



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 12, 2018 – 11:21 AM EDT

PDB ID : 4RVY
Title : Serial Time resolved crystallography of Photosystem II using a femtosecond X-ray laser. The S state after two flashes (S3)
Authors : Kupitz, C.; Basu, S.; Grotjohann, I.; Fromme, R.; Zatsepin, N.; Rendek, K.N.; Hunter, M.; Shoeman, R.L.; White, T.A.; Wang, D.; James, D.; Yang, J.-H.; Cobb, D.E.; Reeder, B.; Sierra, R.G.; Liu, H.; Barty, A.; Aquila, A.; Deponte, D.; Kirian, R.; Bari, S.; Bergkamp, J.J.; Beyerlein, K.; Bogan, M.J.; Caleman, C.; Chao, T.-C.; Conrad, C.E.; Davis, K.M.; Fleckenstein, H.; Galli, L.; Hau-Riege, S.P.; Kassemeyer, S.; Laksmono, H.; Liang, M.; Lomb, L.; Marchesini, S.; Martin, A.V.; Messerschmidt, M.; Milathianaki, D.; Nass, K.; Ros, A.; Roy-Chowdhury, S.; Schmidt, K.; Seibert, M.; Steinbrener, J.; Stellato, F.; Yan, L.; Yoon, C.; Moore, T.A.; Moore, A.L.; Pushkar, Y.; Williams, G.J.; Boutet, S.; Doak, R.B.; Weierstall, U.; Frank, M.; Chapman, H.N.; Spence, J.C.H.; Fromme, P.
Deposited on : 2014-11-29
Resolution : 5.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : rb-20031172

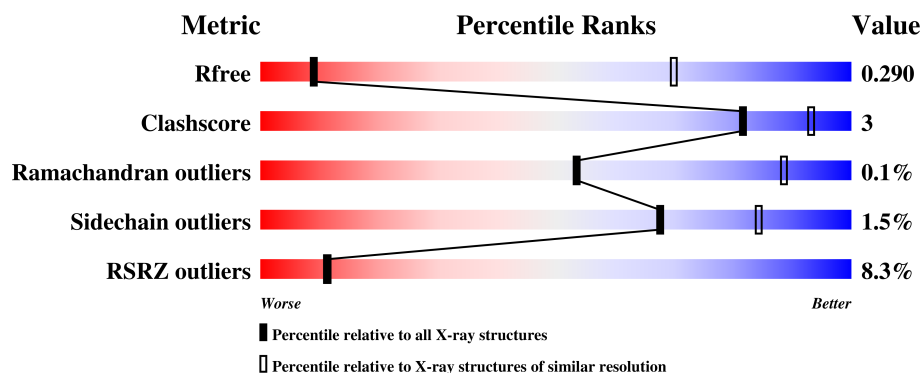
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.50 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 111664 | 1015 (7.20-3.80) |
| Clashscore | 122126 | 1090 (7.20-3.80) |
| Ramachandran outliers | 120053 | 1020 (7.20-3.80) |
| Sidechain outliers | 120020 | 1010 (7.20-3.78) |
| RSRZ outliers | 108989 | 1025 (7.32-3.66) |

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 | 334 | <div> <div>6%</div> <div>94%</div> <div>6%</div> </div> |
| 1 | a | 334 | <div> <div>8%</div> <div>100%</div> </div> |

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Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
 Refmac : 5.8.0158
 CCP4 : 7.0 (Gargrove)
 Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : rb-20031172

