-CHC | 2.91 | 1.47 | 1.40 |
| 24 | C | 509 | CLA | C4C-C3C | 2.91 | 1.50 | 1.45 |
| 24 | C | 503 | CLA | C4B-CHC | 2.91 | 1.47 | 1.40 |
| 24 | d | 402 | CLA | C1B-CHB | 2.91 | 1.47 | 1.40 |
| 24 | b | 606 | CLA | C4B-CHC | 2.91 | 1.47 | 1.40 |
| 24 | B | 611 | CLA | C1B-CHB | 2.91 | 1.47 | 1.40 |
| 24 | B | 602 | CLA | C4B-CHC | 2.92 | 1.47 | 1.40 |
| 24 | a | 407 | CLA | C4B-CHC | 2.92 | 1.47 | 1.40 |
| 24 | B | 604 | CLA | C1B-CHB | 2.93 | 1.47 | 1.40 |
| 24 | B | 614 | CLA | C1B-CHB | 2.93 | 1.47 | 1.40 |
| 24 | b | 608 | CLA | C4B-CHC | 2.95 | 1.48 | 1.40 |
| 24 | c | 514 | CLA | C4B-CHC | 2.95 | 1.48 | 1.40 |
| 24 | b | 608 | CLA | C1C-C2C | 2.95 | 1.50 | 1.44 |
| 24 | B | 614 | CLA | C4C-C3C | 2.96 | 1.50 | 1.45 |
| 24 | c | 506 | CLA | C1C-C2C | 2.96 | 1.50 | 1.44 |
| 24 | b | 617 | CLA | C4B-CHC | 2.96 | 1.48 | 1.40 |
| 24 | b | 610 | CLA | C4B-CHC | 2.97 | 1.48 | 1.40 |
| 24 | b | 616 | CLA | C4B-CHC | 2.98 | 1.48 | 1.40 |
| 24 | D | 403 | CLA | C1C-C2C | 2.98 | 1.50 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 24 | b | 611 | CLA | C4B-CHC | 2.98 | 1.48 | 1.40 |
| 25 | A | 407 | PHO | CHC-C4B | 2.99 | 1.47 | 1.40 |
| 24 | B | 612 | CLA | C4B-CHC | 2.99 | 1.48 | 1.40 |
| 24 | c | 504 | CLA | C1B-CHB | 2.99 | 1.48 | 1.40 |
| 24 | B | 613 | CLA | C4C-C3C | 3.00 | 1.50 | 1.45 |
| 24 | c | 507 | CLA | C4C-C3C | 3.00 | 1.50 | 1.45 |
| 24 | C | 512 | CLA | C1B-CHB | 3.00 | 1.48 | 1.40 |
| 24 | B | 613 | CLA | C1B-CHB | 3.00 | 1.48 | 1.40 |
| 25 | d | 403 | PHO | C3B-C4B | 3.01 | 1.49 | 1.43 |
| 24 | b | 613 | CLA | C4B-CHC | 3.01 | 1.48 | 1.40 |
| 24 | B | 604 | CLA | C1C-C2C | 3.01 | 1.50 | 1.44 |
| 25 | a | 408 | PHO | CHD-C4C | 3.01 | 1.47 | 1.40 |
| 24 | c | 505 | CLA | C4B-CHC | 3.01 | 1.48 | 1.40 |
| 24 | C | 509 | CLA | C1B-CHB | 3.02 | 1.48 | 1.40 |
| 24 | C | 506 | CLA | C1B-CHB | 3.02 | 1.48 | 1.40 |
| 24 | d | 404 | CLA | C4B-CHC | 3.03 | 1.48 | 1.40 |
| 25 | d | 403 | PHO | CHB-C4A | 3.03 | 1.47 | 1.40 |
| 24 | A | 405 | CLA | C4C-C3C | 3.03 | 1.50 | 1.45 |
| 24 | C | 514 | CLA | C1B-CHB | 3.03 | 1.48 | 1.40 |
| 24 | b | 615 | CLA | C4B-CHC | 3.04 | 1.48 | 1.40 |
| 24 | d | 401 | CLA | C1B-CHB | 3.04 | 1.48 | 1.40 |
| 24 | C | 511 | CLA | C1B-CHB | 3.04 | 1.48 | 1.40 |
| 24 | b | 616 | CLA | C1B-CHB | 3.04 | 1.48 | 1.40 |
| 24 | c | 509 | CLA | C1B-CHB | 3.04 | 1.48 | 1.40 |
| 24 | b | 614 | CLA | C1B-CHB | 3.04 | 1.48 | 1.40 |
| 24 | C | 508 | CLA | C4B-CHC | 3.04 | 1.48 | 1.40 |
| 24 | B | 607 | CLA | C1C-C2C | 3.05 | 1.50 | 1.44 |
| 24 | c | 510 | CLA | C4B-CHC | 3.05 | 1.48 | 1.40 |
| 24 | b | 621 | CLA | C1B-CHB | 3.06 | 1.48 | 1.40 |
| 25 | A | 407 | PHO | C3B-C4B | 3.07 | 1.49 | 1.43 |
| 24 | b | 615 | CLA | C1C-C2C | 3.07 | 1.50 | 1.44 |
| 24 | B | 617 | CLA | C1B-CHB | 3.08 | 1.48 | 1.40 |
| 24 | c | 513 | CLA | C1B-CHB | 3.08 | 1.48 | 1.40 |
| 24 | A | 405 | CLA | C1B-CHB | 3.08 | 1.48 | 1.40 |
| 24 | B | 605 | CLA | C1B-CHB | 3.09 | 1.48 | 1.40 |
| 25 | d | 403 | PHO | CHC-C4B | 3.10 | 1.47 | 1.40 |
| 25 | A | 407 | PHO | CHD-C4C | 3.11 | 1.47 | 1.40 |
| 24 | b | 617 | CLA | C1B-CHB | 3.11 | 1.48 | 1.40 |
| 24 | A | 406 | CLA | C1B-CHB | 3.11 | 1.48 | 1.40 |
| 24 | C | 503 | CLA | C1B-CHB | 3.11 | 1.48 | 1.40 |
| 24 | C | 507 | CLA | C1B-CHB | 3.12 | 1.48 | 1.40 |
| 24 | b | 609 | CLA | C1B-CHB | 3.13 | 1.48 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 24 | b | 618 | CLA | C1B-CHB | 3.13 | 1.48 | 1.40 |
| 24 | B | 608 | CLA | C4B-CHC | 3.14 | 1.48 | 1.40 |
| 24 | b | 615 | CLA | C1B-CHB | 3.15 | 1.48 | 1.40 |
| 24 | B | 610 | CLA | C1B-CHB | 3.15 | 1.48 | 1.40 |
| 24 | C | 510 | CLA | C1B-CHB | 3.16 | 1.48 | 1.40 |
| 25 | A | 408 | PHO | CHD-C4C | 3.17 | 1.48 | 1.40 |
| 24 | a | 406 | CLA | C1B-CHB | 3.17 | 1.48 | 1.40 |
| 24 | b | 609 | CLA | C4B-CHC | 3.20 | 1.48 | 1.40 |
| 24 | A | 409 | CLA | C4B-CHC | 3.21 | 1.48 | 1.40 |
| 25 | d | 403 | PHO | CHD-C4C | 3.21 | 1.48 | 1.40 |
| 24 | c | 503 | CLA | C1B-CHB | 3.21 | 1.48 | 1.40 |
| 24 | c | 510 | CLA | C1C-C2C | 3.23 | 1.50 | 1.44 |
| 24 | B | 608 | CLA | C1B-CHB | 3.23 | 1.48 | 1.40 |
| 24 | B | 611 | CLA | C4B-CHC | 3.26 | 1.48 | 1.40 |
| 25 | d | 403 | PHO | OBD-CAD | 3.27 | 1.28 | 1.22 |
| 24 | D | 403 | CLA | C1B-CHB | 3.27 | 1.48 | 1.40 |
| 37 | d | 408 | LHG | O7-C7 | 3.29 | 1.43 | 1.34 |
| 24 | C | 505 | CLA | C1B-CHB | 3.31 | 1.48 | 1.40 |
| 25 | A | 408 | PHO | C3B-C4B | 3.32 | 1.50 | 1.43 |
| 37 | D | 408 | LHG | O7-C7 | 3.35 | 1.44 | 1.34 |
| 24 | c | 512 | CLA | C1B-CHB | 3.37 | 1.49 | 1.40 |
| 37 | D | 409 | LHG | O7-C7 | 3.38 | 1.44 | 1.34 |
| 25 | a | 408 | PHO | OBD-CAD | 3.42 | 1.28 | 1.22 |
| 24 | B | 605 | CLA | OBD-CAD | 3.44 | 1.27 | 1.22 |
| 37 | D | 409 | LHG | O8-C23 | 3.50 | 1.43 | 1.33 |
| 36 | C | 519 | DGD | O2G-C1B | 3.50 | 1.44 | 1.34 |
| 24 | b | 609 | CLA | C1C-C2C | 3.51 | 1.51 | 1.44 |
| 24 | a | 406 | CLA | O2A-CGA | 3.51 | 1.43 | 1.33 |
| 37 | d | 409 | LHG | O7-C7 | 3.51 | 1.44 | 1.34 |
| 25 | a | 408 | PHO | C3D-C2D | 3.52 | 1.48 | 1.38 |
| 25 | A | 408 | PHO | OBD-CAD | 3.55 | 1.28 | 1.22 |
| 25 | a | 408 | PHO | C3B-C4B | 3.57 | 1.51 | 1.43 |
| 24 | B | 605 | CLA | C3D-C2D | 3.58 | 1.47 | 1.39 |
| 34 | b | 625 | LMG | O7-C10 | 3.59 | 1.44 | 1.34 |
| 37 | L | 101 | LHG | O7-C7 | 3.62 | 1.44 | 1.34 |
| 36 | c | 518 | DGD | O2G-C1B | 3.62 | 1.44 | 1.34 |
| 34 | J | 101 | LMG | O7-C10 | 3.63 | 1.44 | 1.34 |
| 37 | D | 408 | LHG | O8-C23 | 3.63 | 1.44 | 1.33 |
| 34 | c | 501 | LMG | O7-C10 | 3.65 | 1.44 | 1.34 |
| 24 | B | 603 | CLA | O2A-CGA | 3.65 | 1.44 | 1.33 |
| 25 | A | 408 | PHO | O2A-CGA | 3.66 | 1.44 | 1.33 |
| 24 | d | 402 | CLA | OBD-CAD | 3.66 | 1.27 | 1.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 24 | A | 405 | CLA | O2A-CGA | 3.67 | 1.44 | 1.33 |
| 25 | A | 408 | PHO | CHC-C4B | 3.67 | 1.49 | 1.40 |
| 24 | b | 612 | CLA | O2A-CGA | 3.67 | 1.44 | 1.33 |
| 34 | J | 101 | LMG | O8-C28 | 3.69 | 1.44 | 1.33 |
| 24 | c | 507 | CLA | O2A-CGA | 3.70 | 1.44 | 1.33 |
| 25 | a | 408 | PHO | CHC-C4B | 3.71 | 1.49 | 1.40 |
| 36 | h | 102 | DGD | O2G-C1B | 3.71 | 1.45 | 1.34 |
| 36 | C | 517 | DGD | O1G-C1A | 3.76 | 1.44 | 1.33 |
| 24 | C | 509 | CLA | OBD-CAD | 3.76 | 1.27 | 1.22 |
| 36 | c | 517 | DGD | O1G-C1A | 3.77 | 1.44 | 1.33 |
| 27 | A | 411 | SQD | O47-C7 | 3.79 | 1.45 | 1.34 |
| 24 | B | 615 | CLA | O2A-CGA | 3.79 | 1.44 | 1.33 |
| 34 | j | 101 | LMG | O7-C10 | 3.80 | 1.45 | 1.34 |
| 27 | a | 411 | SQD | O47-C7 | 3.80 | 1.45 | 1.34 |
| 24 | A | 406 | CLA | O2A-CGA | 3.80 | 1.44 | 1.33 |
| 25 | A | 407 | PHO | C3D-C2D | 3.81 | 1.49 | 1.38 |
| 36 | C | 518 | DGD | O2G-C1B | 3.81 | 1.45 | 1.34 |
| 36 | C | 519 | DGD | O1G-C1A | 3.83 | 1.44 | 1.33 |
| 27 | A | 411 | SQD | O48-C23 | 3.83 | 1.44 | 1.33 |
| 24 | A | 409 | CLA | O2A-CGA | 3.84 | 1.44 | 1.33 |
| 37 | d | 410 | LHG | O7-C7 | 3.84 | 1.45 | 1.34 |
| 37 | L | 101 | LHG | O8-C23 | 3.85 | 1.44 | 1.33 |
| 24 | d | 401 | CLA | CHC-C1C | 3.85 | 1.46 | 1.35 |
| 24 | b | 607 | CLA | O2A-CGA | 3.85 | 1.44 | 1.33 |
| 25 | A | 408 | PHO | CHD-C1D | 3.85 | 1.46 | 1.38 |
| 24 | b | 615 | CLA | O2A-CGA | 3.85 | 1.44 | 1.33 |
| 36 | c | 519 | DGD | O2G-C1B | 3.85 | 1.45 | 1.34 |
| 25 | A | 407 | PHO | O2A-CGA | 3.85 | 1.44 | 1.33 |
| 36 | c | 517 | DGD | O2G-C1B | 3.86 | 1.45 | 1.34 |
| 24 | D | 404 | CLA | O2A-CGA | 3.86 | 1.44 | 1.33 |
| 37 | d | 408 | LHG | O8-C23 | 3.86 | 1.44 | 1.33 |
| 24 | B | 602 | CLA | OBD-CAD | 3.88 | 1.27 | 1.22 |
| 24 | B | 605 | CLA | O2A-CGA | 3.89 | 1.44 | 1.33 |
| 37 | D | 410 | LHG | O8-C23 | 3.91 | 1.44 | 1.33 |
| 27 | a | 411 | SQD | O48-C23 | 3.92 | 1.44 | 1.33 |
| 24 | B | 614 | CLA | O2A-CGA | 3.93 | 1.44 | 1.33 |
| 36 | H | 102 | DGD | O1G-C1A | 3.93 | 1.44 | 1.33 |
| 34 | j | 101 | LMG | O8-C28 | 3.93 | 1.44 | 1.33 |
| 24 | B | 613 | CLA | OBD-CAD | 3.93 | 1.28 | 1.22 |
| 24 | c | 507 | CLA | C3D-C2D | 3.93 | 1.48 | 1.39 |
| 24 | B | 606 | CLA | CHC-C1C | 3.94 | 1.46 | 1.35 |
| 24 | B | 612 | CLA | O2A-CGA | 3.94 | 1.44 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 24 | c | 505 | CLA | O2A-CGA | 3.94 | 1.44 | 1.33 |
| 34 | B | 621 | LMG | O7-C10 | 3.94 | 1.45 | 1.34 |
| 36 | C | 517 | DGD | O2G-C1B | 3.94 | 1.45 | 1.34 |
| 34 | c | 520 | LMG | O7-C10 | 3.95 | 1.45 | 1.34 |
| 24 | c | 513 | CLA | O2A-CGA | 3.95 | 1.45 | 1.33 |
| 24 | C | 507 | CLA | OBD-CAD | 3.95 | 1.28 | 1.22 |
| 25 | d | 403 | PHO | C3D-C2D | 3.95 | 1.49 | 1.38 |
| 34 | C | 520 | LMG | O7-C10 | 3.95 | 1.45 | 1.34 |
| 27 | a | 402 | SQD | O47-C7 | 3.96 | 1.45 | 1.34 |
| 37 | l | 102 | LHG | O7-C7 | 3.96 | 1.45 | 1.34 |
| 24 | b | 620 | CLA | O2A-CGA | 3.96 | 1.45 | 1.33 |
| 36 | H | 102 | DGD | O2G-C1B | 3.98 | 1.45 | 1.34 |
| 24 | b | 606 | CLA | OBD-CAD | 3.99 | 1.28 | 1.22 |
| 25 | A | 408 | PHO | C3D-C2D | 3.99 | 1.49 | 1.38 |
| 37 | E | 101 | LHG | O7-C7 | 4.00 | 1.45 | 1.34 |
| 24 | B | 606 | CLA | OBD-CAD | 4.00 | 1.28 | 1.22 |
| 24 | c | 506 | CLA | O2A-CGA | 4.00 | 1.45 | 1.33 |
| 24 | b | 611 | CLA | O2A-CGA | 4.01 | 1.45 | 1.33 |
| 27 | l | 101 | SQD | O48-C23 | 4.01 | 1.45 | 1.33 |
| 24 | B | 609 | CLA | OBD-CAD | 4.01 | 1.28 | 1.22 |
| 24 | B | 611 | CLA | O2A-CGA | 4.01 | 1.45 | 1.33 |
| 25 | a | 408 | PHO | O2A-CGA | 4.02 | 1.45 | 1.33 |
| 24 | B | 613 | CLA | O2A-CGA | 4.03 | 1.45 | 1.33 |
| 24 | C | 511 | CLA | O2A-CGA | 4.03 | 1.45 | 1.33 |
| 27 | l | 101 | SQD | O47-C7 | 4.03 | 1.46 | 1.34 |
| 24 | d | 402 | CLA | CHC-C1C | 4.03 | 1.47 | 1.35 |
| 24 | D | 401 | CLA | O2A-CGA | 4.03 | 1.45 | 1.33 |
| 24 | C | 503 | CLA | OBD-CAD | 4.04 | 1.28 | 1.22 |
| 34 | B | 621 | LMG | O8-C28 | 4.04 | 1.45 | 1.33 |
| 37 | D | 410 | LHG | O7-C7 | 4.04 | 1.46 | 1.34 |
| 27 | b | 601 | SQD | O48-C23 | 4.04 | 1.45 | 1.33 |
| 34 | c | 501 | LMG | O8-C28 | 4.04 | 1.45 | 1.33 |
| 24 | B | 607 | CLA | O2A-CGA | 4.04 | 1.45 | 1.33 |
| 36 | h | 102 | DGD | O1G-C1A | 4.04 | 1.45 | 1.33 |
| 24 | b | 618 | CLA | O2A-CGA | 4.05 | 1.45 | 1.33 |
| 24 | a | 406 | CLA | CHC-C1C | 4.05 | 1.47 | 1.35 |
| 24 | c | 508 | CLA | OBD-CAD | 4.05 | 1.28 | 1.22 |
| 34 | z | 101 | LMG | O7-C10 | 4.05 | 1.46 | 1.34 |
| 25 | d | 403 | PHO | O2A-CGA | 4.05 | 1.45 | 1.33 |
| 25 | A | 407 | PHO | OBD-CAD | 4.06 | 1.29 | 1.22 |
| 24 | C | 503 | CLA | O2A-CGA | 4.06 | 1.45 | 1.33 |
| 24 | c | 505 | CLA | OBD-CAD | 4.06 | 1.28 | 1.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 37 | e | 101 | LHG | O7-C7 | 4.07 | 1.46 | 1.34 |
| 24 | C | 505 | CLA | O2A-CGA | 4.07 | 1.45 | 1.33 |
| 24 | b | 617 | CLA | C3D-C2D | 4.07 | 1.48 | 1.39 |
| 24 | B | 605 | CLA | O2D-CGD | 4.07 | 1.43 | 1.33 |
| 24 | b | 612 | CLA | OBD-CAD | 4.08 | 1.28 | 1.22 |
| 37 | d | 410 | LHG | O8-C23 | 4.08 | 1.45 | 1.33 |
| 24 | b | 608 | CLA | C3D-C2D | 4.08 | 1.48 | 1.39 |
| 24 | b | 614 | CLA | CHC-C1C | 4.08 | 1.47 | 1.35 |
| 24 | c | 503 | CLA | C3D-C2D | 4.08 | 1.48 | 1.39 |
| 24 | b | 608 | CLA | O2A-CGA | 4.08 | 1.45 | 1.33 |
| 24 | B | 614 | CLA | CHC-C1C | 4.09 | 1.47 | 1.35 |
| 24 | a | 409 | CLA | CHC-C1C | 4.09 | 1.47 | 1.35 |
| 24 | C | 512 | CLA | O2A-CGA | 4.09 | 1.45 | 1.33 |
| 24 | C | 513 | CLA | OBD-CAD | 4.09 | 1.28 | 1.22 |
| 24 | B | 617 | CLA | CHC-C1C | 4.09 | 1.47 | 1.35 |
| 24 | b | 618 | CLA | CHC-C1C | 4.09 | 1.47 | 1.35 |
| 27 | A | 416 | SQD | O47-C7 | 4.09 | 1.46 | 1.34 |
| 37 | d | 409 | LHG | O8-C23 | 4.09 | 1.45 | 1.33 |
| 24 | b | 609 | CLA | O2A-CGA | 4.09 | 1.45 | 1.33 |
| 24 | B | 615 | CLA | C3D-C2D | 4.10 | 1.48 | 1.39 |
| 24 | C | 508 | CLA | C3D-C2D | 4.10 | 1.48 | 1.39 |
| 34 | Z | 101 | LMG | O7-C10 | 4.10 | 1.46 | 1.34 |
| 24 | C | 507 | CLA | CHC-C1C | 4.10 | 1.47 | 1.35 |
| 24 | b | 621 | CLA | O2A-CGA | 4.10 | 1.45 | 1.33 |
| 24 | B | 617 | CLA | O2A-CGA | 4.11 | 1.45 | 1.33 |
| 24 | D | 403 | CLA | CHC-C1C | 4.11 | 1.47 | 1.35 |
| 24 | b | 619 | CLA | O2A-CGA | 4.11 | 1.45 | 1.33 |
| 24 | b | 614 | CLA | O2A-CGA | 4.11 | 1.45 | 1.33 |
| 24 | c | 509 | CLA | OBD-CAD | 4.11 | 1.28 | 1.22 |
| 24 | B | 617 | CLA | C3D-C2D | 4.12 | 1.48 | 1.39 |
| 24 | b | 609 | CLA | CHC-C1C | 4.12 | 1.47 | 1.35 |
| 24 | b | 610 | CLA | O2A-CGA | 4.12 | 1.45 | 1.33 |
| 24 | d | 404 | CLA | O2A-CGA | 4.12 | 1.45 | 1.33 |
| 24 | C | 510 | CLA | CHC-C1C | 4.12 | 1.47 | 1.35 |
| 24 | c | 503 | CLA | CHC-C1C | 4.12 | 1.47 | 1.35 |
| 37 | l | 102 | LHG | O8-C23 | 4.13 | 1.45 | 1.33 |
| 36 | c | 518 | DGD | O1G-C1A | 4.13 | 1.45 | 1.33 |
| 24 | C | 511 | CLA | CHC-C1C | 4.13 | 1.47 | 1.35 |
| 24 | C | 504 | CLA | O2A-CGA | 4.13 | 1.45 | 1.33 |
| 24 | c | 512 | CLA | O2A-CGA | 4.13 | 1.45 | 1.33 |
| 24 | c | 511 | CLA | O2A-CGA | 4.13 | 1.45 | 1.33 |
| 24 | b | 612 | CLA | CHC-C1C | 4.14 | 1.47 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 24 | c | 508 | CLA | CHC-C1C | 4.14 | 1.47 | 1.35 |
| 24 | b | 618 | CLA | OBD-CAD | 4.14 | 1.28 | 1.22 |
| 24 | B | 607 | CLA | OBD-CAD | 4.14 | 1.28 | 1.22 |
| 27 | F | 101 | SQD | O48-C23 | 4.15 | 1.45 | 1.33 |
| 34 | b | 625 | LMG | O8-C28 | 4.15 | 1.45 | 1.33 |
| 24 | b | 610 | CLA | C3D-C2D | 4.15 | 1.48 | 1.39 |
| 24 | c | 512 | CLA | OBD-CAD | 4.15 | 1.28 | 1.22 |
| 24 | B | 610 | CLA | O2A-CGA | 4.15 | 1.45 | 1.33 |
| 24 | c | 504 | CLA | OBD-CAD | 4.15 | 1.28 | 1.22 |
| 24 | C | 514 | CLA | O2A-CGA | 4.15 | 1.45 | 1.33 |
| 24 | C | 502 | CLA | CHC-C1C | 4.15 | 1.47 | 1.35 |
| 27 | f | 101 | SQD | O48-C23 | 4.15 | 1.45 | 1.33 |
| 24 | c | 512 | CLA | C3D-C2D | 4.15 | 1.48 | 1.39 |
| 24 | b | 610 | CLA | O2D-CGD | 4.16 | 1.43 | 1.33 |
| 24 | b | 621 | CLA | CHC-C1C | 4.16 | 1.47 | 1.35 |
| 24 | b | 616 | CLA | O2A-CGA | 4.16 | 1.45 | 1.33 |
| 24 | C | 506 | CLA | O2A-CGA | 4.16 | 1.45 | 1.33 |
| 24 | D | 401 | CLA | CHC-C1C | 4.16 | 1.47 | 1.35 |
| 24 | c | 504 | CLA | O2A-CGA | 4.17 | 1.45 | 1.33 |
| 24 | C | 509 | CLA | O2A-CGA | 4.17 | 1.45 | 1.33 |
| 24 | C | 507 | CLA | O2A-CGA | 4.17 | 1.45 | 1.33 |
| 24 | b | 620 | CLA | CHC-C1C | 4.17 | 1.47 | 1.35 |
| 34 | c | 521 | LMG | O8-C28 | 4.17 | 1.45 | 1.33 |
| 27 | b | 601 | SQD | O47-C7 | 4.17 | 1.46 | 1.34 |
| 24 | B | 606 | CLA | C3D-C2D | 4.17 | 1.48 | 1.39 |
| 24 | B | 611 | CLA | CHC-C1C | 4.18 | 1.47 | 1.35 |
| 34 | C | 521 | LMG | O8-C28 | 4.18 | 1.45 | 1.33 |
| 24 | b | 619 | CLA | CHC-C1C | 4.18 | 1.47 | 1.35 |
| 24 | c | 513 | CLA | C3D-C2D | 4.19 | 1.49 | 1.39 |
| 24 | B | 609 | CLA | O2A-CGA | 4.19 | 1.45 | 1.33 |
| 24 | C | 506 | CLA | C3D-C2D | 4.20 | 1.49 | 1.39 |
| 24 | c | 509 | CLA | CHC-C1C | 4.20 | 1.47 | 1.35 |
| 24 | b | 613 | CLA | CHC-C1C | 4.20 | 1.47 | 1.35 |
| 34 | c | 521 | LMG | O7-C10 | 4.20 | 1.46 | 1.34 |
| 24 | B | 608 | CLA | O2A-CGA | 4.21 | 1.45 | 1.33 |
| 24 | B | 613 | CLA | C3D-C2D | 4.21 | 1.49 | 1.39 |
| 24 | B | 608 | CLA | CHC-C1C | 4.21 | 1.47 | 1.35 |
| 24 | C | 509 | CLA | CHC-C1C | 4.21 | 1.47 | 1.35 |
| 24 | c | 508 | CLA | O2A-CGA | 4.22 | 1.45 | 1.33 |
| 24 | B | 611 | CLA | OBD-CAD | 4.22 | 1.28 | 1.22 |
| 24 | C | 502 | CLA | O2A-CGA | 4.22 | 1.45 | 1.33 |
| 24 | d | 404 | CLA | OBD-CAD | 4.22 | 1.28 | 1.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 36 | C | 518 | DGD | O1G-C1A | 4.22 | 1.45 | 1.33 |
| 34 | c | 520 | LMG | O8-C28 | 4.23 | 1.45 | 1.33 |
| 24 | a | 407 | CLA | O2D-CGD | 4.23 | 1.43 | 1.33 |
| 24 | c | 503 | CLA | O2A-CGA | 4.23 | 1.45 | 1.33 |
| 34 | C | 501 | LMG | O8-C28 | 4.23 | 1.45 | 1.33 |
| 24 | c | 514 | CLA | O2A-CGA | 4.24 | 1.45 | 1.33 |
| 24 | d | 401 | CLA | O2A-CGA | 4.24 | 1.45 | 1.33 |
| 34 | C | 521 | LMG | O7-C10 | 4.24 | 1.46 | 1.34 |
| 24 | D | 403 | CLA | O2D-CGD | 4.24 | 1.43 | 1.33 |
| 24 | b | 617 | CLA | OBD-CAD | 4.24 | 1.28 | 1.22 |
| 24 | c | 513 | CLA | CHC-C1C | 4.24 | 1.47 | 1.35 |
| 24 | c | 506 | CLA | CHC-C1C | 4.24 | 1.47 | 1.35 |
| 24 | c | 504 | CLA | CHC-C1C | 4.24 | 1.47 | 1.35 |
| 24 | a | 409 | CLA | OBD-CAD | 4.24 | 1.28 | 1.22 |
| 36 | c | 519 | DGD | O1G-C1A | 4.25 | 1.45 | 1.33 |
| 24 | b | 617 | CLA | O2A-CGA | 4.25 | 1.45 | 1.33 |
| 27 | F | 101 | SQD | O47-C7 | 4.25 | 1.46 | 1.34 |
| 24 | C | 513 | CLA | CHC-C1C | 4.25 | 1.47 | 1.35 |
| 24 | B | 604 | CLA | CHC-C1C | 4.25 | 1.47 | 1.35 |
| 24 | a | 406 | CLA | OBD-CAD | 4.25 | 1.28 | 1.22 |
| 24 | c | 515 | CLA | O2A-CGA | 4.25 | 1.45 | 1.33 |
| 24 | C | 504 | CLA | CHC-C1C | 4.25 | 1.47 | 1.35 |
| 24 | C | 512 | CLA | C3D-C2D | 4.25 | 1.49 | 1.39 |
| 24 | b | 616 | CLA | OBD-CAD | 4.25 | 1.28 | 1.22 |
| 24 | c | 511 | CLA | CHC-C1C | 4.26 | 1.47 | 1.35 |
| 24 | b | 606 | CLA | O2A-CGA | 4.26 | 1.45 | 1.33 |
| 37 | E | 101 | LHG | O8-C23 | 4.26 | 1.45 | 1.33 |
| 24 | B | 609 | CLA | CHC-C1C | 4.26 | 1.47 | 1.35 |
| 24 | c | 514 | CLA | OBD-CAD | 4.26 | 1.28 | 1.22 |
| 24 | C | 508 | CLA | O2A-CGA | 4.26 | 1.45 | 1.33 |
| 24 | C | 514 | CLA | CHC-C1C | 4.27 | 1.47 | 1.35 |
| 24 | B | 604 | CLA | O2A-CGA | 4.27 | 1.45 | 1.33 |
| 36 | D | 407 | DGD | O2G-C1B | 4.27 | 1.46 | 1.34 |
| 24 | b | 609 | CLA | C3D-C2D | 4.27 | 1.49 | 1.39 |
| 36 | d | 407 | DGD | O1G-C1A | 4.28 | 1.45 | 1.33 |
| 24 | B | 604 | CLA | OBD-CAD | 4.28 | 1.28 | 1.22 |
| 24 | C | 513 | CLA | O2A-CGA | 4.28 | 1.45 | 1.33 |
| 27 | f | 101 | SQD | O47-C7 | 4.28 | 1.46 | 1.34 |
| 24 | b | 610 | CLA | CHC-C1C | 4.29 | 1.47 | 1.35 |
| 24 | B | 606 | CLA | O2A-CGA | 4.29 | 1.46 | 1.33 |
| 34 | C | 501 | LMG | O7-C10 | 4.29 | 1.46 | 1.34 |
| 24 | b | 611 | CLA | OBD-CAD | 4.29 | 1.28 | 1.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 24 | B | 607 | CLA | CHC-C1C | 4.29 | 1.47 | 1.35 |
| 24 | B | 614 | CLA | C3D-C2D | 4.29 | 1.49 | 1.39 |
| 24 | b | 621 | CLA | OBD-CAD | 4.29 | 1.28 | 1.22 |
| 24 | D | 403 | CLA | C3D-C2D | 4.29 | 1.49 | 1.39 |
| 24 | C | 512 | CLA | CHC-C1C | 4.29 | 1.47 | 1.35 |
| 24 | B | 608 | CLA | O2D-CGD | 4.29 | 1.44 | 1.33 |
| 24 | B | 603 | CLA | CHC-C1C | 4.30 | 1.47 | 1.35 |
| 24 | b | 619 | CLA | OBD-CAD | 4.30 | 1.28 | 1.22 |
| 36 | d | 407 | DGD | O2G-C1B | 4.31 | 1.46 | 1.34 |
| 24 | B | 605 | CLA | CHC-C1C | 4.31 | 1.47 | 1.35 |
| 24 | c | 512 | CLA | CHC-C1C | 4.31 | 1.47 | 1.35 |
| 24 | B | 608 | CLA | C3D-C2D | 4.31 | 1.49 | 1.39 |
| 24 | B | 612 | CLA | CHC-C1C | 4.31 | 1.47 | 1.35 |
| 24 | C | 506 | CLA | CHC-C1C | 4.31 | 1.47 | 1.35 |
| 24 | C | 508 | CLA | CHC-C1C | 4.31 | 1.47 | 1.35 |
| 24 | b | 615 | CLA | O2D-CGD | 4.32 | 1.44 | 1.33 |
| 24 | c | 507 | CLA | CHC-C1C | 4.32 | 1.47 | 1.35 |
| 24 | b | 608 | CLA | OBD-CAD | 4.32 | 1.28 | 1.22 |
| 24 | C | 505 | CLA | CHC-C1C | 4.33 | 1.48 | 1.35 |
| 24 | b | 618 | CLA | C3D-C2D | 4.33 | 1.49 | 1.39 |
| 24 | a | 406 | CLA | C3D-C2D | 4.33 | 1.49 | 1.39 |
| 24 | A | 406 | CLA | CHC-C1C | 4.34 | 1.48 | 1.35 |
| 24 | D | 404 | CLA | CHC-C1C | 4.34 | 1.48 | 1.35 |
| 24 | b | 613 | CLA | OBD-CAD | 4.35 | 1.28 | 1.22 |
| 24 | C | 502 | CLA | OBD-CAD | 4.35 | 1.28 | 1.22 |
| 24 | B | 603 | CLA | C3D-C2D | 4.35 | 1.49 | 1.39 |
| 24 | D | 404 | CLA | C3D-C2D | 4.35 | 1.49 | 1.39 |
| 24 | d | 404 | CLA | C3D-C2D | 4.35 | 1.49 | 1.39 |
| 37 | e | 101 | LHG | O8-C23 | 4.35 | 1.46 | 1.33 |
| 24 | C | 514 | CLA | C3D-C2D | 4.35 | 1.49 | 1.39 |
| 24 | d | 404 | CLA | CHC-C1C | 4.35 | 1.48 | 1.35 |
| 24 | c | 509 | CLA | O2A-CGA | 4.35 | 1.46 | 1.33 |
| 24 | a | 409 | CLA | O2A-CGA | 4.36 | 1.46 | 1.33 |
| 24 | A | 405 | CLA | CHC-C1C | 4.36 | 1.48 | 1.35 |
| 24 | a | 407 | CLA | O2A-CGA | 4.36 | 1.46 | 1.33 |
| 24 | B | 610 | CLA | C3D-C2D | 4.36 | 1.49 | 1.39 |
| 24 | c | 508 | CLA | C3D-C2D | 4.36 | 1.49 | 1.39 |
| 24 | a | 407 | CLA | C3D-C2D | 4.36 | 1.49 | 1.39 |
| 24 | B | 612 | CLA | OBD-CAD | 4.37 | 1.28 | 1.22 |
| 24 | b | 613 | CLA | C3D-C2D | 4.37 | 1.49 | 1.39 |
| 27 | a | 402 | SQD | O48-C23 | 4.37 | 1.46 | 1.33 |
| 24 | B | 610 | CLA | O2D-CGD | 4.37 | 1.44 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 34 | C | 520 | LMG | O8-C28 | 4.37 | 1.46 | 1.33 |
| 24 | b | 611 | CLA | C3D-C2D | 4.38 | 1.49 | 1.39 |
| 24 | b | 606 | CLA | CHC-C1C | 4.38 | 1.48 | 1.35 |
| 24 | B | 614 | CLA | OBD-CAD | 4.38 | 1.28 | 1.22 |
| 24 | a | 409 | CLA | C3D-C2D | 4.38 | 1.49 | 1.39 |
| 24 | c | 510 | CLA | CHC-C1C | 4.39 | 1.48 | 1.35 |
| 24 | c | 510 | CLA | O2A-CGA | 4.39 | 1.46 | 1.33 |
| 24 | A | 409 | CLA | CHC-C1C | 4.39 | 1.48 | 1.35 |
| 24 | c | 505 | CLA | C3D-C2D | 4.39 | 1.49 | 1.39 |
| 24 | c | 511 | CLA | C3D-C2D | 4.40 | 1.49 | 1.39 |
| 24 | A | 405 | CLA | OBD-CAD | 4.40 | 1.28 | 1.22 |
| 24 | b | 615 | CLA | CHC-C1C | 4.40 | 1.48 | 1.35 |
| 24 | B | 615 | CLA | CHC-C1C | 4.40 | 1.48 | 1.35 |
| 24 | C | 512 | CLA | OBD-CAD | 4.41 | 1.28 | 1.22 |
| 24 | B | 602 | CLA | O2A-CGA | 4.41 | 1.46 | 1.33 |
| 24 | b | 614 | CLA | C3D-C2D | 4.42 | 1.49 | 1.39 |
| 24 | c | 509 | CLA | C3D-C2D | 4.42 | 1.49 | 1.39 |
| 24 | C | 503 | CLA | CHC-C1C | 4.42 | 1.48 | 1.35 |
| 24 | c | 514 | CLA | CHC-C1C | 4.42 | 1.48 | 1.35 |
| 27 | A | 416 | SQD | O48-C23 | 4.42 | 1.46 | 1.33 |
| 24 | d | 401 | CLA | O2D-CGD | 4.43 | 1.44 | 1.33 |
| 24 | d | 402 | CLA | C3D-C2D | 4.43 | 1.49 | 1.39 |
| 24 | c | 503 | CLA | OBD-CAD | 4.43 | 1.28 | 1.22 |
| 24 | B | 616 | CLA | OBD-CAD | 4.43 | 1.28 | 1.22 |
| 24 | c | 515 | CLA | C3D-C2D | 4.43 | 1.49 | 1.39 |
| 24 | B | 616 | CLA | CHC-C1C | 4.44 | 1.48 | 1.35 |
| 24 | B | 602 | CLA | CHC-C1C | 4.44 | 1.48 | 1.35 |
| 24 | C | 510 | CLA | O2A-CGA | 4.44 | 1.46 | 1.33 |
| 24 | C | 504 | CLA | C3D-C2D | 4.44 | 1.49 | 1.39 |
| 24 | a | 407 | CLA | CHC-C1C | 4.44 | 1.48 | 1.35 |
| 36 | D | 407 | DGD | O1G-C1A | 4.44 | 1.46 | 1.33 |
| 24 | b | 621 | CLA | C3D-C2D | 4.44 | 1.49 | 1.39 |
| 24 | C | 506 | CLA | OBD-CAD | 4.44 | 1.28 | 1.22 |
| 24 | b | 608 | CLA | CHC-C1C | 4.44 | 1.48 | 1.35 |
| 24 | a | 407 | CLA | OBD-CAD | 4.45 | 1.28 | 1.22 |
| 24 | B | 602 | CLA | C3D-C2D | 4.45 | 1.49 | 1.39 |
| 24 | b | 607 | CLA | CHC-C1C | 4.45 | 1.48 | 1.35 |
| 24 | d | 402 | CLA | O2D-CGD | 4.45 | 1.44 | 1.33 |
| 24 | b | 616 | CLA | CHC-C1C | 4.46 | 1.48 | 1.35 |
| 24 | c | 505 | CLA | CHC-C1C | 4.46 | 1.48 | 1.35 |
| 24 | B | 604 | CLA | C3D-C2D | 4.46 | 1.49 | 1.39 |
| 24 | c | 515 | CLA | CHC-C1C | 4.46 | 1.48 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 24 | C | 505 | CLA | O2D-CGD | 4.47 | 1.44 | 1.33 |
| 24 | c | 507 | CLA | O2D-CGD | 4.47 | 1.44 | 1.33 |
| 24 | B | 611 | CLA | C3D-C2D | 4.47 | 1.49 | 1.39 |
| 24 | b | 611 | CLA | CHC-C1C | 4.47 | 1.48 | 1.35 |
| 24 | A | 406 | CLA | C3D-C2D | 4.48 | 1.49 | 1.39 |
| 24 | D | 403 | CLA | OBD-CAD | 4.48 | 1.28 | 1.22 |
| 24 | C | 511 | CLA | OBD-CAD | 4.49 | 1.28 | 1.22 |
| 24 | B | 616 | CLA | O2A-CGA | 4.49 | 1.46 | 1.33 |
| 24 | B | 612 | CLA | O2D-CGD | 4.49 | 1.44 | 1.33 |
| 24 | b | 612 | CLA | C3D-C2D | 4.49 | 1.49 | 1.39 |
| 24 | D | 404 | CLA | OBD-CAD | 4.49 | 1.28 | 1.22 |
| 24 | c | 514 | CLA | C3D-C2D | 4.50 | 1.49 | 1.39 |
| 24 | c | 504 | CLA | O2D-CGD | 4.50 | 1.44 | 1.33 |
| 24 | b | 613 | CLA | O2A-CGA | 4.50 | 1.46 | 1.33 |
| 24 | C | 504 | CLA | O2D-CGD | 4.50 | 1.44 | 1.33 |
| 24 | B | 611 | CLA | O2D-CGD | 4.51 | 1.44 | 1.33 |
| 24 | B | 607 | CLA | C3D-C2D | 4.51 | 1.49 | 1.39 |
| 34 | z | 101 | LMG | O8-C28 | 4.51 | 1.46 | 1.33 |
| 24 | c | 513 | CLA | OBD-CAD | 4.51 | 1.28 | 1.22 |
| 24 | C | 505 | CLA | C3D-C2D | 4.51 | 1.49 | 1.39 |
| 24 | b | 617 | CLA | CHC-C1C | 4.52 | 1.48 | 1.35 |
| 24 | b | 609 | CLA | C3C-C2C | 4.52 | 1.46 | 1.36 |
| 24 | C | 511 | CLA | O2D-CGD | 4.52 | 1.44 | 1.33 |
| 25 | A | 408 | PHO | O2D-CGD | 4.53 | 1.44 | 1.33 |
| 24 | C | 513 | CLA | C3D-C2D | 4.53 | 1.49 | 1.39 |
| 24 | B | 615 | CLA | OBD-CAD | 4.54 | 1.28 | 1.22 |
| 24 | c | 506 | CLA | C3D-C2D | 4.54 | 1.49 | 1.39 |
| 24 | B | 613 | CLA | CHC-C1C | 4.54 | 1.48 | 1.35 |
| 24 | b | 609 | CLA | OBD-CAD | 4.54 | 1.28 | 1.22 |
| 24 | c | 510 | CLA | O2D-CGD | 4.54 | 1.44 | 1.33 |
| 24 | C | 502 | CLA | O2D-CGD | 4.55 | 1.44 | 1.33 |
| 24 | C | 503 | CLA | O2D-CGD | 4.55 | 1.44 | 1.33 |
| 24 | C | 505 | CLA | OBD-CAD | 4.55 | 1.28 | 1.22 |
| 24 | C | 510 | CLA | C3D-C2D | 4.56 | 1.49 | 1.39 |
| 24 | B | 605 | CLA | C3C-C2C | 4.56 | 1.46 | 1.36 |
| 24 | b | 606 | CLA | C3D-C2D | 4.57 | 1.49 | 1.39 |
| 24 | D | 403 | CLA | O2A-CGA | 4.57 | 1.46 | 1.33 |
| 24 | A | 405 | CLA | O2D-CGD | 4.58 | 1.44 | 1.33 |
| 24 | b | 615 | CLA | C3D-C2D | 4.58 | 1.49 | 1.39 |
| 24 | C | 511 | CLA | C3D-C2D | 4.59 | 1.49 | 1.39 |
| 24 | B | 610 | CLA | CHC-C1C | 4.59 | 1.48 | 1.35 |
| 24 | b | 619 | CLA | C3D-C2D | 4.59 | 1.49 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 25 | a | 408 | PHO | CHD-C1D | 4.60 | 1.47 | 1.38 |
| 24 | A | 409 | CLA | OBD-CAD | 4.61 | 1.29 | 1.22 |
| 24 | c | 515 | CLA | OBD-CAD | 4.61 | 1.29 | 1.22 |
| 24 | c | 510 | CLA | OBD-CAD | 4.61 | 1.29 | 1.22 |
| 24 | D | 404 | CLA | O2D-CGD | 4.62 | 1.44 | 1.33 |
| 24 | c | 508 | CLA | O2D-CGD | 4.62 | 1.44 | 1.33 |
| 24 | C | 508 | CLA | OBD-CAD | 4.62 | 1.29 | 1.22 |
| 24 | b | 610 | CLA | OBD-CAD | 4.63 | 1.29 | 1.22 |
| 24 | b | 607 | CLA | OBD-CAD | 4.63 | 1.29 | 1.22 |
| 24 | b | 615 | CLA | OBD-CAD | 4.64 | 1.29 | 1.22 |
| 25 | A | 407 | PHO | O2D-CGD | 4.64 | 1.45 | 1.33 |
| 24 | C | 502 | CLA | C3D-C2D | 4.64 | 1.49 | 1.39 |
| 24 | c | 505 | CLA | O2D-CGD | 4.64 | 1.45 | 1.33 |
| 24 | C | 508 | CLA | O2D-CGD | 4.64 | 1.45 | 1.33 |
| 24 | A | 405 | CLA | C3D-C2D | 4.65 | 1.50 | 1.39 |
| 24 | C | 514 | CLA | O2D-CGD | 4.65 | 1.45 | 1.33 |
| 24 | b | 612 | CLA | O2D-CGD | 4.65 | 1.45 | 1.33 |
| 24 | B | 603 | CLA | OBD-CAD | 4.65 | 1.29 | 1.22 |
| 24 | b | 608 | CLA | O2D-CGD | 4.65 | 1.45 | 1.33 |
| 24 | d | 402 | CLA | O2A-CGA | 4.66 | 1.47 | 1.33 |
| 24 | c | 504 | CLA | C3D-C2D | 4.66 | 1.50 | 1.39 |
| 24 | B | 613 | CLA | O2D-CGD | 4.66 | 1.45 | 1.33 |
| 24 | D | 401 | CLA | O2D-CGD | 4.67 | 1.45 | 1.33 |
| 24 | B | 603 | CLA | O2D-CGD | 4.68 | 1.45 | 1.33 |
| 24 | B | 612 | CLA | C3D-C2D | 4.68 | 1.50 | 1.39 |
| 24 | c | 509 | CLA | O2D-CGD | 4.68 | 1.45 | 1.33 |
| 24 | C | 504 | CLA | OBD-CAD | 4.69 | 1.29 | 1.22 |
| 24 | b | 611 | CLA | O2D-CGD | 4.69 | 1.45 | 1.33 |
| 24 | b | 619 | CLA | O2D-CGD | 4.70 | 1.45 | 1.33 |
| 24 | C | 513 | CLA | O2D-CGD | 4.70 | 1.45 | 1.33 |
| 24 | c | 506 | CLA | OBD-CAD | 4.70 | 1.29 | 1.22 |
| 24 | B | 609 | CLA | O2D-CGD | 4.70 | 1.45 | 1.33 |
| 24 | b | 620 | CLA | C3D-C2D | 4.70 | 1.50 | 1.39 |
| 24 | B | 614 | CLA | O2D-CGD | 4.71 | 1.45 | 1.33 |
| 24 | C | 506 | CLA | O2D-CGD | 4.72 | 1.45 | 1.33 |
| 24 | c | 510 | CLA | C3D-C2D | 4.72 | 1.50 | 1.39 |
| 24 | D | 401 | CLA | C3D-C2D | 4.72 | 1.50 | 1.39 |
| 24 | B | 616 | CLA | C3C-C2C | 4.73 | 1.46 | 1.36 |
| 25 | A | 408 | PHO | CHB-C1B | 4.73 | 1.48 | 1.38 |
| 24 | d | 404 | CLA | O2D-CGD | 4.74 | 1.45 | 1.33 |
| 24 | A | 409 | CLA | O2D-CGD | 4.74 | 1.45 | 1.33 |
| 24 | C | 509 | CLA | C3D-C2D | 4.74 | 1.50 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 25 | d | 403 | PHO | CHD-C1D | 4.75 | 1.48 | 1.38 |
| 24 | A | 409 | CLA | C3D-C2D | 4.75 | 1.50 | 1.39 |
| 24 | a | 409 | CLA | O2D-CGD | 4.75 | 1.45 | 1.33 |
| 24 | B | 604 | CLA | O2D-CGD | 4.76 | 1.45 | 1.33 |
| 24 | b | 620 | CLA | O2D-CGD | 4.76 | 1.45 | 1.33 |
| 24 | B | 616 | CLA | C3D-C2D | 4.77 | 1.50 | 1.39 |
| 24 | c | 503 | CLA | O2D-CGD | 4.77 | 1.45 | 1.33 |
| 24 | d | 401 | CLA | C3D-C2D | 4.78 | 1.50 | 1.39 |
| 24 | C | 507 | CLA | C3D-C2D | 4.78 | 1.50 | 1.39 |
| 24 | B | 615 | CLA | O2D-CGD | 4.78 | 1.45 | 1.33 |
| 25 | A | 407 | PHO | CHC-C1C | 4.78 | 1.48 | 1.38 |
| 24 | A | 406 | CLA | O2D-CGD | 4.78 | 1.45 | 1.33 |
| 24 | b | 617 | CLA | O2D-CGD | 4.78 | 1.45 | 1.33 |
| 24 | D | 403 | CLA | C3C-C2C | 4.78 | 1.47 | 1.36 |
| 25 | d | 403 | PHO | O2D-CGD | 4.79 | 1.45 | 1.33 |
| 24 | b | 616 | CLA | O2D-CGD | 4.79 | 1.45 | 1.33 |
| 24 | C | 509 | CLA | O2D-CGD | 4.79 | 1.45 | 1.33 |
| 24 | C | 512 | CLA | O2D-CGD | 4.80 | 1.45 | 1.33 |
| 24 | b | 616 | CLA | C3D-C2D | 4.80 | 1.50 | 1.39 |
| 24 | C | 510 | CLA | OBD-CAD | 4.80 | 1.29 | 1.22 |
| 24 | b | 619 | CLA | C3C-C2C | 4.81 | 1.47 | 1.36 |
| 24 | c | 513 | CLA | O2D-CGD | 4.82 | 1.45 | 1.33 |
| 24 | c | 514 | CLA | O2D-CGD | 4.83 | 1.45 | 1.33 |
| 24 | c | 507 | CLA | OBD-CAD | 4.84 | 1.29 | 1.22 |
| 25 | A | 407 | PHO | CHD-C1D | 4.84 | 1.48 | 1.38 |
| 24 | b | 607 | CLA | O2D-CGD | 4.85 | 1.45 | 1.33 |
| 24 | C | 514 | CLA | C3C-C2C | 4.85 | 1.47 | 1.36 |
| 24 | b | 609 | CLA | O2D-CGD | 4.85 | 1.45 | 1.33 |
| 24 | c | 512 | CLA | O2D-CGD | 4.86 | 1.45 | 1.33 |
| 24 | C | 503 | CLA | C3D-C2D | 4.86 | 1.50 | 1.39 |
| 24 | B | 616 | CLA | O2D-CGD | 4.87 | 1.45 | 1.33 |
| 25 | A | 408 | PHO | CHC-C1C | 4.87 | 1.48 | 1.38 |
| 25 | a | 408 | PHO | O2D-CGD | 4.87 | 1.45 | 1.33 |
| 24 | C | 507 | CLA | O2D-CGD | 4.87 | 1.45 | 1.33 |
| 24 | B | 610 | CLA | OBD-CAD | 4.88 | 1.29 | 1.22 |
| 24 | B | 608 | CLA | C3C-C2C | 4.88 | 1.47 | 1.36 |
| 24 | B | 609 | CLA | C3D-C2D | 4.88 | 1.50 | 1.39 |
| 24 | a | 406 | CLA | O2D-CGD | 4.89 | 1.45 | 1.33 |
| 24 | B | 607 | CLA | O2D-CGD | 4.89 | 1.45 | 1.33 |
| 24 | d | 404 | CLA | C3C-C2C | 4.89 | 1.47 | 1.36 |
| 24 | b | 613 | CLA | O2D-CGD | 4.90 | 1.45 | 1.33 |
| 24 | c | 511 | CLA | OBD-CAD | 4.90 | 1.29 | 1.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 24 | B | 617 | CLA | OBD-CAD | 4.90 | 1.29 | 1.22 |
| 24 | b | 620 | CLA | OBD-CAD | 4.91 | 1.29 | 1.22 |
| 24 | A | 405 | CLA | C3C-C2C | 4.92 | 1.47 | 1.36 |
| 24 | c | 515 | CLA | O2D-CGD | 4.92 | 1.45 | 1.33 |
| 24 | C | 502 | CLA | C3C-C2C | 4.93 | 1.47 | 1.36 |
| 24 | b | 621 | CLA | O2D-CGD | 4.94 | 1.45 | 1.33 |
| 24 | b | 618 | CLA | O2D-CGD | 4.95 | 1.45 | 1.33 |
| 24 | B | 617 | CLA | O2D-CGD | 4.96 | 1.45 | 1.33 |
| 24 | C | 514 | CLA | OBD-CAD | 4.96 | 1.29 | 1.22 |
| 24 | C | 508 | CLA | C3C-C2C | 4.97 | 1.47 | 1.36 |
| 24 | b | 607 | CLA | C3D-C2D | 4.97 | 1.50 | 1.39 |
| 24 | c | 506 | CLA | O2D-CGD | 4.97 | 1.45 | 1.33 |
| 24 | b | 610 | CLA | C3C-C2C | 4.97 | 1.47 | 1.36 |
| 24 | c | 511 | CLA | O2D-CGD | 4.98 | 1.45 | 1.33 |
| 24 | B | 606 | CLA | C3C-C2C | 4.98 | 1.47 | 1.36 |
| 25 | a | 408 | PHO | CHB-C1B | 5.00 | 1.48 | 1.38 |
| 24 | d | 401 | CLA | OBD-CAD | 5.00 | 1.29 | 1.22 |
| 24 | B | 602 | CLA | O2D-CGD | 5.00 | 1.45 | 1.33 |
| 25 | d | 403 | PHO | CHB-C1B | 5.01 | 1.48 | 1.38 |
| 24 | B | 615 | CLA | C3C-C2C | 5.01 | 1.47 | 1.36 |
| 24 | b | 611 | CLA | C3C-C2C | 5.02 | 1.47 | 1.36 |
| 24 | b | 621 | CLA | C3C-C2C | 5.02 | 1.47 | 1.36 |
| 24 | B | 617 | CLA | C3C-C2C | 5.03 | 1.47 | 1.36 |
| 24 | B | 607 | CLA | C3C-C2C | 5.05 | 1.47 | 1.36 |
| 24 | b | 606 | CLA | O2D-CGD | 5.05 | 1.46 | 1.33 |
| 24 | B | 606 | CLA | O2D-CGD | 5.05 | 1.46 | 1.33 |
| 24 | B | 614 | CLA | C3C-C2C | 5.05 | 1.47 | 1.36 |
| 24 | b | 616 | CLA | C3C-C2C | 5.06 | 1.47 | 1.36 |
| 24 | C | 510 | CLA | O2D-CGD | 5.06 | 1.46 | 1.33 |
| 24 | c | 508 | CLA | C3C-C2C | 5.07 | 1.47 | 1.36 |
| 24 | C | 512 | CLA | C3C-C2C | 5.08 | 1.47 | 1.36 |
| 24 | d | 401 | CLA | C3C-C2C | 5.08 | 1.47 | 1.36 |
| 24 | B | 613 | CLA | C3C-C2C | 5.09 | 1.47 | 1.36 |
| 24 | a | 407 | CLA | C3C-C2C | 5.10 | 1.47 | 1.36 |
| 24 | c | 507 | CLA | C3B-C2B | 5.10 | 1.47 | 1.40 |
| 24 | c | 513 | CLA | C3C-C2C | 5.11 | 1.47 | 1.36 |
| 24 | c | 507 | CLA | C3C-C2C | 5.11 | 1.47 | 1.36 |
| 24 | b | 612 | CLA | C3C-C2C | 5.11 | 1.47 | 1.36 |
| 24 | B | 603 | CLA | C3C-C2C | 5.12 | 1.47 | 1.36 |
| 24 | B | 608 | CLA | OBD-CAD | 5.12 | 1.29 | 1.22 |
| 24 | A | 406 | CLA | C3C-C2C | 5.12 | 1.47 | 1.36 |
| 24 | D | 401 | CLA | C3C-C2C | 5.13 | 1.47 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 24 | c | 515 | CLA | C3C-C2C | 5.13 | 1.47 | 1.36 |
| 24 | B | 616 | CLA | C3B-C2B | 5.13 | 1.47 | 1.40 |
| 24 | c | 505 | CLA | C3C-C2C | 5.13 | 1.47 | 1.36 |
| 24 | b | 614 | CLA | O2D-CGD | 5.14 | 1.46 | 1.33 |
| 25 | A | 407 | PHO | CHB-C1B | 5.14 | 1.48 | 1.38 |
| 24 | b | 608 | CLA | C3C-C2C | 5.14 | 1.47 | 1.36 |
| 24 | B | 610 | CLA | C3C-C2C | 5.14 | 1.47 | 1.36 |
| 24 | b | 614 | CLA | OBD-CAD | 5.15 | 1.29 | 1.22 |
| 24 | b | 615 | CLA | C3C-C2C | 5.16 | 1.47 | 1.36 |
| 24 | C | 507 | CLA | C3C-C2C | 5.17 | 1.47 | 1.36 |
| 24 | C | 505 | CLA | C3C-C2C | 5.18 | 1.47 | 1.36 |
| 24 | b | 614 | CLA | C3C-C2C | 5.20 | 1.47 | 1.36 |
| 24 | D | 401 | CLA | OBD-CAD | 5.20 | 1.29 | 1.22 |
| 24 | C | 511 | CLA | C3C-C2C | 5.20 | 1.47 | 1.36 |
| 24 | B | 604 | CLA | C3C-C2C | 5.21 | 1.47 | 1.36 |
| 24 | c | 510 | CLA | C3C-C2C | 5.21 | 1.47 | 1.36 |
| 24 | b | 607 | CLA | C3C-C2C | 5.22 | 1.47 | 1.36 |
| 24 | C | 513 | CLA | C3C-C2C | 5.23 | 1.48 | 1.36 |
| 24 | c | 509 | CLA | C3C-C2C | 5.25 | 1.48 | 1.36 |
| 24 | C | 510 | CLA | C3C-C2C | 5.25 | 1.48 | 1.36 |
| 24 | a | 409 | CLA | C3C-C2C | 5.27 | 1.48 | 1.36 |
| 24 | c | 504 | CLA | C3C-C2C | 5.27 | 1.48 | 1.36 |
| 24 | d | 402 | CLA | C3C-C2C | 5.27 | 1.48 | 1.36 |
| 24 | b | 613 | CLA | C3C-C2C | 5.28 | 1.48 | 1.36 |
| 24 | c | 512 | CLA | C3C-C2C | 5.29 | 1.48 | 1.36 |
| 24 | c | 514 | CLA | C3C-C2C | 5.29 | 1.48 | 1.36 |
| 24 | b | 618 | CLA | C3C-C2C | 5.29 | 1.48 | 1.36 |
| 24 | D | 404 | CLA | C3C-C2C | 5.30 | 1.48 | 1.36 |
| 24 | b | 617 | CLA | C3C-C2C | 5.30 | 1.48 | 1.36 |
| 24 | a | 406 | CLA | C3C-C2C | 5.30 | 1.48 | 1.36 |
| 25 | d | 403 | PHO | CHC-C1C | 5.31 | 1.49 | 1.38 |
| 24 | c | 503 | CLA | C3C-C2C | 5.32 | 1.48 | 1.36 |
| 24 | b | 620 | CLA | C3C-C2C | 5.33 | 1.48 | 1.36 |
| 24 | C | 504 | CLA | C3C-C2C | 5.33 | 1.48 | 1.36 |
| 24 | c | 511 | CLA | C3C-C2C | 5.34 | 1.48 | 1.36 |
| 24 | C | 503 | CLA | C3C-C2C | 5.35 | 1.48 | 1.36 |
| 24 | c | 506 | CLA | C3C-C2C | 5.37 | 1.48 | 1.36 |
| 24 | C | 506 | CLA | C3C-C2C | 5.37 | 1.48 | 1.36 |
| 25 | a | 408 | PHO | CHC-C1C | 5.39 | 1.49 | 1.38 |
| 24 | C | 509 | CLA | C3C-C2C | 5.40 | 1.48 | 1.36 |
| 24 | B | 611 | CLA | C3C-C2C | 5.40 | 1.48 | 1.36 |
| 24 | b | 610 | CLA | C3B-C2B | 5.42 | 1.47 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 24 | A | 406 | CLA | OBD-CAD | 5.43 | 1.30 | 1.22 |
| 24 | B | 602 | CLA | C3C-C2C | 5.45 | 1.48 | 1.36 |
| 24 | B | 612 | CLA | C3C-C2C | 5.45 | 1.48 | 1.36 |
| 25 | d | 403 | PHO | C3C-C2C | 5.50 | 1.48 | 1.36 |
| 25 | A | 408 | PHO | C3C-C2C | 5.52 | 1.48 | 1.36 |
| 24 | B | 610 | CLA | C3B-C2B | 5.54 | 1.47 | 1.40 |
| 24 | A | 409 | CLA | C3C-C2C | 5.54 | 1.48 | 1.36 |
| 24 | B | 609 | CLA | C3C-C2C | 5.55 | 1.48 | 1.36 |
| 24 | c | 504 | CLA | C3B-C2B | 5.56 | 1.47 | 1.40 |
| 24 | b | 606 | CLA | C3C-C2C | 5.61 | 1.48 | 1.36 |
| 24 | c | 505 | CLA | C3B-C2B | 5.62 | 1.47 | 1.40 |
| 24 | B | 606 | CLA | C3B-C2B | 5.63 | 1.47 | 1.40 |
| 24 | a | 409 | CLA | C3B-C2B | 5.69 | 1.47 | 1.40 |
| 24 | d | 404 | CLA | C3B-C2B | 5.69 | 1.47 | 1.40 |
| 24 | C | 512 | CLA | C3B-C2B | 5.75 | 1.47 | 1.40 |
| 24 | B | 615 | CLA | C3B-C2B | 5.77 | 1.48 | 1.40 |
| 24 | b | 614 | CLA | C3B-C2B | 5.79 | 1.48 | 1.40 |
| 25 | a | 408 | PHO | C3C-C2C | 5.86 | 1.49 | 1.36 |
| 25 | A | 407 | PHO | C3C-C2C | 5.88 | 1.49 | 1.36 |
| 24 | b | 616 | CLA | C3B-C2B | 5.92 | 1.48 | 1.40 |
| 24 | C | 505 | CLA | C3B-C2B | 5.93 | 1.48 | 1.40 |
| 24 | b | 612 | CLA | C3B-C2B | 5.99 | 1.48 | 1.40 |
| 24 | A | 409 | CLA | C3B-C2B | 6.01 | 1.48 | 1.40 |
| 24 | A | 406 | CLA | C3B-C2B | 6.04 | 1.48 | 1.40 |
| 24 | c | 509 | CLA | C3B-C2B | 6.04 | 1.48 | 1.40 |
| 24 | C | 507 | CLA | C3B-C2B | 6.04 | 1.48 | 1.40 |
| 24 | a | 407 | CLA | C3B-C2B | 6.04 | 1.48 | 1.40 |
| 24 | c | 515 | CLA | C3B-C2B | 6.05 | 1.48 | 1.40 |
| 24 | D | 403 | CLA | C3B-C2B | 6.08 | 1.48 | 1.40 |
| 24 | c | 514 | CLA | C3B-C2B | 6.10 | 1.48 | 1.40 |
| 24 | b | 613 | CLA | C3B-C2B | 6.12 | 1.48 | 1.40 |
| 24 | c | 506 | CLA | C3B-C2B | 6.14 | 1.48 | 1.40 |
| 24 | c | 508 | CLA | C3B-C2B | 6.15 | 1.48 | 1.40 |
| 24 | c | 512 | CLA | C3B-C2B | 6.16 | 1.48 | 1.40 |
| 24 | D | 404 | CLA | C3B-C2B | 6.17 | 1.48 | 1.40 |
| 24 | b | 617 | CLA | C3B-C2B | 6.18 | 1.48 | 1.40 |
| 24 | C | 503 | CLA | C3B-C2B | 6.19 | 1.48 | 1.40 |
| 24 | C | 510 | CLA | C3B-C2B | 6.20 | 1.48 | 1.40 |
| 24 | a | 406 | CLA | C3B-C2B | 6.20 | 1.48 | 1.40 |
| 24 | B | 607 | CLA | C3B-C2B | 6.21 | 1.48 | 1.40 |
| 24 | c | 513 | CLA | C3B-C2B | 6.22 | 1.48 | 1.40 |
| 24 | B | 611 | CLA | C3B-C2B | 6.24 | 1.48 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 24 | b | 609 | CLA | C3B-C2B | 6.27 | 1.48 | 1.40 |
| 24 | b | 611 | CLA | C3B-C2B | 6.28 | 1.48 | 1.40 |
| 24 | C | 502 | CLA | C3B-C2B | 6.28 | 1.48 | 1.40 |
| 24 | b | 620 | CLA | C3B-C2B | 6.30 | 1.48 | 1.40 |
| 24 | B | 608 | CLA | C3B-C2B | 6.30 | 1.48 | 1.40 |
| 24 | b | 606 | CLA | C3B-C2B | 6.32 | 1.48 | 1.40 |
| 24 | b | 607 | CLA | C3B-C2B | 6.35 | 1.48 | 1.40 |
| 24 | C | 514 | CLA | C3B-C2B | 6.35 | 1.48 | 1.40 |
| 24 | C | 509 | CLA | C3B-C2B | 6.36 | 1.48 | 1.40 |
| 24 | d | 401 | CLA | C3B-C2B | 6.38 | 1.48 | 1.40 |
| 24 | d | 402 | CLA | C3B-C2B | 6.38 | 1.48 | 1.40 |
| 24 | D | 401 | CLA | C3B-C2B | 6.39 | 1.48 | 1.40 |
| 25 | A | 407 | PHO | C3B-C2B | 6.40 | 1.49 | 1.37 |
| 25 | a | 408 | PHO | C3B-C2B | 6.44 | 1.49 | 1.37 |
| 24 | b | 619 | CLA | C3B-C2B | 6.45 | 1.48 | 1.40 |
| 24 | b | 615 | CLA | C3B-C2B | 6.45 | 1.48 | 1.40 |
| 24 | B | 605 | CLA | C3B-C2B | 6.47 | 1.48 | 1.40 |
| 24 | C | 513 | CLA | C3B-C2B | 6.48 | 1.48 | 1.40 |
| 25 | A | 408 | PHO | C3B-C2B | 6.49 | 1.49 | 1.37 |
| 24 | C | 506 | CLA | C3B-C2B | 6.49 | 1.48 | 1.40 |
| 24 | B | 602 | CLA | C3B-C2B | 6.50 | 1.48 | 1.40 |
| 24 | c | 503 | CLA | C3B-C2B | 6.52 | 1.49 | 1.40 |
| 24 | B | 604 | CLA | C3B-C2B | 6.53 | 1.49 | 1.40 |
| 24 | b | 608 | CLA | C3B-C2B | 6.53 | 1.49 | 1.40 |
| 24 | C | 508 | CLA | C3B-C2B | 6.54 | 1.49 | 1.40 |
| 24 | B | 612 | CLA | C3B-C2B | 6.55 | 1.49 | 1.40 |
| 25 | d | 403 | PHO | C3B-C2B | 6.59 | 1.49 | 1.37 |
| 24 | B | 603 | CLA | C3B-C2B | 6.59 | 1.49 | 1.40 |
| 24 | B | 614 | CLA | C3B-C2B | 6.61 | 1.49 | 1.40 |
| 24 | B | 613 | CLA | C3B-C2B | 6.62 | 1.49 | 1.40 |
| 24 | b | 621 | CLA | C3B-C2B | 6.63 | 1.49 | 1.40 |
| 24 | C | 504 | CLA | C3B-C2B | 6.69 | 1.49 | 1.40 |
| 24 | b | 618 | CLA | C3B-C2B | 6.70 | 1.49 | 1.40 |
| 24 | c | 510 | CLA | C3B-C2B | 6.72 | 1.49 | 1.40 |
| 24 | B | 609 | CLA | C3B-C2B | 6.74 | 1.49 | 1.40 |
| 24 | A | 405 | CLA | C3B-C2B | 6.79 | 1.49 | 1.40 |
| 24 | C | 511 | CLA | C3B-C2B | 6.89 | 1.49 | 1.40 |
| 24 | B | 617 | CLA | C3B-C2B | 6.96 | 1.49 | 1.40 |
| 24 | c | 511 | CLA | C3B-C2B | 6.97 | 1.49 | 1.40 |

All (2080) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24 | B | 605 | CLA | C1C-NC-C4C | -7.67 | 102.65 | 107.06 |
| 24 | b | 612 | CLA | C1C-NC-C4C | -7.57 | 102.70 | 107.06 |
| 24 | A | 405 | CLA | C1C-NC-C4C | -7.48 | 102.75 | 107.06 |
| 24 | b | 609 | CLA | C1C-NC-C4C | -7.36 | 102.82 | 107.06 |
| 24 | D | 403 | CLA | C1C-NC-C4C | -7.11 | 102.97 | 107.06 |
| 24 | b | 618 | CLA | C1C-NC-C4C | -6.87 | 103.11 | 107.06 |
| 24 | B | 606 | CLA | C1C-NC-C4C | -6.76 | 103.17 | 107.06 |
| 24 | b | 616 | CLA | C1C-NC-C4C | -6.75 | 103.17 | 107.06 |
| 24 | B | 607 | CLA | C1C-NC-C4C | -6.72 | 103.19 | 107.06 |
| 24 | d | 402 | CLA | C1C-NC-C4C | -6.66 | 103.22 | 107.06 |
| 24 | c | 509 | CLA | C1C-NC-C4C | -6.64 | 103.23 | 107.06 |
| 24 | c | 507 | CLA | C1C-NC-C4C | -6.64 | 103.24 | 107.06 |
| 24 | b | 616 | CLA | CHD-C4C-C3C | -6.53 | 115.08 | 124.92 |
| 24 | B | 610 | CLA | CHD-C4C-C3C | -6.52 | 115.09 | 124.92 |
| 24 | b | 618 | CLA | CHD-C4C-C3C | -6.49 | 115.14 | 124.92 |
| 24 | B | 608 | CLA | C1C-NC-C4C | -6.45 | 103.35 | 107.06 |
| 24 | C | 504 | CLA | C1C-NC-C4C | -6.39 | 103.38 | 107.06 |
| 24 | b | 612 | CLA | CHD-C4C-C3C | -6.37 | 115.31 | 124.92 |
| 24 | C | 508 | CLA | CHD-C4C-C3C | -6.34 | 115.36 | 124.92 |
| 24 | B | 607 | CLA | CHD-C4C-C3C | -6.34 | 115.37 | 124.92 |
| 24 | b | 610 | CLA | CHD-C4C-C3C | -6.32 | 115.40 | 124.92 |
| 24 | B | 614 | CLA | C1C-NC-C4C | -6.28 | 103.44 | 107.06 |
| 24 | A | 409 | CLA | CHD-C4C-C3C | -6.26 | 115.49 | 124.92 |
| 24 | C | 506 | CLA | C1C-NC-C4C | -6.23 | 103.47 | 107.06 |
| 24 | B | 604 | CLA | C1C-NC-C4C | -6.23 | 103.47 | 107.06 |
| 24 | B | 605 | CLA | CHD-C4C-C3C | -6.21 | 115.56 | 124.92 |
| 24 | a | 406 | CLA | C1C-NC-C4C | -6.21 | 103.48 | 107.06 |
| 24 | b | 606 | CLA | CHD-C4C-C3C | -6.20 | 115.57 | 124.92 |
| 24 | B | 606 | CLA | CHD-C4C-C3C | -6.18 | 115.61 | 124.92 |
| 24 | c | 510 | CLA | CHD-C4C-C3C | -6.17 | 115.61 | 124.92 |
| 24 | B | 604 | CLA | CHD-C4C-C3C | -6.15 | 115.64 | 124.92 |
| 24 | c | 510 | CLA | C1C-NC-C4C | -6.15 | 103.52 | 107.06 |
| 24 | B | 609 | CLA | CHD-C4C-C3C | -6.09 | 115.75 | 124.92 |
| 24 | b | 611 | CLA | CHD-C4C-C3C | -6.08 | 115.75 | 124.92 |
| 24 | B | 611 | CLA | C1C-NC-C4C | -6.08 | 103.56 | 107.06 |
| 24 | c | 505 | CLA | C1C-NC-C4C | -6.06 | 103.57 | 107.06 |
| 24 | b | 614 | CLA | C1C-NC-C4C | -6.03 | 103.59 | 107.06 |
| 24 | c | 505 | CLA | CHD-C4C-C3C | -6.02 | 115.84 | 124.92 |
| 24 | c | 509 | CLA | CHD-C4C-C3C | -6.02 | 115.85 | 124.92 |
| 24 | B | 609 | CLA | C1C-NC-C4C | -6.00 | 103.60 | 107.06 |
| 24 | B | 612 | CLA | CHD-C4C-C3C | -6.00 | 115.88 | 124.92 |
| 24 | b | 609 | CLA | CHD-C4C-C3C | -5.99 | 115.89 | 124.92 |
| 24 | C | 504 | CLA | CHD-C4C-C3C | -5.97 | 115.93 | 124.92 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24 | B | 613 | CLA | C1C-NC-C4C | -5.95 | 103.63 | 107.06 |
| 24 | C | 508 | CLA | C1C-NC-C4C | -5.93 | 103.64 | 107.06 |
| 24 | c | 512 | CLA | CHD-C4C-C3C | -5.93 | 115.99 | 124.92 |
| 24 | b | 617 | CLA | CHD-C4C-C3C | -5.93 | 115.99 | 124.92 |
| 24 | C | 503 | CLA | C1C-NC-C4C | -5.92 | 103.65 | 107.06 |
| 24 | d | 404 | CLA | CHD-C4C-C3C | -5.91 | 116.02 | 124.92 |
| 24 | D | 404 | CLA | CHD-C4C-C3C | -5.91 | 116.02 | 124.92 |
| 24 | b | 607 | CLA | CHD-C4C-C3C | -5.90 | 116.03 | 124.92 |
| 24 | B | 602 | CLA | CHD-C4C-C3C | -5.87 | 116.07 | 124.92 |
| 24 | B | 616 | CLA | C1C-NC-C4C | -5.86 | 103.68 | 107.06 |
| 24 | b | 615 | CLA | CHD-C4C-C3C | -5.86 | 116.09 | 124.92 |
| 24 | C | 511 | CLA | CHD-C4C-C3C | -5.86 | 116.09 | 124.92 |
| 24 | d | 401 | CLA | C1C-NC-C4C | -5.85 | 103.69 | 107.06 |
| 24 | C | 502 | CLA | C1C-NC-C4C | -5.84 | 103.69 | 107.06 |
| 24 | b | 615 | CLA | C1C-NC-C4C | -5.83 | 103.70 | 107.06 |
| 24 | b | 621 | CLA | C1C-NC-C4C | -5.80 | 103.72 | 107.06 |
| 24 | b | 611 | CLA | C1C-NC-C4C | -5.79 | 103.72 | 107.06 |
| 24 | B | 603 | CLA | CHD-C4C-C3C | -5.78 | 116.21 | 124.92 |
| 24 | B | 612 | CLA | C1C-NC-C4C | -5.77 | 103.73 | 107.06 |
| 24 | B | 615 | CLA | CHD-C4C-C3C | -5.76 | 116.24 | 124.92 |
| 24 | a | 407 | CLA | CHD-C4C-C3C | -5.75 | 116.25 | 124.92 |
| 24 | b | 619 | CLA | C1C-NC-C4C | -5.75 | 103.75 | 107.06 |
| 24 | B | 617 | CLA | CHD-C4C-C3C | -5.74 | 116.27 | 124.92 |
| 24 | C | 503 | CLA | CHD-C4C-C3C | -5.74 | 116.28 | 124.92 |
| 24 | B | 616 | CLA | CHD-C4C-C3C | -5.73 | 116.28 | 124.92 |
| 24 | b | 610 | CLA | C1C-NC-C4C | -5.73 | 103.76 | 107.06 |
| 24 | C | 512 | CLA | CHD-C4C-C3C | -5.72 | 116.30 | 124.92 |
| 24 | C | 513 | CLA | CHD-C4C-C3C | -5.72 | 116.30 | 124.92 |
| 24 | B | 617 | CLA | C1C-NC-C4C | -5.70 | 103.77 | 107.06 |
| 24 | C | 510 | CLA | C1C-NC-C4C | -5.68 | 103.79 | 107.06 |
| 24 | D | 403 | CLA | CHD-C4C-C3C | -5.64 | 116.43 | 124.92 |
| 24 | c | 506 | CLA | C1C-NC-C4C | -5.62 | 103.82 | 107.06 |
| 24 | C | 506 | CLA | CHD-C4C-C3C | -5.59 | 116.49 | 124.92 |
| 24 | C | 509 | CLA | C1C-NC-C4C | -5.59 | 103.84 | 107.06 |
| 24 | C | 514 | CLA | C1C-NC-C4C | -5.59 | 103.84 | 107.06 |
| 24 | b | 614 | CLA | CHD-C4C-C3C | -5.58 | 116.51 | 124.92 |
| 24 | c | 504 | CLA | CHD-C4C-C3C | -5.56 | 116.53 | 124.92 |
| 25 | A | 408 | PHO | C3D-C2D-C1D | -5.55 | 97.58 | 105.82 |
| 24 | B | 611 | CLA | CHD-C4C-C3C | -5.54 | 116.57 | 124.92 |
| 24 | d | 404 | CLA | C1C-NC-C4C | -5.53 | 103.87 | 107.06 |
| 24 | C | 507 | CLA | C1C-NC-C4C | -5.50 | 103.89 | 107.06 |
| 24 | c | 508 | CLA | C1C-NC-C4C | -5.50 | 103.89 | 107.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24 | C | 511 | CLA | C1C-NC-C4C | -5.50 | 103.89 | 107.06 |
| 24 | C | 507 | CLA | CHD-C4C-C3C | -5.49 | 116.64 | 124.92 |
| 24 | c | 511 | CLA | C1C-NC-C4C | -5.48 | 103.90 | 107.06 |
| 24 | C | 513 | CLA | C1C-NC-C4C | -5.48 | 103.90 | 107.06 |
| 24 | B | 608 | CLA | CHD-C4C-C3C | -5.47 | 116.68 | 124.92 |
| 24 | a | 409 | CLA | CHD-C4C-C3C | -5.46 | 116.68 | 124.92 |
| 24 | b | 608 | CLA | CHD-C4C-C3C | -5.46 | 116.69 | 124.92 |
| 24 | c | 513 | CLA | CHD-C4C-C3C | -5.46 | 116.69 | 124.92 |
| 24 | c | 514 | CLA | CHD-C4C-C3C | -5.43 | 116.73 | 124.92 |
| 24 | c | 503 | CLA | CHD-C4C-C3C | -5.43 | 116.73 | 124.92 |
| 24 | c | 506 | CLA | CHD-C4C-C3C | -5.43 | 116.74 | 124.92 |
| 24 | b | 620 | CLA | CHD-C4C-C3C | -5.42 | 116.75 | 124.92 |
| 24 | c | 511 | CLA | CHD-C4C-C3C | -5.41 | 116.76 | 124.92 |
| 24 | C | 514 | CLA | CHD-C4C-C3C | -5.41 | 116.77 | 124.92 |
| 24 | c | 508 | CLA | CHD-C4C-C3C | -5.40 | 116.78 | 124.92 |
| 24 | b | 607 | CLA | C1C-NC-C4C | -5.40 | 103.95 | 107.06 |
| 25 | a | 408 | PHO | C3D-C2D-C1D | -5.38 | 97.84 | 105.82 |
| 24 | C | 510 | CLA | CHD-C4C-C3C | -5.38 | 116.81 | 124.92 |
| 24 | C | 502 | CLA | CHD-C4C-C3C | -5.38 | 116.81 | 124.92 |
| 24 | c | 515 | CLA | CHD-C4C-C3C | -5.38 | 116.81 | 124.92 |
| 24 | B | 603 | CLA | C1C-NC-C4C | -5.35 | 103.98 | 107.06 |
| 24 | c | 503 | CLA | C1C-NC-C4C | -5.34 | 103.98 | 107.06 |
| 24 | C | 512 | CLA | C1C-NC-C4C | -5.32 | 103.99 | 107.06 |
| 24 | b | 620 | CLA | C1C-NC-C4C | -5.31 | 104.00 | 107.06 |
| 24 | b | 613 | CLA | CHD-C4C-C3C | -5.30 | 116.93 | 124.92 |
| 24 | b | 617 | CLA | C1C-NC-C4C | -5.30 | 104.00 | 107.06 |
| 24 | b | 613 | CLA | C1C-NC-C4C | -5.30 | 104.01 | 107.06 |
| 24 | a | 409 | CLA | C1C-NC-C4C | -5.27 | 104.02 | 107.06 |
| 25 | d | 403 | PHO | C3D-C2D-C1D | -5.27 | 98.00 | 105.82 |
| 24 | c | 504 | CLA | C1C-NC-C4C | -5.23 | 104.05 | 107.06 |
| 24 | B | 610 | CLA | C1C-NC-C4C | -5.21 | 104.06 | 107.06 |
| 24 | b | 608 | CLA | C1C-NC-C4C | -5.17 | 104.08 | 107.06 |
| 24 | C | 509 | CLA | CHD-C4C-C3C | -5.16 | 117.14 | 124.92 |
| 24 | d | 402 | CLA | CHD-C4C-C3C | -5.16 | 117.15 | 124.92 |
| 24 | c | 515 | CLA | C1C-NC-C4C | -5.14 | 104.10 | 107.06 |
| 24 | c | 507 | CLA | CHD-C4C-C3C | -5.13 | 117.19 | 124.92 |
| 24 | b | 619 | CLA | C1-C2-C3 | -5.12 | 116.53 | 125.96 |
| 24 | B | 614 | CLA | CHD-C4C-C3C | -5.10 | 117.23 | 124.92 |
| 24 | c | 513 | CLA | C1C-NC-C4C | -5.08 | 104.13 | 107.06 |
| 24 | A | 406 | CLA | CHD-C4C-C3C | -5.06 | 117.30 | 124.92 |
| 24 | c | 512 | CLA | C1C-NC-C4C | -5.05 | 104.15 | 107.06 |
| 24 | B | 602 | CLA | C1C-NC-C4C | -5.05 | 104.15 | 107.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24 | b | 619 | CLA | CHD-C4C-C3C | -5.03 | 117.33 | 124.92 |
| 24 | d | 401 | CLA | CHD-C4C-C3C | -5.00 | 117.39 | 124.92 |
| 26 | D | 405 | BCR | C24-C23-C22 | -4.98 | 118.73 | 126.21 |
| 24 | b | 621 | CLA | CHD-C4C-C3C | -4.96 | 117.44 | 124.92 |
| 24 | A | 409 | CLA | C1C-NC-C4C | -4.94 | 104.22 | 107.06 |
| 24 | C | 505 | CLA | C1C-NC-C4C | -4.92 | 104.22 | 107.06 |
| 24 | B | 613 | CLA | CHD-C4C-C3C | -4.91 | 117.51 | 124.92 |
| 24 | A | 405 | CLA | CHD-C4C-C3C | -4.91 | 117.51 | 124.92 |
| 24 | B | 615 | CLA | C1C-NC-C4C | -4.89 | 104.24 | 107.06 |
| 24 | a | 407 | CLA | C1C-NC-C4C | -4.85 | 104.27 | 107.06 |
| 24 | b | 618 | CLA | C1-C2-C3 | -4.84 | 117.04 | 125.96 |
| 24 | D | 401 | CLA | CHD-C4C-C3C | -4.82 | 117.65 | 124.92 |
| 24 | D | 404 | CLA | C1C-NC-C4C | -4.82 | 104.28 | 107.06 |
| 24 | D | 401 | CLA | C1C-NC-C4C | -4.80 | 104.29 | 107.06 |
| 24 | a | 406 | CLA | CHD-C4C-C3C | -4.80 | 117.68 | 124.92 |
| 24 | C | 505 | CLA | CHD-C4C-C3C | -4.73 | 117.79 | 124.92 |
| 25 | d | 403 | PHO | C1-C2-C3 | -4.68 | 117.34 | 125.96 |
| 25 | A | 407 | PHO | C3D-C2D-C1D | -4.63 | 98.96 | 105.82 |
| 26 | D | 405 | BCR | C7-C8-C9 | -4.58 | 119.33 | 126.21 |
| 24 | D | 401 | CLA | C1C-C2C-C3C | -4.58 | 101.84 | 106.92 |
| 26 | y | 101 | BCR | C33-C5-C6 | -4.56 | 119.40 | 124.51 |
| 24 | b | 606 | CLA | C1C-NC-C4C | -4.54 | 104.44 | 107.06 |
| 38 | e | 102 | HEM | CBA-CAA-C2A | -4.44 | 103.99 | 112.48 |
| 26 | k | 103 | BCR | C24-C23-C22 | -4.31 | 119.73 | 126.21 |
| 26 | Y | 101 | BCR | C33-C5-C6 | -4.31 | 119.68 | 124.51 |
| 25 | a | 408 | PHO | C4C-C3C-C2C | -4.25 | 102.04 | 106.81 |
| 24 | c | 505 | CLA | C1D-CHD-C4C | -4.25 | 116.68 | 122.48 |
| 26 | b | 622 | BCR | C33-C5-C6 | -4.23 | 119.77 | 124.51 |
| 27 | A | 411 | SQD | C5-C6-S | -4.21 | 108.47 | 114.34 |
| 26 | D | 405 | BCR | C38-C26-C25 | -4.21 | 119.80 | 124.51 |
| 24 | b | 609 | CLA | C1C-C2C-C3C | -4.20 | 102.26 | 106.92 |
| 24 | B | 607 | CLA | C1D-CHD-C4C | -4.17 | 116.78 | 122.48 |
| 26 | d | 405 | BCR | C38-C26-C25 | -4.14 | 119.87 | 124.51 |
| 24 | A | 405 | CLA | C1C-C2C-C3C | -4.12 | 102.35 | 106.92 |
| 26 | y | 101 | BCR | C15-C14-C13 | -4.11 | 121.44 | 127.31 |
| 24 | b | 608 | CLA | C1D-CHD-C4C | -4.10 | 116.89 | 122.48 |
| 24 | c | 503 | CLA | O2D-CGD-O1D | -4.09 | 115.60 | 123.82 |
| 32 | A | 419 | PL9 | C32-C33-C34 | -4.08 | 117.42 | 127.68 |
| 24 | B | 614 | CLA | C1C-C2C-C3C | -4.07 | 102.40 | 106.92 |
| 26 | d | 405 | BCR | C15-C14-C13 | -4.07 | 121.50 | 127.31 |
| 26 | H | 101 | BCR | C38-C26-C25 | -4.06 | 119.96 | 124.51 |
| 26 | c | 516 | BCR | C7-C8-C9 | -4.06 | 120.12 | 126.21 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24 | B | 605 | CLA | C1C-C2C-C3C | -4.04 | 102.44 | 106.92 |
| 24 | A | 406 | CLA | C1C-NC-C4C | -4.03 | 104.73 | 107.06 |
| 38 | E | 103 | HEM | CBD-CAD-C3D | -4.02 | 104.79 | 112.47 |
| 25 | A | 408 | PHO | C1-C2-C3 | -4.02 | 118.55 | 125.96 |
| 24 | C | 505 | CLA | C1C-C2C-C3C | -4.02 | 102.46 | 106.92 |
| 24 | b | 610 | CLA | C1C-C2C-C3C | -4.01 | 102.47 | 106.92 |
| 24 | C | 510 | CLA | O2D-CGD-O1D | -4.00 | 115.77 | 123.82 |
| 24 | C | 503 | CLA | O2D-CGD-O1D | -3.99 | 115.79 | 123.82 |
| 24 | c | 511 | CLA | C1D-CHD-C4C | -3.98 | 117.04 | 122.48 |
| 24 | C | 504 | CLA | C1D-CHD-C4C | -3.98 | 117.05 | 122.48 |
| 26 | C | 516 | BCR | C7-C8-C9 | -3.98 | 120.24 | 126.21 |
| 24 | a | 406 | CLA | C1C-C2C-C3C | -3.96 | 102.53 | 106.92 |
| 26 | C | 515 | BCR | C33-C5-C6 | -3.95 | 120.09 | 124.51 |
| 24 | d | 401 | CLA | C1C-C2C-C3C | -3.94 | 102.55 | 106.92 |
| 24 | b | 610 | CLA | O2D-CGD-O1D | -3.93 | 115.91 | 123.82 |
| 26 | d | 405 | BCR | C7-C8-C9 | -3.92 | 120.31 | 126.21 |
| 24 | b | 619 | CLA | C1C-C2C-C3C | -3.92 | 102.58 | 106.92 |
| 24 | d | 402 | CLA | O2D-CGD-O1D | -3.91 | 115.95 | 123.82 |
| 24 | B | 608 | CLA | C1C-C2C-C3C | -3.91 | 102.58 | 106.92 |
| 24 | c | 514 | CLA | C1C-NC-C4C | -3.90 | 104.81 | 107.06 |
| 24 | c | 514 | CLA | C1C-C2C-C3C | -3.88 | 102.61 | 106.92 |
| 24 | C | 507 | CLA | C1C-C2C-C3C | -3.88 | 102.61 | 106.92 |
| 24 | c | 503 | CLA | C1C-C2C-C3C | -3.86 | 102.64 | 106.92 |
| 24 | B | 606 | CLA | C1C-C2C-C3C | -3.82 | 102.69 | 106.92 |
| 24 | b | 614 | CLA | C1C-C2C-C3C | -3.82 | 102.69 | 106.92 |
| 26 | C | 515 | BCR | C7-C8-C9 | -3.81 | 120.48 | 126.21 |
| 26 | c | 526 | BCR | C33-C5-C6 | -3.81 | 120.24 | 124.51 |
| 26 | B | 618 | BCR | C33-C5-C6 | -3.80 | 120.25 | 124.51 |
| 24 | A | 406 | CLA | C1C-C2C-C3C | -3.80 | 102.70 | 106.92 |
| 24 | c | 506 | CLA | C1C-C2C-C3C | -3.80 | 102.70 | 106.92 |
| 26 | d | 405 | BCR | C33-C5-C6 | -3.80 | 120.25 | 124.51 |
| 34 | c | 501 | LMG | C8-O7-C10 | -3.79 | 108.93 | 117.88 |
| 24 | b | 608 | CLA | O2A-CGA-O1A | -3.78 | 114.16 | 123.55 |
| 24 | d | 402 | CLA | C1C-C2C-C3C | -3.77 | 102.74 | 106.92 |
| 27 | a | 411 | SQD | C1-O5-C5 | -3.77 | 106.62 | 113.72 |
| 24 | B | 615 | CLA | C1C-C2C-C3C | -3.76 | 102.75 | 106.92 |
| 24 | b | 616 | CLA | C1D-CHD-C4C | -3.76 | 117.35 | 122.48 |
| 24 | b | 607 | CLA | C1D-CHD-C4C | -3.76 | 117.35 | 122.48 |
| 24 | B | 610 | CLA | C1D-CHD-C4C | -3.75 | 117.36 | 122.48 |
| 26 | K | 101 | BCR | C33-C5-C6 | -3.74 | 120.32 | 124.51 |
| 24 | c | 504 | CLA | O2D-CGD-O1D | -3.73 | 116.31 | 123.82 |
| 24 | b | 618 | CLA | C1C-C2C-C3C | -3.73 | 102.79 | 106.92 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24 | b | 617 | CLA | C4C-C3C-C2C | -3.72 | 101.20 | 106.91 |
| 24 | B | 609 | CLA | C1C-C2C-C3C | -3.72 | 102.79 | 106.92 |
| 24 | a | 409 | CLA | C1D-CHD-C4C | -3.72 | 117.41 | 122.48 |
| 26 | T | 102 | BCR | C33-C5-C6 | -3.71 | 120.35 | 124.51 |
| 34 | c | 501 | LMG | C7-O1-C1 | -3.71 | 106.15 | 113.76 |
| 24 | D | 401 | CLA | CAA-C2A-C3A | -3.71 | 102.65 | 112.81 |
| 24 | C | 506 | CLA | C1D-CHD-C4C | -3.70 | 117.43 | 122.48 |
| 26 | D | 405 | BCR | C33-C5-C6 | -3.70 | 120.37 | 124.51 |
| 25 | A | 407 | PHO | CHC-C1C-C2C | -3.70 | 117.14 | 125.62 |
| 24 | c | 513 | CLA | C1D-CHD-C4C | -3.70 | 117.43 | 122.48 |
| 38 | e | 102 | HEM | CBD-CAD-C3D | -3.69 | 105.44 | 112.47 |
| 24 | C | 513 | CLA | C1C-C2C-C3C | -3.67 | 102.84 | 106.92 |
| 24 | B | 615 | CLA | O2D-CGD-O1D | -3.67 | 116.44 | 123.82 |
| 24 | c | 509 | CLA | C1C-C2C-C3C | -3.67 | 102.85 | 106.92 |
| 24 | b | 608 | CLA | C1C-C2C-C3C | -3.65 | 102.87 | 106.92 |
| 27 | f | 101 | SQD | C5-C6-S | -3.65 | 109.26 | 114.34 |
| 24 | a | 406 | CLA | C1D-CHD-C4C | -3.63 | 117.52 | 122.48 |
| 27 | a | 411 | SQD | C1-C2-C3 | -3.63 | 103.23 | 109.98 |
| 24 | d | 401 | CLA | CHC-C1C-C2C | -3.62 | 116.77 | 126.65 |
| 24 | A | 409 | CLA | C1C-C2C-C3C | -3.62 | 102.90 | 106.92 |
| 24 | C | 511 | CLA | C1D-CHD-C4C | -3.62 | 117.54 | 122.48 |
| 24 | b | 620 | CLA | O2D-CGD-O1D | -3.62 | 116.54 | 123.82 |
| 24 | b | 608 | CLA | O2D-CGD-O1D | -3.61 | 116.55 | 123.82 |
| 26 | d | 405 | BCR | C24-C23-C22 | -3.61 | 120.79 | 126.21 |
| 24 | c | 511 | CLA | O2D-CGD-O1D | -3.61 | 116.56 | 123.82 |
| 24 | b | 613 | CLA | C1C-C2C-C3C | -3.60 | 102.92 | 106.92 |
| 24 | B | 606 | CLA | C1D-CHD-C4C | -3.60 | 117.56 | 122.48 |
| 24 | c | 508 | CLA | C1D-CHD-C4C | -3.59 | 117.58 | 122.48 |
| 24 | C | 509 | CLA | C1C-C2C-C3C | -3.58 | 102.95 | 106.92 |
| 24 | B | 615 | CLA | O2A-CGA-O1A | -3.58 | 114.67 | 123.55 |
| 24 | B | 609 | CLA | C1D-CHD-C4C | -3.57 | 117.60 | 122.48 |
| 24 | B | 604 | CLA | C1C-C2C-C3C | -3.57 | 102.96 | 106.92 |
| 24 | c | 513 | CLA | C1C-C2C-C3C | -3.57 | 102.97 | 106.92 |
| 24 | D | 403 | CLA | C1C-C2C-C3C | -3.56 | 102.97 | 106.92 |
| 24 | c | 510 | CLA | C1C-C2C-C3C | -3.56 | 102.97 | 106.92 |
| 24 | B | 604 | CLA | C1D-CHD-C4C | -3.55 | 117.63 | 122.48 |
| 24 | C | 508 | CLA | C1D-CHD-C4C | -3.54 | 117.64 | 122.48 |
| 32 | A | 419 | PL9 | C27-C28-C29 | -3.54 | 118.80 | 127.68 |
| 24 | c | 512 | CLA | C1C-C2C-C3C | -3.54 | 103.00 | 106.92 |
| 24 | C | 502 | CLA | O2D-CGD-O1D | -3.53 | 116.71 | 123.82 |
| 24 | D | 404 | CLA | O2D-CGD-O1D | -3.52 | 116.74 | 123.82 |
| 26 | h | 101 | BCR | C38-C26-C25 | -3.52 | 120.57 | 124.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24 | b | 608 | CLA | CAA-C2A-C3A | -3.51 | 103.19 | 112.81 |
| 24 | B | 613 | CLA | C4C-C3C-C2C | -3.51 | 101.53 | 106.91 |
| 24 | c | 507 | CLA | O2D-CGD-O1D | -3.50 | 116.77 | 123.82 |
| 24 | A | 406 | CLA | CBC-CAC-C3C | -3.50 | 102.47 | 112.41 |
| 24 | a | 407 | CLA | C1D-CHD-C4C | -3.50 | 117.70 | 122.48 |
| 24 | c | 504 | CLA | C1C-C2C-C3C | -3.50 | 103.04 | 106.92 |
| 25 | d | 403 | PHO | C4C-C3C-C2C | -3.49 | 102.89 | 106.81 |
| 24 | b | 612 | CLA | C1D-CHD-C4C | -3.49 | 117.72 | 122.48 |
| 32 | a | 416 | PL9 | C22-C23-C24 | -3.49 | 118.92 | 127.68 |
| 24 | C | 503 | CLA | C1C-C2C-C3C | -3.47 | 103.07 | 106.92 |
| 25 | A | 407 | PHO | C4C-C3C-C2C | -3.46 | 102.92 | 106.81 |
| 24 | b | 612 | CLA | C1C-C2C-C3C | -3.46 | 103.08 | 106.92 |
| 24 | c | 515 | CLA | C1C-C2C-C3C | -3.46 | 103.08 | 106.92 |
| 27 | a | 411 | SQD | C5-C6-S | -3.45 | 109.53 | 114.34 |
| 24 | b | 611 | CLA | C1D-CHD-C4C | -3.45 | 117.77 | 122.48 |
| 24 | b | 619 | CLA | CHC-C1C-C2C | -3.45 | 117.25 | 126.65 |