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2 | B | 504 | |
| 2 | b | 504 | |
| 3 | C | 461 | |
| 3 | c | 461 | |
| 4 | D | 342 | |
| 4 | d | 342 | |
| 5 | E | 81 | |
| 5 | e | 81 | |
| 6 | F | 34 | |
| 6 | f | 34 | |
| 7 | H | 65 | |
| 7 | h | 65 | |
| 8 | I | 38 | |
| 8 | i | 38 | |
| 9 | J | 40 | |
| 9 | j | 40 | |
| 10 | K | 37 | |
| 10 | k | 37 | |
| 11 | L | 37 | |
| 11 | l | 37 | |
| 12 | M | 34 | |
| 12 | m | 34 | |
| 13 | O | 243 | |
| 13 | o | 243 | |
| 14 | T | 30 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 14 | t | 30 | |
| 15 | U | 97 | |
| 15 | u | 97 | |
| 16 | V | 137 | |
| 16 | v | 137 | |
| 17 | X | 39 | |
| 17 | x | 39 | |
| 18 | Y | 29 | |
| 18 | y | 29 | |
| 19 | Z | 62 | |
| 19 | z | 62 | |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 22 | CLA | A | 603 | X | - | - | X |
| 22 | CLA | A | 604 | X | - | - | X |
| 22 | CLA | A | 607 | X | - | - | - |
| 22 | CLA | B | 602 | X | - | - | X |
| 22 | CLA | B | 603 | X | - | - | - |
| 22 | CLA | B | 604 | X | - | - | - |
| 22 | CLA | B | 605 | X | - | - | - |
| 22 | CLA | B | 606 | X | - | - | - |
| 22 | CLA | B | 607 | X | - | - | X |
| 22 | CLA | B | 608 | X | - | - | - |
| 22 | CLA | B | 609 | X | - | - | - |
| 22 | CLA | B | 610 | X | - | - | - |
| 22 | CLA | B | 611 | X | - | - | - |
| 22 | CLA | B | 612 | X | - | - | - |
| 22 | CLA | B | 613 | X | - | - | - |
| 22 | CLA | B | 614 | X | - | - | - |
| 22 | CLA | B | 615 | X | - | - | - |
| 22 | CLA | B | 616 | X | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 22 | CLA | B | 617 | X | - | - | X |
| 22 | CLA | C | 501 | X | - | - | X |
| 22 | CLA | C | 502 | X | - | - | - |
| 22 | CLA | C | 503 | X | - | - | - |
| 22 | CLA | C | 504 | X | - | - | - |
| 22 | CLA | C | 505 | X | - | - | - |
| 22 | CLA | C | 506 | X | - | - | X |
| 22 | CLA | C | 507 | X | - | - | X |
| 22 | CLA | C | 508 | X | - | - | X |
| 22 | CLA | C | 509 | X | - | - | - |
| 22 | CLA | C | 510 | X | - | - | - |
| 22 | CLA | C | 511 | X | - | - | - |
| 22 | CLA | C | 512 | X | - | - | X |
| 22 | CLA | C | 513 | X | - | - | X |
| 22 | CLA | D | 401 | X | - | - | - |
| 22 | CLA | D | 402 | X | - | - | X |
| 22 | CLA | D | 403 | X | - | - | X |
| 22 | CLA | a | 603 | X | - | - | X |
| 22 | CLA | a | 604 | X | - | - | X |
| 22 | CLA | a | 607 | X | - | - | X |
| 22 | CLA | b | 602 | X | - | - | X |
| 22 | CLA | b | 603 | X | - | - | - |
| 22 | CLA | b | 604 | X | - | - | - |
| 22 | CLA | b | 605 | X | - | - | - |
| 22 | CLA | b | 606 | X | - | - | X |
| 22 | CLA | b | 607 | X | - | - | X |
| 22 | CLA | b | 608 | X | - | - | - |
| 22 | CLA | b | 609 | X | - | - | - |
| 22 | CLA | b | 610 | X | - | - | - |
| 22 | CLA | b | 611 | X | - | - | - |
| 22 | CLA | b | 612 | X | - | - | X |
| 22 | CLA | b | 613 | X | - | - | - |
| 22 | CLA | b | 614 | X | - | - | X |
| 22 | CLA | b | 615 | X | - | - | X |
| 22 | CLA | b | 616 | X | - | - | - |
| 22 | CLA | b | 617 | X | - | - | X |
| 22 | CLA | c | 501 | X | - | - | X |
| 22 | CLA | c | 502 | X | - | - | X |
| 22 | CLA | c | 503 | X | - | - | - |
| 22 | CLA | c | 504 | X | - | - | - |
| 22 | CLA | c | 505 | X | - | - | - |
| 22 | CLA | c | 506 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 22 | CLA | c | 507 | X | - | - | X |
| 22 | CLA | c | 508 | X | - | - | - |
| 22 | CLA | c | 509 | X | - | - | - |
| 22 | CLA | c | 510 | X | - | - | - |
| 22 | CLA | c | 511 | X | - | - | - |
| 22 | CLA | c | 512 | X | - | - | X |
| 22 | CLA | c | 513 | X | - | - | X |
| 22 | CLA | d | 401 | X | - | - | - |
| 22 | CLA | d | 402 | X | - | - | X |
| 22 | CLA | d | 403 | X | - | - | X |
| 23 | PHO | A | 605 | - | - | - | X |
| 24 | BCR | A | 608 | - | - | - | X |
| 24 | BCR | B | 622 | - | - | - | X |
| 24 | BCR | C | 514 | - | - | - | X |
| 24 | BCR | C | 515 | - | - | - | X |
| 24 | BCR | D | 404 | - | - | - | X |
| 24 | BCR | H | 101 | - | - | - | X |
| 24 | BCR | K | 101 | - | - | - | X |
| 24 | BCR | T | 101 | - | - | - | X |
| 24 | BCR | T | 102 | - | - | - | X |
| 24 | BCR | a | 608 | - | - | - | X |
| 24 | BCR | b | 618 | - | - | - | X |
| 24 | BCR | b | 622 | - | - | - | X |
| 24 | BCR | c | 514 | - | - | - | X |
| 24 | BCR | c | 515 | - | - | - | X |
| 24 | BCR | d | 404 | - | - | - | X |
| 24 | BCR | k | 101 | - | - | - | X |
| 24 | BCR | k | 102 | - | - | - | X |
| 24 | BCR | t | 101 | - | - | - | X |
| 25 | SQD | A | 609 | - | - | - | X |
| 25 | SQD | D | 411 | - | - | - | X |
| 25 | SQD | L | 101 | - | - | - | X |
| 25 | SQD | a | 609 | - | - | - | X |
| 25 | SQD | b | 601 | - | - | - | X |
| 25 | SQD | b | 621 | - | - | - | X |
| 25 | SQD | d | 411 | - | - | - | X |
| 26 | CL | a | 610 | - | - | - | X |
| 28 | PL9 | A | 613 | - | - | - | X |
| 28 | PL9 | D | 408 | - | - | - | X |
| 28 | PL9 | a | 613 | - | - | - | X |
| 28 | PL9 | d | 408 | - | - | - | X |
| 29 | LMG | A | 614 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 29 | LMG | C | 519 | - | - | - | X |
| 29 | LMG | C | 520 | - | - | - | X |
| 29 | LMG | D | 406 | - | - | - | X |
| 29 | LMG | Z | 101 | - | - | - | X |
| 29 | LMG | a | 614 | - | - | - | X |
| 29 | LMG | c | 520 | - | - | - | X |
| 29 | LMG | d | 406 | - | - | - | X |
| 29 | LMG | z | 101 | - | - | - | X |
| 30 | CA | B | 621 | - | - | - | X |
| 30 | CA | F | 102 | - | - | - | X |
| 30 | CA | b | 620 | - | - | - | X |
| 30 | CA | f | 102 | - | - | - | X |
| 31 | DGD | C | 518 | - | - | - | X |
| 31 | DGD | D | 410 | - | - | - | X |
| 31 | DGD | d | 410 | - | - | - | X |
| 32 | LHG | D | 409 | - | - | - | X |
| 32 | LHG | E | 101 | - | - | - | X |
| 32 | LHG | d | 409 | - | - | - | X |
| 32 | LHG | e | 101 | - | - | - | X |