| 24 | B | 607 | CLA | C1C-C2C-C3C | -3.45 | 103.10 | 106.92 |
| 24 | a | 409 | CLA | O2D-CGD-O1D | -3.45 | 116.89 | 123.82 |
| 24 | C | 505 | CLA | O2D-CGD-O1D | -3.44 | 116.89 | 123.82 |
| 24 | B | 612 | CLA | C1-C2-C3 | -3.44 | 119.61 | 125.96 |
| 25 | A | 408 | PHO | C4C-C3C-C2C | -3.44 | 102.94 | 106.81 |
| 27 | A | 411 | SQD | C1-C2-C3 | -3.44 | 103.58 | 109.98 |
| 24 | C | 508 | CLA | C1C-C2C-C3C | -3.44 | 103.11 | 106.92 |
| 24 | b | 619 | CLA | O2D-CGD-O1D | -3.44 | 116.90 | 123.82 |
| 26 | B | 620 | BCR | C38-C26-C25 | -3.44 | 120.66 | 124.51 |
| 24 | c | 511 | CLA | C1C-C2C-C3C | -3.44 | 103.11 | 106.92 |
| 32 | a | 416 | PL9 | C17-C18-C19 | -3.43 | 119.06 | 127.68 |
| 24 | a | 406 | CLA | CHC-C1C-C2C | -3.43 | 117.30 | 126.65 |
| 24 | B | 610 | CLA | C1C-C2C-C3C | -3.43 | 103.12 | 106.92 |
| 24 | b | 620 | CLA | C1C-C2C-C3C | -3.43 | 103.12 | 106.92 |
| 26 | t | 101 | BCR | C33-C5-C6 | -3.42 | 120.68 | 124.51 |
| 24 | b | 606 | CLA | C1C-C2C-C3C | -3.42 | 103.13 | 106.92 |
| 24 | C | 511 | CLA | C1C-C2C-C3C | -3.41 | 103.13 | 106.92 |
| 24 | B | 603 | CLA | CAA-C2A-C3A | -3.41 | 103.45 | 112.81 |
| 26 | b | 622 | BCR | C7-C8-C9 | -3.41 | 121.08 | 126.21 |
| 24 | C | 510 | CLA | C1-C2-C3 | -3.41 | 119.67 | 125.96 |
| 24 | C | 510 | CLA | C1C-C2C-C3C | -3.40 | 103.15 | 106.92 |
| 24 | D | 401 | CLA | CHC-C1C-C2C | -3.40 | 117.38 | 126.65 |
| 24 | a | 409 | CLA | C1C-C2C-C3C | -3.40 | 103.15 | 106.92 |
| 24 | b | 606 | CLA | C1D-CHD-C4C | -3.40 | 117.84 | 122.48 |
| 24 | C | 506 | CLA | C1C-C2C-C3C | -3.39 | 103.16 | 106.92 |
| 24 | b | 615 | CLA | C1C-C2C-C3C | -3.39 | 103.16 | 106.92 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32 | A | 419 | PL9 | C22-C23-C24 | -3.39 | 119.17 | 127.68 |
| 26 | C | 515 | BCR | C38-C26-C25 | -3.38 | 120.73 | 124.51 |
| 24 | C | 502 | CLA | C1C-C2C-C3C | -3.38 | 103.18 | 106.92 |
| 24 | a | 406 | CLA | O2A-CGA-O1A | -3.37 | 115.17 | 123.55 |
| 24 | B | 614 | CLA | C1-C2-C3 | -3.37 | 119.75 | 125.96 |
| 25 | d | 403 | PHO | O2D-CGD-O1D | -3.37 | 117.04 | 123.82 |
| 24 | B | 612 | CLA | O2D-CGD-O1D | -3.37 | 117.04 | 123.82 |
| 26 | Y | 101 | BCR | C38-C26-C25 | -3.37 | 120.74 | 124.51 |
| 32 | a | 416 | PL9 | C32-C33-C34 | -3.37 | 119.22 | 127.68 |
| 24 | D | 403 | CLA | C1-C2-C3 | -3.37 | 119.75 | 125.96 |
| 24 | c | 514 | CLA | CBC-CAC-C3C | -3.36 | 102.86 | 112.41 |
| 24 | C | 509 | CLA | O2A-CGA-O1A | -3.36 | 115.21 | 123.55 |
| 24 | c | 510 | CLA | O2D-CGD-O1D | -3.36 | 117.06 | 123.82 |
| 24 | B | 602 | CLA | C1C-C2C-C3C | -3.36 | 103.20 | 106.92 |
| 24 | c | 511 | CLA | C1-C2-C3 | -3.35 | 119.78 | 125.96 |
| 24 | C | 504 | CLA | C1C-C2C-C3C | -3.35 | 103.20 | 106.92 |
| 24 | B | 612 | CLA | C1D-CHD-C4C | -3.35 | 117.90 | 122.48 |
| 24 | C | 506 | CLA | O2D-CGD-O1D | -3.34 | 117.09 | 123.82 |
| 24 | b | 607 | CLA | O2D-CGD-O1D | -3.34 | 117.10 | 123.82 |
| 24 | c | 510 | CLA | C1D-CHD-C4C | -3.33 | 117.93 | 122.48 |
| 36 | C | 519 | DGD | O3G-C3G-C2G | -3.33 | 103.07 | 110.99 |
| 24 | b | 607 | CLA | CAA-C2A-C3A | -3.33 | 103.69 | 112.81 |
| 24 | A | 405 | CLA | CAA-C2A-C3A | -3.32 | 103.70 | 112.81 |
| 24 | c | 508 | CLA | C1C-C2C-C3C | -3.32 | 103.23 | 106.92 |
| 26 | c | 516 | BCR | C38-C26-C25 | -3.32 | 120.79 | 124.51 |
| 24 | b | 621 | CLA | CHC-C1C-C2C | -3.32 | 117.60 | 126.65 |
| 27 | a | 411 | SQD | C45-O47-C7 | -3.32 | 110.04 | 117.88 |
| 24 | D | 404 | CLA | C1C-C2C-C3C | -3.31 | 103.24 | 106.92 |
| 24 | b | 618 | CLA | C1D-CHD-C4C | -3.31 | 117.96 | 122.48 |
| 24 | b | 610 | CLA | C1D-CHD-C4C | -3.31 | 117.96 | 122.48 |
| 24 | B | 617 | CLA | C4C-C3C-C2C | -3.31 | 101.84 | 106.91 |
| 24 | b | 607 | CLA | C4C-C3C-C2C | -3.31 | 101.84 | 106.91 |
| 37 | D | 408 | LHG | O8-C23-O10 | -3.30 | 115.34 | 123.55 |
| 24 | B | 617 | CLA | C1D-CHD-C4C | -3.30 | 117.97 | 122.48 |
| 24 | d | 404 | CLA | C1C-C2C-C3C | -3.29 | 103.27 | 106.92 |
| 24 | b | 610 | CLA | OBD-CAD-C3D | -3.29 | 121.96 | 128.03 |
| 24 | b | 609 | CLA | O1D-CGD-CBD | -3.29 | 118.70 | 124.60 |
| 24 | B | 617 | CLA | CHC-C1C-C2C | -3.29 | 117.69 | 126.65 |
| 24 | C | 514 | CLA | C1D-CHD-C4C | -3.28 | 118.00 | 122.48 |
| 24 | B | 603 | CLA | C1D-CHD-C4C | -3.28 | 118.00 | 122.48 |
| 25 | d | 403 | PHO | CHC-C1C-C2C | -3.27 | 118.11 | 125.62 |
| 24 | a | 407 | CLA | C1C-C2C-C3C | -3.27 | 103.29 | 106.92 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32 | A | 419 | PL9 | C37-C38-C39 | -3.27 | 119.46 | 127.68 |
| 24 | D | 403 | CLA | C4C-C3C-C2C | -3.27 | 101.89 | 106.91 |
| 24 | a | 409 | CLA | CHC-C1C-C2C | -3.27 | 117.73 | 126.65 |
| 24 | A | 406 | CLA | C1D-CHD-C4C | -3.27 | 118.02 | 122.48 |
| 32 | a | 416 | PL9 | C7-C8-C9 | -3.27 | 121.25 | 126.71 |
| 24 | B | 604 | CLA | CAA-C2A-C3A | -3.27 | 103.86 | 112.81 |
| 24 | C | 513 | CLA | C1D-CHD-C4C | -3.27 | 118.02 | 122.48 |
| 24 | C | 512 | CLA | C1C-C2C-C3C | -3.26 | 103.30 | 106.92 |
| 24 | c | 508 | CLA | CHC-C1C-C2C | -3.26 | 117.75 | 126.65 |
| 24 | b | 614 | CLA | C1D-CHD-C4C | -3.26 | 118.03 | 122.48 |
| 25 | A | 407 | PHO | C1-C2-C3 | -3.26 | 119.95 | 125.96 |
| 24 | b | 615 | CLA | C1D-CHD-C4C | -3.26 | 118.03 | 122.48 |
| 24 | d | 401 | CLA | CMA-C3A-C2A | -3.26 | 100.55 | 113.77 |
| 24 | B | 611 | CLA | C4C-C3C-C2C | -3.26 | 101.91 | 106.91 |
| 24 | C | 503 | CLA | O2A-CGA-O1A | -3.25 | 115.47 | 123.55 |
| 24 | b | 610 | CLA | O2A-CGA-O1A | -3.25 | 115.49 | 123.55 |
| 24 | c | 513 | CLA | CHC-C1C-C2C | -3.24 | 117.80 | 126.65 |
| 24 | C | 509 | CLA | CHC-C1C-C2C | -3.24 | 117.81 | 126.65 |
| 24 | C | 512 | CLA | C1D-CHD-C4C | -3.23 | 118.07 | 122.48 |
| 24 | B | 602 | CLA | C1D-CHD-C4C | -3.23 | 118.07 | 122.48 |
| 24 | B | 603 | CLA | C4C-C3C-C2C | -3.23 | 101.96 | 106.91 |
| 26 | C | 516 | BCR | C24-C23-C22 | -3.22 | 121.38 | 126.21 |
| 32 | a | 416 | PL9 | C37-C38-C39 | -3.22 | 119.60 | 127.68 |
| 25 | A | 408 | PHO | C4D-ND-C1D | -3.21 | 101.18 | 106.98 |
| 24 | B | 614 | CLA | CHC-C1C-C2C | -3.21 | 117.90 | 126.65 |
| 24 | B | 605 | CLA | C1D-CHD-C4C | -3.20 | 118.11 | 122.48 |
| 27 | A | 411 | SQD | C45-O47-C7 | -3.20 | 110.32 | 117.88 |
| 24 | b | 615 | CLA | CAA-C2A-C3A | -3.20 | 104.05 | 112.81 |
| 24 | b | 613 | CLA | C1-C2-C3 | -3.19 | 120.09 | 125.96 |
| 24 | b | 611 | CLA | C1C-C2C-C3C | -3.18 | 103.39 | 106.92 |
| 24 | B | 616 | CLA | C4C-C3C-C2C | -3.18 | 102.03 | 106.91 |
| 24 | b | 621 | CLA | C1C-C2C-C3C | -3.18 | 103.39 | 106.92 |
| 24 | B | 611 | CLA | O2D-CGD-O1D | -3.18 | 117.42 | 123.82 |
| 24 | C | 507 | CLA | C1D-CHD-C4C | -3.18 | 118.14 | 122.48 |
| 24 | B | 603 | CLA | CHC-C1C-C2C | -3.18 | 117.98 | 126.65 |
| 24 | B | 612 | CLA | C1C-C2C-C3C | -3.18 | 103.40 | 106.92 |
| 24 | b | 618 | CLA | C4C-C3C-C2C | -3.17 | 102.04 | 106.91 |
| 24 | A | 406 | CLA | CAA-C2A-C3A | -3.16 | 104.14 | 112.81 |
| 24 | C | 514 | CLA | C1C-C2C-C3C | -3.16 | 103.42 | 106.92 |
| 24 | b | 616 | CLA | C1C-C2C-C3C | -3.16 | 103.42 | 106.92 |
| 24 | c | 505 | CLA | C1C-C2C-C3C | -3.16 | 103.42 | 106.92 |
| 24 | B | 604 | CLA | C4C-C3C-C2C | -3.16 | 102.07 | 106.91 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24 | c | 507 | CLA | C4C-C3C-C2C | -3.16 | 102.07 | 106.91 |
| 24 | b | 612 | CLA | C4C-C3C-C2C | -3.15 | 102.08 | 106.91 |
| 24 | a | 409 | CLA | C4C-C3C-C2C | -3.15 | 102.08 | 106.91 |
| 24 | c | 515 | CLA | C1D-CHD-C4C | -3.14 | 118.19 | 122.48 |
| 24 | b | 611 | CLA | O2D-CGD-O1D | -3.14 | 117.50 | 123.82 |
| 24 | C | 507 | CLA | CHC-C1C-C2C | -3.14 | 118.08 | 126.65 |
| 24 | b | 616 | CLA | C4C-C3C-C2C | -3.14 | 102.09 | 106.91 |
| 24 | B | 606 | CLA | O2D-CGD-O1D | -3.14 | 117.50 | 123.82 |
| 24 | B | 616 | CLA | C1C-C2C-C3C | -3.14 | 103.44 | 106.92 |
| 24 | b | 621 | CLA | C1D-CHD-C4C | -3.13 | 118.20 | 122.48 |
| 24 | B | 605 | CLA | O2A-CGA-O1A | -3.13 | 115.78 | 123.55 |
| 25 | A | 408 | PHO | CHC-C1C-C2C | -3.13 | 118.44 | 125.62 |
| 24 | a | 407 | CLA | CAA-C2A-C3A | -3.13 | 104.23 | 112.81 |
| 24 | C | 506 | CLA | C4C-C3C-C2C | -3.13 | 102.11 | 106.91 |
| 24 | B | 611 | CLA | C1C-C2C-C3C | -3.13 | 103.45 | 106.92 |
| 24 | C | 509 | CLA | C1D-CHD-C4C | -3.12 | 118.22 | 122.48 |
| 24 | a | 406 | CLA | CAA-C2A-C3A | -3.12 | 104.26 | 112.81 |
| 32 | D | 406 | PL9 | C42-C43-C44 | -3.12 | 119.85 | 127.68 |
| 26 | k | 103 | BCR | C33-C5-C6 | -3.12 | 121.02 | 124.51 |
| 24 | c | 506 | CLA | C1D-CHD-C4C | -3.12 | 118.23 | 122.48 |
| 32 | A | 419 | PL9 | C7-C8-C9 | -3.11 | 121.50 | 126.71 |
| 24 | B | 603 | CLA | C1C-C2C-C3C | -3.11 | 103.47 | 106.92 |
| 26 | d | 405 | BCR | C3-C4-C5 | -3.11 | 108.44 | 113.78 |
| 24 | C | 509 | CLA | O2D-CGD-O1D | -3.11 | 117.57 | 123.82 |
| 26 | H | 101 | BCR | C7-C8-C9 | -3.11 | 121.55 | 126.21 |
| 24 | b | 614 | CLA | O2D-CGD-O1D | -3.10 | 117.57 | 123.82 |
| 24 | c | 508 | CLA | CAA-C2A-C3A | -3.09 | 104.34 | 112.81 |
| 24 | b | 618 | CLA | CHC-C1C-C2C | -3.09 | 118.23 | 126.65 |
| 24 | c | 504 | CLA | CHC-C1C-C2C | -3.08 | 118.24 | 126.65 |
| 24 | c | 509 | CLA | C4C-C3C-C2C | -3.08 | 102.18 | 106.91 |
| 24 | c | 507 | CLA | C1C-C2C-C3C | -3.08 | 103.50 | 106.92 |
| 24 | c | 504 | CLA | C1-C2-C3 | -3.08 | 120.28 | 125.96 |
| 24 | A | 406 | CLA | O2A-CGA-O1A | -3.08 | 115.90 | 123.55 |
| 24 | b | 612 | CLA | CAA-C2A-C3A | -3.08 | 104.37 | 112.81 |
| 24 | b | 620 | CLA | CHC-C1C-C2C | -3.08 | 118.26 | 126.65 |
| 24 | D | 401 | CLA | CBC-CAC-C3C | -3.07 | 103.68 | 112.41 |
| 24 | B | 609 | CLA | CMA-C3A-C4A | -3.07 | 103.51 | 111.77 |
| 24 | C | 504 | CLA | C4C-C3C-C2C | -3.07 | 102.19 | 106.91 |
| 24 | C | 503 | CLA | C1D-CHD-C4C | -3.07 | 118.29 | 122.48 |
| 25 | A | 408 | PHO | CHD-C1D-C2D | -3.07 | 118.58 | 125.62 |
| 24 | d | 402 | CLA | C1-C2-C3 | -3.07 | 120.31 | 125.96 |
| 24 | b | 621 | CLA | C4C-C3C-C2C | -3.06 | 102.21 | 106.91 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24 | a | 409 | CLA | C1-C2-C3 | -3.06 | 120.32 | 125.96 |
| 24 | C | 506 | CLA | CHC-C1C-C2C | -3.05 | 118.32 | 126.65 |
| 24 | b | 615 | CLA | C4C-C3C-C2C | -3.05 | 102.23 | 106.91 |
| 24 | b | 617 | CLA | O2D-CGD-O1D | -3.05 | 117.69 | 123.82 |
| 26 | K | 101 | BCR | C20-C21-C22 | -3.04 | 122.97 | 127.31 |
| 32 | a | 416 | PL9 | C27-C28-C29 | -3.04 | 120.05 | 127.68 |
| 24 | B | 615 | CLA | C2A-C1A-CHA | -3.04 | 118.53 | 123.92 |
| 24 | c | 503 | CLA | C1D-CHD-C4C | -3.04 | 118.33 | 122.48 |
| 24 | C | 505 | CLA | C1D-CHD-C4C | -3.03 | 118.34 | 122.48 |
| 24 | a | 407 | CLA | O2D-CGD-O1D | -3.03 | 117.72 | 123.82 |
| 24 | B | 616 | CLA | CHC-C1C-C2C | -3.03 | 118.38 | 126.65 |
| 26 | k | 103 | BCR | C38-C26-C25 | -3.03 | 121.11 | 124.51 |
| 26 | c | 526 | BCR | C15-C14-C13 | -3.03 | 122.98 | 127.31 |
| 24 | D | 404 | CLA | C4C-C3C-C2C | -3.03 | 102.26 | 106.91 |
| 24 | C | 511 | CLA | O1D-CGD-CBD | -3.03 | 119.16 | 124.60 |
| 27 | A | 411 | SQD | C1-O5-C5 | -3.03 | 108.01 | 113.72 |
| 24 | d | 402 | CLA | O2A-CGA-O1A | -3.02 | 116.05 | 123.55 |
| 24 | B | 611 | CLA | CAA-C2A-C3A | -3.02 | 104.53 | 112.81 |
| 24 | C | 512 | CLA | CHC-C1C-C2C | -3.02 | 118.41 | 126.65 |
| 24 | B | 610 | CLA | O2D-CGD-O1D | -3.02 | 117.74 | 123.82 |
| 24 | D | 401 | CLA | O2A-CGA-O1A | -3.02 | 116.06 | 123.55 |
| 24 | C | 510 | CLA | CHC-C1C-C2C | -3.02 | 118.42 | 126.65 |
| 26 | A | 410 | BCR | C33-C5-C6 | -3.02 | 121.13 | 124.51 |
| 36 | c | 518 | DGD | C2G-O2G-C1B | -3.02 | 110.75 | 117.88 |
| 24 | C | 512 | CLA | C4C-C3C-C2C | -3.02 | 102.28 | 106.91 |
| 32 | a | 416 | PL9 | C42-C43-C44 | -3.01 | 120.11 | 127.68 |
| 24 | B | 603 | CLA | O2D-CGD-O1D | -3.01 | 117.76 | 123.82 |
| 24 | b | 616 | CLA | CHC-C1C-C2C | -3.01 | 118.44 | 126.65 |
| 24 | c | 512 | CLA | C1D-CHD-C4C | -3.01 | 118.37 | 122.48 |
| 24 | c | 503 | CLA | CHC-C1C-C2C | -3.01 | 118.45 | 126.65 |
| 27 | F | 101 | SQD | C1-C2-C3 | -3.00 | 104.39 | 109.98 |
| 24 | c | 507 | CLA | C1D-CHD-C4C | -3.00 | 118.38 | 122.48 |
| 24 | B | 617 | CLA | O2D-CGD-O1D | -3.00 | 117.78 | 123.82 |
| 24 | b | 614 | CLA | CHC-C1C-C2C | -3.00 | 118.46 | 126.65 |
| 24 | A | 405 | CLA | C4C-C3C-C2C | -3.00 | 102.31 | 106.91 |
| 24 | b | 617 | CLA | C2A-C1A-CHA | -3.00 | 118.61 | 123.92 |
| 24 | b | 612 | CLA | CHC-C1C-C2C | -2.99 | 118.48 | 126.65 |
| 25 | A | 407 | PHO | C1C-C2C-C3C | -2.99 | 103.04 | 106.51 |
| 26 | c | 516 | BCR | C31-C1-C6 | -2.99 | 105.46 | 110.31 |
| 27 | A | 416 | SQD | C5-C6-S | -2.99 | 110.17 | 114.34 |
| 27 | b | 601 | SQD | C1-C2-C3 | -2.99 | 104.43 | 109.98 |
| 24 | B | 613 | CLA | C1C-C2C-C3C | -2.98 | 103.61 | 106.92 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24 | B | 609 | CLA | CHC-C1C-C2C | -2.98 | 118.52 | 126.65 |
| 24 | B | 612 | CLA | C4C-C3C-C2C | -2.98 | 102.34 | 106.91 |
| 25 | a | 408 | PHO | O1D-CGD-CBD | -2.98 | 119.25 | 124.60 |
| 37 | D | 409 | LHG | O8-C23-O10 | -2.98 | 116.16 | 123.55 |
| 24 | A | 406 | CLA | CHC-C1C-C2C | -2.98 | 118.53 | 126.65 |
| 24 | c | 503 | CLA | OBD-CAD-C3D | -2.97 | 122.55 | 128.03 |
| 26 | A | 410 | BCR | C15-C14-C13 | -2.97 | 123.07 | 127.31 |
| 24 | c | 511 | CLA | CHC-C1C-C2C | -2.97 | 118.54 | 126.65 |
| 24 | C | 514 | CLA | C1-C2-C3 | -2.97 | 120.48 | 125.96 |
| 24 | B | 613 | CLA | O2D-CGD-O1D | -2.97 | 117.84 | 123.82 |
| 24 | A | 405 | CLA | CAA-C2A-C1A | -2.97 | 102.25 | 111.97 |
| 36 | c | 517 | DGD | C2G-O2G-C1B | -2.96 | 110.88 | 117.88 |
| 24 | c | 505 | CLA | C4C-C3C-C2C | -2.96 | 102.37 | 106.91 |
| 25 | A | 407 | PHO | C4D-ND-C1D | -2.96 | 101.64 | 106.98 |
| 34 | Z | 101 | LMG | C7-O1-C1 | -2.96 | 107.69 | 113.76 |
| 24 | B | 616 | CLA | O2D-CGD-O1D | -2.96 | 117.87 | 123.82 |
| 24 | B | 610 | CLA | CHC-C1C-C2C | -2.96 | 118.59 | 126.65 |
| 24 | d | 404 | CLA | CAA-C2A-C3A | -2.96 | 104.71 | 112.81 |
| 24 | C | 503 | CLA | C4C-C3C-C2C | -2.95 | 102.38 | 106.91 |
| 24 | B | 604 | CLA | O2A-CGA-O1A | -2.95 | 116.22 | 123.55 |
| 24 | C | 510 | CLA | C4C-C3C-C2C | -2.95 | 102.38 | 106.91 |
| 24 | C | 511 | CLA | C1-C2-C3 | -2.95 | 120.52 | 125.96 |
| 24 | c | 504 | CLA | C1D-CHD-C4C | -2.95 | 118.45 | 122.48 |
| 24 | B | 602 | CLA | C4C-C3C-C2C | -2.95 | 102.39 | 106.91 |
| 24 | b | 617 | CLA | C1-C2-C3 | -2.94 | 120.53 | 125.96 |
| 24 | d | 402 | CLA | CHC-C1C-C2C | -2.94 | 118.63 | 126.65 |
| 24 | B | 609 | CLA | C4C-C3C-C2C | -2.94 | 102.40 | 106.91 |
| 24 | C | 514 | CLA | C4C-C3C-C2C | -2.94 | 102.40 | 106.91 |
| 26 | B | 620 | BCR | C24-C23-C22 | -2.94 | 121.80 | 126.21 |
| 24 | d | 402 | CLA | C2A-C1A-CHA | -2.93 | 118.72 | 123.92 |
| 24 | C | 504 | CLA | CHC-C1C-C2C | -2.93 | 118.65 | 126.65 |
| 24 | C | 507 | CLA | CAA-C2A-C3A | -2.93 | 104.77 | 112.81 |
| 24 | c | 509 | CLA | CHC-C1C-C2C | -2.93 | 118.66 | 126.65 |
| 24 | B | 611 | CLA | CHC-C1C-C2C | -2.93 | 118.66 | 126.65 |
| 24 | B | 607 | CLA | O2D-CGD-O1D | -2.93 | 117.93 | 123.82 |
| 24 | d | 401 | CLA | C2A-C1A-CHA | -2.93 | 118.73 | 123.92 |
| 26 | Y | 101 | BCR | C15-C14-C13 | -2.92 | 123.14 | 127.31 |
| 24 | c | 506 | CLA | CHC-C1C-C2C | -2.92 | 118.68 | 126.65 |
| 24 | c | 514 | CLA | O2D-CGD-O1D | -2.92 | 117.94 | 123.82 |
| 24 | C | 514 | CLA | O2D-CGD-O1D | -2.92 | 117.95 | 123.82 |
| 24 | A | 409 | CLA | C2A-C1A-CHA | -2.92 | 118.74 | 123.92 |
| 24 | C | 502 | CLA | C4C-C3C-C2C | -2.92 | 102.43 | 106.91 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24 | A | 405 | CLA | C2A-C1A-CHA | -2.92 | 118.75 | 123.92 |
| 26 | Y | 101 | BCR | C16-C17-C18 | -2.91 | 123.15 | 127.31 |
| 24 | C | 507 | CLA | O2D-CGD-O1D | -2.91 | 117.96 | 123.82 |
| 24 | c | 504 | CLA | C4C-C3C-C2C | -2.91 | 102.44 | 106.91 |
| 24 | B | 605 | CLA | C1-C2-C3 | -2.91 | 120.59 | 125.96 |
| 24 | c | 510 | CLA | C4C-C3C-C2C | -2.91 | 102.44 | 106.91 |
| 24 | c | 507 | CLA | CHC-C1C-C2C | -2.91 | 118.72 | 126.65 |
| 24 | b | 620 | CLA | C4C-C3C-C2C | -2.91 | 102.45 | 106.91 |
| 32 | A | 419 | PL9 | C42-C43-C44 | -2.90 | 120.39 | 127.68 |
| 37 | L | 101 | LHG | C6-C5-C4 | -2.90 | 105.32 | 111.86 |
| 24 | B | 612 | CLA | CHC-C1C-C2C | -2.90 | 118.75 | 126.65 |
| 24 | b | 611 | CLA | C4C-C3C-C2C | -2.90 | 102.46 | 106.91 |
| 24 | C | 508 | CLA | C4C-C3C-C2C | -2.90 | 102.47 | 106.91 |
| 24 | D | 404 | CLA | C1D-CHD-C4C | -2.90 | 118.53 | 122.48 |
| 24 | b | 610 | CLA | CHC-C1C-C2C | -2.90 | 118.75 | 126.65 |
| 24 | c | 515 | CLA | CHC-C1C-C2C | -2.90 | 118.75 | 126.65 |
| 26 | D | 405 | BCR | C28-C27-C26 | -2.89 | 108.81 | 113.78 |
| 24 | B | 608 | CLA | CAA-C2A-C3A | -2.89 | 104.89 | 112.81 |
| 24 | B | 611 | CLA | C1-C2-C3 | -2.89 | 120.64 | 125.96 |
| 24 | C | 509 | CLA | C4C-C3C-C2C | -2.89 | 102.48 | 106.91 |
| 25 | a | 408 | PHO | C4D-ND-C1D | -2.89 | 101.77 | 106.98 |
| 26 | C | 515 | BCR | C16-C17-C18 | -2.88 | 123.19 | 127.31 |
| 24 | B | 617 | CLA | C1C-C2C-C3C | -2.88 | 103.72 | 106.92 |
| 24 | c | 509 | CLA | O1D-CGD-CBD | -2.88 | 119.44 | 124.60 |
| 26 | K | 101 | BCR | C37-C22-C21 | -2.87 | 118.90 | 122.92 |
| 26 | b | 624 | BCR | C38-C26-C25 | -2.87 | 121.29 | 124.51 |
| 24 | c | 515 | CLA | CAA-C2A-C3A | -2.87 | 104.94 | 112.81 |
| 24 | B | 616 | CLA | C1D-CHD-C4C | -2.87 | 118.56 | 122.48 |
| 32 | d | 406 | PL9 | C7-C3-C4 | -2.86 | 114.55 | 116.88 |
| 24 | b | 606 | CLA | C4C-C3C-C2C | -2.86 | 102.52 | 106.91 |
| 37 | E | 101 | LHG | C5-O7-C7 | -2.86 | 111.12 | 117.88 |
| 24 | D | 404 | CLA | CHC-C1C-C2C | -2.86 | 118.86 | 126.65 |
| 24 | d | 401 | CLA | CAA-C2A-C3A | -2.85 | 104.99 | 112.81 |
| 26 | b | 622 | BCR | C15-C14-C13 | -2.85 | 123.24 | 127.31 |
| 30 | I | 102 | LMT | C2'-C3'-C4' | -2.85 | 103.69 | 109.61 |
| 24 | B | 610 | CLA | C4C-C3C-C2C | -2.85 | 102.53 | 106.91 |
| 24 | b | 608 | CLA | CMA-C3A-C2A | -2.85 | 102.21 | 113.77 |
| 24 | a | 407 | CLA | OBD-CAD-C3D | -2.85 | 122.78 | 128.03 |
| 32 | d | 406 | PL9 | C7-C8-C9 | -2.85 | 121.95 | 126.71 |
| 24 | c | 508 | CLA | C4C-C3C-C2C | -2.85 | 102.54 | 106.91 |
| 24 | b | 608 | CLA | C2A-C1A-CHA | -2.84 | 118.88 | 123.92 |
| 24 | B | 610 | CLA | CMA-C3A-C4A | -2.84 | 104.14 | 111.77 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 26 | h | 101 | BCR | C16-C17-C18 | -2.84 | 123.25 | 127.31 |
| 24 | a | 407 | CLA | CBC-CAC-C3C | -2.84 | 104.34 | 112.41 |
| 24 | C | 505 | CLA | CHC-C1C-C2C | -2.84 | 118.91 | 126.65 |
| 24 | B | 605 | CLA | O2D-CGD-O1D | -2.84 | 118.11 | 123.82 |
| 24 | B | 605 | CLA | CHC-C1C-C2C | -2.84 | 118.92 | 126.65 |
| 24 | d | 402 | CLA | C4C-C3C-C2C | -2.83 | 102.57 | 106.91 |
| 24 | d | 404 | CLA | C4C-C3C-C2C | -2.83 | 102.57 | 106.91 |
| 27 | b | 601 | SQD | C44-O6-C1 | -2.83 | 107.96 | 113.76 |
| 24 | C | 502 | CLA | CBC-CAC-C3C | -2.82 | 104.39 | 112.41 |
| 24 | b | 617 | CLA | OBD-CAD-C3D | -2.82 | 122.83 | 128.03 |
| 24 | B | 606 | CLA | CHC-C1C-C2C | -2.82 | 118.95 | 126.65 |
| 24 | b | 607 | CLA | C1C-C2C-C3C | -2.82 | 103.79 | 106.92 |
| 24 | c | 503 | CLA | O2A-CGA-O1A | -2.82 | 116.55 | 123.55 |
| 24 | b | 619 | CLA | C1D-CHD-C4C | -2.82 | 118.63 | 122.48 |
| 24 | c | 509 | CLA | C1D-CHD-C4C | -2.82 | 118.63 | 122.48 |
| 24 | c | 513 | CLA | C1-C2-C3 | -2.82 | 120.77 | 125.96 |
| 24 | b | 616 | CLA | O2D-CGD-O1D | -2.82 | 118.15 | 123.82 |
| 30 | m | 102 | LMT | C1'-O5'-C5' | -2.81 | 108.41 | 113.72 |
| 24 | b | 606 | CLA | CHC-C1C-C2C | -2.81 | 118.98 | 126.65 |
| 24 | D | 403 | CLA | CHC-C1C-C2C | -2.81 | 118.98 | 126.65 |
| 24 | c | 514 | CLA | CHC-C1C-C2C | -2.81 | 118.99 | 126.65 |
| 24 | c | 514 | CLA | C1D-CHD-C4C | -2.81 | 118.64 | 122.48 |
| 24 | b | 615 | CLA | CHC-C1C-C2C | -2.81 | 119.00 | 126.65 |
| 24 | B | 608 | CLA | CHC-C1C-C2C | -2.81 | 119.00 | 126.65 |
| 24 | C | 513 | CLA | CHC-C1C-C2C | -2.80 | 119.00 | 126.65 |
| 24 | c | 503 | CLA | C4C-C3C-C2C | -2.80 | 102.61 | 106.91 |
| 24 | C | 511 | CLA | C4C-C3C-C2C | -2.80 | 102.61 | 106.91 |
| 38 | E | 103 | HEM | CBA-CAA-C2A | -2.80 | 107.13 | 112.48 |
| 24 | c | 509 | CLA | O2A-CGA-O1A | -2.80 | 116.60 | 123.55 |
| 26 | y | 101 | BCR | C28-C27-C26 | -2.80 | 108.97 | 113.78 |
| 27 | A | 411 | SQD | C44-O6-C1 | -2.79 | 108.03 | 113.76 |
| 24 | b | 616 | CLA | C1-C2-C3 | -2.79 | 120.82 | 125.96 |
| 24 | b | 613 | CLA | C4C-C3C-C2C | -2.79 | 102.63 | 106.91 |
| 24 | b | 620 | CLA | C1D-CHD-C4C | -2.79 | 118.67 | 122.48 |
| 34 | j | 101 | LMG | O8-C28-O10 | -2.79 | 116.63 | 123.55 |
| 24 | c | 511 | CLA | C4C-C3C-C2C | -2.79 | 102.63 | 106.91 |
| 24 | d | 402 | CLA | C4A-NA-C1A | -2.79 | 102.99 | 106.45 |
| 24 | B | 615 | CLA | CHC-C1C-C2C | -2.79 | 119.05 | 126.65 |
| 24 | c | 512 | CLA | O1D-CGD-CBD | -2.78 | 119.60 | 124.60 |
| 24 | d | 404 | CLA | C1D-CHD-C4C | -2.78 | 118.68 | 122.48 |
| 24 | B | 606 | CLA | C4C-C3C-C2C | -2.78 | 102.64 | 106.91 |
| 24 | C | 514 | CLA | CHC-C1C-C2C | -2.78 | 119.08 | 126.65 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24 | a | 409 | CLA | CAA-C2A-C3A | -2.78 | 105.20 | 112.81 |
| 24 | c | 515 | CLA | C4C-C3C-C2C | -2.78 | 102.65 | 106.91 |
| 25 | d | 403 | PHO | CHD-C1D-C2D | -2.77 | 119.26 | 125.62 |
| 26 | h | 101 | BCR | C11-C10-C9 | -2.77 | 123.35 | 127.31 |
| 24 | a | 406 | CLA | CAA-C2A-C1A | -2.77 | 102.89 | 111.97 |
| 24 | C | 510 | CLA | C1D-CHD-C4C | -2.77 | 118.69 | 122.48 |
| 24 | C | 502 | CLA | CHC-C1C-C2C | -2.77 | 119.09 | 126.65 |
| 24 | C | 502 | CLA | O2A-CGA-O1A | -2.77 | 116.67 | 123.55 |
| 24 | B | 608 | CLA | OBD-CAD-C3D | -2.77 | 122.92 | 128.03 |
| 24 | C | 503 | CLA | CHC-C1C-C2C | -2.77 | 119.10 | 126.65 |
| 24 | A | 409 | CLA | C4C-C3C-C2C | -2.77 | 102.66 | 106.91 |
| 24 | B | 608 | CLA | C2A-C1A-CHA | -2.77 | 119.01 | 123.92 |
| 24 | B | 604 | CLA | C2A-C1A-CHA | -2.77 | 119.02 | 123.92 |
| 24 | B | 602 | CLA | CHC-C1C-C2C | -2.76 | 119.12 | 126.65 |
| 24 | b | 606 | CLA | O2D-CGD-O1D | -2.76 | 118.27 | 123.82 |
| 34 | C | 521 | LMG | C8-O7-C10 | -2.76 | 111.36 | 117.88 |
| 26 | c | 516 | BCR | C15-C14-C13 | -2.75 | 123.38 | 127.31 |
| 24 | b | 616 | CLA | C2A-C1A-CHA | -2.75 | 119.04 | 123.92 |
| 26 | y | 101 | BCR | C16-C17-C18 | -2.75 | 123.39 | 127.31 |
| 24 | B | 607 | CLA | C4C-C3C-C2C | -2.75 | 102.69 | 106.91 |
| 24 | D | 404 | CLA | O2A-CGA-O1A | -2.75 | 116.73 | 123.55 |
| 24 | B | 606 | CLA | C2A-C1A-CHA | -2.75 | 119.05 | 123.92 |
| 36 | C | 517 | DGD | O1G-C1A-O1A | -2.74 | 116.74 | 123.55 |
| 24 | A | 409 | CLA | CAA-C2A-C3A | -2.74 | 105.29 | 112.81 |
| 24 | B | 610 | CLA | C1-C2-C3 | -2.74 | 120.90 | 125.96 |
| 24 | B | 613 | CLA | CHC-C1C-C2C | -2.74 | 119.17 | 126.65 |
| 24 | C | 507 | CLA | CBC-CAC-C3C | -2.74 | 104.63 | 112.41 |
| 24 | C | 503 | CLA | C1-C2-C3 | -2.74 | 120.91 | 125.96 |
| 24 | a | 407 | CLA | C4C-C3C-C2C | -2.74 | 102.71 | 106.91 |
| 36 | c | 517 | DGD | O1G-C1A-O1A | -2.74 | 116.75 | 123.55 |
| 24 | C | 513 | CLA | C4C-C3C-C2C | -2.74 | 102.71 | 106.91 |
| 24 | b | 607 | CLA | CHC-C1C-C2C | -2.74 | 119.19 | 126.65 |
| 24 | C | 511 | CLA | CHC-C1C-C2C | -2.74 | 119.19 | 126.65 |
| 37 | D | 409 | LHG | C5-O7-C7 | -2.73 | 111.41 | 117.88 |
| 24 | c | 512 | CLA | CHC-C1C-C2C | -2.73 | 119.19 | 126.65 |
| 24 | b | 617 | CLA | C1D-CHD-C4C | -2.73 | 118.75 | 122.48 |
| 24 | c | 512 | CLA | CBC-CAC-C3C | -2.73 | 104.66 | 112.41 |
| 24 | C | 514 | CLA | C2A-C1A-CHA | -2.73 | 119.08 | 123.92 |
| 24 | b | 610 | CLA | C2A-C1A-CHA | -2.73 | 119.08 | 123.92 |
| 24 | A | 405 | CLA | CHC-C1C-C2C | -2.73 | 119.21 | 126.65 |
| 26 | D | 405 | BCR | C15-C14-C13 | -2.73 | 123.42 | 127.31 |
| 24 | b | 613 | CLA | O2D-CGD-O1D | -2.72 | 118.34 | 123.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25 | d | 403 | PHO | C1C-C2C-C3C | -2.72 | 103.35 | 106.51 |
| 24 | d | 401 | CLA | C4C-C3C-C2C | -2.72 | 102.74 | 106.91 |
| 24 | A | 405 | CLA | C4A-NA-C1A | -2.72 | 103.08 | 106.45 |
| 24 | B | 613 | CLA | C2A-C1A-CHA | -2.72 | 119.10 | 123.92 |
| 24 | c | 512 | CLA | C4C-C3C-C2C | -2.72 | 102.74 | 106.91 |
| 25 | A | 408 | PHO | O2D-CGD-O1D | -2.72 | 118.35 | 123.82 |
| 24 | b | 609 | CLA | C4C-C3C-C2C | -2.71 | 102.75 | 106.91 |
| 26 | K | 101 | BCR | C24-C23-C22 | -2.71 | 122.14 | 126.21 |
| 24 | b | 612 | CLA | O2A-CGA-O1A | -2.71 | 116.82 | 123.55 |
| 24 | c | 505 | CLA | O2A-CGA-O1A | -2.71 | 116.82 | 123.55 |
| 27 | a | 411 | SQD | C44-O6-C1 | -2.71 | 108.20 | 113.76 |
| 24 | B | 615 | CLA | CBC-CAC-C3C | -2.71 | 104.72 | 112.41 |
| 24 | b | 606 | CLA | C2A-C1A-CHA | -2.71 | 119.11 | 123.92 |
| 27 | b | 601 | SQD | O47-C7-O49 | -2.71 | 116.93 | 123.68 |
| 24 | B | 605 | CLA | C4C-C3C-C2C | -2.71 | 102.76 | 106.91 |
| 24 | C | 502 | CLA | C1D-CHD-C4C | -2.70 | 118.79 | 122.48 |
| 24 | b | 613 | CLA | CHC-C1C-C2C | -2.70 | 119.28 | 126.65 |
| 26 | b | 623 | BCR | C38-C26-C25 | -2.70 | 121.48 | 124.51 |
| 24 | C | 508 | CLA | OBD-CAD-C3D | -2.70 | 123.06 | 128.03 |
| 24 | a | 407 | CLA | CHC-C1C-C2C | -2.70 | 119.30 | 126.65 |
| 26 | c | 526 | BCR | C7-C8-C9 | -2.70 | 122.16 | 126.21 |
| 25 | a | 408 | PHO | CHC-C1C-C2C | -2.69 | 119.44 | 125.62 |
| 24 | B | 604 | CLA | O2D-CGD-O1D | -2.69 | 118.40 | 123.82 |
| 24 | C | 503 | CLA | C2A-C1A-CHA | -2.69 | 119.14 | 123.92 |
| 24 | B | 614 | CLA | C4C-C3C-C2C | -2.69 | 102.78 | 106.91 |
| 24 | C | 507 | CLA | C4C-C3C-C2C | -2.69 | 102.78 | 106.91 |
| 24 | b | 611 | CLA | O2A-CGA-O1A | -2.69 | 116.87 | 123.55 |
| 24 | b | 609 | CLA | CHC-C1C-C2C | -2.69 | 119.31 | 126.65 |
| 27 | A | 411 | SQD | O48-C23-O10 | -2.69 | 116.87 | 123.55 |
| 25 | d | 403 | PHO | C4D-ND-C1D | -2.69 | 102.13 | 106.98 |
| 26 | K | 101 | BCR | C7-C8-C9 | -2.69 | 122.17 | 126.21 |
| 24 | c | 508 | CLA | CBC-CAC-C3C | -2.69 | 104.78 | 112.41 |
| 24 | B | 611 | CLA | OBD-CAD-C3D | -2.69 | 123.08 | 128.03 |
| 24 | C | 513 | CLA | C1-C2-C3 | -2.68 | 121.02 | 125.96 |
| 24 | b | 621 | CLA | O1D-CGD-CBD | -2.67 | 119.81 | 124.60 |
| 24 | B | 608 | CLA | CBC-CAC-C3C | -2.67 | 104.84 | 112.41 |
| 37 | d | 408 | LHG | O8-C23-O10 | -2.66 | 116.94 | 123.55 |
| 24 | D | 401 | CLA | C1D-CHD-C4C | -2.66 | 118.85 | 122.48 |
| 24 | C | 509 | CLA | C2A-C1A-CHA | -2.66 | 119.21 | 123.92 |
| 24 | b | 609 | CLA | C1-C2-C3 | -2.65 | 121.07 | 125.96 |
| 24 | a | 406 | CLA | C4C-C3C-C2C | -2.65 | 102.84 | 106.91 |
| 24 | c | 513 | CLA | CBC-CAC-C3C | -2.65 | 104.89 | 112.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24 | A | 409 | CLA | O2A-CGA-O1A | -2.65 | 116.97 | 123.55 |
| 24 | A | 406 | CLA | C1-C2-C3 | -2.65 | 121.08 | 125.96 |
| 24 | c | 510 | CLA | CHC-C1C-C2C | -2.65 | 119.43 | 126.65 |
| 26 | B | 618 | BCR | C7-C8-C9 | -2.65 | 122.23 | 126.21 |
| 24 | B | 615 | CLA | C1D-CHD-C4C | -2.65 | 118.87 | 122.48 |
| 24 | b | 607 | CLA | C1-C2-C3 | -2.65 | 121.08 | 125.96 |
| 24 | A | 405 | CLA | CMA-C3A-C2A | -2.65 | 103.04 | 113.77 |
| 24 | b | 613 | CLA | C2A-C1A-CHA | -2.64 | 119.23 | 123.92 |
| 24 | b | 610 | CLA | CBC-CAC-C3C | -2.64 | 104.93 | 112.41 |
| 24 | a | 407 | CLA | O2A-CGA-O1A | -2.63 | 117.01 | 123.55 |
| 24 | c | 508 | CLA | O2A-CGA-O1A | -2.63 | 117.01 | 123.55 |
| 24 | b | 619 | CLA | O2A-CGA-O1A | -2.63 | 117.01 | 123.55 |
| 24 | b | 611 | CLA | CHC-C1C-C2C | -2.63 | 119.47 | 126.65 |
| 24 | B | 617 | CLA | O1D-CGD-CBD | -2.63 | 119.87 | 124.60 |
| 24 | c | 506 | CLA | C4C-C3C-C2C | -2.63 | 102.87 | 106.91 |
| 26 | T | 102 | BCR | C29-C28-C27 | -2.63 | 105.07 | 111.34 |
| 26 | B | 620 | BCR | C28-C27-C26 | -2.63 | 109.26 | 113.78 |
| 26 | T | 102 | BCR | C28-C27-C26 | -2.63 | 109.26 | 113.78 |
| 26 | d | 405 | BCR | C28-C27-C26 | -2.62 | 109.28 | 113.78 |
| 24 | D | 401 | CLA | CMA-C3A-C4A | -2.62 | 104.74 | 111.77 |
| 24 | b | 614 | CLA | C4C-C3C-C2C | -2.61 | 102.90 | 106.91 |
| 24 | B | 609 | CLA | CAA-C2A-C3A | -2.61 | 105.65 | 112.81 |
| 25 | A | 408 | PHO | O2A-CGA-O1A | -2.61 | 117.07 | 123.55 |
| 32 | d | 406 | PL9 | C37-C38-C39 | -2.61 | 121.13 | 127.68 |
| 25 | A | 407 | PHO | CHD-C1D-C2D | -2.61 | 119.64 | 125.62 |
| 24 | d | 404 | CLA | CHC-C1C-C2C | -2.60 | 119.55 | 126.65 |
| 26 | h | 101 | BCR | C10-C11-C12 | -2.60 | 115.24 | 123.23 |
| 24 | b | 608 | CLA | CHC-C1C-C2C | -2.60 | 119.56 | 126.65 |
| 24 | c | 509 | CLA | O2D-CGD-O1D | -2.60 | 118.60 | 123.82 |
| 24 | D | 401 | CLA | CMA-C3A-C2A | -2.60 | 103.24 | 113.77 |
| 24 | D | 403 | CLA | O2D-CGD-O1D | -2.59 | 118.60 | 123.82 |
| 24 | b | 617 | CLA | C1C-C2C-C3C | -2.59 | 104.05 | 106.92 |
| 24 | C | 508 | CLA | CBC-CAC-C3C | -2.59 | 105.05 | 112.41 |
| 24 | b | 617 | CLA | CHC-C1C-C2C | -2.59 | 119.59 | 126.65 |
| 24 | b | 619 | CLA | C2A-C1A-CHA | -2.59 | 119.33 | 123.92 |
| 24 | B | 616 | CLA | CBC-CAC-C3C | -2.58 | 105.08 | 112.41 |
| 24 | d | 401 | CLA | CBC-CAC-C3C | -2.58 | 105.08 | 112.41 |
| 24 | C | 505 | CLA | CAA-C2A-C3A | -2.58 | 105.73 | 112.81 |
| 26 | a | 410 | BCR | C15-C14-C13 | -2.58 | 123.62 | 127.31 |
| 26 | c | 526 | BCR | C11-C10-C9 | -2.58 | 123.63 | 127.31 |
| 24 | B | 608 | CLA | O2D-CGD-O1D | -2.58 | 118.63 | 123.82 |
| 24 | A | 405 | CLA | C1D-CHD-C4C | -2.58 | 118.96 | 122.48 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24 | a | 407 | CLA | C1-C2-C3 | -2.58 | 121.21 | 125.96 |
| 24 | C | 508 | CLA | O1D-CGD-CBD | -2.58 | 119.97 | 124.60 |
| 24 | d | 401 | CLA | O2A-CGA-O1A | -2.58 | 117.15 | 123.55 |
| 24 | C | 509 | CLA | C1-C2-C3 | -2.57 | 121.22 | 125.96 |
| 27 | a | 411 | SQD | O47-C7-O49 | -2.57 | 117.26 | 123.68 |
| 24 | a | 406 | CLA | C2A-C1A-CHA | -2.57 | 119.36 | 123.92 |
| 24 | b | 619 | CLA | C4C-C3C-C2C | -2.57 | 102.97 | 106.91 |
| 24 | C | 513 | CLA | O1D-CGD-CBD | -2.57 | 119.99 | 124.60 |
| 24 | b | 621 | CLA | O2A-CGA-O1A | -2.57 | 117.18 | 123.55 |
| 24 | B | 612 | CLA | C2A-C1A-CHA | -2.57 | 119.37 | 123.92 |
| 24 | B | 607 | CLA | CHC-C1C-C2C | -2.56 | 119.66 | 126.65 |
| 25 | d | 403 | PHO | C4D-CHA-C1A | -2.56 | 119.37 | 125.06 |
| 24 | D | 404 | CLA | CAA-C2A-C3A | -2.56 | 105.80 | 112.81 |
| 24 | B | 615 | CLA | C4C-C3C-C2C | -2.56 | 102.99 | 106.91 |
| 24 | B | 610 | CLA | C2A-C1A-CHA | -2.56 | 119.39 | 123.92 |
| 26 | B | 620 | BCR | C36-C18-C17 | -2.55 | 119.35 | 122.92 |
| 24 | b | 616 | CLA | OBD-CAD-C3D | -2.55 | 123.32 | 128.03 |
| 26 | A | 410 | BCR | C7-C8-C9 | -2.55 | 122.38 | 126.21 |
| 30 | m | 103 | LMT | C1-O1'-C1' | -2.55 | 109.48 | 113.87 |
| 27 | l | 101 | SQD | C1-O5-C5 | -2.55 | 108.91 | 113.72 |
| 24 | B | 607 | CLA | CBC-CAC-C3C | -2.55 | 105.19 | 112.41 |
| 24 | a | 406 | CLA | CMA-C3A-C4A | -2.54 | 104.93 | 111.77 |
| 26 | c | 526 | BCR | C20-C21-C22 | -2.54 | 123.69 | 127.31 |
| 26 | c | 516 | BCR | C3-C4-C5 | -2.54 | 109.42 | 113.78 |
| 24 | b | 621 | CLA | C1-C2-C3 | -2.53 | 121.29 | 125.96 |
| 26 | t | 101 | BCR | C11-C10-C9 | -2.53 | 123.70 | 127.31 |
| 25 | A | 407 | PHO | O1D-CGD-CBD | -2.53 | 120.06 | 124.60 |
| 34 | c | 521 | LMG | C8-O7-C10 | -2.52 | 111.92 | 117.88 |
| 24 | D | 403 | CLA | CMA-C3A-C2A | -2.52 | 103.54 | 113.77 |
| 24 | C | 509 | CLA | CAA-C2A-C3A | -2.52 | 105.90 | 112.81 |
| 24 | A | 409 | CLA | CHC-C1C-C2C | -2.52 | 119.78 | 126.65 |
| 24 | c | 510 | CLA | CAA-C2A-C3A | -2.52 | 105.91 | 112.81 |
| 24 | B | 616 | CLA | OBD-CAD-C3D | -2.52 | 123.39 | 128.03 |
| 26 | C | 516 | BCR | C33-C5-C6 | -2.51 | 121.70 | 124.51 |
| 24 | B | 611 | CLA | CMA-C3A-C4A | -2.51 | 105.03 | 111.77 |
| 24 | B | 607 | CLA | CAA-C2A-C3A | -2.51 | 105.94 | 112.81 |
| 24 | B | 602 | CLA | C1-C2-C3 | -2.51 | 121.34 | 125.96 |
| 24 | d | 404 | CLA | O2D-CGD-O1D | -2.51 | 118.78 | 123.82 |
| 24 | A | 405 | CLA | CMA-C3A-C4A | -2.51 | 105.04 | 111.77 |
| 26 | c | 526 | BCR | C38-C26-C25 | -2.51 | 121.70 | 124.51 |
| 26 | c | 526 | BCR | C24-C23-C22 | -2.50 | 122.45 | 126.21 |
| 24 | b | 619 | CLA | CAA-C2A-C3A | -2.50 | 105.96 | 112.81 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24 | b | 608 | CLA | C4C-C3C-C2C | -2.50 | 103.08 | 106.91 |
| 36 | C | 518 | DGD | O2G-C1B-O1B | -2.50 | 117.44 | 123.68 |
| 24 | c | 505 | CLA | O2D-CGD-O1D | -2.50 | 118.80 | 123.82 |
| 24 | B | 603 | CLA | CBC-CAC-C3C | -2.49 | 105.33 | 112.41 |
| 24 | C | 504 | CLA | O2A-CGA-O1A | -2.49 | 117.36 | 123.55 |
| 24 | c | 515 | CLA | C1-C2-C3 | -2.49 | 121.37 | 125.96 |
| 24 | C | 513 | CLA | CBC-CAC-C3C | -2.49 | 105.34 | 112.41 |
| 27 | b | 601 | SQD | O48-C23-O10 | -2.49 | 117.38 | 123.55 |
| 24 | C | 508 | CLA | CHC-C1C-C2C | -2.49 | 119.87 | 126.65 |
| 24 | D | 403 | CLA | C2A-C1A-CHA | -2.48 | 119.51 | 123.92 |
| 26 | a | 410 | BCR | C34-C9-C10 | -2.48 | 119.44 | 122.92 |
| 24 | D | 404 | CLA | C2A-C1A-CHA | -2.48 | 119.52 | 123.92 |
| 24 | B | 608 | CLA | C4C-C3C-C2C | -2.48 | 103.10 | 106.91 |
| 24 | A | 409 | CLA | C1D-CHD-C4C | -2.48 | 119.09 | 122.48 |
| 24 | b | 607 | CLA | O2A-CGA-O1A | -2.48 | 117.40 | 123.55 |
| 24 | b | 607 | CLA | C2A-C1A-CHA | -2.48 | 119.53 | 123.92 |
| 24 | c | 505 | CLA | CHC-C1C-C2C | -2.48 | 119.90 | 126.65 |
| 24 | d | 402 | CLA | CMA-C3A-C2A | -2.48 | 103.73 | 113.77 |
| 24 | c | 514 | CLA | CBA-CAA-C2A | -2.47 | 106.39 | 113.80 |
| 24 | b | 610 | CLA | C4C-C3C-C2C | -2.47 | 103.11 | 106.91 |
| 26 | B | 619 | BCR | C28-C27-C26 | -2.47 | 109.53 | 113.78 |
| 24 | b | 613 | CLA | C1D-CHD-C4C | -2.47 | 119.11 | 122.48 |
| 25 | A | 408 | PHO | C3B-C2B-C1B | -2.47 | 101.31 | 106.30 |
| 24 | C | 507 | CLA | C1-C2-C3 | -2.47 | 121.41 | 125.96 |
| 36 | c | 517 | DGD | O3G-C3G-C2G | -2.47 | 105.11 | 110.99 |
| 24 | c | 510 | CLA | C2A-C1A-CHA | -2.47 | 119.54 | 123.92 |
| 24 | c | 510 | CLA | C1-C2-C3 | -2.47 | 121.41 | 125.96 |
| 25 | A | 407 | PHO | C4D-CHA-C1A | -2.47 | 119.58 | 125.06 |
| 24 | A | 406 | CLA | C2A-C1A-CHA | -2.46 | 119.55 | 123.92 |
| 30 | a | 417 | LMT | C1-O1'-C1' | -2.46 | 109.64 | 113.87 |
| 24 | b | 615 | CLA | O2A-CGA-O1A | -2.46 | 117.44 | 123.55 |
| 35 | V | 204 | HTG | C1-C2-C3 | -2.45 | 105.44 | 110.69 |
| 24 | b | 619 | CLA | CBC-CAC-C3C | -2.45 | 105.44 | 112.41 |
| 24 | B | 608 | CLA | O2A-CGA-O1A | -2.45 | 117.46 | 123.55 |
| 37 | D | 410 | LHG | O8-C23-O10 | -2.45 | 117.46 | 123.55 |
| 24 | B | 604 | CLA | CHC-C1C-C2C | -2.45 | 119.96 | 126.65 |
| 24 | B | 603 | CLA | CAA-CBA-CGA | -2.45 | 105.97 | 113.35 |
| 26 | B | 620 | BCR | C15-C14-C13 | -2.45 | 123.82 | 127.31 |
| 36 | h | 102 | DGD | O1G-C1A-O1A | -2.45 | 117.48 | 123.55 |
| 36 | h | 102 | DGD | O4D-C4D-C3D | -2.45 | 105.04 | 110.36 |
| 24 | b | 617 | CLA | O2A-CGA-O1A | -2.44 | 117.49 | 123.55 |
| 24 | a | 406 | CLA | OBD-CAD-C3D | -2.44 | 123.53 | 128.03 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24 | c | 515 | CLA | C2A-C1A-CHA | -2.44 | 119.59 | 123.92 |
| 24 | B | 602 | CLA | O1D-CGD-CBD | -2.44 | 120.22 | 124.60 |
| 24 | D | 403 | CLA | OBD-CAD-C3D | -2.44 | 123.53 | 128.03 |
| 26 | D | 405 | BCR | C10-C11-C12 | -2.44 | 115.75 | 123.23 |
| 24 | C | 514 | CLA | CAA-C2A-C3A | -2.43 | 106.14 | 112.81 |
| 26 | h | 101 | BCR | C7-C8-C9 | -2.43 | 122.55 | 126.21 |
| 25 | A | 408 | PHO | C1C-C2C-C3C | -2.43 | 103.69 | 106.51 |
| 24 | b | 611 | CLA | CAA-C2A-C3A | -2.43 | 106.14 | 112.81 |
| 24 | d | 402 | CLA | C1D-CHD-C4C | -2.43 | 119.16 | 122.48 |
| 37 | d | 409 | LHG | C5-O7-C7 | -2.43 | 112.13 | 117.88 |
| 25 | A | 408 | PHO | C4D-CHA-C1A | -2.43 | 119.66 | 125.06 |
| 26 | B | 618 | BCR | C34-C9-C10 | -2.43 | 119.52 | 122.92 |
| 24 | A | 406 | CLA | CMA-C3A-C2A | -2.43 | 103.93 | 113.77 |
| 32 | D | 406 | PL9 | C7-C8-C9 | -2.42 | 122.66 | 126.71 |
| 24 | b | 614 | CLA | C1-C2-C3 | -2.42 | 121.50 | 125.96 |
| 37 | D | 409 | LHG | O7-C7-O9 | -2.42 | 117.65 | 123.68 |
| 26 | B | 618 | BCR | C11-C10-C9 | -2.41 | 123.87 | 127.31 |
| 26 | A | 410 | BCR | C37-C22-C21 | -2.41 | 119.55 | 122.92 |
| 24 | b | 613 | CLA | CMA-C3A-C2A | -2.41 | 104.00 | 113.77 |
| 24 | A | 409 | CLA | CMA-C3A-C2A | -2.41 | 104.00 | 113.77 |
| 34 | Z | 101 | LMG | C9-C8-C7 | -2.41 | 106.42 | 111.86 |
| 32 | d | 406 | PL9 | C42-C43-C44 | -2.41 | 121.63 | 127.68 |
| 37 | d | 410 | LHG | O8-C23-O10 | -2.41 | 117.58 | 123.55 |
| 26 | B | 620 | BCR | C3-C4-C5 | -2.41 | 109.64 | 113.78 |
| 24 | B | 610 | CLA | CBC-CAC-C3C | -2.40 | 105.58 | 112.41 |
| 24 | B | 605 | CLA | C2A-C1A-CHA | -2.40 | 119.66 | 123.92 |
| 24 | B | 612 | CLA | C4A-NA-C1A | -2.40 | 103.47 | 106.45 |
| 24 | B | 616 | CLA | C4A-NA-C1A | -2.40 | 103.47 | 106.45 |
| 24 | d | 404 | CLA | C2A-C1A-CHA | -2.40 | 119.66 | 123.92 |
| 24 | c | 512 | CLA | C1-C2-C3 | -2.40 | 121.53 | 125.96 |
| 24 | b | 607 | CLA | CMA-C3A-C4A | -2.40 | 105.32 | 111.77 |
| 24 | C | 505 | CLA | C4C-C3C-C2C | -2.40 | 103.23 | 106.91 |
| 26 | B | 620 | BCR | C7-C8-C9 | -2.40 | 122.61 | 126.21 |
| 24 | c | 513 | CLA | C4C-C3C-C2C | -2.40 | 103.23 | 106.91 |
| 24 | B | 614 | CLA | O2A-CGA-O1A | -2.39 | 117.61 | 123.55 |
| 24 | B | 608 | CLA | C1D-CHD-C4C | -2.39 | 119.22 | 122.48 |
| 24 | B | 607 | CLA | C1-C2-C3 | -2.39 | 121.55 | 125.96 |
| 26 | C | 516 | BCR | C21-C20-C19 | -2.39 | 115.90 | 123.23 |
| 34 | B | 621 | LMG | C9-C8-C7 | -2.39 | 106.47 | 111.86 |
| 24 | B | 603 | CLA | CMA-C3A-C4A | -2.39 | 105.35 | 111.77 |
| 24 | b | 609 | CLA | O2A-CGA-O1A | -2.39 | 117.63 | 123.55 |
| 26 | H | 101 | BCR | C37-C22-C21 | -2.39 | 119.58 | 122.92 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24 | a | 406 | CLA | CMA-C3A-C2A | -2.38 | 104.11 | 113.77 |
| 24 | C | 502 | CLA | C2A-C1A-CHA | -2.38 | 119.70 | 123.92 |
| 24 | c | 506 | CLA | OBD-CAD-C3D | -2.38 | 123.64 | 128.03 |
| 26 | a | 410 | BCR | C33-C5-C6 | -2.38 | 121.84 | 124.51 |
| 24 | C | 504 | CLA | C1-C2-C3 | -2.38 | 121.57 | 125.96 |
| 24 | c | 513 | CLA | O2A-CGA-O1A | -2.38 | 117.65 | 123.55 |
| 24 | b | 613 | CLA | CAA-C2A-C3A | -2.38 | 106.29 | 112.81 |
| 24 | c | 513 | CLA | O2D-CGD-O1D | -2.38 | 119.04 | 123.82 |
| 34 | c | 501 | LMG | O7-C10-O9 | -2.38 | 117.75 | 123.68 |
| 24 | D | 401 | CLA | OBD-CAD-C3D | -2.37 | 123.65 | 128.03 |
| 26 | y | 101 | BCR | C10-C11-C12 | -2.37 | 115.95 | 123.23 |
| 24 | c | 503 | CLA | C2A-C1A-CHA | -2.37 | 119.72 | 123.92 |
| 36 | H | 102 | DGD | O1G-C1A-O1A | -2.37 | 117.67 | 123.55 |
| 24 | C | 504 | CLA | C2A-C1A-CHA | -2.37 | 119.72 | 123.92 |
| 24 | A | 409 | CLA | C1-C2-C3 | -2.36 | 121.60 | 125.96 |
| 27 | a | 402 | SQD | O48-C23-O10 | -2.36 | 117.68 | 123.55 |
| 36 | C | 518 | DGD | O1G-C1A-O1A | -2.36 | 117.68 | 123.55 |
| 24 | b | 615 | CLA | CMA-C3A-C4A | -2.36 | 105.42 | 111.77 |
| 34 | J | 101 | LMG | O8-C28-O10 | -2.36 | 117.68 | 123.55 |
| 24 | B | 607 | CLA | C4A-NA-C1A | -2.36 | 103.52 | 106.45 |
| 27 | F | 101 | SQD | C1-O5-C5 | -2.36 | 109.27 | 113.72 |
| 24 | A | 409 | CLA | CMA-C3A-C4A | -2.36 | 105.44 | 111.77 |
| 24 | D | 403 | CLA | C4A-NA-C1A | -2.36 | 103.53 | 106.45 |
| 24 | D | 401 | CLA | O2D-CGD-O1D | -2.35 | 119.08 | 123.82 |
| 24 | C | 507 | CLA | O2A-CGA-O1A | -2.35 | 117.70 | 123.55 |
| 24 | c | 503 | CLA | CBC-CAC-C3C | -2.35 | 105.73 | 112.41 |
| 32 | D | 406 | PL9 | C37-C38-C39 | -2.35 | 121.77 | 127.68 |
| 24 | b | 612 | CLA | CBC-CAC-C3C | -2.35 | 105.73 | 112.41 |
| 24 | B | 606 | CLA | CAA-C2A-C3A | -2.35 | 106.36 | 112.81 |
| 24 | c | 511 | CLA | O2A-CGA-O1A | -2.35 | 117.72 | 123.55 |
| 24 | c | 506 | CLA | O2A-CGA-O1A | -2.35 | 117.72 | 123.55 |
| 26 | Y | 101 | BCR | C10-C11-C12 | -2.35 | 116.04 | 123.23 |
| 24 | d | 404 | CLA | CGD-CBD-CAD | -2.34 | 102.86 | 110.71 |
| 26 | A | 410 | BCR | C38-C26-C25 | -2.34 | 121.88 | 124.51 |
| 24 | b | 612 | CLA | O2D-CGD-O1D | -2.34 | 119.10 | 123.82 |
| 24 | c | 505 | CLA | C2A-C1A-CHA | -2.34 | 119.76 | 123.92 |
| 25 | d | 403 | PHO | C3B-C2B-C1B | -2.34 | 101.57 | 106.30 |
| 24 | b | 620 | CLA | C4A-NA-C1A | -2.34 | 103.55 | 106.45 |
| 24 | c | 505 | CLA | C1-C2-C3 | -2.34 | 121.65 | 125.96 |
| 24 | c | 514 | CLA | C1-C2-C3 | -2.33 | 121.66 | 125.96 |
| 26 | a | 410 | BCR | C35-C13-C14 | -2.33 | 119.65 | 122.92 |
| 34 | J | 101 | LMG | C9-C8-C7 | -2.33 | 106.59 | 111.86 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24 | B | 611 | CLA | C1D-CHD-C4C | -2.33 | 119.30 | 122.48 |
| 24 | C | 508 | CLA | O2A-CGA-O1A | -2.33 | 117.76 | 123.55 |
| 24 | c | 514 | CLA | C2A-C1A-CHA | -2.33 | 119.79 | 123.92 |
| 26 | B | 620 | BCR | C16-C17-C18 | -2.33 | 123.99 | 127.31 |
| 26 | t | 101 | BCR | C15-C16-C17 | -2.33 | 118.49 | 123.46 |
| 24 | b | 614 | CLA | CBC-CAC-C3C | -2.33 | 105.81 | 112.41 |
| 25 | A | 407 | PHO | CBA-CAA-C2A | -2.33 | 106.84 | 113.80 |
| 37 | d | 408 | LHG | O7-C7-O9 | -2.32 | 117.88 | 123.68 |
| 32 | d | 406 | PL9 | O1-C4-C3 | -2.32 | 118.08 | 120.71 |
| 26 | C | 516 | BCR | C11-C10-C9 | -2.32 | 124.00 | 127.31 |
| 24 | b | 620 | CLA | O2A-CGA-O1A | -2.32 | 117.78 | 123.55 |
| 24 | C | 513 | CLA | O2D-CGD-O1D | -2.32 | 119.16 | 123.82 |
| 27 | a | 402 | SQD | C45-O47-C7 | -2.31 | 112.41 | 117.88 |
| 34 | C | 520 | LMG | O8-C28-O10 | -2.31 | 117.81 | 123.55 |
| 26 | a | 410 | BCR | C37-C22-C21 | -2.31 | 119.69 | 122.92 |
| 35 | V | 204 | HTG | O5-C1-C2 | -2.31 | 107.11 | 110.28 |
| 26 | h | 101 | BCR | C31-C1-C6 | -2.31 | 106.57 | 110.31 |
| 24 | b | 611 | CLA | C1-C2-C3 | -2.31 | 121.71 | 125.96 |
| 26 | T | 102 | BCR | C7-C6-C5 | -2.30 | 116.05 | 121.54 |
| 24 | B | 606 | CLA | O2A-CGA-O1A | -2.30 | 117.83 | 123.55 |
| 26 | C | 516 | BCR | C3-C4-C5 | -2.30 | 109.82 | 113.78 |
| 24 | c | 508 | CLA | CGD-CBD-CAD | -2.30 | 103.00 | 110.71 |
| 24 | a | 409 | CLA | CMA-C3A-C4A | -2.30 | 105.59 | 111.77 |
| 24 | B | 602 | CLA | O2D-CGD-O1D | -2.30 | 119.20 | 123.82 |
| 24 | C | 512 | CLA | O2D-CGD-O1D | -2.30 | 119.20 | 123.82 |
| 24 | c | 505 | CLA | CBC-CAC-C3C | -2.30 | 105.89 | 112.41 |
| 24 | c | 505 | CLA | C4A-NA-C1A | -2.29 | 103.61 | 106.45 |
| 24 | c | 511 | CLA | OBD-CAD-C3D | -2.29 | 123.81 | 128.03 |
| 24 | b | 608 | CLA | OBD-CAD-C3D | -2.29 | 123.81 | 128.03 |
| 26 | b | 624 | BCR | C16-C17-C18 | -2.29 | 124.04 | 127.31 |
| 24 | c | 506 | CLA | O2D-CGD-O1D | -2.29 | 119.21 | 123.82 |
| 24 | d | 401 | CLA | O2D-CGD-O1D | -2.29 | 119.22 | 123.82 |
| 24 | c | 504 | CLA | C2A-C1A-CHA | -2.29 | 119.87 | 123.92 |
| 24 | c | 512 | CLA | C2A-C1A-CHA | -2.28 | 119.87 | 123.92 |
| 25 | a | 408 | PHO | CHD-C1D-C2D | -2.28 | 120.38 | 125.62 |
| 37 | d | 408 | LHG | C5-O7-C7 | -2.28 | 112.48 | 117.88 |
| 24 | b | 618 | CLA | O2A-CGA-O1A | -2.28 | 117.89 | 123.55 |
| 30 | A | 417 | LMT | C1B-O1B-C4' | -2.28 | 112.44 | 118.00 |
| 26 | D | 405 | BCR | C37-C22-C21 | -2.28 | 119.73 | 122.92 |
| 24 | a | 409 | CLA | C2A-C1A-CHA | -2.28 | 119.88 | 123.92 |
| 24 | B | 609 | CLA | O2D-CGD-O1D | -2.28 | 119.24 | 123.82 |
| 24 | b | 613 | CLA | O2A-CGA-O1A | -2.28 | 117.90 | 123.55 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 26 | Y | 101 | BCR | C40-C30-C25 | -2.28 | 106.62 | 110.31 |
| 32 | D | 406 | PL9 | C12-C13-C14 | -2.27 | 121.97 | 127.68 |
| 24 | C | 505 | CLA | CBC-CAC-C3C | -2.27 | 105.96 | 112.41 |
| 26 | b | 623 | BCR | C37-C22-C21 | -2.26 | 119.75 | 122.92 |
| 24 | d | 401 | CLA | C1D-CHD-C4C | -2.26 | 119.39 | 122.48 |
| 24 | b | 608 | CLA | C1B-CHB-C4A | -2.26 | 125.64 | 130.12 |
| 37 | D | 408 | LHG | O7-C7-O9 | -2.26 | 118.03 | 123.68 |
| 27 | A | 411 | SQD | O47-C7-O49 | -2.26 | 118.04 | 123.68 |
| 24 | B | 602 | CLA | CAA-C2A-C3A | -2.26 | 106.62 | 112.81 |
| 24 | c | 514 | CLA | C4C-C3C-C2C | -2.26 | 103.45 | 106.91 |
| 24 | C | 510 | CLA | C2A-C1A-CHA | -2.26 | 119.92 | 123.92 |
| 27 | f | 101 | SQD | O47-C7-O49 | -2.26 | 118.05 | 123.68 |
| 24 | C | 505 | CLA | C2A-C1A-CHA | -2.25 | 119.92 | 123.92 |
| 24 | A | 409 | CLA | O2D-CGD-O1D | -2.25 | 119.29 | 123.82 |
| 24 | b | 615 | CLA | C1-C2-C3 | -2.25 | 121.81 | 125.96 |
| 24 | B | 607 | CLA | O1D-CGD-CBD | -2.25 | 120.56 | 124.60 |
| 30 | m | 102 | LMT | C3'-C4'-C5' | -2.25 | 106.11 | 110.88 |
| 32 | d | 406 | PL9 | C22-C23-C24 | -2.24 | 122.04 | 127.68 |
| 24 | C | 502 | CLA | CAA-C2A-C3A | -2.24 | 106.67 | 112.81 |
| 25 | a | 408 | PHO | C3B-C2B-C1B | -2.24 | 101.78 | 106.30 |
| 24 | c | 507 | CLA | C4A-NA-C1A | -2.24 | 103.67 | 106.45 |
| 24 | b | 618 | CLA | CMA-C3A-C4A | -2.24 | 105.76 | 111.77 |
| 24 | B | 616 | CLA | C11-C10-C8 | -2.23 | 108.40 | 115.73 |
| 24 | b | 616 | CLA | O2A-CGA-O1A | -2.23 | 118.00 | 123.55 |
| 24 | c | 511 | CLA | C2A-C1A-CHA | -2.23 | 119.96 | 123.92 |
| 24 | B | 603 | CLA | C2A-C1A-CHA | -2.23 | 119.96 | 123.92 |
| 24 | c | 514 | CLA | O1D-CGD-CBD | -2.23 | 120.60 | 124.60 |
| 24 | a | 406 | CLA | C1B-CHB-C4A | -2.23 | 125.70 | 130.12 |
| 24 | b | 612 | CLA | C2A-C1A-CHA | -2.23 | 119.97 | 123.92 |
| 24 | C | 504 | CLA | C4A-NA-C1A | -2.23 | 103.69 | 106.45 |
| 27 | A | 416 | SQD | O48-C23-O10 | -2.23 | 118.02 | 123.55 |
| 24 | b | 613 | CLA | CBC-CAC-C3C | -2.22 | 106.10 | 112.41 |
| 26 | T | 102 | BCR | C21-C20-C19 | -2.22 | 116.41 | 123.23 |
| 24 | C | 503 | CLA | CBC-CAC-C3C | -2.22 | 106.10 | 112.41 |
| 26 | k | 103 | BCR | C11-C10-C9 | -2.22 | 124.14 | 127.31 |
| 24 | c | 506 | CLA | CAA-C2A-C3A | -2.22 | 106.72 | 112.81 |
| 24 | B | 603 | CLA | O2A-CGA-O1A | -2.22 | 118.04 | 123.55 |
| 24 | B | 603 | CLA | C1-C2-C3 | -2.22 | 121.87 | 125.96 |
| 37 | L | 101 | LHG | O8-C23-O10 | -2.22 | 118.04 | 123.55 |
| 24 | b | 620 | CLA | C11-C10-C8 | -2.22 | 108.45 | 115.73 |
| 26 | B | 620 | BCR | C10-C11-C12 | -2.22 | 116.44 | 123.23 |
| 26 | a | 410 | BCR | C38-C26-C25 | -2.21 | 122.03 | 124.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 26 | d | 405 | BCR | C16-C17-C18 | -2.21 | 124.15 | 127.31 |
| 27 | F | 101 | SQD | C44-O6-C1 | -2.21 | 109.22 | 113.76 |
| 26 | y | 101 | BCR | C21-C20-C19 | -2.21 | 116.44 | 123.23 |
| 24 | B | 610 | CLA | O2A-CGA-O1A | -2.21 | 118.06 | 123.55 |
| 26 | t | 101 | BCR | C21-C20-C19 | -2.21 | 116.45 | 123.23 |
| 36 | h | 102 | DGD | O2G-C1B-O1B | -2.21 | 118.17 | 123.68 |
| 24 | d | 404 | CLA | O2A-CGA-O1A | -2.20 | 118.08 | 123.55 |
| 34 | B | 621 | LMG | C30-C29-C28 | -2.20 | 105.54 | 113.58 |
| 26 | Y | 101 | BCR | C21-C20-C19 | -2.20 | 116.48 | 123.23 |
| 26 | K | 101 | BCR | C11-C10-C9 | -2.20 | 124.17 | 127.31 |
| 24 | b | 614 | CLA | C2A-C1A-CHA | -2.20 | 120.02 | 123.92 |
| 24 | b | 607 | CLA | C4A-NA-C1A | -2.20 | 103.72 | 106.45 |
| 24 | b | 613 | CLA | C11-C10-C8 | -2.20 | 108.52 | 115.73 |
| 37 | d | 409 | LHG | O8-C23-O10 | -2.20 | 118.10 | 123.55 |
| 37 | l | 102 | LHG | C6-C5-C4 | -2.20 | 106.90 | 111.86 |
| 24 | b | 614 | CLA | CGD-CBD-CAD | -2.19 | 103.37 | 110.71 |
| 25 | a | 408 | PHO | O2D-CGD-O1D | -2.19 | 119.41 | 123.82 |
| 24 | D | 404 | CLA | CMA-C3A-C2A | -2.19 | 104.89 | 113.77 |
| 24 | a | 406 | CLA | O2D-CGD-O1D | -2.19 | 119.42 | 123.82 |
| 26 | y | 101 | BCR | C35-C13-C14 | -2.19 | 119.86 | 122.92 |
| 24 | B | 613 | CLA | C1D-CHD-C4C | -2.18 | 119.50 | 122.48 |
| 24 | C | 506 | CLA | C2A-C1A-CHA | -2.18 | 120.05 | 123.92 |
| 24 | d | 404 | CLA | C4A-NA-C1A | -2.18 | 103.75 | 106.45 |
| 24 | c | 504 | CLA | O2A-CGA-O1A | -2.18 | 118.14 | 123.55 |
| 24 | B | 603 | CLA | C4A-NA-C1A | -2.18 | 103.75 | 106.45 |
| 24 | c | 510 | CLA | O2A-CGA-O1A | -2.18 | 118.15 | 123.55 |
| 24 | c | 514 | CLA | OBD-CAD-C3D | -2.17 | 124.02 | 128.03 |
| 24 | B | 605 | CLA | OBD-CAD-C3D | -2.17 | 124.03 | 128.03 |
| 24 | b | 606 | CLA | CAA-C2A-C3A | -2.17 | 106.86 | 112.81 |
| 24 | c | 515 | CLA | O2A-CGA-O1A | -2.17 | 118.16 | 123.55 |
| 24 | b | 615 | CLA | O1D-CGD-CBD | -2.17 | 120.70 | 124.60 |
| 24 | A | 406 | CLA | C4C-C3C-C2C | -2.17 | 103.59 | 106.91 |
| 26 | b | 624 | BCR | C3-C4-C5 | -2.17 | 110.06 | 113.78 |
| 26 | T | 102 | BCR | C19-C18-C17 | -2.17 | 115.62 | 118.94 |
| 24 | C | 503 | CLA | OBD-CAD-C3D | -2.16 | 124.04 | 128.03 |
| 24 | b | 619 | CLA | C4-C3-C2 | -2.16 | 117.92 | 123.69 |
| 24 | b | 613 | CLA | OBD-CAD-C3D | -2.16 | 124.04 | 128.03 |
| 24 | C | 509 | CLA | C4A-NA-C1A | -2.16 | 103.77 | 106.45 |
| 27 | l | 101 | SQD | C45-O47-C7 | -2.16 | 112.78 | 117.88 |
| 24 | B | 617 | CLA | OBD-CAD-C3D | -2.16 | 124.05 | 128.03 |
| 24 | B | 607 | CLA | C2A-C1A-CHA | -2.15 | 120.10 | 123.92 |
| 24 | A | 406 | CLA | O2D-CGD-O1D | -2.15 | 119.48 | 123.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 26 | a | 410 | BCR | C40-C30-C25 | -2.15 | 106.82 | 110.31 |
| 36 | C | 518 | DGD | O6D-C1D-O3G | -2.15 | 104.91 | 110.02 |
| 24 | B | 602 | CLA | C2A-C1A-CHA | -2.15 | 120.11 | 123.92 |
| 26 | c | 526 | BCR | C16-C17-C18 | -2.15 | 124.24 | 127.31 |
| 32 | D | 406 | PL9 | C27-C28-C29 | -2.14 | 122.29 | 127.68 |
| 32 | D | 406 | PL9 | C40-C39-C38 | -2.14 | 117.97 | 123.69 |
| 27 | a | 402 | SQD | C5-C6-S | -2.14 | 111.35 | 114.34 |
| 24 | b | 611 | CLA | CBC-CAC-C3C | -2.14 | 106.34 | 112.41 |
| 32 | A | 419 | PL9 | C35-C34-C33 | -2.14 | 117.98 | 123.69 |
| 38 | V | 203 | HEM | CBA-CAA-C2A | -2.14 | 108.40 | 112.48 |
| 24 | b | 608 | CLA | C4A-NA-C1A | -2.14 | 103.80 | 106.45 |
| 24 | B | 612 | CLA | O2A-CGA-O1A | -2.14 | 118.25 | 123.55 |
| 26 | c | 516 | BCR | C35-C13-C14 | -2.14 | 119.93 | 122.92 |
| 24 | C | 511 | CLA | CMA-C3A-C4A | -2.13 | 106.03 | 111.77 |
| 27 | l | 101 | SQD | C1-C2-C3 | -2.13 | 106.01 | 109.98 |
| 24 | b | 607 | CLA | CMA-C3A-C2A | -2.13 | 105.12 | 113.77 |
| 24 | B | 609 | CLA | C1-C2-C3 | -2.13 | 122.03 | 125.96 |
| 24 | B | 617 | CLA | C2A-C1A-CHA | -2.13 | 120.14 | 123.92 |
| 26 | b | 624 | BCR | C10-C11-C12 | -2.13 | 116.70 | 123.23 |
| 24 | A | 405 | CLA | C1B-CHB-C4A | -2.13 | 125.90 | 130.12 |
| 34 | c | 521 | LMG | O8-C28-O10 | -2.13 | 118.27 | 123.55 |
| 38 | V | 203 | HEM | CMA-C3A-C4A | -2.13 | 125.19 | 128.46 |
| 26 | h | 101 | BCR | C36-C18-C17 | -2.13 | 119.94 | 122.92 |
| 26 | y | 101 | BCR | C24-C23-C22 | -2.13 | 123.02 | 126.21 |
| 26 | K | 101 | BCR | C16-C17-C18 | -2.12 | 124.28 | 127.31 |
| 36 | c | 519 | DGD | O1G-C1A-O1A | -2.12 | 118.28 | 123.55 |
| 24 | D | 403 | CLA | O2A-CGA-O1A | -2.12 | 118.28 | 123.55 |
| 26 | C | 515 | BCR | C15-C14-C13 | -2.12 | 124.28 | 127.31 |
| 24 | c | 508 | CLA | OBD-CAD-C3D | -2.12 | 124.12 | 128.03 |
| 26 | c | 516 | BCR | C33-C5-C6 | -2.12 | 122.14 | 124.51 |
| 24 | B | 611 | CLA | C2A-C1A-CHA | -2.12 | 120.17 | 123.92 |
| 24 | D | 403 | CLA | CBC-CAC-C3C | -2.11 | 106.41 | 112.41 |
| 27 | a | 411 | SQD | O48-C23-O10 | -2.11 | 118.31 | 123.55 |
| 24 | B | 602 | CLA | C4A-NA-C1A | -2.11 | 103.83 | 106.45 |
| 24 | b | 611 | CLA | C2A-C1A-CHA | -2.11 | 120.19 | 123.92 |
| 24 | B | 613 | CLA | C4A-NA-C1A | -2.10 | 103.84 | 106.45 |
| 24 | B | 606 | CLA | C4A-NA-C1A | -2.10 | 103.84 | 106.45 |
| 24 | B | 616 | CLA | CHA-C1A-NA | -2.10 | 121.29 | 126.18 |
| 26 | t | 101 | BCR | C7-C6-C5 | -2.10 | 116.53 | 121.54 |
| 24 | c | 514 | CLA | CMA-C3A-C4A | -2.10 | 106.12 | 111.77 |
| 24 | b | 609 | CLA | C1D-CHD-C4C | -2.10 | 119.61 | 122.48 |
| 36 | H | 102 | DGD | C3G-C2G-C1G | -2.10 | 107.12 | 111.86 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24 | C | 513 | CLA | CBA-CAA-C2A | -2.10 | 107.52 | 113.80 |
| 34 | c | 521 | LMG | O7-C10-O9 | -2.10 | 118.44 | 123.68 |
| 24 | B | 614 | CLA | CMA-C3A-C4A | -2.09 | 106.15 | 111.77 |
| 30 | a | 417 | LMT | C1B-O1B-C4' | -2.09 | 112.90 | 118.00 |
| 38 | E | 103 | HEM | C3C-C4C-NC | -2.09 | 107.00 | 110.94 |
| 24 | c | 512 | CLA | CMA-C3A-C4A | -2.09 | 106.16 | 111.77 |
| 26 | b | 624 | BCR | C15-C14-C13 | -2.09 | 124.33 | 127.31 |
| 26 | K | 101 | BCR | C31-C1-C6 | -2.08 | 106.93 | 110.31 |
| 37 | L | 101 | LHG | O7-C7-O9 | -2.08 | 118.48 | 123.68 |
| 24 | D | 401 | CLA | C4C-C3C-C2C | -2.08 | 103.72 | 106.91 |
| 26 | d | 405 | BCR | C29-C28-C27 | -2.08 | 106.39 | 111.34 |
| 24 | b | 608 | CLA | C7-C6-C5 | -2.08 | 107.33 | 113.11 |
| 26 | H | 101 | BCR | C24-C23-C22 | -2.08 | 123.09 | 126.21 |
| 34 | b | 625 | LMG | O8-C28-O10 | -2.08 | 118.39 | 123.55 |
| 24 | C | 514 | CLA | CBC-CAC-C3C | -2.08 | 106.52 | 112.41 |
| 24 | b | 613 | CLA | CMA-C3A-C4A | -2.08 | 106.19 | 111.77 |
| 26 | B | 620 | BCR | C23-C24-C25 | -2.08 | 121.44 | 127.25 |
| 27 | l | 101 | SQD | O47-C7-O49 | -2.07 | 118.51 | 123.68 |
| 26 | B | 618 | BCR | C21-C20-C19 | -2.07 | 116.88 | 123.23 |
| 36 | h | 102 | DGD | C3G-O3G-C1D | -2.07 | 109.51 | 113.76 |
| 37 | d | 409 | LHG | O7-C7-O9 | -2.07 | 118.51 | 123.68 |
| 26 | C | 516 | BCR | C40-C30-C25 | -2.07 | 106.95 | 110.31 |
| 24 | B | 610 | CLA | CGD-CBD-CAD | -2.07 | 103.78 | 110.71 |
| 24 | b | 609 | CLA | O2D-CGD-O1D | -2.07 | 119.66 | 123.82 |
| 24 | D | 401 | CLA | C1-C2-C3 | -2.07 | 122.15 | 125.96 |
| 26 | A | 410 | BCR | C8-C7-C6 | -2.07 | 121.47 | 127.25 |
| 24 | B | 616 | CLA | C2A-C1A-CHA | -2.07 | 120.26 | 123.92 |
| 34 | C | 520 | LMG | C30-C29-C28 | -2.07 | 106.04 | 113.58 |
| 26 | c | 516 | BCR | C28-C27-C26 | -2.06 | 110.23 | 113.78 |
| 24 | b | 619 | CLA | OBD-CAD-C3D | -2.06 | 124.22 | 128.03 |
| 24 | a | 409 | CLA | CMA-C3A-C2A | -2.06 | 105.40 | 113.77 |
| 26 | y | 101 | BCR | C40-C30-C25 | -2.06 | 106.96 | 110.31 |
| 30 | M | 101 | LMT | C6'-C5'-C4' | -2.06 | 107.61 | 113.24 |
| 24 | B | 611 | CLA | CAA-CBA-CGA | -2.06 | 107.14 | 113.35 |
| 25 | d | 403 | PHO | O2A-CGA-O1A | -2.06 | 118.43 | 123.55 |
| 24 | B | 604 | CLA | CAA-C2A-C1A | -2.06 | 105.22 | 111.97 |
| 24 | B | 613 | CLA | C11-C10-C8 | -2.06 | 108.97 | 115.73 |
| 32 | D | 406 | PL9 | C15-C14-C13 | -2.06 | 118.20 | 123.69 |
| 26 | c | 526 | BCR | C21-C20-C19 | -2.06 | 116.92 | 123.23 |
| 24 | C | 514 | CLA | OBD-CAD-C3D | -2.06 | 124.24 | 128.03 |
| 24 | A | 405 | CLA | O2A-CGA-O1A | -2.06 | 118.45 | 123.55 |
| 24 | d | 402 | CLA | CAA-C2A-C3A | -2.05 | 107.18 | 112.81 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 26 | d | 405 | BCR | C40-C30-C25 | -2.05 | 106.98 | 110.31 |
| 24 | B | 609 | CLA | O2A-CGA-O1A | -2.05 | 118.46 | 123.55 |
| 24 | C | 507 | CLA | C2A-C1A-CHA | -2.05 | 120.28 | 123.92 |
| 24 | C | 508 | CLA | C11-C12-C13 | -2.05 | 109.01 | 115.73 |
| 26 | D | 405 | BCR | C29-C28-C27 | -2.05 | 106.46 | 111.34 |
| 26 | b | 624 | BCR | C21-C20-C19 | -2.05 | 116.95 | 123.23 |
| 24 | a | 409 | CLA | OBD-CAD-C3D | -2.05 | 124.26 | 128.03 |
| 24 | A | 405 | CLA | CAA-CBA-CGA | -2.05 | 107.19 | 113.35 |
| 24 | B | 604 | CLA | C1B-CHB-C4A | -2.04 | 126.07 | 130.12 |
| 24 | c | 515 | CLA | O2D-CGD-O1D | -2.04 | 119.71 | 123.82 |
| 24 | b | 607 | CLA | C1B-CHB-C4A | -2.04 | 126.07 | 130.12 |
| 24 | b | 610 | CLA | C5-C3-C2 | -2.04 | 116.93 | 121.10 |
| 24 | C | 513 | CLA | CMA-C3A-C4A | -2.04 | 106.29 | 111.77 |
| 24 | B | 614 | CLA | OBD-CAD-C3D | -2.04 | 124.27 | 128.03 |
| 24 | B | 612 | CLA | OBD-CAD-C3D | -2.04 | 124.28 | 128.03 |
| 34 | C | 521 | LMG | O7-C10-O9 | -2.04 | 118.60 | 123.68 |
| 24 | c | 508 | CLA | O2D-CGD-O1D | -2.03 | 119.72 | 123.82 |
| 24 | B | 603 | CLA | CMA-C3A-C2A | -2.03 | 105.53 | 113.77 |
| 24 | B | 614 | CLA | CMA-C3A-C2A | -2.03 | 105.53 | 113.77 |
| 24 | B | 614 | CLA | C2A-C1A-CHA | -2.03 | 120.32 | 123.92 |
| 26 | b | 623 | BCR | C11-C12-C13 | -2.03 | 120.71 | 126.42 |
| 26 | k | 103 | BCR | C20-C21-C22 | -2.03 | 124.41 | 127.31 |
| 24 | B | 608 | CLA | C1-C2-C3 | -2.03 | 122.22 | 125.96 |
| 24 | b | 621 | CLA | O2D-CGD-O1D | -2.03 | 119.74 | 123.82 |
| 24 | b | 621 | CLA | C2A-C1A-CHA | -2.03 | 120.33 | 123.92 |
| 24 | C | 507 | CLA | CGD-CBD-CAD | -2.03 | 103.93 | 110.71 |
| 37 | e | 101 | LHG | O8-C23-O10 | -2.02 | 118.53 | 123.55 |
| 24 | b | 608 | CLA | C5-C3-C2 | -2.02 | 116.96 | 121.10 |
| 24 | C | 511 | CLA | CAA-C2A-C3A | -2.02 | 107.27 | 112.81 |
| 24 | c | 514 | CLA | O2A-CGA-O1A | -2.02 | 118.53 | 123.55 |
| 36 | C | 517 | DGD | C3G-C2G-C1G | -2.02 | 107.30 | 111.86 |
| 24 | C | 507 | CLA | OBD-CAD-C3D | -2.02 | 124.31 | 128.03 |
| 24 | D | 404 | CLA | CBC-CAC-C3C | -2.02 | 106.68 | 112.41 |
| 36 | D | 407 | DGD | O2G-C1B-O1B | -2.02 | 118.64 | 123.68 |
| 24 | c | 508 | CLA | C1B-CHB-C4A | -2.01 | 126.13 | 130.12 |
| 24 | C | 502 | CLA | OBD-CAD-C3D | -2.01 | 124.32 | 128.03 |
| 24 | b | 612 | CLA | OBD-CAD-C3D | -2.01 | 124.32 | 128.03 |
| 24 | b | 614 | CLA | O2A-CGA-O1A | -2.01 | 118.56 | 123.55 |