2 Entry composition [i](#)

There are 34 unique types of molecules in this entry. The entry contains 49594 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 II protein D1 1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 334 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2620 | 1716 | 431 | 458 | 15 | | | |
| 1 | a | 334 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2620 | 1716 | 431 | 458 | 15 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| A | 286 | ALA | THR | CONFLICT | UNP P0A444 |
| a | 286 | ALA | THR | CONFLICT | UNP P0A444 |

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2 | B | 504 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3969 | 2605 | 661 | 690 | 13 | | | |
| 2 | b | 504 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3969 | 2605 | 661 | 690 | 13 | | | |

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3 | C | 451 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3486 | 2281 | 584 | 608 | 13 | | | |
| 3 | c | 451 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3486 | 2281 | 584 | 608 | 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 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 4 | d | 342 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2726 | 1805 | 445 | 464 | 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 | 0 | 0 |
| | | | 662 | 432 | 107 | 123 | | | | |
| 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 | 34 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 275 | 187 | 45 | 42 | 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 | 0 | 0 |
| | | | 511 | 341 | 82 | 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 |
| | | | 312 | 210 | 48 | 53 | 1 | | | |
| 8 | i | 38 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 312 | 210 | 48 | 53 | 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 | 38 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 272 | 182 | 42 | 47 | 1 | | | |

- 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 | | | |
| 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 | 0 | 0 |
| | | | 304 | 202 | 48 | 53 | 1 | | | |
| 11 | l | 37 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 304 | 202 | 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 | 0 | 0 |
| | | | 267 | 178 | 40 | 48 | 1 | | | |
| 12 | m | 34 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 267 | 178 | 40 | 48 | 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 | 0 | 0 |
| | | | 1865 | 1165 | 315 | 381 | 4 | | | |
| 13 | o | 243 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1865 | 1165 | 315 | 381 | 4 | | | |