| 25 | d | 403 | PHO | C4-C3-C2 | -2.01 | 118.32 | 123.69 |
| 26 | A | 410 | BCR | C36-C18-C17 | -2.01 | 120.11 | 122.92 |
| 24 | c | 508 | CLA | C2A-C1A-CHA | -2.01 | 120.35 | 123.92 |
| 24 | B | 614 | CLA | CBC-CAC-C3C | -2.01 | 106.71 | 112.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 34 | J | 101 | LMG | C7-O1-C1 | -2.01 | 109.64 | 113.76 |
| 26 | a | 410 | BCR | C20-C21-C22 | -2.01 | 124.45 | 127.31 |
| 27 | f | 101 | SQD | O48-C23-O10 | -2.01 | 118.57 | 123.55 |
| 24 | c | 506 | CLA | C2A-C1A-CHA | -2.01 | 120.36 | 123.92 |
| 34 | b | 625 | LMG | O7-C10-O9 | -2.01 | 118.67 | 123.68 |
| 26 | K | 101 | BCR | C38-C26-C25 | -2.00 | 122.27 | 124.51 |
| 30 | D | 402 | LMT | O1B-C4'-C5' | -2.00 | 104.42 | 109.34 |
| 24 | C | 504 | CLA | O2D-CGD-O1D | -2.00 | 119.79 | 123.82 |
| 24 | c | 510 | CLA | OBD-CAD-C3D | -2.00 | 124.34 | 128.03 |
| 37 | D | 408 | LHG | C6-O8-C23 | 2.00 | 123.16 | 117.13 |
| 24 | b | 617 | CLA | CHB-C4A-NA | 2.00 | 127.28 | 124.51 |
| 26 | K | 101 | BCR | C33-C5-C4 | 2.00 | 117.25 | 113.45 |
| 25 | A | 408 | PHO | CBD-CHA-C1A | 2.00 | 131.08 | 126.36 |
| 24 | B | 614 | CLA | CHB-C4A-NA | 2.00 | 127.28 | 124.51 |
| 24 | B | 613 | CLA | C1-O2A-CGA | 2.01 | 121.58 | 116.77 |
| 32 | a | 416 | PL9 | C51-C49-C50 | 2.01 | 119.29 | 114.60 |
| 24 | b | 615 | CLA | CHB-C4A-NA | 2.01 | 127.29 | 124.51 |
| 24 | a | 406 | CLA | CMC-C2C-C1C | 2.02 | 128.08 | 125.02 |
| 36 | c | 517 | DGD | C1E-O6E-C5E | 2.02 | 117.52 | 113.72 |
| 24 | B | 604 | CLA | C6-C5-C3 | 2.02 | 117.24 | 112.66 |
| 35 | c | 523 | HTG | C1-O5-C5 | 2.02 | 116.58 | 112.69 |
| 24 | C | 509 | CLA | C3D-CAD-CBD | 2.02 | 110.45 | 107.60 |
| 26 | t | 101 | BCR | C35-C13-C12 | 2.02 | 121.32 | 118.10 |
| 35 | B | 622 | HTG | O5-C1-C2 | 2.03 | 113.06 | 110.28 |
| 24 | c | 504 | CLA | CHB-C4A-NA | 2.03 | 127.32 | 124.51 |
| 32 | d | 406 | PL9 | C2-C1-C6 | 2.03 | 121.23 | 117.82 |
| 24 | c | 504 | CLA | CMC-C2C-C1C | 2.03 | 128.10 | 125.02 |
| 24 | D | 401 | CLA | CAA-CBA-CGA | 2.04 | 119.48 | 113.35 |
| 24 | b | 621 | CLA | C4-C3-C5 | 2.04 | 118.82 | 115.29 |
| 32 | A | 419 | PL9 | C40-C39-C41 | 2.04 | 118.83 | 115.29 |
| 27 | A | 416 | SQD | O7-S-C6 | 2.04 | 108.57 | 106.83 |
| 38 | V | 203 | HEM | CMB-C2B-C3B | 2.04 | 128.69 | 124.89 |
| 24 | c | 509 | CLA | CAA-C2A-C1A | 2.04 | 118.68 | 111.97 |
| 24 | a | 409 | CLA | CED-O2D-CGD | 2.05 | 120.77 | 115.97 |
| 30 | a | 401 | LMT | O5B-C5B-C4B | 2.05 | 113.43 | 109.66 |
| 36 | d | 407 | DGD | O6D-C5D-C6D | 2.05 | 110.72 | 106.64 |
| 36 | h | 102 | DGD | C6D-C5D-C4D | 2.05 | 116.36 | 112.00 |
| 24 | C | 509 | CLA | C4-C3-C5 | 2.05 | 118.84 | 115.29 |
| 24 | C | 513 | CLA | CHB-C4A-NA | 2.05 | 127.35 | 124.51 |
| 24 | B | 615 | CLA | CED-O2D-CGD | 2.05 | 120.79 | 115.97 |
| 24 | c | 508 | CLA | CHB-C4A-NA | 2.06 | 127.35 | 124.51 |
| 26 | D | 405 | BCR | C29-C30-C25 | 2.06 | 113.70 | 110.48 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 32 | D | 406 | PL9 | C10-C9-C11 | 2.06 | 118.86 | 115.29 |
| 24 | b | 618 | CLA | CED-O2D-CGD | 2.06 | 120.80 | 115.97 |
| 24 | B | 602 | CLA | CHB-C4A-NA | 2.06 | 127.36 | 124.51 |
| 30 | M | 102 | LMT | O5B-C5B-C6B | 2.06 | 111.35 | 106.41 |
| 24 | b | 621 | CLA | CED-O2D-CGD | 2.06 | 120.81 | 115.97 |
| 24 | B | 606 | CLA | CMB-C2B-C1B | 2.06 | 131.64 | 128.46 |
| 24 | B | 604 | CLA | CAA-CBA-CGA | 2.06 | 119.56 | 113.35 |
| 35 | B | 623 | HTG | C1-C2-C3 | 2.06 | 115.11 | 110.69 |
| 24 | c | 506 | CLA | CMB-C2B-C3B | 2.07 | 128.73 | 124.89 |
| 30 | M | 101 | LMT | O1B-C1B-C2B | 2.07 | 112.77 | 108.11 |
| 24 | c | 510 | CLA | CHB-C4A-NA | 2.07 | 127.38 | 124.51 |
| 30 | D | 402 | LMT | C3B-C4B-C5B | 2.07 | 113.87 | 110.22 |
| 24 | C | 503 | CLA | C3D-CAD-CBD | 2.07 | 110.53 | 107.60 |
| 24 | B | 609 | CLA | CHB-C4A-NA | 2.08 | 127.38 | 124.51 |
| 24 | c | 512 | CLA | C1-O2A-CGA | 2.08 | 121.75 | 116.77 |
| 32 | D | 406 | PL9 | C20-C19-C21 | 2.08 | 118.89 | 115.29 |
| 24 | b | 611 | CLA | CHB-C4A-NA | 2.08 | 127.38 | 124.51 |
| 24 | c | 512 | CLA | CHB-C4A-NA | 2.08 | 127.39 | 124.51 |
| 24 | b | 620 | CLA | O2A-CGA-CBA | 2.09 | 117.97 | 111.90 |
| 35 | B | 631 | HTG | C1-O5-C5 | 2.09 | 116.72 | 112.69 |
| 24 | D | 404 | CLA | CMB-C2B-C3B | 2.10 | 128.78 | 124.89 |
| 24 | d | 401 | CLA | CMB-C2B-C3B | 2.10 | 128.78 | 124.89 |
| 26 | c | 516 | BCR | C2-C1-C6 | 2.10 | 113.77 | 110.48 |
| 24 | B | 603 | CLA | O2A-CGA-CBA | 2.10 | 118.02 | 111.90 |
| 26 | B | 619 | BCR | C2-C1-C6 | 2.11 | 113.77 | 110.48 |
| 25 | a | 408 | PHO | C4D-C3D-CAD | 2.11 | 109.33 | 105.41 |
| 25 | A | 407 | PHO | C2A-C1A-NA | 2.11 | 114.47 | 111.91 |
| 25 | a | 408 | PHO | CMC-C2C-C1C | 2.12 | 128.34 | 125.04 |
| 24 | B | 610 | CLA | C6-C5-C3 | 2.12 | 117.46 | 112.66 |
| 24 | C | 513 | CLA | CED-O2D-CGD | 2.12 | 120.94 | 115.97 |
| 24 | B | 604 | CLA | CED-O2D-CGD | 2.12 | 120.95 | 115.97 |
| 24 | b | 614 | CLA | CED-O2D-CGD | 2.13 | 120.95 | 115.97 |
| 24 | b | 610 | CLA | CMB-C2B-C1B | 2.13 | 131.74 | 128.46 |
| 26 | y | 101 | BCR | C1-C6-C7 | 2.13 | 121.73 | 115.73 |
| 24 | c | 510 | CLA | C1-O2A-CGA | 2.13 | 121.89 | 116.77 |
| 24 | b | 619 | CLA | CHB-C4A-NA | 2.14 | 127.47 | 124.51 |
| 26 | d | 405 | BCR | C38-C26-C27 | 2.15 | 117.52 | 113.45 |
| 35 | B | 622 | HTG | C1-O5-C5 | 2.15 | 116.83 | 112.69 |
| 35 | b | 627 | HTG | C1-C2-C3 | 2.15 | 115.29 | 110.69 |
| 24 | B | 609 | CLA | C1-O2A-CGA | 2.15 | 121.94 | 116.77 |
| 36 | C | 517 | DGD | O6D-C5D-C6D | 2.15 | 110.94 | 106.64 |
| 24 | C | 514 | CLA | CHB-C4A-NA | 2.16 | 127.49 | 124.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 34 | c | 501 | LMG | O1-C1-C2 | 2.16 | 111.75 | 108.23 |
| 24 | B | 606 | CLA | O2A-CGA-CBA | 2.16 | 118.18 | 111.90 |
| 34 | J | 101 | LMG | O8-C28-C29 | 2.16 | 118.18 | 111.90 |
| 32 | a | 416 | PL9 | C45-C44-C46 | 2.16 | 119.04 | 115.29 |
| 30 | I | 102 | LMT | C1B-C2B-C3B | 2.16 | 114.00 | 109.98 |
| 24 | c | 506 | CLA | C1-O2A-CGA | 2.16 | 121.97 | 116.77 |
| 36 | d | 407 | DGD | O5D-C1E-C2E | 2.17 | 111.78 | 108.23 |
| 36 | C | 519 | DGD | O1G-C1A-C2A | 2.17 | 118.22 | 111.90 |
| 34 | C | 521 | LMG | O6-C5-C6 | 2.17 | 111.61 | 106.41 |
| 35 | c | 522 | HTG | C1-O5-C5 | 2.17 | 116.87 | 112.69 |
| 35 | C | 522 | HTG | O5-C1-C2 | 2.18 | 113.26 | 110.28 |
| 26 | K | 101 | BCR | C29-C30-C25 | 2.18 | 113.89 | 110.48 |
| 26 | b | 623 | BCR | C29-C30-C25 | 2.18 | 113.89 | 110.48 |
| 24 | C | 507 | CLA | CMB-C2B-C3B | 2.18 | 128.94 | 124.89 |
| 24 | A | 406 | CLA | CED-O2D-CGD | 2.18 | 121.09 | 115.97 |
| 24 | c | 508 | CLA | CMC-C2C-C1C | 2.19 | 128.34 | 125.02 |
| 26 | B | 620 | BCR | C34-C9-C8 | 2.19 | 121.59 | 118.10 |
| 25 | d | 403 | PHO | C3C-C4C-NC | 2.19 | 113.77 | 110.19 |
| 38 | V | 203 | HEM | C4A-C3A-C2A | 2.19 | 108.52 | 107.00 |
| 24 | B | 604 | CLA | C1-O2A-CGA | 2.19 | 122.04 | 116.77 |
| 26 | b | 622 | BCR | C29-C30-C25 | 2.20 | 113.92 | 110.48 |
| 30 | D | 402 | LMT | O5'-C5'-C4' | 2.20 | 114.26 | 109.75 |
| 24 | b | 612 | CLA | O2A-CGA-CBA | 2.21 | 118.32 | 111.90 |
| 26 | c | 526 | BCR | C2-C1-C6 | 2.21 | 113.93 | 110.48 |
| 24 | b | 607 | CLA | CMC-C2C-C1C | 2.21 | 128.37 | 125.02 |
| 25 | a | 408 | PHO | CMB-C2B-C1B | 2.21 | 128.48 | 125.04 |
| 24 | C | 510 | CLA | CMC-C2C-C1C | 2.21 | 128.37 | 125.02 |
| 24 | a | 407 | CLA | CHB-C4A-NA | 2.21 | 127.57 | 124.51 |
| 26 | T | 102 | BCR | C29-C30-C25 | 2.21 | 113.94 | 110.48 |
| 24 | A | 406 | CLA | CAA-CBA-CGA | 2.22 | 120.02 | 113.35 |
| 24 | B | 610 | CLA | CMB-C2B-C1B | 2.22 | 131.88 | 128.46 |
| 24 | c | 515 | CLA | CHB-C4A-NA | 2.22 | 127.59 | 124.51 |
| 24 | B | 603 | CLA | CAC-C3C-C4C | 2.22 | 127.97 | 124.83 |
| 24 | b | 606 | CLA | CMC-C2C-C1C | 2.22 | 128.39 | 125.02 |
| 34 | C | 520 | LMG | O6-C5-C6 | 2.23 | 111.74 | 106.41 |
| 24 | c | 510 | CLA | CAC-C3C-C4C | 2.23 | 127.97 | 124.83 |
| 32 | d | 406 | PL9 | C35-C34-C36 | 2.23 | 119.16 | 115.29 |
| 24 | B | 616 | CLA | CED-O2D-CGD | 2.23 | 121.21 | 115.97 |
| 24 | c | 503 | CLA | C1-O2A-CGA | 2.24 | 122.14 | 116.77 |
| 24 | c | 514 | CLA | CED-O2D-CGD | 2.24 | 121.22 | 115.97 |
| 36 | d | 407 | DGD | C1E-O6E-C5E | 2.24 | 117.93 | 113.72 |
| 26 | h | 101 | BCR | C29-C30-C25 | 2.24 | 113.98 | 110.48 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 24 | c | 508 | CLA | C4-C3-C5 | 2.24 | 119.18 | 115.29 |
| 24 | c | 512 | CLA | CAC-C3C-C4C | 2.25 | 128.00 | 124.83 |
| 24 | B | 610 | CLA | C4-C3-C5 | 2.25 | 119.19 | 115.29 |
| 24 | b | 612 | CLA | C1-O2A-CGA | 2.25 | 122.17 | 116.77 |
| 27 | b | 601 | SQD | O8-S-C6 | 2.25 | 108.76 | 106.01 |
| 24 | b | 618 | CLA | CMC-C2C-C1C | 2.26 | 128.44 | 125.02 |
| 32 | A | 419 | PL9 | C2-C1-C6 | 2.26 | 121.61 | 117.82 |
| 26 | T | 102 | BCR | C35-C13-C12 | 2.27 | 121.72 | 118.10 |
| 24 | c | 503 | CLA | C4-C3-C5 | 2.27 | 119.23 | 115.29 |
| 24 | B | 613 | CLA | O2A-CGA-CBA | 2.27 | 118.52 | 111.90 |
| 24 | B | 608 | CLA | CMB-C2B-C3B | 2.27 | 129.11 | 124.89 |
| 36 | D | 407 | DGD | O6D-C5D-C6D | 2.27 | 111.18 | 106.64 |
| 24 | b | 615 | CLA | CMB-C2B-C3B | 2.28 | 129.12 | 124.89 |
| 24 | A | 409 | CLA | CHB-C4A-NA | 2.28 | 127.66 | 124.51 |
| 24 | B | 616 | CLA | O2A-CGA-CBA | 2.28 | 118.53 | 111.90 |
| 24 | b | 609 | CLA | C4-C3-C5 | 2.28 | 119.25 | 115.29 |
| 24 | b | 616 | CLA | C4-C3-C5 | 2.29 | 119.25 | 115.29 |
| 24 | A | 409 | CLA | CMB-C2B-C3B | 2.29 | 129.14 | 124.89 |
| 24 | c | 514 | CLA | CHB-C4A-NA | 2.29 | 127.68 | 124.51 |
| 24 | c | 515 | CLA | C4-C3-C5 | 2.29 | 119.26 | 115.29 |
| 32 | D | 406 | PL9 | C2-C1-C6 | 2.29 | 121.67 | 117.82 |
| 24 | D | 404 | CLA | CMC-C2C-C1C | 2.30 | 128.50 | 125.02 |
| 24 | C | 503 | CLA | C4-C3-C5 | 2.30 | 119.28 | 115.29 |
| 27 | A | 416 | SQD | O5-C5-C4 | 2.31 | 113.91 | 109.66 |
| 30 | m | 103 | LMT | O1'-C1'-C2' | 2.31 | 112.01 | 108.23 |
| 24 | C | 504 | CLA | CMC-C2C-C1C | 2.31 | 128.53 | 125.02 |
| 24 | b | 607 | CLA | CMB-C2B-C3B | 2.31 | 129.18 | 124.89 |
| 24 | B | 611 | CLA | CMC-C2C-C1C | 2.31 | 128.53 | 125.02 |
| 24 | B | 602 | CLA | CAC-C3C-C4C | 2.32 | 128.10 | 124.83 |
| 24 | B | 614 | CLA | CMC-C2C-C1C | 2.32 | 128.54 | 125.02 |
| 24 | B | 613 | CLA | C4-C3-C5 | 2.32 | 119.32 | 115.29 |
| 24 | B | 616 | CLA | C4-C3-C5 | 2.32 | 119.32 | 115.29 |
| 25 | A | 407 | PHO | C3C-C4C-NC | 2.33 | 114.00 | 110.19 |
| 24 | B | 614 | CLA | O2D-CGD-CBD | 2.33 | 115.46 | 111.30 |
| 24 | B | 607 | CLA | CMB-C2B-C3B | 2.33 | 129.22 | 124.89 |
| 24 | b | 607 | CLA | C1-O2A-CGA | 2.34 | 122.38 | 116.77 |
| 24 | C | 506 | CLA | C4-C3-C5 | 2.34 | 119.35 | 115.29 |
| 25 | d | 403 | PHO | CBD-CHA-C1A | 2.35 | 131.90 | 126.36 |
| 24 | d | 402 | CLA | CAC-C3C-C4C | 2.35 | 128.15 | 124.83 |
| 26 | d | 405 | BCR | C29-C30-C25 | 2.36 | 114.16 | 110.48 |
| 25 | A | 407 | PHO | CBD-CHA-C1A | 2.36 | 131.91 | 126.36 |
| 36 | D | 407 | DGD | O6E-C5E-C4E | 2.36 | 114.01 | 109.66 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 24 | c | 506 | CLA | O2A-CGA-CBA | 2.36 | 118.77 | 111.90 |
| 24 | B | 614 | CLA | CMB-C2B-C3B | 2.36 | 129.28 | 124.89 |
| 24 | b | 621 | CLA | CMB-C2B-C3B | 2.37 | 129.28 | 124.89 |
| 24 | C | 511 | CLA | O2A-CGA-CBA | 2.37 | 118.79 | 111.90 |
| 24 | b | 612 | CLA | CAA-CBA-CGA | 2.37 | 120.49 | 113.35 |
| 24 | a | 407 | CLA | C4-C3-C5 | 2.37 | 119.41 | 115.29 |
| 24 | C | 513 | CLA | CAC-C3C-C4C | 2.38 | 128.18 | 124.83 |
| 24 | b | 614 | CLA | CAC-C3C-C4C | 2.38 | 128.18 | 124.83 |
| 26 | D | 405 | BCR | C30-C25-C24 | 2.38 | 122.41 | 115.73 |
| 24 | B | 611 | CLA | CMB-C2B-C3B | 2.38 | 129.31 | 124.89 |
| 24 | c | 503 | CLA | CMC-C2C-C1C | 2.38 | 128.63 | 125.02 |
| 24 | c | 506 | CLA | C6-C5-C3 | 2.38 | 118.05 | 112.66 |
| 24 | b | 618 | CLA | CAC-C3C-C4C | 2.38 | 128.19 | 124.83 |
| 24 | c | 511 | CLA | C4-C3-C5 | 2.39 | 119.43 | 115.29 |
| 26 | t | 101 | BCR | C2-C1-C6 | 2.39 | 114.21 | 110.48 |
| 24 | d | 401 | CLA | CAA-CBA-CGA | 2.39 | 120.53 | 113.35 |
| 24 | c | 514 | CLA | C4-C3-C5 | 2.39 | 119.44 | 115.29 |
| 34 | j | 101 | LMG | O8-C28-C29 | 2.39 | 118.86 | 111.90 |
| 26 | b | 624 | BCR | C2-C1-C6 | 2.40 | 114.22 | 110.48 |
| 24 | b | 614 | CLA | O2A-CGA-CBA | 2.40 | 118.88 | 111.90 |
| 24 | C | 505 | CLA | C1-O2A-CGA | 2.40 | 122.53 | 116.77 |
| 24 | b | 606 | CLA | CMB-C2B-C3B | 2.40 | 129.35 | 124.89 |
| 24 | b | 611 | CLA | O2A-CGA-CBA | 2.40 | 118.89 | 111.90 |
| 26 | K | 101 | BCR | C2-C1-C6 | 2.40 | 114.23 | 110.48 |
| 30 | a | 401 | LMT | C1'-O5'-C5' | 2.40 | 118.24 | 113.72 |
| 24 | c | 504 | CLA | CAC-C3C-C4C | 2.40 | 128.22 | 124.83 |
| 24 | B | 605 | CLA | CAC-C3C-C4C | 2.40 | 128.22 | 124.83 |
| 24 | b | 620 | CLA | CMC-C2C-C1C | 2.40 | 128.67 | 125.02 |
| 24 | b | 611 | CLA | C4-C3-C5 | 2.41 | 119.46 | 115.29 |
| 24 | B | 610 | CLA | O2A-CGA-CBA | 2.41 | 118.90 | 111.90 |
| 24 | D | 401 | CLA | CHB-C4A-NA | 2.41 | 127.84 | 124.51 |
| 24 | b | 614 | CLA | C4-C3-C5 | 2.41 | 119.47 | 115.29 |
| 24 | b | 614 | CLA | C1-O2A-CGA | 2.41 | 122.56 | 116.77 |
| 36 | d | 407 | DGD | O6E-C5E-C4E | 2.42 | 114.11 | 109.66 |
| 24 | D | 401 | CLA | O2A-CGA-CBA | 2.42 | 118.94 | 111.90 |
| 24 | B | 608 | CLA | CAC-C3C-C4C | 2.42 | 128.25 | 124.83 |
| 24 | C | 504 | CLA | CMB-C2B-C3B | 2.42 | 129.39 | 124.89 |
| 26 | d | 405 | BCR | C37-C22-C23 | 2.43 | 121.97 | 118.10 |
| 24 | C | 506 | CLA | O2A-CGA-CBA | 2.43 | 118.97 | 111.90 |
| 36 | C | 519 | DGD | O2G-C1B-C2B | 2.43 | 116.60 | 111.55 |
| 24 | c | 512 | CLA | CMB-C2B-C3B | 2.43 | 129.41 | 124.89 |
| 25 | A | 408 | PHO | O2A-CGA-CBA | 2.44 | 118.99 | 111.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 35 | b | 627 | HTG | C1-O5-C5 | 2.44 | 117.39 | 112.69 |
| 24 | C | 510 | CLA | O2A-CGA-CBA | 2.45 | 119.03 | 111.90 |
| 24 | B | 604 | CLA | CAC-C3C-C4C | 2.45 | 128.29 | 124.83 |
| 32 | a | 416 | PL9 | C35-C34-C36 | 2.45 | 119.55 | 115.29 |
| 26 | t | 101 | BCR | C1-C6-C7 | 2.46 | 122.64 | 115.73 |
| 24 | C | 509 | CLA | CMB-C2B-C3B | 2.46 | 129.46 | 124.89 |
| 24 | C | 513 | CLA | C1-O2A-CGA | 2.46 | 122.68 | 116.77 |
| 30 | b | 602 | LMT | O5'-C1'-C2' | 2.46 | 115.05 | 110.30 |
| 24 | C | 505 | CLA | C4-C3-C5 | 2.47 | 119.56 | 115.29 |
| 24 | B | 602 | CLA | C4-C3-C5 | 2.47 | 119.57 | 115.29 |
| 24 | b | 613 | CLA | CMB-C2B-C3B | 2.47 | 129.47 | 124.89 |
| 36 | H | 102 | DGD | O1G-C1A-C2A | 2.47 | 119.08 | 111.90 |
| 24 | C | 512 | CLA | CMC-C2C-C1C | 2.47 | 128.76 | 125.02 |
| 24 | C | 508 | CLA | C3B-C4B-NB | 2.47 | 112.40 | 109.21 |
| 32 | A | 419 | PL9 | C7-C3-C4 | 2.47 | 118.89 | 116.88 |
| 24 | c | 510 | CLA | O2A-CGA-CBA | 2.48 | 119.11 | 111.90 |
| 30 | a | 401 | LMT | O5'-C5'-C4' | 2.48 | 114.83 | 109.75 |
| 24 | C | 506 | CLA | CMC-C2C-C1C | 2.48 | 128.78 | 125.02 |
| 30 | m | 103 | LMT | C1B-O5B-C5B | 2.48 | 118.39 | 113.72 |
| 24 | B | 606 | CLA | C1-O2A-CGA | 2.48 | 122.73 | 116.77 |
| 24 | B | 617 | CLA | O2A-CGA-CBA | 2.49 | 119.14 | 111.90 |
| 30 | m | 103 | LMT | O5B-C5B-C4B | 2.49 | 114.25 | 109.66 |
| 24 | d | 402 | CLA | CMB-C2B-C3B | 2.49 | 129.52 | 124.89 |
| 34 | B | 621 | LMG | O8-C28-C29 | 2.50 | 119.16 | 111.90 |
| 24 | c | 508 | CLA | CED-O2D-CGD | 2.50 | 121.82 | 115.97 |
| 26 | D | 405 | BCR | C37-C22-C23 | 2.50 | 122.08 | 118.10 |
| 32 | d | 406 | PL9 | C8-C7-C3 | 2.50 | 119.12 | 111.73 |
| 26 | H | 101 | BCR | C29-C30-C25 | 2.50 | 114.38 | 110.48 |
| 24 | b | 616 | CLA | O2A-CGA-CBA | 2.50 | 119.17 | 111.90 |
| 24 | B | 602 | CLA | CMC-C2C-C1C | 2.50 | 128.81 | 125.02 |
| 35 | b | 628 | HTG | C1-O5-C5 | 2.50 | 117.51 | 112.69 |
| 32 | A | 419 | PL9 | C30-C29-C31 | 2.50 | 119.63 | 115.29 |
| 36 | C | 517 | DGD | O1G-C1A-C2A | 2.51 | 119.19 | 111.90 |
| 27 | A | 416 | SQD | O8-S-C6 | 2.51 | 109.07 | 106.01 |
| 24 | C | 504 | CLA | CAC-C3C-C4C | 2.51 | 128.37 | 124.83 |
| 24 | d | 401 | CLA | O2A-CGA-CBA | 2.51 | 119.21 | 111.90 |
| 24 | C | 508 | CLA | CMB-C2B-C3B | 2.51 | 129.55 | 124.89 |
| 24 | D | 401 | CLA | CMC-C2C-C1C | 2.51 | 128.83 | 125.02 |
| 24 | b | 619 | CLA | C4-C3-C5 | 2.51 | 119.65 | 115.29 |
| 24 | C | 507 | CLA | CMC-C2C-C1C | 2.52 | 128.84 | 125.02 |
| 32 | D | 406 | PL9 | C15-C14-C16 | 2.52 | 119.66 | 115.29 |
| 24 | B | 617 | CLA | CMB-C2B-C3B | 2.52 | 129.57 | 124.89 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 26 | T | 102 | BCR | C1-C6-C7 | 2.52 | 122.81 | 115.73 |
| 24 | c | 515 | CLA | CMB-C2B-C3B | 2.52 | 129.57 | 124.89 |
| 32 | d | 406 | PL9 | C20-C19-C21 | 2.53 | 119.67 | 115.29 |
| 24 | d | 404 | CLA | CMB-C2B-C3B | 2.53 | 129.58 | 124.89 |
| 24 | c | 511 | CLA | CMC-C2C-C1C | 2.53 | 128.85 | 125.02 |
| 24 | b | 612 | CLA | CAC-C3C-C4C | 2.53 | 128.40 | 124.83 |
| 24 | C | 510 | CLA | CMB-C2B-C3B | 2.53 | 129.59 | 124.89 |
| 36 | d | 407 | DGD | O1G-C1A-C2A | 2.54 | 119.28 | 111.90 |
| 24 | D | 404 | CLA | C4-C3-C5 | 2.54 | 119.70 | 115.29 |
| 24 | C | 503 | CLA | CAC-C3C-C4C | 2.55 | 128.42 | 124.83 |
| 24 | B | 616 | CLA | C1-O2A-CGA | 2.55 | 122.89 | 116.77 |
| 24 | B | 609 | CLA | CMC-C2C-C1C | 2.55 | 128.89 | 125.02 |
| 32 | a | 416 | PL9 | C40-C39-C41 | 2.55 | 119.72 | 115.29 |
| 24 | a | 406 | CLA | O2D-CGD-CBD | 2.56 | 115.87 | 111.30 |
| 24 | d | 402 | CLA | CMC-C2C-C1C | 2.56 | 128.90 | 125.02 |
| 36 | c | 518 | DGD | O1G-C1A-C2A | 2.56 | 119.35 | 111.90 |
| 24 | c | 511 | CLA | CMB-C2B-C3B | 2.56 | 129.65 | 124.89 |
| 24 | b | 617 | CLA | CAC-C3C-C4C | 2.56 | 128.44 | 124.83 |
| 24 | B | 615 | CLA | CMB-C2B-C3B | 2.56 | 129.65 | 124.89 |
| 37 | l | 102 | LHG | O8-C23-C24 | 2.56 | 119.36 | 111.90 |
| 24 | C | 510 | CLA | CAC-C3C-C4C | 2.57 | 128.45 | 124.83 |
| 24 | A | 406 | CLA | O2A-CGA-CBA | 2.57 | 119.37 | 111.90 |
| 24 | B | 612 | CLA | O2A-CGA-CBA | 2.57 | 119.38 | 111.90 |
| 25 | A | 408 | PHO | C2A-C1A-NA | 2.57 | 115.03 | 111.91 |
| 24 | B | 606 | CLA | C4-C3-C5 | 2.57 | 119.75 | 115.29 |
| 24 | B | 616 | CLA | CAC-C3C-C4C | 2.58 | 128.46 | 124.83 |
| 25 | A | 407 | PHO | C4D-C3D-CAD | 2.58 | 110.19 | 105.41 |
| 32 | D | 406 | PL9 | C25-C24-C26 | 2.58 | 119.76 | 115.29 |
| 24 | c | 510 | CLA | C4-C3-C5 | 2.58 | 119.77 | 115.29 |
| 24 | B | 607 | CLA | CAC-C3C-C4C | 2.58 | 128.47 | 124.83 |
| 24 | D | 404 | CLA | O2A-CGA-CBA | 2.58 | 119.41 | 111.90 |
| 24 | A | 406 | CLA | CMC-C2C-C1C | 2.58 | 128.94 | 125.02 |
| 24 | b | 615 | CLA | CMC-C2C-C1C | 2.59 | 128.95 | 125.02 |
| 25 | A | 408 | PHO | C3C-C4C-NC | 2.59 | 114.43 | 110.19 |
| 24 | B | 612 | CLA | C4-C3-C5 | 2.59 | 119.79 | 115.29 |
| 25 | A | 408 | PHO | C2C-C1C-NC | 2.60 | 113.66 | 109.82 |
| 32 | A | 419 | PL9 | C35-C34-C36 | 2.60 | 119.79 | 115.29 |
| 24 | B | 606 | CLA | CAC-C3C-C4C | 2.60 | 128.49 | 124.83 |
| 24 | C | 502 | CLA | O2A-CGA-CBA | 2.60 | 119.46 | 111.90 |
| 24 | C | 510 | CLA | C4-C3-C5 | 2.60 | 119.80 | 115.29 |
| 24 | C | 511 | CLA | CMB-C2B-C3B | 2.60 | 129.72 | 124.89 |
| 30 | A | 417 | LMT | C1'-O5'-C5' | 2.60 | 118.62 | 113.72 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 32 | d | 406 | PL9 | C15-C14-C16 | 2.60 | 119.81 | 115.29 |
| 24 | a | 409 | CLA | CHB-C4A-NA | 2.61 | 128.12 | 124.51 |
| 27 | a | 411 | SQD | O7-S-C6 | 2.61 | 109.06 | 106.83 |
| 24 | d | 404 | CLA | O2A-CGA-CBA | 2.61 | 119.49 | 111.90 |
| 32 | A | 419 | PL9 | C45-C44-C46 | 2.61 | 119.82 | 115.29 |
| 25 | A | 407 | PHO | C2B-C1B-NB | 2.62 | 113.70 | 109.82 |
| 34 | z | 101 | LMG | C3-C4-C5 | 2.62 | 114.83 | 110.22 |
| 24 | C | 508 | CLA | CAC-C3C-C4C | 2.62 | 128.53 | 124.83 |
| 24 | c | 508 | CLA | O2A-CGA-CBA | 2.62 | 119.53 | 111.90 |
| 24 | C | 511 | CLA | CAC-C3C-C4C | 2.63 | 128.53 | 124.83 |
| 24 | b | 611 | CLA | CMB-C2B-C3B | 2.63 | 129.77 | 124.89 |
| 24 | c | 507 | CLA | C1-O2A-CGA | 2.63 | 123.08 | 116.77 |
| 25 | d | 403 | PHO | O2A-CGA-CBA | 2.63 | 119.55 | 111.90 |
| 30 | D | 402 | LMT | O1B-C4'-C3' | 2.63 | 113.52 | 107.19 |
| 24 | C | 508 | CLA | O2A-CGA-CBA | 2.63 | 119.56 | 111.90 |
| 24 | c | 507 | CLA | CMC-C2C-C1C | 2.64 | 129.02 | 125.02 |
| 24 | B | 604 | CLA | CMB-C2B-C3B | 2.64 | 129.79 | 124.89 |
| 24 | B | 611 | CLA | C4-C3-C5 | 2.64 | 119.88 | 115.29 |
| 24 | d | 401 | CLA | CAC-C3C-C4C | 2.65 | 128.56 | 124.83 |
| 24 | c | 513 | CLA | O2A-CGA-CBA | 2.65 | 119.60 | 111.90 |
| 32 | a | 416 | PL9 | C25-C24-C26 | 2.65 | 119.88 | 115.29 |
| 24 | a | 409 | CLA | O2A-CGA-CBA | 2.65 | 119.61 | 111.90 |
| 24 | C | 514 | CLA | O2A-CGA-CBA | 2.65 | 119.61 | 111.90 |
| 34 | C | 501 | LMG | O8-C28-C29 | 2.65 | 119.61 | 111.90 |
| 24 | C | 511 | CLA | C1-O2A-CGA | 2.65 | 123.14 | 116.77 |
| 24 | b | 618 | CLA | C4-C3-C5 | 2.66 | 119.90 | 115.29 |
| 24 | c | 503 | CLA | CAC-C3C-C4C | 2.66 | 128.58 | 124.83 |
| 26 | B | 620 | BCR | C2-C1-C6 | 2.67 | 114.65 | 110.48 |
| 24 | c | 508 | CLA | CMB-C2B-C3B | 2.67 | 129.85 | 124.89 |
| 37 | d | 409 | LHG | O8-C23-C24 | 2.67 | 119.68 | 111.90 |
| 34 | c | 520 | LMG | O8-C28-C29 | 2.67 | 119.68 | 111.90 |
| 26 | Y | 101 | BCR | C37-C22-C23 | 2.68 | 122.36 | 118.10 |
| 24 | b | 615 | CLA | CAC-C3C-C4C | 2.68 | 128.61 | 124.83 |
| 24 | C | 504 | CLA | O2A-CGA-CBA | 2.68 | 119.70 | 111.90 |
| 24 | b | 607 | CLA | O2A-CGA-CBA | 2.68 | 119.70 | 111.90 |
| 34 | z | 101 | LMG | O6-C5-C4 | 2.68 | 114.60 | 109.66 |
| 24 | b | 612 | CLA | C4-C3-C5 | 2.69 | 119.95 | 115.29 |
| 24 | C | 510 | CLA | C1-O2A-CGA | 2.69 | 123.22 | 116.77 |
| 24 | A | 405 | CLA | O2A-CGA-CBA | 2.69 | 119.72 | 111.90 |
| 24 | C | 513 | CLA | C4-C3-C5 | 2.69 | 119.96 | 115.29 |
| 24 | c | 509 | CLA | C4-C3-C5 | 2.69 | 119.96 | 115.29 |
| 24 | B | 617 | CLA | C1-O2A-CGA | 2.69 | 123.23 | 116.77 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 24 | B | 605 | CLA | C4-C3-C5 | 2.70 | 119.97 | 115.29 |
| 34 | c | 501 | LMG | O8-C28-C29 | 2.70 | 119.75 | 111.90 |
| 25 | A | 408 | PHO | CMC-C2C-C1C | 2.70 | 129.25 | 125.04 |
| 24 | C | 504 | CLA | C4-C3-C5 | 2.71 | 119.99 | 115.29 |
| 30 | b | 602 | LMT | O5'-C5'-C4' | 2.71 | 115.29 | 109.75 |
| 25 | a | 408 | PHO | C3C-C4C-NC | 2.71 | 114.62 | 110.19 |
| 38 | v | 202 | HEM | CAD-CBD-CGD | 2.71 | 117.29 | 112.66 |
| 24 | b | 608 | CLA | CMB-C2B-C3B | 2.71 | 129.92 | 124.89 |
| 24 | c | 512 | CLA | O2A-CGA-CBA | 2.71 | 119.79 | 111.90 |
| 25 | d | 403 | PHO | C2C-C1C-NC | 2.71 | 113.83 | 109.82 |
| 24 | c | 513 | CLA | CMB-C2B-C3B | 2.72 | 129.94 | 124.89 |
| 26 | T | 102 | BCR | C2-C1-C6 | 2.72 | 114.73 | 110.48 |
| 37 | D | 409 | LHG | O8-C23-C24 | 2.72 | 119.81 | 111.90 |
| 24 | A | 409 | CLA | O2A-CGA-CBA | 2.72 | 119.82 | 111.90 |
| 24 | c | 510 | CLA | CMC-C2C-C1C | 2.74 | 129.17 | 125.02 |
| 24 | b | 613 | CLA | CAC-C3C-C4C | 2.74 | 128.70 | 124.83 |
| 24 | D | 401 | CLA | CMB-C2B-C3B | 2.74 | 129.98 | 124.89 |
| 36 | D | 407 | DGD | O1G-C1A-C2A | 2.75 | 119.90 | 111.90 |
| 24 | b | 610 | CLA | O2A-CGA-CBA | 2.76 | 119.92 | 111.90 |
| 24 | C | 503 | CLA | CMC-C2C-C1C | 2.76 | 129.20 | 125.02 |
| 35 | B | 624 | HTG | C1-C2-C3 | 2.76 | 116.58 | 110.69 |
| 24 | D | 404 | CLA | CAC-C3C-C4C | 2.76 | 128.72 | 124.83 |
| 32 | A | 419 | PL9 | C8-C7-C3 | 2.76 | 119.89 | 111.73 |
| 24 | D | 403 | CLA | CAC-C3C-C4C | 2.76 | 128.72 | 124.83 |
| 24 | b | 608 | CLA | CAC-C3C-C4C | 2.76 | 128.73 | 124.83 |
| 24 | A | 406 | CLA | C4-C3-C5 | 2.76 | 120.08 | 115.29 |
| 24 | c | 514 | CLA | CMC-C2C-C1C | 2.77 | 129.22 | 125.02 |
| 24 | A | 406 | CLA | CAC-C3C-C4C | 2.77 | 128.74 | 124.83 |
| 25 | d | 403 | PHO | CAC-C3C-C4C | 2.77 | 128.46 | 125.21 |
| 25 | A | 407 | PHO | CAC-C3C-C4C | 2.77 | 128.47 | 125.21 |
| 27 | A | 416 | SQD | C3-C4-C5 | 2.77 | 115.10 | 110.22 |
| 24 | c | 503 | CLA | O2A-CGA-CBA | 2.77 | 119.97 | 111.90 |
| 26 | b | 624 | BCR | C37-C22-C23 | 2.78 | 122.53 | 118.10 |
| 34 | Z | 101 | LMG | C4-C3-C2 | 2.78 | 115.74 | 110.84 |
| 37 | E | 101 | LHG | O8-C23-C24 | 2.79 | 120.02 | 111.90 |
| 24 | b | 616 | CLA | CAC-C3C-C4C | 2.79 | 128.76 | 124.83 |
| 24 | a | 407 | CLA | CMC-C2C-C1C | 2.79 | 129.25 | 125.02 |
| 24 | B | 604 | CLA | C4-C3-C5 | 2.79 | 120.13 | 115.29 |
| 24 | C | 511 | CLA | C4-C3-C5 | 2.79 | 120.13 | 115.29 |
| 24 | C | 508 | CLA | C4-C3-C5 | 2.79 | 120.14 | 115.29 |
| 24 | C | 513 | CLA | CMC-C2C-C1C | 2.79 | 129.26 | 125.02 |
| 27 | F | 101 | SQD | O48-C23-C24 | 2.80 | 120.04 | 111.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 24 | C | 507 | CLA | O2A-CGA-CBA | 2.80 | 120.04 | 111.90 |
| 32 | a | 416 | PL9 | C53-C6-C1 | 2.80 | 120.78 | 114.84 |
| 24 | B | 608 | CLA | O2A-CGA-CBA | 2.80 | 120.06 | 111.90 |
| 36 | c | 517 | DGD | O1G-C1A-C2A | 2.81 | 120.06 | 111.90 |
| 24 | a | 407 | CLA | CAC-C3C-C4C | 2.81 | 128.79 | 124.83 |
| 25 | a | 408 | PHO | C1-O2A-CGA | 2.81 | 123.52 | 116.77 |
| 27 | F | 101 | SQD | C3-C4-C5 | 2.81 | 115.17 | 110.22 |
| 24 | B | 607 | CLA | C4-C3-C5 | 2.81 | 120.17 | 115.29 |
| 34 | C | 521 | LMG | O8-C28-C29 | 2.81 | 120.08 | 111.90 |
| 24 | C | 513 | CLA | O2A-CGA-CBA | 2.82 | 120.09 | 111.90 |
| 24 | C | 514 | CLA | C4-C3-C5 | 2.82 | 120.17 | 115.29 |
| 24 | B | 614 | CLA | C4-C3-C5 | 2.82 | 120.18 | 115.29 |
| 25 | a | 408 | PHO | CAC-C3C-C4C | 2.82 | 128.52 | 125.21 |
| 24 | c | 511 | CLA | O2A-CGA-CBA | 2.82 | 120.10 | 111.90 |
| 24 | b | 613 | CLA | CMC-C2C-C1C | 2.82 | 129.29 | 125.02 |
| 24 | B | 613 | CLA | CMB-C2B-C3B | 2.82 | 130.12 | 124.89 |
| 34 | c | 521 | LMG | O8-C28-C29 | 2.82 | 120.10 | 111.90 |
| 24 | B | 611 | CLA | C3B-C4B-NB | 2.82 | 112.86 | 109.21 |
| 32 | d | 406 | PL9 | C53-C6-C1 | 2.82 | 120.83 | 114.84 |
| 24 | B | 605 | CLA | O2A-CGA-CBA | 2.83 | 120.12 | 111.90 |
| 24 | d | 404 | CLA | C4-C3-C5 | 2.83 | 120.19 | 115.29 |
| 24 | b | 606 | CLA | C4-C3-C5 | 2.83 | 120.20 | 115.29 |
| 24 | a | 409 | CLA | CAC-C3C-C4C | 2.83 | 128.82 | 124.83 |
| 34 | b | 625 | LMG | O7-C10-C11 | 2.83 | 117.44 | 111.55 |
| 27 | a | 402 | SQD | O8-S-C6 | 2.83 | 109.47 | 106.01 |
| 24 | b | 616 | CLA | CMC-C2C-C1C | 2.84 | 129.32 | 125.02 |
| 24 | c | 515 | CLA | O2A-CGA-CBA | 2.84 | 120.16 | 111.90 |
| 24 | d | 404 | CLA | CAC-C3C-C4C | 2.84 | 128.84 | 124.83 |
| 24 | C | 507 | CLA | C4-C3-C5 | 2.85 | 120.24 | 115.29 |
| 27 | l | 101 | SQD | O48-C23-C24 | 2.85 | 120.20 | 111.90 |
| 24 | b | 609 | CLA | CAC-C3C-C4C | 2.86 | 128.86 | 124.83 |
| 24 | C | 503 | CLA | C3B-C4B-NB | 2.86 | 112.91 | 109.21 |
| 24 | B | 613 | CLA | CMC-C2C-C1C | 2.86 | 129.36 | 125.02 |
| 32 | A | 419 | PL9 | C53-C6-C1 | 2.87 | 120.93 | 114.84 |
| 26 | B | 619 | BCR | C29-C30-C25 | 2.87 | 114.96 | 110.48 |
| 24 | b | 609 | CLA | O2A-CGA-CBA | 2.87 | 120.26 | 111.90 |
| 24 | d | 402 | CLA | C4-C3-C5 | 2.87 | 120.28 | 115.29 |
| 24 | b | 618 | CLA | O2A-CGA-CBA | 2.87 | 120.26 | 111.90 |
| 32 | A | 419 | PL9 | C25-C24-C26 | 2.88 | 120.28 | 115.29 |
| 24 | B | 614 | CLA | O2A-CGA-CBA | 2.88 | 120.28 | 111.90 |
| 24 | a | 407 | CLA | C3B-C4B-NB | 2.88 | 112.93 | 109.21 |
| 32 | d | 406 | PL9 | C40-C39-C41 | 2.88 | 120.29 | 115.29 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 24 | B | 614 | CLA | CAC-C3C-C4C | 2.88 | 128.90 | 124.83 |
| 24 | b | 607 | CLA | C4-C3-C5 | 2.89 | 120.30 | 115.29 |
| 24 | C | 509 | CLA | CAC-C3C-C4C | 2.89 | 128.90 | 124.83 |
| 24 | c | 504 | CLA | O2A-CGA-CBA | 2.89 | 120.30 | 111.90 |
| 24 | c | 505 | CLA | O2A-CGA-CBA | 2.89 | 120.31 | 111.90 |
| 24 | A | 409 | CLA | C3B-C4B-NB | 2.89 | 112.95 | 109.21 |
| 24 | b | 619 | CLA | CMC-C2C-C1C | 2.90 | 129.41 | 125.02 |
| 36 | h | 102 | DGD | O1G-C1A-C2A | 2.90 | 120.33 | 111.90 |
| 32 | D | 406 | PL9 | C53-C6-C1 | 2.90 | 121.00 | 114.84 |
| 24 | B | 608 | CLA | C4-C3-C5 | 2.90 | 120.32 | 115.29 |
| 32 | d | 406 | PL9 | C10-C9-C11 | 2.90 | 120.32 | 115.29 |
| 27 | A | 411 | SQD | O48-C23-C24 | 2.90 | 120.34 | 111.90 |
| 24 | c | 509 | CLA | CAC-C3C-C4C | 2.91 | 128.93 | 124.83 |
| 24 | b | 607 | CLA | CAC-C3C-C4C | 2.91 | 128.93 | 124.83 |
| 24 | C | 507 | CLA | CAC-C3C-C4C | 2.91 | 128.94 | 124.83 |
| 30 | A | 417 | LMT | O5'-C5'-C4' | 2.92 | 115.72 | 109.75 |