- 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 | 0 | 0 |
| | | | 256 | 180 | 36 | 38 | 2 | | | |
| 14 | t | 30 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 256 | 180 | 36 | 38 | 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 | 0 | 0 |
| | | | 1064 | 675 | 177 | 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 X protein.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 17 | X | 39 | Total | C | N | O | 0 | 0 | 0 |
| | | | 287 | 191 | 46 | 50 | | | |
| 17 | x | 39 | Total | C | N | O | 0 | 0 | 0 |
| | | | 287 | 191 | 46 | 50 | | | |

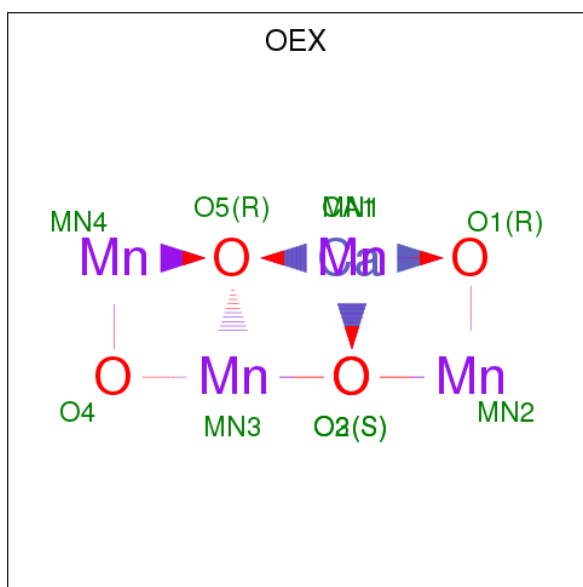
- Molecule 18 is a protein called Photosystem II reaction center protein Ycf12.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 18 | Y | 29 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 215 | 142 | 37 | 33 | 3 | | | |
| 18 | y | 29 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 215 | 142 | 37 | 33 | 3 | | | |

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

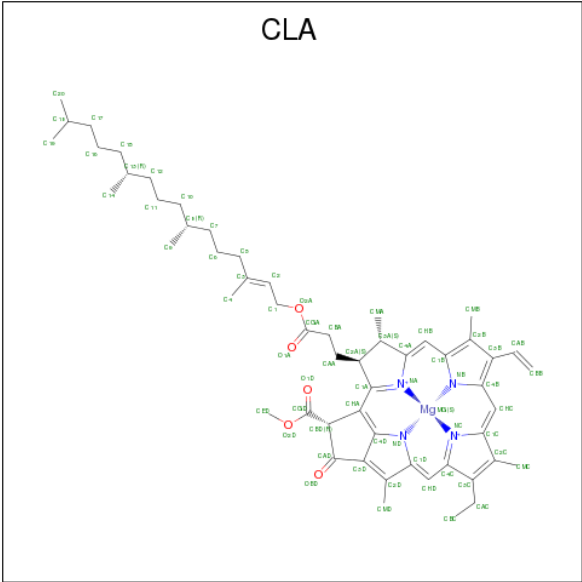


| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 20 | A | 1 | Total | Ca | Mn | O | 0 | 0 |
| | | | 10 | 1 | 4 | 5 | | |
| 20 | a | 1 | Total | Ca | Mn | O | 0 | 0 |
| | | | 10 | 1 | 4 | 5 | | |

- 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 | | |
| 21 | a | 1 | Total | Fe | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 22 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 22 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 22 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 22 | a | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 22 | a | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 22 | a | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 22 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 22 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 22 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 22 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 22 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 22 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 22 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 22 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |

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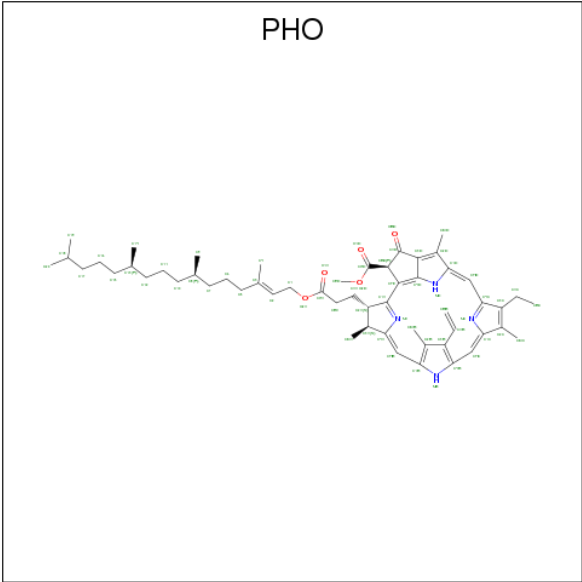
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 22 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |

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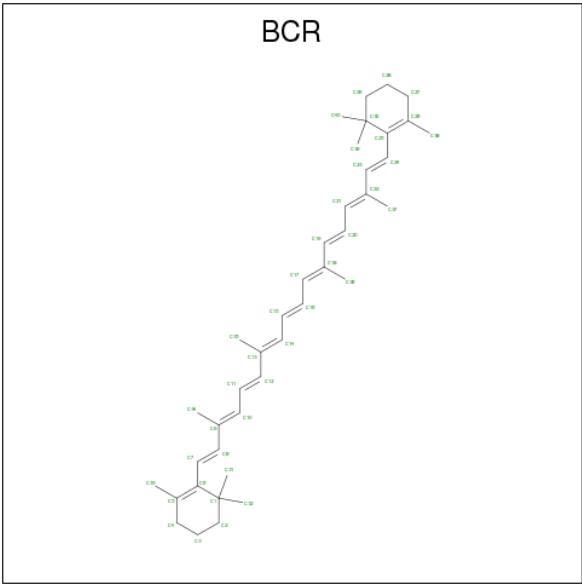
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 22 | c | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 22 | c | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 22 | c | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 22 | c | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 22 | c | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 22 | c | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 22 | D | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 22 | D | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 22 | D | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 22 | d | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 22 | d | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 22 | d | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |

- Molecule 23 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



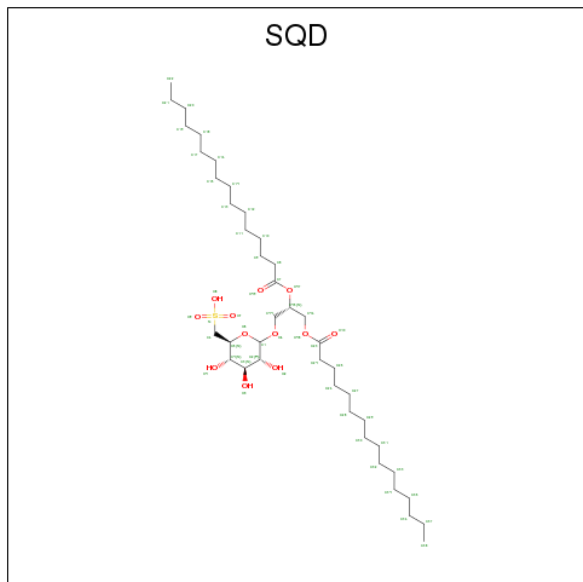
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 23 | A | 1 | Total | C | N | O | 0 | 0 |
| | | | 64 | 55 | 4 | 5 | | |
| 23 | A | 1 | Total | C | N | O | 0 | 0 |
| | | | 64 | 55 | 4 | 5 | | |
| 23 | a | 1 | Total | C | N | O | 0 | 0 |
| | | | 64 | 55 | 4 | 5 | | |
| 23 | a | 1 | Total | C | N | O | 0 | 0 |
| | | | 64 | 55 | 4 | 5 | | |

- Molecule 24 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 24 | A | 1 | Total C 40 40 | 0 | 0 |
| 24 | a | 1 | Total C 40 40 | 0 | 0 |
| 24 | B | 1 | Total C 40 40 | 0 | 0 |
| 24 | B | 1 | Total C 40 40 | 0 | 0 |
| 24 | B | 1 | Total C 40 40 | 0 | 0 |
| 24 | b | 1 | Total C 40 40 | 0 | 0 |
| 24 | b | 1 | Total C 40 40 | 0 | 0 |
| 24 | C | 1 | Total C 40 40 | 0 | 0 |
| 24 | C | 1 | Total C 40 40 | 0 | 0 |
| 24 | c | 1 | Total C 40 40 | 0 | 0 |
| 24 | c | 1 | Total C 40 40 | 0 | 0 |
| 24 | D | 1 | Total C 40 40 | 0 | 0 |
| 24 | d | 1 | Total C 40 40 | 0 | 0 |
| 24 | H | 1 | Total C 40 40 | 0 | 0 |
| 24 | h | 1 | Total C 40 40 | 0 | 0 |
| 24 | K | 1 | Total C 40 40 | 0 | 0 |
| 24 | K | 1 | Total C 40 40 | 0 | 0 |
| 24 | k | 1 | Total C 40 40 | 0 | 0 |
| 24 | k | 1 | Total C 40 40 | 0 | 0 |
| 24 | T | 1 | Total C 40 40 | 0 | 0 |
| 24 | T | 1 | Total C 40 40 | 0 | 0 |
| 24 | t | 1 | Total C 40 40 | 0 | 0 |

- Molecule 25 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).