| 24 | c | 515 | CLA | CAC-C3C-C4C | 2.92 | 128.94 | 124.83 |
| 24 | B | 604 | CLA | O2A-CGA-CBA | 2.92 | 120.40 | 111.90 |
| 27 | a | 411 | SQD | O48-C23-C24 | 2.92 | 120.40 | 111.90 |
| 36 | C | 518 | DGD | O1G-C1A-C2A | 2.92 | 120.41 | 111.90 |
| 24 | b | 606 | CLA | C3B-C4B-NB | 2.92 | 112.99 | 109.21 |
| 24 | c | 506 | CLA | CAC-C3C-C4C | 2.93 | 128.96 | 124.83 |
| 24 | A | 405 | CLA | CMC-C2C-C1C | 2.93 | 129.47 | 125.02 |
| 24 | c | 512 | CLA | C4-C3-C5 | 2.93 | 120.38 | 115.29 |
| 27 | f | 101 | SQD | O5-C5-C4 | 2.94 | 115.07 | 109.66 |
| 24 | B | 609 | CLA | O2A-CGA-CBA | 2.94 | 120.46 | 111.90 |
| 24 | B | 612 | CLA | CMC-C2C-C1C | 2.95 | 129.49 | 125.02 |
| 27 | f | 101 | SQD | O48-C23-C24 | 2.95 | 120.47 | 111.90 |
| 24 | b | 614 | CLA | CMC-C2C-C1C | 2.95 | 129.49 | 125.02 |
| 24 | B | 609 | CLA | CMB-C2B-C3B | 2.95 | 130.37 | 124.89 |
| 37 | D | 410 | LHG | O8-C23-C24 | 2.96 | 120.51 | 111.90 |
| 24 | c | 505 | CLA | C3B-C4B-NB | 2.96 | 113.04 | 109.21 |
| 24 | C | 512 | CLA | CAC-C3C-C4C | 2.97 | 129.02 | 124.83 |
| 24 | b | 611 | CLA | C3B-C4B-NB | 2.97 | 113.05 | 109.21 |
| 24 | c | 514 | CLA | C3B-C4B-NB | 2.97 | 113.05 | 109.21 |
| 25 | a | 408 | PHO | C2B-C1B-NB | 2.97 | 114.22 | 109.82 |
| 25 | A | 407 | PHO | C2C-C1C-NC | 2.98 | 114.22 | 109.82 |
| 24 | a | 409 | CLA | C4-C3-C5 | 2.98 | 120.45 | 115.29 |
| 24 | B | 612 | CLA | CAC-C3C-C4C | 2.98 | 129.03 | 124.83 |
| 24 | c | 515 | CLA | CMC-C2C-C1C | 2.98 | 129.54 | 125.02 |
| 24 | B | 602 | CLA | O2A-CGA-CBA | 2.98 | 120.58 | 111.90 |
| 24 | b | 619 | CLA | O2A-CGA-CBA | 2.98 | 120.58 | 111.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 37 | d | 408 | LHG | O8-C23-C24 | 2.99 | 120.59 | 111.90 |
| 24 | b | 609 | CLA | C3B-C4B-NB | 2.99 | 113.08 | 109.21 |
| 24 | b | 610 | CLA | C4-C3-C5 | 2.99 | 120.48 | 115.29 |
| 38 | V | 203 | HEM | CAD-CBD-CGD | 2.99 | 117.78 | 112.66 |
| 24 | A | 406 | CLA | CMB-C2B-C3B | 2.99 | 130.45 | 124.89 |
| 34 | z | 101 | LMG | O8-C28-C29 | 3.00 | 120.63 | 111.90 |
| 24 | c | 509 | CLA | CMC-C2C-C1C | 3.00 | 129.57 | 125.02 |
| 24 | c | 513 | CLA | CAC-C3C-C4C | 3.01 | 129.07 | 124.83 |
| 32 | A | 419 | PL9 | C20-C19-C21 | 3.01 | 120.51 | 115.29 |
| 36 | c | 519 | DGD | O2G-C1B-C2B | 3.01 | 117.81 | 111.55 |
| 24 | C | 509 | CLA | O2A-CGA-CBA | 3.02 | 120.68 | 111.90 |
| 24 | C | 503 | CLA | O2A-CGA-CBA | 3.02 | 120.69 | 111.90 |
| 24 | C | 512 | CLA | C4-C3-C5 | 3.02 | 120.53 | 115.29 |
| 24 | b | 606 | CLA | O2A-CGA-CBA | 3.02 | 120.70 | 111.90 |
| 24 | B | 608 | CLA | C1-O2A-CGA | 3.03 | 124.03 | 116.77 |
| 24 | c | 513 | CLA | CMC-C2C-C1C | 3.03 | 129.62 | 125.02 |
| 35 | C | 523 | HTG | O5-C5-C4 | 3.04 | 115.26 | 109.66 |
| 37 | d | 410 | LHG | O8-C23-C24 | 3.04 | 120.75 | 111.90 |
| 24 | c | 505 | CLA | CAC-C3C-C4C | 3.04 | 129.12 | 124.83 |
| 24 | a | 407 | CLA | O2A-CGA-CBA | 3.04 | 120.76 | 111.90 |
| 37 | L | 101 | LHG | O8-C23-C24 | 3.05 | 120.77 | 111.90 |
| 24 | B | 614 | CLA | CED-O2D-CGD | 3.05 | 123.13 | 115.97 |
| 25 | d | 403 | PHO | C2B-C1B-NB | 3.06 | 114.34 | 109.82 |
| 27 | A | 416 | SQD | O9-S-C6 | 3.06 | 109.44 | 106.83 |
| 24 | B | 603 | CLA | CMB-C2B-C3B | 3.06 | 130.57 | 124.89 |
| 24 | D | 401 | CLA | CAC-C3C-C4C | 3.06 | 129.15 | 124.83 |
| 24 | B | 607 | CLA | C1-O2A-CGA | 3.07 | 124.13 | 116.77 |
| 32 | a | 416 | PL9 | C10-C9-C11 | 3.07 | 120.61 | 115.29 |
| 24 | D | 403 | CLA | CMC-C2C-C1C | 3.07 | 129.68 | 125.02 |
| 24 | A | 409 | CLA | CMC-C2C-C1C | 3.07 | 129.68 | 125.02 |
| 24 | b | 620 | CLA | CAC-C3C-C4C | 3.08 | 129.17 | 124.83 |
| 32 | a | 416 | PL9 | C7-C3-C4 | 3.08 | 119.38 | 116.88 |
| 32 | a | 416 | PL9 | C30-C29-C31 | 3.08 | 120.63 | 115.29 |
| 24 | c | 514 | CLA | O2A-CGA-CBA | 3.09 | 120.88 | 111.90 |
| 24 | C | 511 | CLA | CMC-C2C-C1C | 3.09 | 129.71 | 125.02 |
| 24 | B | 602 | CLA | CMB-C2B-C3B | 3.09 | 130.63 | 124.89 |
| 24 | b | 617 | CLA | O2A-CGA-CBA | 3.10 | 120.91 | 111.90 |
| 24 | C | 513 | CLA | CMB-C2B-C3B | 3.10 | 130.65 | 124.89 |
| 32 | a | 416 | PL9 | C20-C19-C21 | 3.10 | 120.67 | 115.29 |
| 24 | B | 602 | CLA | C3B-C4B-NB | 3.10 | 113.22 | 109.21 |
| 24 | b | 615 | CLA | O2A-CGA-CBA | 3.11 | 120.94 | 111.90 |
| 24 | A | 405 | CLA | C3B-C4B-NB | 3.12 | 113.24 | 109.21 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 30 | I | 102 | LMT | C1'-O5'-C5' | 3.12 | 119.59 | 113.72 |
| 24 | c | 509 | CLA | C3B-C4B-NB | 3.12 | 113.25 | 109.21 |
| 24 | b | 613 | CLA | C3B-C4B-NB | 3.12 | 113.25 | 109.21 |
| 24 | c | 506 | CLA | CMC-C2C-C1C | 3.12 | 129.76 | 125.02 |
| 24 | c | 509 | CLA | O2A-CGA-CBA | 3.14 | 121.05 | 111.90 |
| 24 | B | 606 | CLA | C3B-C4B-NB | 3.15 | 113.28 | 109.21 |
| 25 | d | 403 | PHO | C4-C3-C5 | 3.15 | 120.76 | 115.29 |
| 24 | A | 405 | CLA | O2D-CGD-CBD | 3.15 | 116.93 | 111.30 |
| 37 | d | 408 | LHG | O7-C7-C8 | 3.16 | 118.11 | 111.55 |
| 36 | c | 519 | DGD | O1G-C1A-C2A | 3.16 | 121.09 | 111.90 |
| 32 | A | 419 | PL9 | C15-C14-C16 | 3.16 | 120.77 | 115.29 |
| 32 | A | 419 | PL9 | C10-C9-C11 | 3.17 | 120.78 | 115.29 |
| 24 | c | 510 | CLA | C3B-C4B-NB | 3.17 | 113.31 | 109.21 |
| 24 | A | 405 | CLA | CAC-C3C-C4C | 3.18 | 129.31 | 124.83 |
| 24 | C | 502 | CLA | CMC-C2C-C1C | 3.18 | 129.84 | 125.02 |
| 24 | c | 507 | CLA | C3B-C4B-NB | 3.18 | 113.32 | 109.21 |
| 24 | B | 608 | CLA | C3B-C4B-NB | 3.18 | 113.32 | 109.21 |
| 24 | B | 610 | CLA | C3B-C4B-NB | 3.18 | 113.33 | 109.21 |
| 24 | c | 512 | CLA | CMC-C2C-C1C | 3.19 | 129.85 | 125.02 |
| 24 | C | 506 | CLA | CAC-C3C-C4C | 3.19 | 129.33 | 124.83 |
| 24 | c | 510 | CLA | CMB-C2B-C3B | 3.20 | 130.82 | 124.89 |
| 24 | B | 615 | CLA | CAC-C3C-C4C | 3.20 | 129.34 | 124.83 |
| 24 | b | 610 | CLA | C3B-C4B-NB | 3.20 | 113.35 | 109.21 |
| 24 | c | 513 | CLA | C4-C3-C5 | 3.20 | 120.84 | 115.29 |
| 35 | D | 411 | HTG | C1'-S1-C1 | 3.20 | 105.03 | 100.28 |
| 36 | H | 102 | DGD | O2G-C1B-C2B | 3.21 | 118.21 | 111.55 |
| 37 | D | 408 | LHG | O8-C23-C24 | 3.21 | 121.23 | 111.90 |
| 24 | B | 611 | CLA | O2A-CGA-CBA | 3.21 | 121.24 | 111.90 |
| 24 | b | 611 | CLA | CAC-C3C-C4C | 3.21 | 129.36 | 124.83 |
| 24 | b | 616 | CLA | C3B-C4B-NB | 3.21 | 113.36 | 109.21 |
| 34 | b | 625 | LMG | O8-C28-C29 | 3.22 | 121.26 | 111.90 |
| 30 | I | 102 | LMT | C1B-O5B-C5B | 3.22 | 119.79 | 113.72 |
| 24 | b | 615 | CLA | C3B-C4B-NB | 3.22 | 113.38 | 109.21 |
| 24 | b | 618 | CLA | O2D-CGD-CBD | 3.22 | 117.06 | 111.30 |
| 24 | B | 607 | CLA | C3B-C4B-NB | 3.24 | 113.40 | 109.21 |
| 24 | c | 508 | CLA | CAC-C3C-C4C | 3.25 | 129.41 | 124.83 |
| 25 | A | 408 | PHO | C2B-C1B-NB | 3.25 | 114.63 | 109.82 |
| 24 | b | 612 | CLA | CMC-C2C-C1C | 3.25 | 129.95 | 125.02 |
| 24 | c | 505 | CLA | C4-C3-C5 | 3.25 | 120.94 | 115.29 |
| 24 | B | 617 | CLA | CAC-C3C-C4C | 3.26 | 129.42 | 124.83 |
| 25 | A | 408 | PHO | C4-C3-C5 | 3.26 | 120.94 | 115.29 |
| 27 | f | 101 | SQD | O9-S-C6 | 3.26 | 109.61 | 106.83 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 24 | b | 608 | CLA | CMC-C2C-C1C | 3.27 | 129.98 | 125.02 |
| 24 | B | 615 | CLA | O2A-CGA-CBA | 3.28 | 121.44 | 111.90 |
| 24 | B | 604 | CLA | CMC-C2C-C1C | 3.28 | 130.00 | 125.02 |
| 35 | b | 628 | HTG | O5-C1-C2 | 3.29 | 114.78 | 110.28 |
| 24 | b | 610 | CLA | CMC-C2C-C1C | 3.29 | 130.00 | 125.02 |
| 24 | b | 617 | CLA | C3B-C4B-NB | 3.29 | 113.46 | 109.21 |
| 24 | B | 603 | CLA | C4-C3-C5 | 3.29 | 121.00 | 115.29 |
| 24 | B | 616 | CLA | C3B-C4B-NB | 3.29 | 113.47 | 109.21 |
| 24 | b | 617 | CLA | C4-C3-C5 | 3.29 | 121.00 | 115.29 |
| 24 | b | 608 | CLA | C4-C3-C5 | 3.30 | 121.01 | 115.29 |
| 27 | a | 411 | SQD | O9-S-C6 | 3.30 | 109.65 | 106.83 |
| 24 | C | 514 | CLA | C3B-C4B-NB | 3.30 | 113.48 | 109.21 |
| 27 | b | 601 | SQD | O9-S-C6 | 3.31 | 109.66 | 106.83 |
| 24 | b | 607 | CLA | C3B-C4B-NB | 3.32 | 113.50 | 109.21 |
| 24 | C | 506 | CLA | C3B-C4B-NB | 3.32 | 113.50 | 109.21 |
| 34 | j | 101 | LMG | O7-C10-C11 | 3.32 | 118.44 | 111.55 |
| 24 | D | 403 | CLA | O2A-CGA-CBA | 3.33 | 121.58 | 111.90 |
| 24 | b | 619 | CLA | CAC-C3C-C4C | 3.33 | 129.53 | 124.83 |
| 24 | B | 612 | CLA | C3B-C4B-NB | 3.33 | 113.52 | 109.21 |
| 36 | D | 407 | DGD | C3D-C4D-C5D | 3.33 | 116.09 | 110.22 |
| 24 | c | 504 | CLA | C3B-C4B-NB | 3.33 | 113.52 | 109.21 |
| 24 | c | 503 | CLA | C3B-C4B-NB | 3.34 | 113.52 | 109.21 |
| 34 | Z | 101 | LMG | O6-C1-C2 | 3.34 | 116.74 | 110.30 |
| 24 | B | 611 | CLA | CAC-C3C-C4C | 3.35 | 129.55 | 124.83 |
| 24 | C | 514 | CLA | CMC-C2C-C1C | 3.35 | 130.10 | 125.02 |
| 37 | e | 101 | LHG | O8-C23-C24 | 3.35 | 121.64 | 111.90 |
| 24 | c | 511 | CLA | CAC-C3C-C4C | 3.35 | 129.56 | 124.83 |
| 24 | d | 404 | CLA | O2D-CGD-CBD | 3.36 | 117.30 | 111.30 |
| 24 | b | 621 | CLA | CAC-C3C-C4C | 3.36 | 129.57 | 124.83 |
| 24 | B | 615 | CLA | CMC-C2C-C1C | 3.36 | 130.12 | 125.02 |
| 24 | C | 513 | CLA | C3B-C4B-NB | 3.37 | 113.56 | 109.21 |
| 27 | b | 601 | SQD | O48-C23-C24 | 3.37 | 121.71 | 111.90 |
| 24 | b | 613 | CLA | O2A-CGA-CBA | 3.38 | 121.72 | 111.90 |
| 24 | C | 502 | CLA | C3B-C4B-NB | 3.38 | 113.58 | 109.21 |
| 24 | D | 403 | CLA | CED-O2D-CGD | 3.39 | 123.91 | 115.97 |
| 24 | c | 506 | CLA | C4-C3-C5 | 3.39 | 121.17 | 115.29 |
| 27 | A | 416 | SQD | O48-C23-C24 | 3.40 | 121.78 | 111.90 |
| 24 | b | 620 | CLA | C4-C3-C5 | 3.41 | 121.20 | 115.29 |
| 24 | A | 409 | CLA | C4-C3-C5 | 3.41 | 121.21 | 115.29 |
| 24 | C | 502 | CLA | CAC-C3C-C4C | 3.41 | 129.65 | 124.83 |
| 24 | B | 605 | CLA | C3B-C4B-NB | 3.41 | 113.62 | 109.21 |
| 24 | c | 515 | CLA | C3B-C4B-NB | 3.41 | 113.62 | 109.21 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 36 | D | 407 | DGD | C1E-O6E-C5E | 3.41 | 120.15 | 113.72 |
| 24 | B | 615 | CLA | C3B-C4B-NB | 3.43 | 113.64 | 109.21 |
| 24 | B | 603 | CLA | C3B-C4B-NB | 3.43 | 113.65 | 109.21 |
| 24 | B | 606 | CLA | CMC-C2C-C1C | 3.43 | 130.23 | 125.02 |
| 24 | D | 404 | CLA | C3B-C4B-NB | 3.43 | 113.65 | 109.21 |
| 24 | c | 505 | CLA | CMC-C2C-C1C | 3.44 | 130.23 | 125.02 |
| 24 | b | 608 | CLA | O2A-CGA-CBA | 3.45 | 121.94 | 111.90 |
| 24 | C | 504 | CLA | C3B-C4B-NB | 3.46 | 113.68 | 109.21 |
| 24 | a | 406 | CLA | O2A-CGA-CBA | 3.46 | 121.98 | 111.90 |
| 24 | d | 404 | CLA | C3B-C4B-NB | 3.48 | 113.71 | 109.21 |
| 24 | B | 615 | CLA | C4-C3-C5 | 3.48 | 121.33 | 115.29 |
| 24 | b | 614 | CLA | C3B-C4B-NB | 3.49 | 113.72 | 109.21 |
| 36 | h | 102 | DGD | O2G-C1B-C2B | 3.49 | 118.81 | 111.55 |
| 24 | b | 608 | CLA | C3B-C4B-NB | 3.50 | 113.73 | 109.21 |
| 27 | l | 101 | SQD | O9-S-C6 | 3.51 | 109.83 | 106.83 |
| 27 | a | 402 | SQD | O48-C23-C24 | 3.51 | 122.13 | 111.90 |
| 32 | D | 406 | PL9 | C40-C39-C41 | 3.53 | 121.42 | 115.29 |
| 24 | d | 404 | CLA | CMC-C2C-C1C | 3.54 | 130.38 | 125.02 |
| 24 | A | 409 | CLA | O2D-CGD-CBD | 3.54 | 117.62 | 111.30 |
| 37 | D | 408 | LHG | O7-C7-C8 | 3.54 | 118.90 | 111.55 |
| 24 | a | 406 | CLA | CAC-C3C-C4C | 3.54 | 129.83 | 124.83 |
| 24 | C | 508 | CLA | CMC-C2C-C1C | 3.54 | 130.40 | 125.02 |
| 24 | c | 506 | CLA | C3B-C4B-NB | 3.54 | 113.79 | 109.21 |
| 24 | B | 608 | CLA | CMC-C2C-C1C | 3.55 | 130.40 | 125.02 |
| 34 | c | 520 | LMG | O7-C10-C11 | 3.56 | 118.95 | 111.55 |
| 37 | L | 101 | LHG | O7-C7-C8 | 3.56 | 118.95 | 111.55 |
| 24 | B | 604 | CLA | C3B-C4B-NB | 3.56 | 113.82 | 109.21 |
| 37 | D | 410 | LHG | O7-C7-C8 | 3.58 | 118.98 | 111.55 |
| 27 | l | 101 | SQD | O8-S-C6 | 3.58 | 110.39 | 106.01 |
| 24 | A | 405 | CLA | CMB-C2B-C3B | 3.58 | 131.54 | 124.89 |
| 24 | b | 621 | CLA | O2A-CGA-CBA | 3.59 | 122.36 | 111.90 |
| 27 | a | 402 | SQD | O9-S-C6 | 3.59 | 109.90 | 106.83 |
| 37 | l | 102 | LHG | O7-C7-C8 | 3.60 | 119.02 | 111.55 |
| 24 | B | 616 | CLA | O2D-CGD-CBD | 3.62 | 117.76 | 111.30 |
| 24 | C | 510 | CLA | C3B-C4B-NB | 3.62 | 113.89 | 109.21 |
| 24 | B | 609 | CLA | C3B-C4B-NB | 3.62 | 113.89 | 109.21 |
| 27 | f | 101 | SQD | C1-O5-C5 | 3.64 | 120.57 | 113.72 |
| 24 | c | 508 | CLA | O2D-CGD-CBD | 3.67 | 117.85 | 111.30 |
| 37 | d | 410 | LHG | O7-C7-C8 | 3.67 | 119.17 | 111.55 |
| 34 | z | 101 | LMG | O7-C10-C11 | 3.68 | 119.19 | 111.55 |
| 24 | A | 406 | CLA | C3C-C4C-NC | 3.69 | 113.94 | 110.21 |
| 24 | b | 620 | CLA | C3B-C4B-NB | 3.69 | 113.98 | 109.21 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 24 | C | 505 | CLA | CAC-C3C-C4C | 3.70 | 130.04 | 124.83 |
| 35 | O | 303 | HTG | C1'-S1-C1 | 3.70 | 105.77 | 100.28 |
| 25 | A | 408 | PHO | CAC-C3C-C4C | 3.71 | 129.57 | 125.21 |
| 32 | a | 416 | PL9 | C15-C14-C16 | 3.72 | 121.75 | 115.29 |
| 36 | D | 407 | DGD | C4D-C3D-C2D | 3.73 | 117.42 | 110.84 |
| 24 | C | 511 | CLA | C3B-C4B-NB | 3.73 | 114.03 | 109.21 |
| 34 | B | 621 | LMG | O7-C10-C11 | 3.74 | 119.32 | 111.55 |
| 27 | l | 101 | SQD | O6-C1-C2 | 3.74 | 114.33 | 108.23 |
| 24 | a | 406 | CLA | C3B-C4B-NB | 3.74 | 114.05 | 109.21 |
| 30 | I | 102 | LMT | O1B-C4'-C3' | 3.75 | 116.21 | 107.19 |
| 24 | D | 403 | CLA | C3B-C4B-NB | 3.75 | 114.06 | 109.21 |
| 24 | C | 509 | CLA | C3B-C4B-NB | 3.75 | 114.06 | 109.21 |
| 24 | B | 614 | CLA | C3B-C4B-NB | 3.75 | 114.06 | 109.21 |
| 27 | A | 416 | SQD | O47-C7-C8 | 3.76 | 119.37 | 111.55 |
| 24 | b | 612 | CLA | C3B-C4B-NB | 3.76 | 114.08 | 109.21 |
| 24 | C | 505 | CLA | CMC-C2C-C1C | 3.77 | 130.73 | 125.02 |
| 24 | c | 513 | CLA | C3B-C4B-NB | 3.78 | 114.09 | 109.21 |
| 24 | b | 609 | CLA | CMC-C2C-C1C | 3.78 | 130.75 | 125.02 |
| 24 | C | 504 | CLA | O2D-CGD-CBD | 3.78 | 118.06 | 111.30 |
| 24 | C | 512 | CLA | C3B-C4B-NB | 3.78 | 114.10 | 109.21 |
| 24 | b | 619 | CLA | C3B-C4B-NB | 3.79 | 114.11 | 109.21 |
| 34 | C | 520 | LMG | O7-C10-C11 | 3.79 | 119.42 | 111.55 |
| 24 | D | 403 | CLA | O2D-CGD-CBD | 3.80 | 118.09 | 111.30 |
| 24 | C | 507 | CLA | C3B-C4B-NB | 3.80 | 114.13 | 109.21 |
| 24 | d | 402 | CLA | C3B-C4B-NB | 3.80 | 114.13 | 109.21 |
| 24 | A | 406 | CLA | C3B-C4B-NB | 3.80 | 114.13 | 109.21 |
| 34 | J | 101 | LMG | O7-C10-C11 | 3.81 | 119.47 | 111.55 |
| 37 | e | 101 | LHG | O7-C7-C8 | 3.83 | 119.50 | 111.55 |
| 24 | b | 611 | CLA | CMC-C2C-C1C | 3.83 | 130.83 | 125.02 |
| 36 | c | 517 | DGD | O2G-C1B-C2B | 3.83 | 119.51 | 111.55 |
| 27 | A | 411 | SQD | O9-S-C6 | 3.86 | 110.12 | 106.83 |
| 24 | C | 512 | CLA | O2D-CGD-CBD | 3.86 | 118.20 | 111.30 |
| 24 | C | 512 | CLA | C1-O2A-CGA | 3.88 | 126.07 | 116.77 |
| 27 | b | 601 | SQD | C3-C4-C5 | 3.88 | 117.06 | 110.22 |
| 24 | d | 402 | CLA | O2A-CGA-CBA | 3.89 | 123.22 | 111.90 |
| 24 | c | 508 | CLA | C3B-C4B-NB | 3.90 | 114.25 | 109.21 |
| 24 | C | 505 | CLA | C3B-C4B-NB | 3.92 | 114.27 | 109.21 |
| 37 | D | 409 | LHG | O7-C7-C8 | 3.92 | 119.69 | 111.55 |
| 24 | B | 609 | CLA | O2D-CGD-CBD | 3.93 | 118.32 | 111.30 |
| 36 | D | 407 | DGD | C1D-C2D-C3D | 3.93 | 117.28 | 109.98 |
| 24 | c | 507 | CLA | CAC-C3C-C4C | 3.93 | 130.38 | 124.83 |
| 24 | D | 401 | CLA | C3C-C4C-NC | 3.94 | 114.20 | 110.21 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 37 | d | 409 | LHG | O7-C7-C8 | 3.94 | 119.74 | 111.55 |
| 24 | c | 515 | CLA | O2D-CGD-CBD | 3.98 | 118.41 | 111.30 |
| 24 | B | 607 | CLA | CMC-C2C-C1C | 3.99 | 131.06 | 125.02 |
| 24 | c | 511 | CLA | C3B-C4B-NB | 3.99 | 114.37 | 109.21 |
| 24 | B | 605 | CLA | CMC-C2C-C1C | 4.00 | 131.08 | 125.02 |
| 24 | B | 613 | CLA | C3B-C4B-NB | 4.01 | 114.39 | 109.21 |
| 24 | c | 513 | CLA | O2D-CGD-CBD | 4.01 | 118.47 | 111.30 |
| 36 | C | 518 | DGD | O2G-C1B-C2B | 4.02 | 119.89 | 111.55 |
| 24 | c | 512 | CLA | C3B-C4B-NB | 4.03 | 114.42 | 109.21 |
| 34 | Z | 101 | LMG | O7-C10-C11 | 4.03 | 119.92 | 111.55 |
| 24 | D | 401 | CLA | C3B-C4B-NB | 4.03 | 114.42 | 109.21 |
| 27 | a | 411 | SQD | O8-S-C6 | 4.03 | 110.93 | 106.01 |
| 37 | E | 101 | LHG | O7-C7-C8 | 4.04 | 119.95 | 111.55 |
| 27 | F | 101 | SQD | O9-S-C6 | 4.05 | 110.29 | 106.83 |
| 24 | b | 618 | CLA | C3B-C4B-NB | 4.05 | 114.45 | 109.21 |
| 24 | C | 514 | CLA | CAC-C3C-C4C | 4.06 | 130.55 | 124.83 |
| 24 | B | 613 | CLA | CAC-C3C-C4C | 4.07 | 130.57 | 124.83 |
| 24 | c | 513 | CLA | C3C-C4C-NC | 4.07 | 114.33 | 110.21 |
| 34 | c | 501 | LMG | O7-C10-C11 | 4.08 | 120.02 | 111.55 |
| 36 | c | 518 | DGD | O2G-C1B-C2B | 4.09 | 120.04 | 111.55 |
| 24 | c | 514 | CLA | C3C-C4C-NC | 4.10 | 114.36 | 110.21 |
| 27 | F | 101 | SQD | O47-C7-C8 | 4.12 | 120.11 | 111.55 |
| 24 | a | 409 | CLA | C3B-C4B-NB | 4.13 | 114.55 | 109.21 |
| 24 | d | 401 | CLA | O2D-CGD-CBD | 4.15 | 118.72 | 111.30 |
| 24 | C | 514 | CLA | O2D-CGD-CBD | 4.16 | 118.72 | 111.30 |
| 24 | B | 608 | CLA | O2D-CGD-CBD | 4.19 | 118.79 | 111.30 |
| 34 | C | 520 | LMG | O8-C28-C29 | 4.21 | 124.15 | 111.90 |
| 27 | A | 411 | SQD | O8-S-C6 | 4.24 | 111.18 | 106.01 |
| 34 | Z | 101 | LMG | C1-C2-C3 | 4.25 | 117.87 | 109.98 |
| 27 | a | 402 | SQD | O47-C7-C8 | 4.28 | 120.43 | 111.55 |
| 35 | B | 624 | HTG | O5-C1-C2 | 4.29 | 116.15 | 110.28 |
| 24 | C | 505 | CLA | C3C-C4C-NC | 4.32 | 114.59 | 110.21 |
| 24 | b | 610 | CLA | O2D-CGD-CBD | 4.33 | 119.04 | 111.30 |
| 24 | A | 406 | CLA | O2D-CGD-CBD | 4.37 | 119.11 | 111.30 |
| 27 | F | 101 | SQD | O6-C1-C2 | 4.40 | 115.41 | 108.23 |
| 24 | b | 615 | CLA | O2D-CGD-CBD | 4.40 | 119.16 | 111.30 |
| 24 | B | 617 | CLA | C3B-C4B-NB | 4.41 | 114.91 | 109.21 |
| 24 | D | 401 | CLA | O2D-CGD-CBD | 4.42 | 119.20 | 111.30 |
| 24 | b | 612 | CLA | O2D-CGD-CBD | 4.43 | 119.22 | 111.30 |
| 25 | A | 408 | PHO | O2D-CGD-CBD | 4.45 | 119.25 | 111.30 |
| 36 | C | 517 | DGD | O2G-C1B-C2B | 4.46 | 120.81 | 111.55 |
| 24 | C | 507 | CLA | O2D-CGD-CBD | 4.47 | 119.28 | 111.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 24 | B | 612 | CLA | O2D-CGD-CBD | 4.48 | 119.30 | 111.30 |
| 24 | a | 407 | CLA | O2D-CGD-CBD | 4.48 | 119.31 | 111.30 |
| 25 | A | 407 | PHO | O2D-CGD-CBD | 4.51 | 119.36 | 111.30 |
| 35 | V | 204 | HTG | C1'-S1-C1 | 4.52 | 106.98 | 100.28 |
| 27 | A | 411 | SQD | O47-C7-C8 | 4.53 | 120.95 | 111.55 |
| 36 | d | 407 | DGD | O2G-C1B-C2B | 4.54 | 120.97 | 111.55 |
| 24 | B | 610 | CLA | O2D-CGD-CBD | 4.54 | 119.42 | 111.30 |
| 35 | C | 523 | HTG | C1-O5-C5 | 4.57 | 121.49 | 112.69 |
| 27 | a | 411 | SQD | O6-C1-C2 | 4.60 | 115.73 | 108.23 |
| 27 | l | 101 | SQD | O47-C7-C8 | 4.60 | 121.10 | 111.55 |
| 27 | F | 101 | SQD | O7-S-C6 | 4.60 | 110.76 | 106.83 |
| 35 | b | 627 | HTG | C1'-S1-C1 | 4.61 | 107.12 | 100.28 |
| 24 | b | 620 | CLA | O2D-CGD-CBD | 4.63 | 119.57 | 111.30 |
| 24 | c | 506 | CLA | O2D-CGD-CBD | 4.65 | 119.61 | 111.30 |
| 24 | C | 508 | CLA | O2D-CGD-CBD | 4.66 | 119.63 | 111.30 |
| 24 | d | 401 | CLA | C3B-C4B-NB | 4.66 | 115.24 | 109.21 |
| 30 | b | 602 | LMT | C1'-O5'-C5' | 4.66 | 122.50 | 113.72 |
| 24 | b | 619 | CLA | C3C-C4C-NC | 4.67 | 114.95 | 110.21 |
| 35 | b | 604 | HTG | C1'-S1-C1 | 4.68 | 107.23 | 100.28 |
| 24 | a | 406 | CLA | C3C-C4C-NC | 4.69 | 114.96 | 110.21 |
| 24 | c | 508 | CLA | C3C-C4C-NC | 4.70 | 114.97 | 110.21 |
| 24 | B | 615 | CLA | C3C-C4C-NC | 4.71 | 114.99 | 110.21 |
| 24 | a | 409 | CLA | O2D-CGD-CBD | 4.72 | 119.73 | 111.30 |
| 24 | B | 603 | CLA | O2D-CGD-CBD | 4.73 | 119.75 | 111.30 |
| 24 | b | 621 | CLA | C3B-C4B-NB | 4.73 | 115.33 | 109.21 |
| 34 | C | 501 | LMG | O7-C10-C11 | 4.74 | 121.39 | 111.55 |
| 24 | a | 407 | CLA | C3C-C4C-NC | 4.75 | 115.02 | 110.21 |
| 35 | B | 623 | HTG | C1'-S1-C1 | 4.75 | 107.33 | 100.28 |
| 24 | c | 515 | CLA | C3C-C4C-NC | 4.78 | 115.06 | 110.21 |
| 24 | b | 621 | CLA | C3C-C4C-NC | 4.78 | 115.06 | 110.21 |
| 27 | f | 101 | SQD | O7-S-C6 | 4.79 | 110.92 | 106.83 |
| 24 | c | 511 | CLA | C3C-C4C-NC | 4.80 | 115.07 | 110.21 |
| 34 | C | 521 | LMG | O7-C10-C11 | 4.82 | 121.56 | 111.55 |
| 24 | d | 401 | CLA | C3C-C4C-NC | 4.82 | 115.09 | 110.21 |
| 24 | C | 507 | CLA | C3C-C4C-NC | 4.83 | 115.11 | 110.21 |
| 34 | c | 521 | LMG | O7-C10-C11 | 4.84 | 121.60 | 111.55 |
| 24 | b | 608 | CLA | C3C-C4C-NC | 4.85 | 115.12 | 110.21 |
| 24 | b | 614 | CLA | O2D-CGD-CBD | 4.85 | 119.96 | 111.30 |
| 24 | c | 512 | CLA | O2D-CGD-CBD | 4.88 | 120.01 | 111.30 |
| 24 | b | 614 | CLA | C3C-C4C-NC | 4.88 | 115.16 | 110.21 |
| 24 | c | 505 | CLA | O2D-CGD-CBD | 4.88 | 120.03 | 111.30 |
| 24 | b | 620 | CLA | C3C-C4C-NC | 4.89 | 115.17 | 110.21 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 24 | b | 617 | CLA | O2D-CGD-CBD | 4.91 | 120.08 | 111.30 |
| 24 | C | 509 | CLA | C3C-C4C-NC | 4.92 | 115.20 | 110.21 |
| 24 | c | 503 | CLA | C3C-C4C-NC | 4.93 | 115.20 | 110.21 |
| 24 | b | 606 | CLA | C3C-C4C-NC | 4.93 | 115.21 | 110.21 |
| 24 | b | 613 | CLA | C3C-C4C-NC | 4.94 | 115.21 | 110.21 |
| 24 | c | 512 | CLA | C3C-C4C-NC | 4.95 | 115.23 | 110.21 |
| 24 | B | 613 | CLA | O2D-CGD-CBD | 4.96 | 120.16 | 111.30 |
| 24 | C | 503 | CLA | O2D-CGD-CBD | 4.96 | 120.17 | 111.30 |
| 27 | a | 411 | SQD | O47-C7-C8 | 4.97 | 121.87 | 111.55 |
| 24 | B | 611 | CLA | O2D-CGD-CBD | 4.97 | 120.19 | 111.30 |
| 24 | C | 511 | CLA | C3C-C4C-NC | 4.99 | 115.26 | 110.21 |
| 24 | a | 409 | CLA | C3C-C4C-NC | 5.00 | 115.28 | 110.21 |
| 27 | l | 101 | SQD | O7-S-C6 | 5.01 | 111.11 | 106.83 |
| 24 | C | 512 | CLA | C3C-C4C-NC | 5.02 | 115.29 | 110.21 |
| 24 | b | 613 | CLA | O2D-CGD-CBD | 5.03 | 120.28 | 111.30 |
| 24 | c | 504 | CLA | C3C-C4C-NC | 5.03 | 115.31 | 110.21 |
| 36 | D | 407 | DGD | O2G-C1B-C2B | 5.03 | 122.00 | 111.55 |
| 24 | c | 506 | CLA | C3C-C4C-NC | 5.04 | 115.31 | 110.21 |
| 27 | f | 101 | SQD | O47-C7-C8 | 5.05 | 122.03 | 111.55 |
| 25 | d | 403 | PHO | C2D-C1D-ND | 5.06 | 117.31 | 109.82 |
| 24 | C | 513 | CLA | C3C-C4C-NC | 5.06 | 115.33 | 110.21 |
| 24 | C | 514 | CLA | C3C-C4C-NC | 5.06 | 115.34 | 110.21 |
| 24 | C | 510 | CLA | C3C-C4C-NC | 5.06 | 115.34 | 110.21 |
| 24 | B | 614 | CLA | C3C-C4C-NC | 5.07 | 115.35 | 110.21 |
| 24 | B | 604 | CLA | O2D-CGD-CBD | 5.09 | 120.39 | 111.30 |
| 24 | b | 610 | CLA | C3C-C4C-NC | 5.09 | 115.37 | 110.21 |
| 27 | b | 601 | SQD | O47-C7-C8 | 5.10 | 122.13 | 111.55 |
| 24 | B | 602 | CLA | C3C-C4C-NC | 5.10 | 115.37 | 110.21 |
| 24 | b | 621 | CLA | O2D-CGD-CBD | 5.11 | 120.43 | 111.30 |
| 24 | C | 511 | CLA | O2D-CGD-CBD | 5.12 | 120.45 | 111.30 |
| 24 | b | 616 | CLA | O2D-CGD-CBD | 5.15 | 120.50 | 111.30 |
| 24 | B | 605 | CLA | O2D-CGD-CBD | 5.15 | 120.50 | 111.30 |
| 24 | A | 409 | CLA | C3C-C4C-NC | 5.15 | 115.43 | 110.21 |
| 27 | b | 601 | SQD | O6-C1-C2 | 5.15 | 116.64 | 108.23 |
| 24 | B | 608 | CLA | C3C-C4C-NC | 5.16 | 115.44 | 110.21 |
| 24 | d | 402 | CLA | O2D-CGD-CBD | 5.19 | 120.57 | 111.30 |
| 24 | B | 602 | CLA | O2D-CGD-CBD | 5.19 | 120.58 | 111.30 |
| 24 | b | 606 | CLA | O2D-CGD-CBD | 5.19 | 120.58 | 111.30 |
| 25 | A | 407 | PHO | C2D-C1D-ND | 5.20 | 117.52 | 109.82 |
| 24 | C | 502 | CLA | C3C-C4C-NC | 5.21 | 115.49 | 110.21 |
| 24 | B | 610 | CLA | C3C-C4C-NC | 5.23 | 115.51 | 110.21 |
| 24 | d | 404 | CLA | C3C-C4C-NC | 5.23 | 115.51 | 110.21 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 24 | B | 617 | CLA | C3C-C4C-NC | 5.23 | 115.51 | 110.21 |
| 24 | D | 404 | CLA | O2D-CGD-CBD | 5.23 | 120.65 | 111.30 |
| 24 | B | 603 | CLA | C3C-C4C-NC | 5.24 | 115.52 | 110.21 |
| 25 | d | 403 | PHO | O2D-CGD-CBD | 5.25 | 120.69 | 111.30 |
| 24 | B | 615 | CLA | O2D-CGD-CBD | 5.26 | 120.69 | 111.30 |
| 25 | A | 408 | PHO | CMD-C2D-C1D | 5.26 | 133.24 | 125.04 |
| 24 | b | 611 | CLA | O2D-CGD-CBD | 5.26 | 120.71 | 111.30 |
| 24 | B | 612 | CLA | C3C-C4C-NC | 5.27 | 115.55 | 110.21 |
| 24 | C | 509 | CLA | O2D-CGD-CBD | 5.28 | 120.73 | 111.30 |
| 24 | D | 404 | CLA | C3C-C4C-NC | 5.28 | 115.56 | 110.21 |
| 24 | c | 510 | CLA | O2D-CGD-CBD | 5.29 | 120.75 | 111.30 |
| 24 | C | 502 | CLA | O2D-CGD-CBD | 5.32 | 120.81 | 111.30 |
| 24 | B | 616 | CLA | C3C-C4C-NC | 5.33 | 115.61 | 110.21 |
| 24 | c | 504 | CLA | O2D-CGD-CBD | 5.33 | 120.83 | 111.30 |
| 24 | C | 513 | CLA | O2D-CGD-CBD | 5.35 | 120.86 | 111.30 |
| 24 | B | 609 | CLA | C3C-C4C-NC | 5.35 | 115.63 | 110.21 |
| 27 | A | 411 | SQD | O6-C1-C2 | 5.35 | 116.97 | 108.23 |
| 24 | C | 506 | CLA | C3C-C4C-NC | 5.36 | 115.64 | 110.21 |
| 24 | C | 503 | CLA | C3C-C4C-NC | 5.36 | 115.65 | 110.21 |
| 24 | b | 607 | CLA | C3C-C4C-NC | 5.39 | 115.68 | 110.21 |
| 24 | b | 619 | CLA | O2D-CGD-CBD | 5.41 | 120.96 | 111.30 |
| 24 | d | 402 | CLA | C3C-C4C-NC | 5.41 | 115.69 | 110.21 |
| 24 | c | 507 | CLA | C3C-C4C-NC | 5.44 | 115.73 | 110.21 |
| 35 | B | 622 | HTG | C1'-S1-C1 | 5.46 | 108.38 | 100.28 |
| 24 | C | 508 | CLA | C3C-C4C-NC | 5.48 | 115.76 | 110.21 |
| 24 | b | 615 | CLA | C3C-C4C-NC | 5.48 | 115.77 | 110.21 |
| 24 | B | 606 | CLA | C3C-C4C-NC | 5.49 | 115.77 | 110.21 |
| 24 | C | 506 | CLA | O2D-CGD-CBD | 5.51 | 121.14 | 111.30 |
| 24 | B | 611 | CLA | C3C-C4C-NC | 5.51 | 115.80 | 110.21 |
| 24 | b | 611 | CLA | C3C-C4C-NC | 5.52 | 115.80 | 110.21 |
| 24 | c | 505 | CLA | C3C-C4C-NC | 5.53 | 115.82 | 110.21 |
| 24 | C | 504 | CLA | C3C-C4C-NC | 5.54 | 115.82 | 110.21 |
| 25 | a | 408 | PHO | C2D-C1D-ND | 5.55 | 118.04 | 109.82 |
| 24 | B | 606 | CLA | O2D-CGD-CBD | 5.59 | 121.29 | 111.30 |
| 24 | c | 503 | CLA | O2D-CGD-CBD | 5.60 | 121.31 | 111.30 |
| 25 | a | 408 | PHO | O2D-CGD-CBD | 5.61 | 121.33 | 111.30 |
| 24 | C | 505 | CLA | O2D-CGD-CBD | 5.62 | 121.34 | 111.30 |
| 24 | B | 607 | CLA | C3C-C4C-NC | 5.64 | 115.93 | 110.21 |
| 24 | b | 607 | CLA | O2D-CGD-CBD | 5.68 | 121.45 | 111.30 |
| 24 | c | 514 | CLA | O2D-CGD-CBD | 5.68 | 121.45 | 111.30 |
| 24 | B | 607 | CLA | O2D-CGD-CBD | 5.69 | 121.47 | 111.30 |
| 24 | c | 511 | CLA | O2D-CGD-CBD | 5.70 | 121.49 | 111.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 24 | b | 609 | CLA | O2D-CGD-CBD | 5.72 | 121.52 | 111.30 |
| 24 | B | 613 | CLA | C3C-C4C-NC | 5.76 | 116.05 | 110.21 |
| 35 | C | 523 | HTG | C1'-S1-C1 | 5.77 | 108.84 | 100.28 |
| 24 | c | 510 | CLA | C3C-C4C-NC | 5.78 | 116.06 | 110.21 |
| 24 | b | 616 | CLA | C3C-C4C-NC | 5.82 | 116.10 | 110.21 |
| 25 | A | 408 | PHO | C2D-C1D-ND | 5.83 | 118.45 | 109.82 |
| 27 | b | 601 | SQD | O7-S-C6 | 5.84 | 111.81 | 106.83 |
| 24 | c | 507 | CLA | O2D-CGD-CBD | 5.85 | 121.76 | 111.30 |
| 24 | c | 509 | CLA | C3C-C4C-NC | 5.87 | 116.16 | 110.21 |
| 24 | B | 604 | CLA | C3C-C4C-NC | 5.94 | 116.23 | 110.21 |
| 24 | B | 605 | CLA | C3C-C4C-NC | 5.95 | 116.24 | 110.21 |
| 24 | c | 509 | CLA | O2D-CGD-CBD | 5.95 | 121.94 | 111.30 |
| 35 | C | 522 | HTG | C1'-S1-C1 | 5.98 | 109.15 | 100.28 |
| 24 | b | 608 | CLA | O2D-CGD-CBD | 5.98 | 121.99 | 111.30 |
| 35 | B | 630 | HTG | C1'-S1-C1 | 5.99 | 109.17 | 100.28 |
| 24 | b | 618 | CLA | C3C-C4C-NC | 6.00 | 116.29 | 110.21 |
| 24 | b | 617 | CLA | C3C-C4C-NC | 6.03 | 116.32 | 110.21 |
| 24 | D | 403 | CLA | C3C-C4C-NC | 6.05 | 116.34 | 110.21 |
| 24 | A | 405 | CLA | C3C-C4C-NC | 6.07 | 116.36 | 110.21 |
| 35 | b | 603 | HTG | C1'-S1-C1 | 6.08 | 109.30 | 100.28 |
| 24 | b | 609 | CLA | C3C-C4C-NC | 6.09 | 116.38 | 110.21 |
| 24 | b | 617 | CLA | C2C-C1C-NC | 6.10 | 114.42 | 110.22 |
| 25 | d | 403 | PHO | CMD-C2D-C1D | 6.14 | 134.60 | 125.04 |
| 24 | C | 510 | CLA | O2D-CGD-CBD | 6.18 | 122.34 | 111.30 |
| 24 | B | 617 | CLA | O2D-CGD-CBD | 6.18 | 122.35 | 111.30 |
| 35 | c | 523 | HTG | C1'-S1-C1 | 6.33 | 109.67 | 100.28 |
| 24 | b | 612 | CLA | C3C-C4C-NC | 6.35 | 116.64 | 110.21 |
| 24 | b | 611 | CLA | C2C-C1C-NC | 6.39 | 114.62 | 110.22 |
| 38 | e | 102 | HEM | CAD-CBD-CGD | 6.43 | 123.65 | 112.66 |
| 24 | D | 404 | CLA | C2C-C1C-NC | 6.43 | 114.65 | 110.22 |
| 24 | b | 606 | CLA | C2C-C1C-NC | 6.50 | 114.69 | 110.22 |
| 35 | B | 631 | HTG | C1'-S1-C1 | 6.51 | 109.93 | 100.28 |
| 24 | a | 407 | CLA | C2C-C1C-NC | 6.53 | 114.71 | 110.22 |
| 25 | a | 408 | PHO | CMD-C2D-C1D | 6.56 | 135.25 | 125.04 |
| 24 | b | 607 | CLA | C2C-C1C-NC | 6.57 | 114.74 | 110.22 |
| 24 | c | 514 | CLA | C2C-C1C-NC | 6.60 | 114.76 | 110.22 |
| 24 | d | 404 | CLA | C2C-C1C-NC | 6.62 | 114.78 | 110.22 |
| 24 | B | 610 | CLA | C2C-C1C-NC | 6.63 | 114.78 | 110.22 |
| 24 | A | 409 | CLA | C2C-C1C-NC | 6.64 | 114.79 | 110.22 |
| 24 | c | 505 | CLA | C2C-C1C-NC | 6.70 | 114.83 | 110.22 |
| 24 | b | 608 | CLA | C2C-C1C-NC | 6.71 | 114.84 | 110.22 |
| 24 | c | 512 | CLA | C2C-C1C-NC | 6.78 | 114.88 | 110.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 24 | B | 602 | CLA | C2C-C1C-NC | 6.78 | 114.88 | 110.22 |
| 25 | A | 407 | PHO | CMD-C2D-C1D | 6.80 | 135.63 | 125.04 |
| 24 | B | 612 | CLA | C2C-C1C-NC | 6.92 | 114.98 | 110.22 |
| 24 | c | 510 | CLA | C2C-C1C-NC | 6.93 | 114.99 | 110.22 |
| 24 | C | 514 | CLA | C2C-C1C-NC | 6.94 | 115.00 | 110.22 |
| 24 | B | 615 | CLA | C2C-C1C-NC | 6.96 | 115.01 | 110.22 |
| 24 | A | 406 | CLA | C2C-C1C-NC | 6.99 | 115.03 | 110.22 |
| 24 | C | 508 | CLA | C2C-C1C-NC | 6.99 | 115.03 | 110.22 |
| 24 | B | 603 | CLA | C2C-C1C-NC | 7.05 | 115.07 | 110.22 |
| 24 | B | 607 | CLA | C2C-C1C-NC | 7.07 | 115.09 | 110.22 |
| 24 | c | 515 | CLA | C2C-C1C-NC | 7.08 | 115.09 | 110.22 |
| 24 | C | 511 | CLA | C2C-C1C-NC | 7.09 | 115.10 | 110.22 |
| 24 | C | 512 | CLA | C2C-C1C-NC | 7.13 | 115.13 | 110.22 |
| 24 | b | 615 | CLA | C2C-C1C-NC | 7.15 | 115.14 | 110.22 |
| 24 | B | 617 | CLA | C2C-C1C-NC | 7.17 | 115.15 | 110.22 |
| 24 | c | 504 | CLA | C2C-C1C-NC | 7.17 | 115.16 | 110.22 |
| 24 | B | 613 | CLA | C2C-C1C-NC | 7.19 | 115.17 | 110.22 |
| 35 | c | 522 | HTG | C1'-S1-C1 | 7.20 | 110.97 | 100.28 |
| 24 | C | 502 | CLA | C2C-C1C-NC | 7.24 | 115.20 | 110.22 |
| 24 | C | 513 | CLA | C2C-C1C-NC | 7.25 | 115.21 | 110.22 |
| 24 | b | 616 | CLA | C2C-C1C-NC | 7.26 | 115.21 | 110.22 |
| 24 | b | 613 | CLA | C2C-C1C-NC | 7.26 | 115.22 | 110.22 |
| 24 | B | 616 | CLA | C2C-C1C-NC | 7.30 | 115.24 | 110.22 |
| 24 | C | 503 | CLA | C2C-C1C-NC | 7.31 | 115.25 | 110.22 |
| 24 | b | 620 | CLA | C2C-C1C-NC | 7.32 | 115.25 | 110.22 |
| 24 | c | 506 | CLA | C2C-C1C-NC | 7.33 | 115.26 | 110.22 |
| 24 | B | 604 | CLA | C2C-C1C-NC | 7.34 | 115.27 | 110.22 |
| 35 | B | 624 | HTG | C1'-S1-C1 | 7.34 | 111.17 | 100.28 |
| 24 | c | 511 | CLA | C2C-C1C-NC | 7.35 | 115.28 | 110.22 |
| 24 | B | 611 | CLA | C2C-C1C-NC | 7.35 | 115.28 | 110.22 |
| 24 | b | 610 | CLA | C2C-C1C-NC | 7.36 | 115.28 | 110.22 |
| 38 | E | 103 | HEM | CAD-CBD-CGD | 7.37 | 125.25 | 112.66 |
| 24 | c | 513 | CLA | C2C-C1C-NC | 7.43 | 115.33 | 110.22 |
| 24 | C | 510 | CLA | C2C-C1C-NC | 7.45 | 115.34 | 110.22 |
| 24 | c | 508 | CLA | C2C-C1C-NC | 7.47 | 115.36 | 110.22 |
| 24 | C | 504 | CLA | C2C-C1C-NC | 7.51 | 115.39 | 110.22 |
| 35 | d | 411 | HTG | C1'-S1-C1 | 7.54 | 111.46 | 100.28 |
| 24 | c | 507 | CLA | C2C-C1C-NC | 7.61 | 115.46 | 110.22 |
| 24 | a | 409 | CLA | C2C-C1C-NC | 7.62 | 115.46 | 110.22 |
| 24 | C | 505 | CLA | C2C-C1C-NC | 7.64 | 115.48 | 110.22 |
| 24 | b | 612 | CLA | C2C-C1C-NC | 7.67 | 115.50 | 110.22 |
| 24 | B | 608 | CLA | C2C-C1C-NC | 7.70 | 115.52 | 110.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|------|-------------|----------|
| 24 | C | 509 | CLA | C2C-C1C-NC | 7.73 | 115.54 | 110.22 |
| 24 | B | 609 | CLA | C2C-C1C-NC | 7.77 | 115.56 | 110.22 |
| 24 | c | 503 | CLA | C2C-C1C-NC | 7.77 | 115.56 | 110.22 |
| 24 | c | 509 | CLA | C2C-C1C-NC | 7.77 | 115.57 | 110.22 |
| 24 | C | 507 | CLA | C2C-C1C-NC | 7.82 | 115.60 | 110.22 |
| 24 | C | 506 | CLA | C2C-C1C-NC | 7.83 | 115.61 | 110.22 |
| 24 | b | 621 | CLA | C2C-C1C-NC | 7.84 | 115.61 | 110.22 |
| 24 | b | 614 | CLA | C2C-C1C-NC | 7.91 | 115.66 | 110.22 |
| 24 | B | 606 | CLA | C2C-C1C-NC | 8.01 | 115.73 | 110.22 |
| 35 | b | 628 | HTG | C1'-S1-C1 | 8.03 | 112.19 | 100.28 |
| 24 | b | 619 | CLA | C2C-C1C-NC | 8.04 | 115.75 | 110.22 |
| 24 | d | 402 | CLA | C2C-C1C-NC | 8.04 | 115.75 | 110.22 |
| 24 | D | 403 | CLA | C2C-C1C-NC | 8.07 | 115.77 | 110.22 |
| 24 | b | 618 | CLA | C2C-C1C-NC | 8.08 | 115.78 | 110.22 |
| 24 | b | 609 | CLA | C2C-C1C-NC | 8.09 | 115.78 | 110.22 |
| 24 | B | 605 | CLA | C2C-C1C-NC | 8.27 | 115.91 | 110.22 |
| 24 | D | 401 | CLA | C2C-C1C-NC | 8.28 | 115.92 | 110.22 |
| 24 | d | 401 | CLA | C2C-C1C-NC | 8.28 | 115.92 | 110.22 |
| 24 | B | 614 | CLA | C2C-C1C-NC | 8.42 | 116.02 | 110.22 |
| 24 | a | 406 | CLA | C2C-C1C-NC | 8.65 | 116.17 | 110.22 |
| 24 | A | 405 | CLA | C2C-C1C-NC | 8.73 | 116.22 | 110.22 |

All (180) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 24 | c | 513 | CLA | NC |
| 24 | c | 513 | CLA | ND |
| 24 | c | 513 | CLA | NA |
| 24 | B | 612 | CLA | NC |
| 24 | D | 403 | CLA | ND |
| 24 | B | 607 | CLA | NC |
| 24 | B | 607 | CLA | ND |
| 24 | B | 607 | CLA | NA |
| 24 | c | 514 | CLA | NC |
| 24 | c | 514 | CLA | ND |
| 24 | c | 514 | CLA | NA |
| 24 | B | 613 | CLA | NC |
| 24 | B | 613 | CLA | ND |
| 24 | B | 613 | CLA | NA |
| 24 | c | 510 | CLA | NC |
| 24 | c | 510 | CLA | ND |
| 24 | c | 510 | CLA | NA |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 24 | B | 603 | CLA | NC |
| 24 | B | 603 | CLA | ND |
| 24 | C | 504 | CLA | NC |
| 24 | C | 504 | CLA | NA |
| 24 | b | 608 | CLA | NC |
| 24 | b | 608 | CLA | ND |
| 24 | d | 404 | CLA | NC |
| 24 | d | 404 | CLA | ND |
| 24 | d | 404 | CLA | NA |
| 24 | b | 620 | CLA | NA |
| 24 | b | 620 | CLA | NC |
| 24 | b | 620 | CLA | ND |
| 24 | C | 513 | CLA | NC |
| 24 | C | 513 | CLA | ND |
| 24 | C | 513 | CLA | NA |
| 24 | C | 506 | CLA | ND |
| 24 | a | 409 | CLA | NC |
| 24 | a | 409 | CLA | ND |
| 24 | a | 409 | CLA | NA |
| 24 | b | 614 | CLA | NC |
| 24 | b | 614 | CLA | ND |
| 24 | B | 604 | CLA | NC |
| 24 | B | 604 | CLA | ND |
| 24 | B | 606 | CLA | NC |
| 24 | B | 606 | CLA | ND |
| 24 | B | 609 | CLA | NC |
| 24 | B | 609 | CLA | NA |
| 24 | b | 621 | CLA | NA |
| 24 | b | 621 | CLA | NC |
| 24 | b | 621 | CLA | ND |
| 24 | B | 614 | CLA | NC |
| 24 | B | 614 | CLA | ND |
| 24 | B | 614 | CLA | NA |
| 24 | D | 404 | CLA | NC |
| 24 | D | 404 | CLA | ND |
| 24 | D | 404 | CLA | NA |
| 24 | B | 610 | CLA | NC |
| 24 | B | 610 | CLA | ND |
| 24 | C | 503 | CLA | NC |
| 24 | C | 503 | CLA | NA |
| 24 | c | 504 | CLA | NC |
| 24 | c | 504 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 24 | c | 504 | CLA | NA |
| 24 | C | 508 | CLA | NC |
| 24 | C | 508 | CLA | ND |
| 24 | C | 508 | CLA | NA |
| 24 | C | 502 | CLA | NC |
| 24 | C | 502 | CLA | ND |
| 24 | C | 502 | CLA | NA |
| 24 | b | 606 | CLA | NC |
| 24 | b | 606 | CLA | ND |
| 24 | b | 606 | CLA | NA |
| 24 | B | 605 | CLA | NC |
| 24 | B | 605 | CLA | ND |
| 24 | B | 605 | CLA | NA |
| 24 | A | 409 | CLA | NC |
| 24 | A | 409 | CLA | NA |
| 24 | A | 406 | CLA | NC |
| 24 | A | 406 | CLA | NA |
| 24 | b | 618 | CLA | NC |
| 24 | b | 618 | CLA | ND |
| 24 | b | 618 | CLA | NA |
| 24 | b | 607 | CLA | NC |
| 24 | b | 607 | CLA | ND |
| 24 | b | 617 | CLA | NC |
| 24 | b | 617 | CLA | ND |
| 24 | b | 617 | CLA | NA |
| 24 | C | 514 | CLA | NC |
| 24 | C | 514 | CLA | NA |
| 24 | a | 407 | CLA | NC |
| 24 | a | 407 | CLA | NA |
| 24 | b | 609 | CLA | NC |
| 24 | b | 609 | CLA | ND |
| 24 | b | 609 | CLA | NA |
| 24 | c | 512 | CLA | NC |
| 24 | c | 512 | CLA | ND |
| 24 | c | 512 | CLA | NA |
| 24 | b | 611 | CLA | NC |
| 24 | b | 611 | CLA | ND |
| 24 | D | 401 | CLA | NC |
| 24 | D | 401 | CLA | ND |
| 24 | D | 401 | CLA | NA |
| 24 | C | 505 | CLA | NC |
| 24 | C | 505 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 24 | C | 505 | CLA | NA |
| 24 | B | 615 | CLA | NC |
| 24 | B | 615 | CLA | ND |
| 24 | c | 507 | CLA | ND |
| 24 | d | 401 | CLA | NC |
| 24 | d | 401 | CLA | ND |
| 24 | d | 401 | CLA | NA |
| 24 | B | 616 | CLA | NA |
| 24 | B | 616 | CLA | NC |
| 24 | B | 616 | CLA | ND |
| 24 | C | 512 | CLA | NC |
| 24 | C | 512 | CLA | ND |
| 24 | C | 512 | CLA | NA |
| 24 | c | 508 | CLA | NC |
| 24 | c | 508 | CLA | ND |
| 24 | c | 508 | CLA | NA |
| 24 | c | 506 | CLA | NC |
| 24 | c | 506 | CLA | ND |
| 24 | c | 506 | CLA | NA |
| 24 | b | 613 | CLA | NC |
| 24 | b | 613 | CLA | NA |
| 24 | a | 406 | CLA | NC |
| 24 | a | 406 | CLA | ND |
| 24 | a | 406 | CLA | NA |
| 24 | B | 602 | CLA | NC |
| 24 | B | 602 | CLA | ND |
| 24 | B | 602 | CLA | NA |
| 24 | b | 615 | CLA | NC |
| 24 | b | 615 | CLA | ND |
| 24 | b | 615 | CLA | NA |
| 24 | b | 610 | CLA | NC |
| 24 | b | 610 | CLA | ND |
| 24 | b | 610 | CLA | NA |
| 24 | B | 617 | CLA | NA |
| 24 | B | 617 | CLA | NC |
| 24 | B | 617 | CLA | ND |
| 24 | d | 402 | CLA | ND |
| 24 | B | 611 | CLA | NC |
| 24 | B | 611 | CLA | ND |
| 24 | B | 611 | CLA | NA |
| 24 | c | 515 | CLA | NC |
| 24 | c | 515 | CLA | NA |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 24 | C | 511 | CLA | NC |
| 24 | C | 511 | CLA | ND |
| 24 | C | 511 | CLA | NA |
| 24 | C | 507 | CLA | NC |
| 24 | C | 507 | CLA | ND |
| 24 | C | 507 | CLA | NA |
| 24 | b | 616 | CLA | NC |
| 24 | b | 616 | CLA | ND |
| 24 | b | 616 | CLA | NA |
| 24 | c | 505 | CLA | NC |
| 24 | c | 505 | CLA | ND |
| 24 | c | 505 | CLA | NA |
| 24 | A | 405 | CLA | NC |
| 24 | A | 405 | CLA | ND |
| 24 | A | 405 | CLA | NA |
| 24 | C | 509 | CLA | NC |
| 24 | C | 509 | CLA | NA |
| 24 | c | 511 | CLA | NC |
| 24 | c | 511 | CLA | ND |
| 24 | c | 511 | CLA | NA |
| 24 | B | 608 | CLA | NC |
| 24 | B | 608 | CLA | ND |
| 24 | B | 608 | CLA | NA |
| 24 | c | 503 | CLA | NC |
| 24 | c | 503 | CLA | ND |
| 24 | c | 503 | CLA | NA |
| 24 | b | 619 | CLA | NC |
| 24 | b | 619 | CLA | ND |
| 24 | b | 619 | CLA | NA |
| 24 | b | 612 | CLA | NC |
| 24 | b | 612 | CLA | ND |
| 24 | c | 509 | CLA | NC |
| 24 | c | 509 | CLA | ND |
| 24 | c | 509 | CLA | NA |
| 24 | C | 510 | CLA | NC |
| 24 | C | 510 | CLA | ND |
| 24 | C | 510 | CLA | NA |

All (5) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|---------------|
| 27 | b | 601 | SQD | C45-O47-C7-C8 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 36 | D | 407 | DGD | C2G-O2G-C1B-C2B |
| 34 | Z | 101 | LMG | C8-O7-C10-C11 |
| 27 | f | 101 | SQD | C45-O47-C7-O49 |
| 27 | f | 101 | SQD | C45-O47-C7-C8 |

There are no ring outliers.

86 monomers are involved in 236 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 24 | A | 405 | CLA | 4 | 0 |
| 24 | A | 406 | CLA | 6 | 0 |
| 25 | A | 408 | PHO | 2 | 0 |
| 24 | A | 409 | CLA | 3 | 0 |
| 26 | A | 410 | BCR | 3 | 0 |
| 27 | A | 411 | SQD | 6 | 0 |
| 28 | A | 412 | GOL | 2 | 0 |
| 28 | A | 413 | GOL | 2 | 0 |
| 27 | A | 416 | SQD | 2 | 0 |
| 32 | A | 419 | PL9 | 4 | 0 |
| 24 | B | 602 | CLA | 1 | 0 |
| 24 | B | 604 | CLA | 3 | 0 |
| 24 | B | 605 | CLA | 1 | 0 |
| 24 | B | 606 | CLA | 6 | 0 |
| 24 | B | 607 | CLA | 2 | 0 |
| 24 | B | 608 | CLA | 2 | 0 |
| 24 | B | 609 | CLA | 2 | 0 |
| 24 | B | 610 | CLA | 7 | 0 |
| 24 | B | 611 | CLA | 4 | 0 |
| 24 | B | 612 | CLA | 1 | 0 |
| 24 | B | 613 | CLA | 5 | 0 |
| 24 | B | 614 | CLA | 5 | 0 |
| 24 | B | 615 | CLA | 4 | 0 |
| 24 | B | 616 | CLA | 1 | 0 |
| 24 | B | 617 | CLA | 10 | 0 |
| 26 | B | 618 | BCR | 2 | 0 |
| 26 | B | 619 | BCR | 1 | 0 |
| 26 | B | 620 | BCR | 3 | 0 |
| 34 | B | 621 | LMG | 2 | 0 |
| 35 | B | 623 | HTG | 1 | 0 |
| 28 | B | 628 | GOL | 1 | 0 |
| 28 | B | 633 | GOL | 1 | 0 |
| 30 | B | 634 | LMT | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 28 | B | 635 | GOL | 2 | 0 |
| 34 | C | 501 | LMG | 5 | 0 |
| 24 | C | 502 | CLA | 4 | 0 |
| 24 | C | 503 | CLA | 7 | 0 |
| 24 | C | 504 | CLA | 4 | 0 |
| 24 | C | 505 | CLA | 4 | 0 |
| 24 | C | 506 | CLA | 1 | 0 |
| 24 | C | 507 | CLA | 7 | 0 |
| 24 | C | 508 | CLA | 6 | 0 |
| 24 | C | 509 | CLA | 6 | 0 |
| 24 | C | 510 | CLA | 4 | 0 |
| 24 | C | 511 | CLA | 6 | 0 |
| 24 | C | 512 | CLA | 4 | 0 |
| 24 | C | 513 | CLA | 6 | 0 |
| 24 | C | 514 | CLA | 9 | 0 |
| 26 | C | 515 | BCR | 3 | 0 |
| 26 | C | 516 | BCR | 4 | 0 |
| 36 | C | 517 | DGD | 4 | 0 |
| 36 | C | 518 | DGD | 3 | 0 |
| 36 | C | 519 | DGD | 3 | 0 |
| 34 | C | 520 | LMG | 4 | 0 |
| 34 | C | 521 | LMG | 2 | 0 |
| 35 | C | 522 | HTG | 1 | 0 |
| 35 | C | 523 | HTG | 2 | 0 |
| 28 | C | 524 | GOL | 1 | 0 |
| 28 | C | 525 | GOL | 2 | 0 |
| 24 | D | 401 | CLA | 6 | 0 |
| 30 | D | 402 | LMT | 1 | 0 |
| 24 | D | 403 | CLA | 1 | 0 |
| 24 | D | 404 | CLA | 4 | 0 |
| 26 | D | 405 | BCR | 4 | 0 |
| 36 | D | 407 | DGD | 6 | 0 |
| 37 | D | 408 | LHG | 2 | 0 |
| 37 | D | 410 | LHG | 10 | 0 |
| 35 | D | 411 | HTG | 3 | 0 |
| 37 | E | 101 | LHG | 6 | 0 |
| 27 | F | 101 | SQD | 5 | 0 |
| 26 | H | 101 | BCR | 6 | 0 |
| 36 | H | 102 | DGD | 2 | 0 |
| 30 | I | 102 | LMT | 2 | 0 |
| 34 | J | 101 | LMG | 3 | 0 |
| 26 | K | 101 | BCR | 2 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 37 | L | 101 | LHG | 1 | 0 |
| 30 | M | 101 | LMT | 1 | 0 |
| 30 | M | 102 | LMT | 2 | 0 |
| 28 | T | 101 | GOL | 1 | 0 |
| 26 | T | 102 | BCR | 5 | 0 |
| 35 | V | 204 | HTG | 1 | 0 |
| 28 | V | 205 | GOL | 2 | 0 |
| 28 | V | 207 | GOL | 1 | 0 |
| 28 | V | 208 | GOL | 1 | 0 |
| 26 | Y | 101 | BCR | 2 | 0 |
| 34 | Z | 101 | LMG | 6 | 0 |

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 1 | A | 334/344 (97%) | 0.67 | 46 (13%) 3 5 | 16, 23, 42, 79 | 0 |
| 1 | a | 334/344 (97%) | 0.84 | 61 (18%) 1 2 | 17, 25, 48, 82 | 0 |
| 2 | B | 504/505 (99%) | 0.27 | 42 (8%) 12 19 | 18, 27, 52, 90 | 0 |
| 2 | b | 504/505 (99%) | 0.47 | 52 (10%) 7 12 | 19, 29, 60, 108 | 0 |
| 3 | C | 451/455 (99%) | 0.24 | 28 (6%) 21 31 | 20, 32, 49, 89 | 0 |
| 3 | c | 455/455 (100%) | 0.44 | 38 (8%) 12 18 | 23, 35, 50, 87 | 0 |
| 4 | D | 342/342 (100%) | 0.88 | 62 (18%) 1 2 | 15, 24, 40, 114 | 0 |
| 4 | d | 341/342 (99%) | 0.59 | 39 (11%) 6 9 | 18, 26, 42, 90 | 0 |
| 5 | E | 81/84 (96%) | 1.22 | 19 (23%) 1 0 | 27, 40, 68, 97 | 0 |
| 5 | e | 81/84 (96%) | 1.09 | 14 (17%) 2 2 | 32, 45, 77, 97 | 0 |
| 6 | F | 34/44 (77%) | 0.34 | 6 (17%) 2 2 | 26, 35, 56, 64 | 0 |
| 6 | f | 32/44 (72%) | 0.42 | 4 (12%) 4 7 | 31, 37, 84, 99 | 0 |
| 7 | H | 65/65 (100%) | 0.34 | 3 (4%) 33 44 | 24, 34, 52, 97 | 0 |
| 7 | h | 65/65 (100%) | 0.56 | 6 (9%) 10 16 | 28, 37, 58, 113 | 0 |
| 8 | I | 37/38 (97%) | 0.82 | 5 (13%) 3 6 | 30, 34, 91, 101 | 0 |
| 8 | i | 37/38 (97%) | 0.74 | 5 (13%) 3 6 | 29, 34, 79, 102 | 0 |
| 9 | J | 38/39 (97%) | 0.74 | 8 (21%) 1 1 | 26, 38, 85, 109 | 0 |
| 9 | j | 38/39 (97%) | 0.25 | 4 (10%) 7 11 | 30, 41, 84, 85 | 0 |
| 10 | K | 37/37 (100%) | 0.16 | 0 100 100 | 31, 38, 55, 64 | 0 |
| 10 | k | 37/37 (100%) | 0.86 | 8 (21%) 1 1 | 33, 42, 56, 66 | 0 |
| 11 | L | 37/37 (100%) | 1.18 | 11 (29%) 1 0 | 16, 20, 66, 91 | 0 |
| 11 | l | 37/37 (100%) | 1.05 | 6 (16%) 2 3 | 17, 21, 61, 91 | 0 |
| 12 | M | 33/36 (91%) | 0.90 | 6 (18%) 1 2 | 18, 23, 44, 100 | 0 |
| 12 | m | 33/36 (91%) | 0.77 | 6 (18%) 1 2 | 19, 23, 44, 100 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 13 | O | 243/244 (99%) | 0.38 | 22 (9%) 10 16 | 16, 34, 65, 113 | 0 |
| 13 | o | 243/244 (99%) | 0.89 | 52 (21%) 1 1 | 18, 35, 75, 122 | 0 |
| 14 | T | 29/31 (93%) | 0.98 | 4 (13%) 3 5 | 17, 23, 48, 85 | 0 |
| 14 | t | 29/31 (93%) | 0.54 | 2 (6%) 18 27 | 17, 23, 49, 85 | 0 |
| 15 | U | 97/104 (93%) | 0.26 | 6 (6%) 21 31 | 22, 33, 53, 85 | 0 |
| 15 | u | 97/104 (93%) | -0.11 | 0 100 100 | 25, 34, 51, 85 | 0 |
| 16 | V | 137/137 (100%) | -0.02 | 0 100 100 | 23, 33, 54, 70 | 0 |
| 16 | v | 137/137 (100%) | 0.49 | 13 (9%) 9 14 | 26, 38, 57, 72 | 0 |
| 17 | Y | 29/30 (96%) | 2.06 | 9 (31%) 0 0 | 38, 50, 91, 107 | 0 |
| 17 | y | 29/30 (96%) | 1.93 | 9 (31%) 0 0 | 41, 54, 91, 107 | 0 |
| 18 | X | 39/40 (97%) | 0.77 | 8 (20%) 1 1 | 32, 42, 80, 92 | 0 |
| 18 | x | 39/40 (97%) | 1.59 | 11 (28%) 1 0 | 35, 45, 93, 96 | 0 |
| 19 | Z | 62/62 (100%) | 1.30 | 18 (29%) 1 0 | 40, 52, 87, 98 | 0 |
| 19 | z | 62/62 (100%) | 2.98 | 36 (58%) 0 0 | 44, 53, 87, 98 | 0 |
| 20 | R | 34/34 (100%) | 9.36 | 34 (100%) 0 0 | 69, 93, 111, 118 | 0 |
| All | All | 5293/5382 (98%) | 0.65 | 703 (13%) 4 6 | 15, 31, 63, 122 | 0 |

All (703) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 20 | R | 18 | TRP | 18.5 |
| 20 | R | 6 | LEU | 14.1 |
| 20 | R | 14 | LEU | 13.4 |
| 20 | R | 31 | VAL | 13.0 |
| 20 | R | 20 | VAL | 12.1 |
| 20 | R | 19 | ALA | 11.4 |
| 20 | R | 16 | ALA | 11.2 |
| 17 | Y | 18 | VAL | 11.2 |
| 20 | R | 25 | PRO | 10.9 |
| 20 | R | 5 | VAL | 10.7 |
| 19 | z | 3 | ILE | 10.5 |
| 20 | R | 32 | GLN | 10.3 |
| 20 | R | 27 | ALA | 10.3 |
| 20 | R | 23 | ILE | 10.2 |
| 20 | R | 15 | ALA | 9.8 |
| 19 | z | 62 | VAL | 9.7 |
| 18 | x | 38 | GLN | 9.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 17 | Y | 19 | ILE | 9.6 |
| 20 | R | 13 | LEU | 9.5 |
| 8 | i | 37 | LEU | 9.5 |
| 20 | R | 34 | LEU | 9.5 |
| 19 | z | 5 | PHE | 9.4 |
| 17 | y | 19 | ILE | 9.4 |
| 20 | R | 21 | ARG | 9.3 |
| 20 | R | 24 | LEU | 9.2 |
| 20 | R | 26 | TYR | 8.9 |
| 20 | R | 10 | LEU | 8.8 |
| 7 | h | 65 | LEU | 8.8 |
| 20 | R | 9 | LEU | 8.7 |
| 17 | y | 18 | VAL | 8.4 |
| 4 | D | 11 | GLU | 8.3 |
| 20 | R | 22 | ASN | 8.3 |
| 20 | R | 29 | LYS | 8.3 |
| 20 | R | 7 | VAL | 8.2 |
| 20 | R | 12 | VAL | 8.1 |
| 1 | A | 11 | ALA | 8.0 |
| 18 | x | 2 | THR | 7.9 |
| 20 | R | 17 | GLY | 7.9 |
| 8 | I | 38 | GLU | 7.9 |
| 20 | R | 28 | VAL | 7.8 |
| 2 | b | 495 | PHE | 7.7 |
| 8 | I | 37 | LEU | 7.6 |
| 19 | z | 4 | LEU | 7.6 |
| 20 | R | 3 | TRP | 7.6 |
| 18 | x | 37 | VAL | 7.4 |
| 19 | z | 60 | PHE | 7.4 |
| 20 | R | 30 | GLN | 7.3 |
| 7 | H | 65 | LEU | 7.3 |
| 20 | R | 11 | PRO | 7.3 |
| 20 | R | 35 | LEU | 7.2 |
| 17 | Y | 22 | LEU | 7.1 |
| 19 | Z | 62 | VAL | 7.0 |
| 2 | B | 85 | GLY | 6.9 |
| 1 | a | 11 | ALA | 6.7 |
| 2 | b | 491 | VAL | 6.4 |
| 19 | z | 42 | LEU | 6.4 |
| 20 | R | 33 | LYS | 6.4 |
| 19 | z | 61 | VAL | 6.3 |
| 2 | b | 486 | LEU | 6.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 13 | O | 60 | ARG | 6.3 |
| 19 | Z | 3 | ILE | 6.3 |
| 17 | y | 20 | ALA | 6.2 |
| 18 | x | 34 | ILE | 6.2 |
| 13 | o | 246 | ALA | 6.2 |
| 5 | e | 5 | THR | 6.1 |
| 2 | b | 499 | VAL | 6.0 |
| 2 | b | 504 | THR | 6.0 |
| 19 | z | 7 | LEU | 6.0 |
| 13 | o | 36 | GLN | 5.9 |
| 2 | b | 293 | ALA | 5.9 |
| 10 | k | 18 | PHE | 5.9 |
| 2 | b | 496 | TYR | 5.7 |
| 6 | f | 14 | PRO | 5.7 |
| 17 | Y | 20 | ALA | 5.7 |
| 6 | f | 15 | ILE | 5.6 |
| 2 | B | 494 | GLY | 5.5 |
| 1 | A | 13 | LEU | 5.5 |
| 5 | E | 84 | LYS | 5.5 |
| 19 | Z | 31 | GLN | 5.4 |
| 2 | b | 487 | SER | 5.4 |
| 2 | B | 495 | PHE | 5.4 |
| 13 | o | 35 | SER | 5.3 |
| 18 | x | 40 | SER | 5.3 |
| 5 | E | 17 | VAL | 5.2 |
| 5 | e | 6 | GLY | 5.2 |
| 2 | b | 493 | TRP | 5.2 |
| 6 | F | 16 | PHE | 5.2 |
| 4 | D | 12 | ARG | 5.2 |
| 9 | J | 2 | SER | 5.2 |
| 19 | z | 33 | TRP | 5.1 |
| 19 | z | 41 | PHE | 5.1 |
| 17 | y | 22 | LEU | 5.1 |
| 7 | H | 66 | GLY | 5.1 |
| 5 | e | 4 | THR | 5.1 |
| 2 | b | 295 | GLY | 5.0 |
| 11 | l | 1 | MET | 5.0 |
| 19 | Z | 36 | SER | 5.0 |
| 2 | b | 505 | ARG | 5.0 |
| 16 | v | 17 | LYS | 5.0 |
| 2 | b | 494 | GLY | 5.0 |
| 8 | I | 36 | ASP | 5.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 19 | z | 39 | LEU | 4.9 |
| 3 | c | 143 | TYR | 4.9 |
| 3 | c | 146 | PHE | 4.9 |
| 5 | E | 21 | VAL | 4.9 |
| 7 | H | 64 | ALA | 4.8 |
| 2 | b | 85 | GLY | 4.8 |
| 18 | x | 39 | ARG | 4.8 |
| 13 | o | 25 | THR | 4.8 |
| 20 | R | 2 | ASP | 4.8 |
| 19 | Z | 7 | LEU | 4.8 |
| 7 | h | 66 | GLY | 4.7 |
| 18 | X | 40 | SER | 4.7 |
| 20 | R | 8 | VAL | 4.7 |
| 6 | f | 16 | PHE | 4.7 |
| 19 | z | 2 | THR | 4.7 |
| 13 | o | 59 | LYS | 4.7 |
| 2 | B | 297 | THR | 4.6 |
| 5 | E | 6 | GLY | 4.6 |
| 5 | e | 25 | ILE | 4.6 |
| 13 | o | 23 | ASP | 4.6 |
| 19 | Z | 35 | ARG | 4.6 |
| 13 | o | 56 | PRO | 4.6 |
| 19 | Z | 33 | TRP | 4.6 |
| 4 | D | 201 | VAL | 4.6 |
| 13 | o | 133 | VAL | 4.6 |
| 13 | o | 34 | SER | 4.5 |
| 2 | b | 502 | VAL | 4.5 |
| 9 | J | 3 | GLU | 4.5 |
| 10 | k | 12 | PRO | 4.5 |
| 8 | i | 34 | ARG | 4.4 |
| 4 | d | 182 | LEU | 4.4 |
| 13 | o | 61 | GLN | 4.4 |
| 2 | b | 86 | ILE | 4.4 |
| 6 | F | 15 | ILE | 4.4 |
| 2 | b | 497 | GLN | 4.4 |
| 19 | z | 9 | LEU | 4.4 |
| 3 | c | 147 | PHE | 4.4 |
| 2 | b | 294 | SER | 4.4 |
| 2 | B | 486 | LEU | 4.3 |
| 4 | D | 156 | VAL | 4.3 |
| 20 | R | 4 | ARG | 4.3 |
| 2 | b | 84 | THR | 4.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-------|------|------|
| 4 | d | 179 | PHE | 4.3 |
| 8 | i | 38 | GLU | 4.3 |
| 13 | o | 87 | VAL | 4.3 |
| 13 | o | 27 | ARG | 4.2 |
| 1 | a | 290 | ILE | 4.2 |
| 17 | Y | 21 | GLN | 4.2 |
| 13 | O | 58 | ASN | 4.2 |
| 2 | b | 485 | GLU | 4.2 |
| 13 | O | 25 | THR | 4.2 |
| 1 | a | 193 | LEU | 4.2 |
| 17 | Y | 25 | ILE | 4.2 |
| 13 | o | 4 | THR | 4.1 |
| 18 | X | 2 | THR | 4.1 |
| 18 | X | 37 | VAL | 4.1 |
| 19 | z | 1 | MET | 4.1 |
| 19 | z | 35 | ARG | 4.1 |
| 13 | o | 58 | ASN | 4.1 |
| 13 | o | 32 | ILE | 4.1 |
| 13 | o | 26 | ALA | 4.1 |
| 2 | b | 126 | PRO | 4.0 |
| 8 | i | 36 | ASP | 4.0 |
| 1 | A | 200 | LEU | 4.0 |
| 19 | z | 59 | PHE | 4.0 |
| 4 | D | 279 | LEU | 4.0 |
| 1 | a | 288 | LEU | 4.0 |
| 1 | A | 288 | LEU | 4.0 |
| 19 | z | 53 | VAL | 4.0 |
| 1 | a | 184 | ILE | 3.9 |
| 13 | o | 38 | TYR | 3.9 |
| 1 | a | 280 | VAL | 3.9 |
| 2 | B | 86[A] | ILE | 3.9 |
| 2 | b | 490 | GLN | 3.9 |
| 1 | a | 197 | PHE | 3.9 |
| 4 | D | 153 | PHE | 3.9 |
| 4 | D | 191 | TRP | 3.9 |
| 2 | B | 84 | THR | 3.9 |
| 12 | M | 33 | GLN | 3.9 |
| 13 | O | 27 | ARG | 3.8 |
| 3 | C | 432 | VAL | 3.8 |
| 14 | t | 29 | ILE | 3.8 |
| 15 | U | 79 | LEU | 3.8 |
| 13 | o | 37 | THR | 3.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | a | 297 | LEU | 3.8 |
| 4 | D | 289 | LEU | 3.8 |
| 19 | Z | 4 | LEU | 3.8 |
| 19 | Z | 32 | ASP | 3.8 |
| 4 | D | 205 | LEU | 3.8 |
| 13 | o | 208 | THR | 3.7 |
| 13 | o | 60 | ARG | 3.7 |
| 14 | T | 30 | THR | 3.7 |
| 15 | U | 8 | GLU | 3.7 |
| 19 | z | 32 | ASP | 3.7 |
| 1 | a | 285 | PHE | 3.7 |
| 12 | m | 34 | LYS | 3.7 |
| 1 | A | 285 | PHE | 3.7 |
| 3 | C | 257 | PHE | 3.7 |
| 2 | b | 127 | ARG | 3.7 |
| 4 | d | 12 | ARG | 3.7 |
| 1 | a | 200 | LEU | 3.7 |
| 1 | a | 192 | ILE | 3.6 |
| 4 | D | 238 | THR | 3.6 |
| 17 | y | 41 | VAL | 3.6 |
| 13 | O | 62 | GLU | 3.6 |
| 3 | c | 134 | ILE | 3.6 |
| 2 | b | 297 | THR | 3.6 |
| 4 | D | 280 | TRP | 3.6 |
| 3 | c | 21 | ILE | 3.6 |
| 2 | B | 489 | GLU | 3.6 |
| 11 | L | 2 | GLU | 3.6 |
| 4 | D | 150 | ILE | 3.6 |
| 13 | o | 33 | ASP | 3.6 |
| 13 | O | 56 | PRO | 3.6 |
| 19 | z | 25 | VAL | 3.6 |
| 2 | b | 290 | ALA | 3.5 |
| 14 | T | 9 | ILE | 3.5 |
| 13 | O | 59 | LYS | 3.5 |
| 5 | E | 4 | THR | 3.5 |
| 4 | D | 152 | VAL | 3.5 |
| 19 | z | 58 | ASN | 3.5 |
| 2 | b | 500 | GLY | 3.5 |
| 4 | D | 196 | PHE | 3.5 |
| 4 | d | 196 | PHE | 3.5 |
| 17 | y | 21 | GLN | 3.5 |
| 4 | D | 149 | PRO | 3.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 18 | X | 38 | GLN | 3.5 |
| 17 | y | 25 | ILE | 3.4 |
| 2 | b | 129 | GLY | 3.4 |
| 4 | D | 286 | VAL | 3.4 |
| 1 | A | 197 | PHE | 3.4 |
| 11 | L | 31 | PHE | 3.4 |
| 2 | b | 484 | PRO | 3.4 |
| 1 | A | 202 | VAL | 3.4 |
| 3 | c | 432 | VAL | 3.4 |
| 1 | A | 287 | ALA | 3.4 |
| 13 | o | 89 | SER | 3.4 |
| 19 | z | 30 | PRO | 3.4 |
| 2 | b | 296 | ALA | 3.4 |
| 3 | C | 262 | ARG | 3.4 |
| 9 | J | 6 | ARG | 3.4 |
| 18 | X | 31 | ILE | 3.4 |
| 3 | c | 145 | SER | 3.4 |
| 5 | e | 84 | LYS | 3.4 |
| 19 | z | 6 | GLN | 3.4 |
| 11 | l | 2 | GLU | 3.4 |
| 1 | a | 161 | TYR | 3.4 |
| 2 | B | 298 | LEU | 3.4 |
| 2 | b | 292 | LEU | 3.4 |
| 4 | D | 293 | LEU | 3.4 |
| 19 | Z | 60 | PHE | 3.3 |
| 13 | o | 132 | ASN | 3.3 |
| 2 | B | 461 | LEU | 3.3 |
| 4 | d | 14 | TRP | 3.3 |
| 5 | e | 59 | GLU | 3.3 |
| 1 | a | 163 | ILE | 3.3 |
| 3 | C | 253 | LEU | 3.3 |
| 4 | D | 276 | VAL | 3.3 |
| 13 | o | 62 | GLU | 3.3 |
| 3 | c | 257 | PHE | 3.3 |
| 3 | c | 259 | TRP | 3.3 |
| 1 | a | 202 | VAL | 3.3 |
| 16 | v | 107 | LEU | 3.3 |
| 19 | Z | 61 | VAL | 3.3 |
| 1 | A | 230 | THR | 3.3 |
| 9 | J | 5 | GLY | 3.2 |
| 4 | D | 204 | VAL | 3.2 |
| 1 | A | 290 | ILE | 3.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-------|------|------|
| 13 | o | 211 | ILE | 3.2 |
| 16 | v | 19 | ILE | 3.2 |
| 1 | a | 157 | VAL | 3.2 |
| 2 | b | 488 | PRO | 3.2 |
| 11 | l | 3 | PRO | 3.2 |
| 4 | D | 160 | TYR | 3.2 |
| 16 | v | 110 | LYS | 3.2 |
| 10 | k | 14 | ALA | 3.2 |
| 2 | B | 457 | VAL | 3.2 |
| 19 | z | 40 | ILE | 3.2 |
| 18 | x | 36 | LYS | 3.2 |
| 6 | F | 14 | PRO | 3.2 |
| 19 | z | 31 | GLN | 3.2 |
| 17 | Y | 43 | ARG | 3.2 |
| 1 | A | 186 | PHE | 3.2 |
| 2 | B | 496 | TYR | 3.1 |
| 13 | O | 28 | GLY | 3.1 |
| 19 | Z | 1 | MET | 3.1 |
| 19 | Z | 39 | LEU | 3.1 |
| 19 | Z | 42 | LEU | 3.1 |
| 13 | o | 91 | GLY | 3.1 |
| 1 | A | 278 | TRP | 3.1 |
| 3 | C | 436 | PHE | 3.1 |
| 4 | D | 175 | VAL | 3.1 |
| 5 | e | 21 | VAL | 3.1 |
| 6 | F | 18 | VAL | 3.1 |
| 12 | M | 16[A] | LEU | 3.1 |
| 2 | b | 501 | ASP | 3.1 |
| 13 | o | 24 | ASP | 3.1 |
| 3 | C | 143 | TYR | 3.1 |
| 4 | D | 148 | ALA | 3.1 |
| 1 | A | 193 | LEU | 3.1 |
| 2 | b | 298 | LEU | 3.1 |
| 11 | L | 29 | LEU | 3.1 |
| 13 | O | 93 | LEU | 3.1 |
| 3 | C | 260 | ALA | 3.1 |
| 19 | Z | 34 | ASP | 3.0 |
| 13 | o | 126 | VAL | 3.0 |
| 11 | L | 1 | MET | 3.0 |
| 14 | T | 13 | ILE | 3.0 |
| 4 | d | 283 | ALA | 3.0 |
| 3 | c | 20 | SER | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 4 | d | 148 | ALA | 3.0 |
| 10 | k | 17 | ILE | 3.0 |
| 13 | o | 135 | SER | 3.0 |
| 15 | U | 70 | ARG | 3.0 |
| 2 | B | 504 | THR | 3.0 |
| 5 | E | 5 | THR | 3.0 |
| 13 | O | 61 | GLN | 3.0 |
| 2 | b | 125 | ASP | 3.0 |
| 2 | B | 499 | VAL | 3.0 |
| 2 | B | 293 | ALA | 3.0 |
| 1 | A | 321 | ILE | 3.0 |
| 3 | C | 431 | PHE | 3.0 |
| 4 | D | 275 | PRO | 3.0 |
| 4 | d | 184 | PHE | 3.0 |
| 4 | d | 325 | ILE | 3.0 |
| 2 | B | 487 | SER | 3.0 |
| 3 | C | 145[A] | SER | 3.0 |
| 3 | c | 411 | ALA | 3.0 |
| 4 | d | 201 | VAL | 3.0 |
| 4 | D | 182 | LEU | 3.0 |
| 4 | d | 205 | LEU | 3.0 |
| 1 | A | 12 | ASN | 3.0 |
| 5 | E | 19 | TYR | 3.0 |
| 19 | z | 29 | SER | 3.0 |
| 4 | d | 175 | VAL | 3.0 |
| 9 | J | 24 | VAL | 3.0 |
| 8 | I | 34 | ARG | 2.9 |
| 1 | a | 182 | PHE | 2.9 |
| 19 | z | 38 | GLN | 2.9 |
| 3 | c | 144 | SER | 2.9 |
| 4 | D | 278 | GLY | 2.9 |
| 4 | d | 178 | ILE | 2.9 |
| 18 | X | 34 | ILE | 2.9 |
| 4 | d | 185 | PHE | 2.9 |
| 16 | v | 26 | TYR | 2.9 |
| 2 | b | 489 | GLU | 2.9 |
| 5 | E | 22 | ILE | 2.9 |
| 11 | l | 31 | PHE | 2.9 |
| 1 | a | 235 | TYR | 2.9 |
| 3 | c | 142 | GLU | 2.9 |
| 18 | x | 30 | ALA | 2.9 |
| 8 | I | 35 | LYS | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2 | b | 492 | GLU | 2.9 |
| 1 | a | 186 | PHE | 2.9 |
| 4 | D | 202 | ALA | 2.9 |
| 1 | a | 284 | TRP | 2.9 |
| 4 | d | 156 | VAL | 2.9 |
| 1 | A | 196 | PRO | 2.9 |
| 1 | a | 286 | ALA | 2.9 |
| 13 | O | 26 | ALA | 2.9 |
| 2 | b | 503 | THR | 2.8 |
| 2 | B | 488 | PRO | 2.8 |
| 2 | B | 460 | LEU | 2.8 |
| 4 | D | 193 | LEU | 2.8 |
| 13 | o | 130 | GLN | 2.8 |
| 9 | J | 7 | ILE | 2.8 |
| 13 | o | 134 | THR | 2.8 |
| 13 | o | 131 | PRO | 2.8 |
| 4 | D | 200 | GLY | 2.8 |
| 19 | z | 49 | ALA | 2.8 |
| 1 | A | 77 | ILE | 2.8 |
| 4 | d | 187 | GLY | 2.8 |
| 1 | a | 293 | MET | 2.8 |
| 1 | a | 205 | VAL | 2.8 |
| 2 | B | 502 | VAL | 2.8 |
| 1 | A | 297 | LEU | 2.8 |
| 1 | a | 326 | LEU | 2.8 |
| 4 | D | 122 | LEU | 2.8 |
| 13 | o | 22 | LEU | 2.8 |
| 1 | A | 192 | ILE | 2.8 |
| 2 | B | 295 | GLY | 2.8 |
| 1 | A | 283 | VAL | 2.8 |
| 7 | h | 22 | ALA | 2.8 |
| 13 | o | 209 | GLY | 2.8 |
| 4 | d | 280 | TRP | 2.8 |
| 9 | j | 6 | ARG | 2.8 |
| 18 | x | 3 | ILE | 2.8 |
| 2 | b | 291 | SER | 2.8 |
| 4 | D | 146 | PHE | 2.8 |
| 4 | D | 119 | ALA | 2.7 |
| 10 | k | 13 | GLU | 2.8 |
| 4 | d | 183 | LEU | 2.7 |
| 5 | E | 83 | LEU | 2.7 |
| 11 | l | 25 | LEU | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | A | 176 | ILE | 2.7 |
| 1 | a | 194 | MET | 2.7 |
| 3 | c | 425 | TRP | 2.7 |
| 4 | D | 325 | ILE | 2.7 |
| 1 | a | 295 | PHE | 2.7 |
| 1 | a | 299 | GLY | 2.7 |
| 4 | D | 183 | LEU | 2.7 |
| 19 | z | 57 | LEU | 2.7 |
| 2 | b | 123 | PHE | 2.7 |
| 2 | B | 503 | THR | 2.7 |
| 3 | c | 428 | THR | 2.7 |
| 11 | l | 27 | LEU | 2.7 |
| 1 | a | 282 | GLY | 2.7 |
| 17 | Y | 30 | ILE | 2.7 |
| 12 | M | 34 | LYS | 2.7 |
| 2 | B | 462 | PHE | 2.7 |
| 2 | B | 464 | PHE | 2.7 |
| 5 | E | 20 | TRP | 2.7 |
| 13 | O | 65 | PHE | 2.7 |
| 13 | o | 63 | ALA | 2.7 |
| 16 | v | 106 | ASN | 2.7 |
| 3 | c | 410 | VAL | 2.7 |
| 5 | e | 61 | ARG | 2.7 |
| 19 | z | 56 | VAL | 2.7 |
| 3 | c | 426 | LEU | 2.7 |
| 4 | D | 199 | MET | 2.7 |
| 11 | L | 23 | LEU | 2.7 |
| 13 | o | 140 | THR | 2.7 |
| 4 | D | 290 | ALA | 2.7 |
| 3 | C | 259 | TRP | 2.7 |
| 1 | A | 205 | VAL | 2.7 |
| 3 | C | 407 | VAL | 2.7 |
| 1 | A | 210 | LEU | 2.7 |
| 3 | c | 404 | LEU | 2.7 |
| 4 | D | 192 | THR | 2.7 |
| 17 | y | 23 | THR | 2.7 |
| 3 | C | 23 | ALA | 2.6 |
| 4 | D | 154 | VAL | 2.6 |
| 13 | o | 30 | TYR | 2.6 |
| 13 | o | 64 | GLU | 2.6 |
| 3 | c | 140 | LEU | 2.6 |
| 2 | b | 483 | ASP | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 19 | Z | 2 | THR | 2.6 |
| 1 | A | 203 | ALA | 2.6 |
| 4 | D | 281 | MET | 2.6 |
| 5 | e | 79 | PHE | 2.6 |
| 13 | o | 139 | SER | 2.6 |
| 3 | C | 255 | THR | 2.6 |
| 4 | D | 116 | LEU | 2.6 |
| 4 | d | 209 | LEU | 2.6 |
| 11 | L | 30 | LEU | 2.6 |
| 13 | o | 21 | THR | 2.6 |
| 3 | c | 155 | ASN | 2.6 |
| 1 | a | 180 | PHE | 2.6 |
| 1 | a | 281 | VAL | 2.6 |
| 2 | b | 457 | VAL | 2.6 |
| 3 | C | 404 | LEU | 2.6 |
| 4 | d | 279 | LEU | 2.6 |
| 1 | a | 287 | ALA | 2.6 |
| 2 | B | 459 | ALA | 2.6 |
| 16 | v | 16 | GLY | 2.6 |
| 19 | z | 10 | ALA | 2.6 |
| 1 | a | 195 | HIS | 2.6 |
| 4 | D | 284 | ILE | 2.6 |
| 1 | A | 184 | ILE | 2.6 |
| 13 | o | 243 | ILE | 2.6 |
| 4 | D | 277 | THR | 2.6 |
| 2 | B | 165 | GLY | 2.6 |
| 1 | a | 324 | ALA | 2.5 |
| 3 | c | 433 | LEU | 2.5 |
| 4 | D | 283 | ALA | 2.5 |
| 9 | j | 2 | SER | 2.5 |
| 9 | J | 4 | GLY | 2.5 |
| 13 | O | 136 | ILE | 2.5 |
| 1 | a | 330 | VAL | 2.5 |
| 4 | d | 152 | VAL | 2.5 |
| 3 | C | 181 | PHE | 2.5 |
| 3 | c | 163 | PHE | 2.5 |
| 4 | d | 188 | PHE | 2.5 |
| 2 | B | 296 | ALA | 2.5 |
| 1 | a | 279 | PRO | 2.5 |
| 2 | b | 413 | ASP | 2.5 |
| 5 | E | 73 | LYS | 2.5 |
| 7 | h | 6 | TRP | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 16 | v | 108 | THR | 2.5 |
| 1 | a | 321 | ILE | 2.5 |
| 5 | E | 81 | GLU | 2.5 |
| 1 | A | 185 | VAL | 2.5 |
| 4 | D | 287 | VAL | 2.5 |
| 13 | O | 133 | VAL | 2.5 |
| 13 | o | 142 | PHE | 2.5 |
| 19 | Z | 30 | PRO | 2.5 |
| 3 | c | 429 | SER | 2.5 |
| 13 | o | 57 | LYS | 2.5 |
| 19 | z | 14 | ILE | 2.5 |
| 2 | B | 456 | ALA | 2.5 |
| 4 | D | 274 | VAL | 2.5 |
| 5 | E | 72 | ALA | 2.5 |
| 13 | o | 245 | PRO | 2.5 |
| 19 | z | 18 | VAL | 2.5 |
| 1 | A | 182 | PHE | 2.5 |
| 1 | A | 201 | GLY | 2.5 |
| 1 | A | 300 | PHE | 2.5 |
| 3 | c | 431 | PHE | 2.5 |
| 4 | d | 281 | MET | 2.5 |
| 4 | d | 193 | LEU | 2.5 |
| 4 | d | 289 | LEU | 2.5 |
| 4 | d | 321 | LEU | 2.5 |
| 14 | t | 30 | THR | 2.5 |
| 13 | O | 88 | ASN | 2.5 |
| 4 | D | 159 | ILE | 2.5 |
| 1 | A | 180 | PHE | 2.5 |
| 4 | D | 181 | PHE | 2.5 |
| 12 | m | 13 | LEU | 2.5 |
| 16 | v | 95 | LEU | 2.5 |
| 1 | A | 160 | ILE | 2.4 |
| 4 | d | 329 | MET | 2.4 |
| 13 | o | 66 | VAL | 2.4 |
| 2 | b | 302 | TRP | 2.4 |
| 18 | X | 39 | ARG | 2.4 |
| 2 | B | 479 | PHE | 2.4 |
| 12 | M | 14 | PHE | 2.4 |
| 1 | a | 191 | ASN | 2.4 |
| 4 | d | 159 | ILE | 2.4 |
| 4 | d | 284 | ILE | 2.4 |
| 13 | o | 136 | ILE | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | a | 185 | VAL | 2.4 |
| 8 | i | 35 | LYS | 2.4 |
| 18 | x | 8 | LYS | 2.4 |
| 3 | C | 425 | TRP | 2.4 |
| 4 | D | 185 | PHE | 2.4 |
| 12 | m | 14 | PHE | 2.4 |
| 4 | D | 203 | GLY | 2.4 |
| 3 | c | 201 | ASN | 2.4 |
| 1 | a | 203 | ALA | 2.4 |
| 7 | h | 64 | ALA | 2.4 |
| 12 | m | 33 | GLN | 2.4 |
| 5 | e | 26 | THR | 2.4 |
| 1 | A | 281 | VAL | 2.4 |
| 1 | A | 16 | ARG | 2.4 |
| 2 | B | 408 | GLY | 2.4 |
| 1 | A | 284 | TRP | 2.4 |
| 1 | a | 278 | TRP | 2.4 |
| 3 | C | 435 | PHE | 2.4 |
| 4 | D | 184 | PHE | 2.4 |
| 13 | O | 137 | THR | 2.4 |
| 2 | B | 127 | ARG | 2.4 |
| 2 | b | 124 | ARG | 2.4 |
| 1 | A | 282 | GLY | 2.4 |
| 1 | a | 190 | HIS | 2.4 |
| 19 | Z | 38 | GLN | 2.4 |
| 4 | d | 74 | LEU | 2.4 |
| 2 | B | 453 | PHE | 2.4 |
| 4 | D | 170 | ALA | 2.4 |
| 3 | c | 200 | THR | 2.4 |
| 7 | h | 23 | PRO | 2.4 |
| 3 | c | 166 | ILE | 2.4 |
| 3 | c | 207 | ARG | 2.3 |
| 3 | c | 253 | LEU | 2.3 |
| 10 | k | 21 | LEU | 2.3 |
| 2 | B | 402 | TYR | 2.3 |
| 2 | B | 463 | PHE | 2.3 |
| 3 | C | 428 | THR | 2.3 |
| 13 | O | 138 | THR | 2.3 |
| 16 | v | 15 | GLU | 2.3 |
| 5 | e | 36 | LEU | 2.3 |
| 13 | o | 199 | LEU | 2.3 |
| 16 | v | 86 | GLN | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-------|------|------|
| 17 | Y | 26 | ALA | 2.3 |
| 4 | d | 328 | TRP | 2.3 |
| 15 | U | 73 | GLN | 2.3 |
| 1 | A | 188 | ALA | 2.3 |
| 1 | a | 188 | ALA | 2.3 |
| 3 | c | 434 | ALA | 2.3 |
| 2 | B | 324 | LEU | 2.3 |
| 13 | O | 24 | ASP | 2.3 |
| 2 | B | 505 | ARG | 2.3 |
| 3 | C | 261 | ARG | 2.3 |
| 1 | A | 198 | HIS | 2.3 |
| 1 | a | 283 | VAL | 2.3 |
| 5 | e | 17 | VAL | 2.3 |
| 1 | A | 324 | ALA | 2.3 |
| 1 | a | 341 | LEU | 2.3 |
| 3 | c | 401 | LEU | 2.3 |
| 2 | B | 497 | GLN | 2.3 |
| 6 | F | 13 | TYR | 2.3 |
| 1 | a | 300 | PHE | 2.3 |
| 2 | b | 363 | PHE | 2.3 |
| 13 | o | 239 | PHE | 2.3 |
| 10 | k | 10 | LYS | 2.3 |
| 19 | z | 47 | TRP | 2.3 |
| 2 | b | 460 | LEU | 2.3 |
| 4 | D | 158 | LEU | 2.3 |
| 4 | D | 291 | LEU | 2.3 |
| 13 | O | 30 | TYR | 2.2 |
| 13 | o | 141 | ASP | 2.3 |
| 2 | B | 325 | PHE | 2.2 |
| 13 | o | 95 | PHE | 2.2 |
| 13 | O | 87 | VAL | 2.2 |
| 1 | A | 211 | PHE | 2.2 |
| 1 | a | 172 | MET | 2.2 |
| 5 | E | 46 | VAL | 2.2 |
| 18 | x | 35 | ASP | 2.2 |
| 4 | D | 197 | HIS | 2.2 |
| 1 | a | 160 | ILE | 2.2 |
| 11 | L | 24[A] | ILE | 2.2 |
| 1 | a | 13 | LEU | 2.2 |
| 3 | C | 433 | LEU | 2.2 |
| 11 | L | 27 | LEU | 2.2 |
| 4 | D | 195 | PRO | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 4 | D | 198 | MET | 2.2 |
| 1 | a | 206 | PHE | 2.2 |
| 11 | L | 35 | PHE | 2.2 |
| 16 | v | 18 | THR | 2.2 |
| 3 | C | 453 | ALA | 2.2 |
| 13 | o | 202 | ALA | 2.2 |
| 13 | o | 194 | LYS | 2.2 |
| 19 | z | 54 | VAL | 2.2 |
| 1 | a | 176 | ILE | 2.2 |
| 1 | a | 298 | ASN | 2.2 |
| 1 | A | 206 | PHE | 2.2 |
| 2 | B | 500 | GLY | 2.2 |
| 4 | D | 174 | GLY | 2.2 |
| 4 | D | 76 | VAL | 2.2 |
| 4 | d | 204 | VAL | 2.2 |
| 15 | U | 59 | GLU | 2.2 |
| 1 | a | 291 | SER | 2.2 |
| 2 | B | 490 | GLN | 2.2 |
| 6 | F | 17 | THR | 2.2 |
| 4 | d | 202 | ALA | 2.2 |
| 1 | A | 249 | VAL | 2.2 |
| 12 | M | 17 | VAL | 2.2 |
| 2 | B | 291 | SER | 2.1 |
| 1 | a | 210 | LEU | 2.1 |
| 1 | a | 229 | GLU | 2.1 |
| 3 | c | 141 | GLU | 2.1 |
| 3 | c | 184 | GLY | 2.1 |
| 3 | C | 152 | LYS | 2.1 |
| 9 | J | 28 | PHE | 2.1 |
| 14 | T | 8 | PHE | 2.1 |
| 3 | C | 256 | PRO | 2.1 |
| 11 | L | 3 | PRO | 2.1 |
| 1 | a | 292 | THR | 2.1 |
| 3 | c | 193 | GLY | 2.1 |
| 18 | X | 3 | ILE | 2.1 |
| 3 | C | 426 | LEU | 2.1 |
| 1 | a | 243 | GLU | 2.1 |
| 4 | d | 296 | TYR | 2.1 |
| 17 | y | 43 | ARG | 2.1 |
| 12 | M | 15 | VAL | 2.1 |
| 19 | z | 34 | ASP | 2.1 |
| 1 | a | 228 | THR | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | a | 224 | ILE | 2.1 |
| 1 | A | 286 | ALA | 2.1 |
| 1 | a | 156 | ALA | 2.1 |
| 2 | b | 304 | ALA | 2.1 |
| 4 | D | 151 | ALA | 2.1 |
| 16 | v | 12 | LEU | 2.1 |
| 3 | C | 155 | ASN | 2.1 |
| 2 | b | 402 | TYR | 2.1 |
| 4 | D | 13 | GLY | 2.1 |
| 6 | f | 17 | THR | 2.1 |
| 3 | c | 262 | ARG | 2.1 |
| 1 | a | 78 | ILE | 2.1 |
| 2 | b | 301 | ALA | 2.1 |
| 2 | b | 120 | LEU | 2.1 |
| 3 | C | 401 | LEU | 2.1 |
| 10 | k | 11 | LEU | 2.1 |
| 5 | E | 59 | GLU | 2.1 |
| 3 | c | 183 | GLY | 2.1 |
| 2 | B | 302 | TRP | 2.1 |
| 3 | c | 112 | PHE | 2.1 |
| 3 | c | 436 | PHE | 2.1 |
| 5 | E | 79 | PHE | 2.1 |
| 5 | e | 37 | PHE | 2.1 |
| 1 | A | 153 | SER | 2.1 |
| 4 | D | 282 | SER | 2.1 |
| 4 | d | 212 | ALA | 2.1 |
| 13 | O | 63 | ALA | 2.1 |
| 4 | D | 321 | LEU | 2.1 |
| 4 | d | 195 | PRO | 2.1 |
| 4 | d | 237 | PRO | 2.1 |
| 2 | B | 349 | LYS | 2.1 |
| 2 | b | 82 | GLY | 2.1 |
| 3 | C | 284 | PHE | 2.0 |
| 4 | d | 191 | TRP | 2.0 |
| 2 | b | 498 | LYS | 2.0 |
| 13 | O | 57 | LYS | 2.0 |
| 9 | j | 4 | GLY | 2.0 |
| 1 | A | 78 | ILE | 2.0 |
| 5 | E | 42 | LEU | 2.0 |
| 11 | L | 25 | LEU | 2.0 |
| 12 | m | 9 | ILE | 2.0 |
| 15 | U | 62 | LEU | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 5 | e | 81 | GLU | 2.0 |
| 2 | b | 223 | GLN | 2.0 |
| 1 | a | 12 | ASN | 2.0 |
| 12 | m | 15 | VAL | 2.0 |
| 3 | C | 434 | ALA | 2.0 |
| 4 | D | 188 | PHE | 2.0 |
| 4 | d | 181 | PHE | 2.0 |
| 5 | E | 77 | GLU | 2.0 |
| 9 | j | 5 | GLY | 2.0 |
| 5 | E | 82 | GLN | 2.0 |
| 19 | z | 12 | LEU | 2.0 |
| 1 | A | 194 | MET | 2.0 |
| 1 | A | 293 | MET | 2.0 |
| 1 | a | 15 | GLU | 2.0 |

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

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|----------------------------|-------|
| 12 | FME | M | 1 | 10/11 | 0.96 | 0.14 | - | 23,34,56,61 | 0 |
| 14 | FME | T | 1 | 10/11 | 0.96 | 0.14 | - | 21,27,45,56 | 0 |
| 12 | FME | m | 1 | 10/11 | 0.93 | 0.15 | - | 25,31,61,62 | 0 |
| 9 | FME | j | 1 | 10/11 | 0.76 | 0.34 | - | 53,71,94,136 | 0 |
| 14 | FME | t | 1 | 10/11 | 0.95 | 0.11 | - | 13,22,33,65 | 0 |
| 8 | FME | i | 1 | 10/11 | 0.97 | 0.15 | - | 23,34,37,42 | 0 |
| 8 | FME | I | 1 | 10/11 | 0.97 | 0.11 | - | 22,34,37,40 | 0 |

5.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-------|----------------------------|-------|
| 29 | UNL | k | 102 | 10/- | 0.58 | 0.61 | 26.13 | 54,83,94,102 | 0 |
| 28 | GOL | b | 633 | 6/6 | 0.95 | 0.29 | 15.05 | 32,54,63,71 | 0 |
| 29 | UNL | j | 103 | 10/- | 0.61 | 0.32 | 12.31 | 44,61,67,73 | 0 |
| 29 | UNL | k | 101 | 32/- | 0.70 | 0.38 | 10.71 | 42,75,105,108 | 0 |
| 30 | LMT | B | 634 | 25/35 | 0.78 | 0.27 | 9.82 | 32,63,105,111 | 0 |
| 28 | GOL | c | 525 | 6/6 | 0.90 | 0.24 | 9.13 | 43,46,61,62 | 0 |
| 28 | GOL | t | 102 | 6/6 | 0.77 | 0.34 | 8.12 | 29,60,65,69 | 0 |
| 27 | SQD | a | 402 | 54/54 | 0.76 | 0.23 | 7.65 | 34,61,79,100 | 0 |
| 30 | LMT | f | 102 | 35/35 | 0.60 | 0.36 | 7.63 | 56,83,109,113 | 0 |
| 28 | GOL | C | 524 | 6/6 | 0.88 | 0.21 | 7.38 | 39,45,57,60 | 0 |
| 36 | DGD | d | 407 | 62/66 | 0.59 | 0.44 | 7.05 | 41,88,117,122 | 0 |
| 28 | GOL | V | 205 | 6/6 | 0.79 | 0.40 | 6.97 | 37,54,59,72 | 0 |
| 28 | GOL | b | 632 | 6/6 | 0.81 | 0.29 | 6.03 | 40,46,68,69 | 0 |
| 32 | PL9 | a | 416 | 55/55 | 0.75 | 0.27 | 5.87 | 50,76,94,95 | 0 |
| 30 | LMT | E | 102 | 35/35 | 0.61 | 0.34 | 5.82 | 43,81,105,107 | 0 |
| 28 | GOL | v | 203 | 6/6 | 0.75 | 0.29 | 5.78 | 50,69,71,78 | 0 |
| 35 | HTG | V | 204 | 19/19 | 0.88 | 0.26 | 5.70 | 40,65,99,175 | 0 |
| 29 | UNL | X | 101 | 10/- | 0.85 | 0.15 | 5.37 | 29,37,41,42 | 0 |
| 35 | HTG | b | 627 | 19/19 | 0.89 | 0.23 | 5.36 | 27,44,80,80 | 0 |
| 30 | LMT | M | 101 | 35/35 | 0.66 | 0.28 | 5.35 | 35,60,79,85 | 0 |
| 29 | UNL | J | 103 | 10/- | 0.71 | 0.43 | 5.30 | 38,53,73,75 | 0 |
| 29 | UNL | I | 101 | 40/- | 0.76 | 0.29 | 5.11 | 27,63,114,119 | 0 |
| 30 | LMT | b | 602 | 25/35 | 0.79 | 0.30 | 5.10 | 22,63,102,106 | 0 |
| 28 | GOL | F | 103 | 6/6 | 0.91 | 0.18 | 4.95 | 52,59,65,68 | 0 |
| 28 | GOL | c | 527 | 6/6 | 0.89 | 0.21 | 4.95 | 36,57,61,63 | 0 |
| 28 | GOL | B | 629 | 6/6 | 0.94 | 0.24 | 4.90 | 24,40,61,78 | 0 |
| 32 | PL9 | A | 419 | 55/55 | 0.68 | 0.29 | 4.81 | 38,66,87,92 | 0 |
| 28 | GOL | B | 628 | 6/6 | 0.88 | 0.23 | 4.66 | 35,46,67,70 | 0 |
| 28 | GOL | B | 627 | 6/6 | 0.85 | 0.22 | 4.59 | 31,35,43,44 | 0 |
| 30 | LMT | m | 103 | 35/35 | 0.65 | 0.27 | 4.55 | 30,60,86,90 | 0 |
| 28 | GOL | a | 413 | 6/6 | 0.79 | 0.23 | 4.18 | 38,67,69,71 | 0 |
| 26 | BCR | B | 619 | 40/40 | 0.90 | 0.16 | 3.93 | 17,25,44,46 | 0 |
| 30 | LMT | a | 417 | 35/35 | 0.76 | 0.42 | 3.77 | 52,76,90,94 | 0 |
| 30 | LMT | a | 401 | 35/35 | 0.82 | 0.19 | 3.67 | 28,61,79,86 | 0 |
| 29 | UNL | i | 101 | 40/- | 0.73 | 0.24 | 3.62 | 36,64,96,108 | 0 |
| 29 | UNL | D | 413 | 40/- | 0.81 | 0.20 | 3.54 | 33,55,105,108 | 0 |
| 24 | CLA | b | 606 | 65/65 | 0.92 | 0.18 | 3.51 | 30,46,82,98 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|-----------------------------|-------|
| 34 | LMG | J | 101 | 51/55 | 0.92 | 0.22 | 3.49 | 20,37,78,86 | 0 |
| 34 | LMG | Z | 101 | 37/55 | 0.62 | 0.32 | 3.46 | 32,81,104,105 | 0 |
| 28 | GOL | A | 414 | 6/6 | 0.78 | 0.19 | 3.45 | 40,60,69,70 | 0 |
| 28 | GOL | V | 208 | 6/6 | 0.86 | 0.27 | 3.35 | 41,56,62,63 | 0 |
| 34 | LMG | j | 101 | 51/55 | 0.90 | 0.19 | 3.33 | 26,39,70,82 | 0 |
| 28 | GOL | A | 413 | 6/6 | 0.86 | 0.19 | 3.31 | 35,38,41,42 | 0 |
| 35 | HTG | C | 523 | 19/19 | 0.75 | 0.29 | 3.28 | 46,75,97,109 | 0 |
| 26 | BCR | d | 405 | 40/40 | 0.87 | 0.16 | 3.27 | 29,35,63,64 | 0 |
| 34 | LMG | z | 101 | 39/55 | 0.72 | 0.39 | 3.25 | 47,74,94,101 | 0 |
| 35 | HTG | c | 523 | 19/19 | 0.83 | 0.31 | 3.08 | 60,84,93,98 | 0 |
| 28 | GOL | f | 104 | 6/6 | 0.92 | 0.22 | 3.07 | 45,51,59,61 | 0 |
| 28 | GOL | a | 412 | 6/6 | 0.91 | 0.16 | 2.97 | 22,37,41,45 | 0 |
| 35 | HTG | D | 411 | 16/19 | 0.69 | 0.25 | 2.86 | 38,100,111,113 | 0 |
| 23 | BCT | a | 418 | 4/4 | 0.95 | 0.17 | 2.84 | 30,33,42,44 | 0 |
| 27 | SQD | l | 101 | 54/54 | 0.68 | 0.25 | 2.77 | 31,67,98,101 | 0 |
| 34 | LMG | C | 501 | 51/55 | 0.84 | 0.19 | 2.62 | 37,54,74,82 | 0 |
| 28 | GOL | B | 625 | 6/6 | 0.92 | 0.14 | 2.61 | 28,43,48,55 | 0 |
| 27 | SQD | A | 416 | 54/54 | 0.80 | 0.18 | 2.59 | 28,52,75,76 | 0 |
| 30 | LMT | A | 417 | 33/35 | 0.85 | 0.19 | 2.55 | 27,65,78,85 | 0 |
| 29 | UNL | d | 413 | 36/- | 0.80 | 0.19 | 2.52 | 35,58,94,99 | 0 |
| 29 | UNL | C | 526 | 34/- | 0.65 | 0.34 | 2.51 | 46,71,82,84 | 0 |
| 24 | CLA | B | 617 | 65/65 | 0.95 | 0.17 | 2.51 | 19,28,88,91 | 0 |
| 26 | BCR | b | 623 | 40/40 | 0.91 | 0.21 | 2.48 | 15,27,40,46 | 0 |
| 34 | LMG | b | 625 | 51/55 | 0.87 | 0.28 | 2.42 | 24,39,59,71 | 0 |
| 24 | CLA | B | 602 | 65/65 | 0.92 | 0.16 | 2.40 | 24,39,82,104 | 0 |
| 35 | HTG | B | 631 | 19/19 | 0.76 | 0.21 | 2.39 | 25,84,104,120 | 0 |
| 28 | GOL | V | 207 | 6/6 | 0.95 | 0.21 | 2.32 | 35,38,41,44 | 0 |
| 39 | MG | j | 102 | 1/1 | 0.98 | 0.16 | 2.30 | 34,34,34,34 | 0 |
| 28 | GOL | B | 626 | 6/6 | 0.89 | 0.21 | 2.24 | 32,37,40,59 | 0 |
| 29 | UNL | d | 412 | 17/- | 0.84 | 0.16 | 2.23 | 31,48,79,85 | 0 |
| 30 | LMT | I | 102 | 35/35 | 0.75 | 0.34 | 2.09 | 59,81,95,100 | 0 |
| 28 | GOL | V | 206 | 6/6 | 0.87 | 0.21 | 2.09 | 21,38,44,48 | 0 |
| 36 | DGD | D | 407 | 62/66 | 0.51 | 0.49 | 2.09 | 44,89,114,119 | 0 |
| 27 | SQD | b | 601 | 54/54 | 0.72 | 0.23 | 1.96 | 36,58,91,95 | 0 |
| 35 | HTG | B | 630 | 19/19 | 0.86 | 0.18 | 1.84 | 30,54,78,81 | 0 |
| 37 | LHG | L | 101 | 49/49 | 0.93 | 0.23 | 1.81 | 15,29,47,58 | 0 |
| 34 | LMG | c | 501 | 51/55 | 0.80 | 0.21 | 1.72 | 39,60,77,85 | 0 |
| 37 | LHG | d | 408 | 49/49 | 0.90 | 0.23 | 1.67 | 26,34,46,50 | 0 |
| 29 | UNL | x | 101 | 10/- | 0.76 | 0.17 | 1.63 | 35,44,57,58 | 0 |
| 27 | SQD | a | 411 | 54/54 | 0.90 | 0.23 | 1.62 | 32,56,75,78 | 0 |
| 29 | UNL | D | 412 | 17/- | 0.91 | 0.16 | 1.59 | 24,45,74,78 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|-----------------------------|-------|
| 37 | LHG | D | 408 | 49/49 | 0.90 | 0.25 | 1.50 | 16,31,43,54 | 0 |
| 34 | LMG | B | 621 | 51/55 | 0.83 | 0.25 | 1.46 | 20,35,52,64 | 0 |
| 28 | GOL | b | 629 | 6/6 | 0.93 | 0.13 | 1.42 | 32,40,48,57 | 0 |
| 32 | PL9 | d | 406 | 55/55 | 0.90 | 0.21 | 1.41 | 16,23,35,47 | 0 |
| 28 | GOL | T | 101 | 6/6 | 0.89 | 0.18 | 1.38 | 35,60,64,65 | 0 |
| 28 | GOL | v | 204 | 6/6 | 0.84 | 0.20 | 1.36 | 47,64,70,92 | 0 |
| 37 | LHG | l | 102 | 49/49 | 0.90 | 0.19 | 1.33 | 19,30,48,57 | 0 |
| 37 | LHG | E | 101 | 42/49 | 0.69 | 0.25 | 1.33 | 38,73,93,103 | 0 |
| 24 | CLA | c | 515 | 65/65 | 0.86 | 0.27 | 1.33 | 37,51,79,88 | 0 |
| 35 | HTG | B | 623 | 19/19 | 0.84 | 0.16 | 1.33 | 29,42,64,71 | 0 |
| 26 | BCR | B | 618 | 40/40 | 0.93 | 0.16 | 1.31 | 15,23,33,41 | 0 |
| 28 | GOL | B | 633 | 6/6 | 0.92 | 0.10 | 1.31 | 27,36,40,41 | 0 |
| 25 | PHO | A | 408 | 64/64 | 0.95 | 0.26 | 1.30 | 16,22,30,32 | 0 |
| 32 | PL9 | D | 406 | 55/55 | 0.91 | 0.24 | 1.28 | 14,23,36,43 | 0 |
| 24 | CLA | A | 409 | 65/65 | 0.95 | 0.12 | 1.28 | 18,27,83,92 | 0 |
| 30 | LMT | b | 626 | 25/35 | 0.69 | 0.30 | 1.23 | 33,67,110,115 | 0 |
| 27 | SQD | f | 101 | 43/54 | 0.82 | 0.30 | 1.23 | 55,82,109,117 | 0 |
| 25 | PHO | d | 403 | 64/64 | 0.94 | 0.21 | 1.21 | 20,25,34,38 | 0 |
| 24 | CLA | B | 611 | 65/65 | 0.95 | 0.12 | 1.21 | 19,26,36,39 | 0 |
| 34 | LMG | C | 521 | 51/55 | 0.79 | 0.23 | 1.21 | 31,74,90,96 | 0 |
| 28 | GOL | b | 630 | 6/6 | 0.92 | 0.16 | 1.15 | 37,48,50,52 | 0 |
| 27 | SQD | A | 411 | 54/54 | 0.90 | 0.21 | 1.14 | 26,51,71,78 | 0 |
| 34 | LMG | C | 520 | 51/55 | 0.77 | 0.28 | 1.13 | 26,61,82,87 | 0 |
| 24 | CLA | c | 510 | 65/65 | 0.93 | 0.16 | 1.13 | 24,31,70,87 | 0 |
| 24 | CLA | A | 405 | 65/65 | 0.94 | 0.26 | 1.12 | 15,18,26,50 | 0 |
| 24 | CLA | b | 612 | 65/65 | 0.93 | 0.21 | 1.12 | 14,23,30,36 | 0 |
| 24 | CLA | D | 403 | 65/65 | 0.96 | 0.28 | 1.10 | 14,19,36,42 | 0 |
| 24 | CLA | A | 406 | 65/65 | 0.95 | 0.26 | 1.09 | 15,19,84,88 | 0 |
| 36 | DGD | C | 519 | 62/66 | 0.93 | 0.23 | 1.08 | 20,30,58,63 | 0 |
| 35 | HTG | d | 411 | 16/19 | 0.67 | 0.27 | 1.05 | 54,73,84,87 | 0 |
| 24 | CLA | C | 509 | 65/65 | 0.91 | 0.16 | 1.01 | 21,29,78,80 | 0 |
| 24 | CLA | d | 402 | 65/65 | 0.96 | 0.24 | 1.00 | 18,22,38,46 | 0 |
| 26 | BCR | D | 405 | 40/40 | 0.91 | 0.14 | 1.00 | 22,31,61,77 | 0 |
| 37 | LHG | D | 409 | 49/49 | 0.94 | 0.18 | 1.00 | 17,27,48,60 | 0 |
| 26 | BCR | b | 622 | 40/40 | 0.91 | 0.17 | 0.98 | 16,26,33,36 | 0 |
| 24 | CLA | a | 407 | 65/65 | 0.94 | 0.26 | 0.98 | 19,25,72,79 | 0 |
| 37 | LHG | d | 409 | 49/49 | 0.93 | 0.14 | 0.97 | 17,26,39,55 | 0 |
| 36 | DGD | h | 102 | 62/66 | 0.87 | 0.17 | 0.97 | 23,35,52,69 | 0 |
| 26 | BCR | Y | 101 | 40/40 | 0.90 | 0.12 | 0.96 | 28,35,49,50 | 0 |
| 34 | LMG | c | 521 | 51/55 | 0.76 | 0.28 | 0.92 | 35,79,91,98 | 0 |
| 36 | DGD | C | 518 | 62/66 | 0.92 | 0.23 | 0.90 | 22,32,76,92 | 0 |
| 35 | HTG | b | 628 | 19/19 | 0.60 | 0.31 | 0.90 | 48,90,106,124 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|-----------------------------|-------|
| 35 | HTG | B | 622 | 19/19 | 0.92 | 0.11 | 0.90 | 26,30,44,56 | 0 |
| 24 | CLA | D | 401 | 65/65 | 0.96 | 0.24 | 0.89 | 13,18,30,32 | 0 |
| 24 | CLA | c | 512 | 65/65 | 0.93 | 0.17 | 0.84 | 26,32,44,59 | 0 |
| 24 | CLA | b | 609 | 65/65 | 0.95 | 0.15 | 0.84 | 16,25,56,66 | 0 |
| 24 | CLA | C | 514 | 65/65 | 0.91 | 0.16 | 0.83 | 32,42,69,72 | 0 |
| 36 | DGD | c | 519 | 62/66 | 0.92 | 0.20 | 0.83 | 26,34,65,72 | 0 |
| 37 | LHG | D | 410 | 49/49 | 0.94 | 0.18 | 0.81 | 20,33,91,95 | 0 |
| 24 | CLA | b | 618 | 65/65 | 0.94 | 0.18 | 0.81 | 15,23,48,56 | 0 |
| 24 | CLA | B | 615 | 65/65 | 0.92 | 0.14 | 0.78 | 15,24,67,78 | 0 |
| 35 | HTG | b | 603 | 19/19 | 0.89 | 0.14 | 0.77 | 34,44,64,67 | 0 |
| 38 | HEM | e | 102 | 43/43 | 0.94 | 0.18 | 0.77 | 38,48,65,84 | 0 |
| 24 | CLA | c | 505 | 65/65 | 0.89 | 0.13 | 0.75 | 29,35,46,60 | 0 |
| 28 | GOL | v | 201 | 6/6 | 0.93 | 0.13 | 0.75 | 31,40,49,50 | 0 |
| 34 | LMG | c | 520 | 51/55 | 0.85 | 0.22 | 0.74 | 33,63,86,88 | 0 |
| 36 | DGD | c | 517 | 62/66 | 0.93 | 0.17 | 0.74 | 23,32,68,76 | 0 |
| 36 | DGD | H | 102 | 62/66 | 0.86 | 0.19 | 0.72 | 20,29,42,58 | 0 |
| 24 | CLA | a | 409 | 65/65 | 0.94 | 0.13 | 0.70 | 20,27,83,88 | 0 |
| 26 | BCR | K | 101 | 40/40 | 0.93 | 0.12 | 0.68 | 27,33,42,47 | 0 |
| 24 | CLA | C | 505 | 65/65 | 0.92 | 0.21 | 0.66 | 22,29,59,77 | 0 |
| 37 | LHG | d | 410 | 49/49 | 0.94 | 0.18 | 0.65 | 23,35,85,104 | 0 |
| 37 | LHG | e | 101 | 42/49 | 0.74 | 0.23 | 0.64 | 49,87,117,128 | 0 |
| 26 | BCR | t | 101 | 40/40 | 0.92 | 0.12 | 0.63 | 15,24,45,49 | 0 |
| 24 | CLA | B | 610 | 65/65 | 0.91 | 0.12 | 0.60 | 19,26,36,40 | 0 |
| 30 | LMT | m | 102 | 35/35 | 0.70 | 0.23 | 0.60 | 16,51,73,79 | 0 |
| 24 | CLA | d | 401 | 65/65 | 0.96 | 0.21 | 0.60 | 16,19,26,42 | 0 |
| 27 | SQD | F | 101 | 43/54 | 0.88 | 0.30 | 0.56 | 39,70,96,105 | 0 |
| 24 | CLA | b | 619 | 65/65 | 0.93 | 0.14 | 0.55 | 15,25,72,77 | 0 |
| 26 | BCR | T | 102 | 40/40 | 0.91 | 0.16 | 0.55 | 14,28,36,42 | 0 |
| 24 | CLA | d | 404 | 65/65 | 0.94 | 0.12 | 0.52 | 27,34,74,81 | 0 |
| 25 | PHO | A | 407 | 64/64 | 0.94 | 0.18 | 0.50 | 15,18,23,28 | 0 |
| 28 | GOL | A | 412 | 6/6 | 0.92 | 0.10 | 0.48 | 29,31,34,37 | 0 |
| 36 | DGD | C | 517 | 62/66 | 0.94 | 0.14 | 0.48 | 22,33,75,83 | 0 |
| 24 | CLA | a | 406 | 65/65 | 0.96 | 0.24 | 0.47 | 17,20,35,51 | 0 |
| 24 | CLA | B | 612 | 65/65 | 0.91 | 0.17 | 0.47 | 15,21,37,41 | 0 |
| 21 | FE2 | a | 403 | 1/1 | 0.99 | 0.11 | 0.46 | 30,30,30,30 | 0 |
| 26 | BCR | k | 103 | 40/40 | 0.86 | 0.17 | 0.46 | 32,40,48,52 | 0 |
| 30 | LMT | M | 102 | 35/35 | 0.78 | 0.20 | 0.44 | 22,50,66,76 | 0 |
| 26 | BCR | C | 515 | 40/40 | 0.92 | 0.12 | 0.43 | 31,42,49,53 | 0 |
| 24 | CLA | b | 616 | 65/65 | 0.93 | 0.13 | 0.41 | 18,26,38,52 | 0 |
| 24 | CLA | B | 607 | 65/65 | 0.93 | 0.11 | 0.41 | 18,26,51,75 | 0 |
| 25 | PHO | a | 408 | 64/64 | 0.95 | 0.18 | 0.40 | 16,21,29,37 | 0 |
| 24 | CLA | b | 611 | 65/65 | 0.94 | 0.10 | 0.40 | 19,31,58,74 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-------|-----------------------------|-------|
| 24 | CLA | b | 614 | 65/65 | 0.89 | 0.12 | 0.37 | 24,31,41,50 | 0 |
| 24 | CLA | C | 507 | 65/65 | 0.92 | 0.16 | 0.36 | 28,42,81,88 | 0 |
| 24 | CLA | B | 604 | 65/65 | 0.91 | 0.12 | 0.35 | 18,25,32,40 | 0 |
| 30 | LMT | D | 402 | 35/35 | 0.68 | 0.25 | 0.34 | 32,75,96,97 | 0 |
| 24 | CLA | b | 610 | 65/65 | 0.95 | 0.11 | 0.33 | 18,24,37,42 | 0 |
| 28 | GOL | V | 201 | 6/6 | 0.92 | 0.11 | 0.31 | 27,29,40,41 | 0 |
| 24 | CLA | B | 614 | 65/65 | 0.94 | 0.17 | 0.30 | 14,22,45,52 | 0 |
| 28 | GOL | v | 205 | 6/6 | 0.93 | 0.17 | 0.28 | 25,39,52,58 | 0 |
| 36 | DGD | c | 518 | 62/66 | 0.90 | 0.19 | 0.28 | 24,35,79,94 | 0 |
| 24 | CLA | b | 621 | 65/65 | 0.92 | 0.15 | 0.27 | 21,35,82,84 | 0 |
| 26 | BCR | c | 516 | 40/40 | 0.91 | 0.12 | 0.26 | 29,36,47,57 | 0 |
| 24 | CLA | b | 608 | 65/65 | 0.94 | 0.11 | 0.24 | 22,29,38,42 | 0 |
| 24 | CLA | B | 608 | 65/65 | 0.92 | 0.18 | 0.24 | 13,20,31,35 | 0 |
| 24 | CLA | B | 616 | 65/65 | 0.95 | 0.11 | 0.22 | 19,28,48,60 | 0 |
| 24 | CLA | c | 514 | 65/65 | 0.90 | 0.18 | 0.22 | 34,43,67,76 | 0 |
| 24 | CLA | c | 507 | 65/65 | 0.91 | 0.12 | 0.22 | 22,31,52,62 | 0 |
| 26 | BCR | H | 101 | 40/40 | 0.88 | 0.13 | 0.19 | 21,32,48,52 | 0 |
| 24 | CLA | C | 504 | 65/65 | 0.92 | 0.12 | 0.17 | 24,33,42,48 | 0 |
| 24 | CLA | b | 617 | 65/65 | 0.94 | 0.11 | 0.17 | 18,26,36,50 | 0 |
| 24 | CLA | C | 510 | 65/65 | 0.95 | 0.11 | 0.16 | 25,32,51,57 | 0 |
| 24 | CLA | c | 506 | 65/65 | 0.90 | 0.17 | 0.15 | 26,33,51,61 | 0 |
| 24 | CLA | C | 511 | 65/65 | 0.93 | 0.15 | 0.15 | 23,29,41,62 | 0 |
| 24 | CLA | c | 503 | 65/65 | 0.93 | 0.11 | 0.13 | 29,34,45,54 | 0 |
| 24 | CLA | b | 607 | 65/65 | 0.92 | 0.12 | 0.10 | 23,30,38,41 | 0 |
| 28 | GOL | b | 631 | 6/6 | 0.91 | 0.11 | 0.09 | 39,46,48,60 | 0 |
| 24 | CLA | B | 605 | 65/65 | 0.94 | 0.14 | 0.08 | 15,22,51,63 | 0 |
| 26 | BCR | y | 101 | 40/40 | 0.92 | 0.12 | 0.06 | 31,40,53,60 | 0 |
| 26 | BCR | b | 624 | 40/40 | 0.92 | 0.10 | 0.05 | 20,32,46,52 | 0 |
| 21 | FE2 | A | 401 | 1/1 | 0.99 | 0.10 | 0.01 | 27,27,27,27 | 0 |
| 26 | BCR | B | 620 | 40/40 | 0.95 | 0.10 | 0.01 | 22,29,42,47 | 0 |
| 24 | CLA | b | 620 | 65/65 | 0.91 | 0.11 | -0.00 | 22,31,51,74 | 0 |
| 24 | CLA | C | 502 | 65/65 | 0.93 | 0.11 | -0.03 | 25,32,47,58 | 0 |
| 24 | CLA | c | 513 | 65/65 | 0.91 | 0.12 | -0.04 | 30,39,50,54 | 0 |
| 24 | CLA | B | 609 | 65/65 | 0.95 | 0.14 | -0.04 | 17,22,32,36 | 0 |
| 24 | CLA | b | 615 | 65/65 | 0.94 | 0.11 | -0.04 | 21,28,39,46 | 0 |
| 24 | CLA | B | 613 | 65/65 | 0.95 | 0.11 | -0.05 | 15,23,32,35 | 0 |
| 24 | CLA | B | 606 | 65/65 | 0.95 | 0.09 | -0.06 | 16,22,34,38 | 0 |
| 24 | CLA | c | 504 | 65/65 | 0.94 | 0.14 | -0.06 | 26,32,45,55 | 0 |
| 24 | CLA | C | 513 | 65/65 | 0.93 | 0.12 | -0.08 | 29,42,67,74 | 0 |
| 38 | HEM | v | 202 | 43/43 | 0.97 | 0.10 | -0.10 | 29,33,40,48 | 0 |
| 24 | CLA | C | 512 | 65/65 | 0.93 | 0.11 | -0.10 | 26,32,41,48 | 0 |
| 24 | CLA | B | 603 | 65/65 | 0.91 | 0.12 | -0.12 | 18,25,32,38 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-------|-----------------------------|-------|
| 24 | CLA | b | 613 | 65/65 | 0.94 | 0.11 | -0.12 | 22,29,38,42 | 0 |
| 26 | BCR | c | 526 | 40/40 | 0.90 | 0.16 | -0.13 | 39,48,59,63 | 0 |
| 24 | CLA | C | 506 | 65/65 | 0.95 | 0.10 | -0.14 | 21,29,45,53 | 0 |
| 26 | BCR | A | 410 | 40/40 | 0.95 | 0.10 | -0.16 | 16,26,33,35 | 0 |
| 24 | CLA | D | 404 | 65/65 | 0.95 | 0.12 | -0.17 | 21,28,73,84 | 0 |
| 28 | GOL | c | 524 | 6/6 | 0.98 | 0.15 | -0.17 | 25,28,30,34 | 0 |
| 23 | BCT | A | 404 | 4/4 | 0.96 | 0.10 | -0.20 | 27,30,39,40 | 0 |
| 26 | BCR | h | 101 | 40/40 | 0.87 | 0.12 | -0.23 | 27,35,46,49 | 0 |
| 35 | HTG | O | 303 | 19/19 | 0.94 | 0.09 | -0.28 | 24,32,47,48 | 0 |
| 28 | GOL | C | 525 | 6/6 | 0.95 | 0.13 | -0.31 | 20,24,26,27 | 0 |
| 26 | BCR | a | 410 | 40/40 | 0.94 | 0.09 | -0.34 | 16,24,31,33 | 0 |
| 24 | CLA | c | 509 | 65/65 | 0.92 | 0.12 | -0.36 | 27,34,49,58 | 0 |
| 24 | CLA | C | 508 | 65/65 | 0.93 | 0.11 | -0.36 | 25,35,48,57 | 0 |
| 38 | HEM | E | 103 | 43/43 | 0.96 | 0.17 | -0.45 | 27,38,50,56 | 0 |
| 24 | CLA | c | 508 | 65/65 | 0.93 | 0.12 | -0.47 | 30,41,65,70 | 0 |
| 26 | BCR | C | 516 | 40/40 | 0.94 | 0.09 | -0.56 | 25,34,43,46 | 0 |
| 24 | CLA | c | 511 | 65/65 | 0.96 | 0.10 | -0.57 | 29,36,49,55 | 0 |
| 24 | CLA | C | 503 | 65/65 | 0.94 | 0.12 | -0.59 | 22,28,40,51 | 0 |
| 22 | CL | a | 405 | 1/1 | 0.99 | 0.12 | -0.92 | 26,26,26,26 | 0 |
| 38 | HEM | V | 203 | 43/43 | 0.97 | 0.08 | -1.09 | 23,26,31,36 | 0 |
| 31 | OEX | A | 418 | 10/10 | 0.99 | 0.09 | -1.53 | 16,23,28,32 | 0 |
| 31 | OEX | a | 415 | 10/10 | 0.99 | 0.11 | -1.57 | 20,24,35,37 | 0 |
| 22 | CL | a | 404 | 1/1 | 1.00 | 0.10 | -2.07 | 20,20,20,20 | 0 |
| 22 | CL | A | 403 | 1/1 | 0.98 | 0.07 | -2.18 | 23,23,23,23 | 0 |
| 22 | CL | A | 402 | 1/1 | 0.99 | 0.10 | -2.49 | 19,19,19,19 | 0 |
| 33 | CA | O | 301 | 1/1 | 0.97 | 0.05 | -2.99 | 56,56,56,56 | 0 |
| 33 | CA | o | 301 | 1/1 | 0.94 | 0.07 | -3.37 | 62,62,62,62 | 0 |
| 33 | CA | c | 502 | 1/1 | 0.96 | 0.04 | -3.41 | 44,44,44,44 | 0 |
| 39 | MG | J | 102 | 1/1 | 0.97 | 0.04 | -3.51 | 28,28,28,28 | 0 |
| 29 | UNL | M | 103 | 10/- | 0.85 | 0.18 | - | 34,42,59,64 | 0 |
| 33 | CA | b | 605 | 1/1 | 0.67 | 0.14 | - | 95,95,95,95 | 0 |
| 22 | CL | V | 202 | 1/1 | 0.95 | 0.05 | - | 63,63,63,63 | 0 |
| 22 | CL | u | 201 | 1/1 | 0.95 | 0.05 | - | 63,63,63,63 | 0 |
| 29 | UNL | B | 632 | 33/- | 0.74 | 0.24 | - | 32,70,105,113 | 0 |
| 29 | UNL | A | 415 | 28/- | 0.62 | 0.31 | - | 55,65,84,90 | 0 |
| 29 | UNL | b | 634 | 33/- | 0.65 | 0.26 | - | 42,71,112,116 | 0 |
| 28 | GOL | T | 103 | 6/6 | 0.69 | 0.31 | - | 63,76,80,81 | 0 |
| 35 | HTG | C | 522 | 19/19 | 0.91 | 0.18 | - | 53,65,89,95 | 0 |
| 35 | HTG | B | 624 | 19/19 | 0.71 | 0.35 | - | 38,95,102,121 | 0 |
| 28 | GOL | O | 302 | 6/6 | 0.68 | 0.18 | - | 52,61,64,70 | 0 |
| 33 | CA | f | 103 | 1/1 | 0.89 | 0.12 | - | 72,72,72,72 | 0 |
| 35 | HTG | c | 522 | 19/19 | 0.86 | 0.17 | - | 63,69,80,85 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|-----------------------------|-------|
| 35 | HTG | b | 604 | 19/19 | 0.62 | 0.19 | - | 50,80,106,112 | 0 |
| 33 | CA | B | 601 | 1/1 | 0.77 | 0.09 | - | 79,79,79,79 | 0 |
| 33 | CA | F | 102 | 1/1 | 0.88 | 0.14 | - | 72,72,72,72 | 0 |
| 29 | UNL | m | 101 | 10/- | 0.86 | 0.25 | - | 37,51,60,62 | 0 |
| 29 | UNL | a | 414 | 30/- | 0.63 | 0.28 | - | 45,65,86,89 | 0 |
| 28 | GOL | B | 635 | 6/6 | 0.22 | 0.43 | - | 82,91,97,98 | 0 |

5.5 Other polymers [i](#)

There are no such residues in this entry.