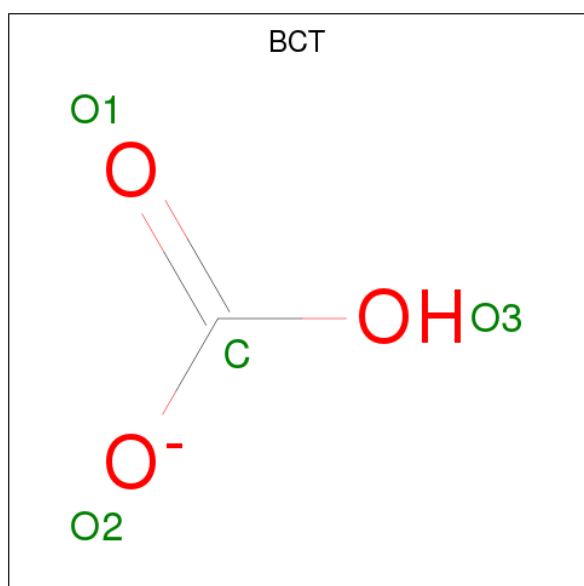


| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 25 | A | 1 | Total | C | O | S | 0 | 0 |
| | | | 54 | 41 | 12 | 1 | | |
| 25 | a | 1 | Total | C | O | S | 0 | 0 |
| | | | 54 | 41 | 12 | 1 | | |
| 25 | B | 1 | Total | C | O | S | 0 | 0 |
| | | | 54 | 41 | 12 | 1 | | |
| 25 | b | 1 | Total | C | O | S | 0 | 0 |
| | | | 54 | 41 | 12 | 1 | | |
| 25 | b | 1 | Total | C | O | S | 0 | 0 |
| | | | 54 | 41 | 12 | 1 | | |
| 25 | D | 1 | Total | C | O | S | 0 | 0 |
| | | | 43 | 30 | 12 | 1 | | |
| 25 | d | 1 | Total | C | O | S | 0 | 0 |
| | | | 43 | 30 | 12 | 1 | | |
| 25 | L | 1 | Total | C | O | S | 0 | 0 |
| | | | 54 | 41 | 12 | 1 | | |
| 25 | l | 1 | Total | C | O | S | 0 | 0 |
| | | | 54 | 41 | 12 | 1 | | |
| 25 | l | 1 | Total | C | O | S | 0 | 0 |
| | | | 54 | 41 | 12 | 1 | | |

- Molecule 26 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

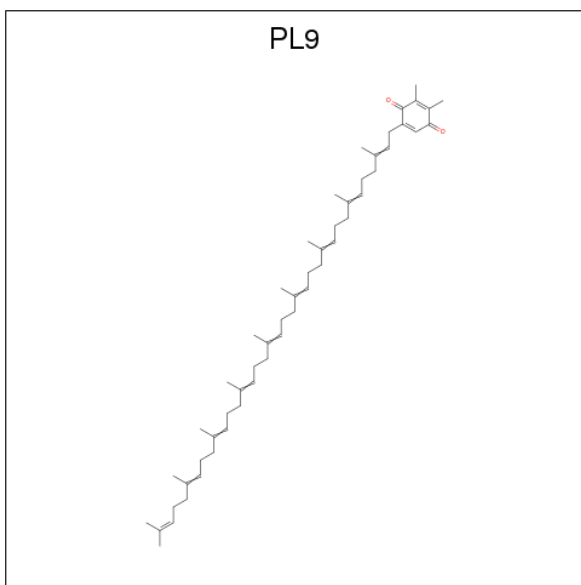
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 26 | A | 2 | Total Cl 2 2 | 0 | 0 |
| 26 | u | 1 | Total Cl 1 1 | 0 | 0 |
| 26 | a | 2 | Total Cl 2 2 | 0 | 0 |
| 26 | U | 1 | Total Cl 1 1 | 0 | 0 |

- Molecule 27 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



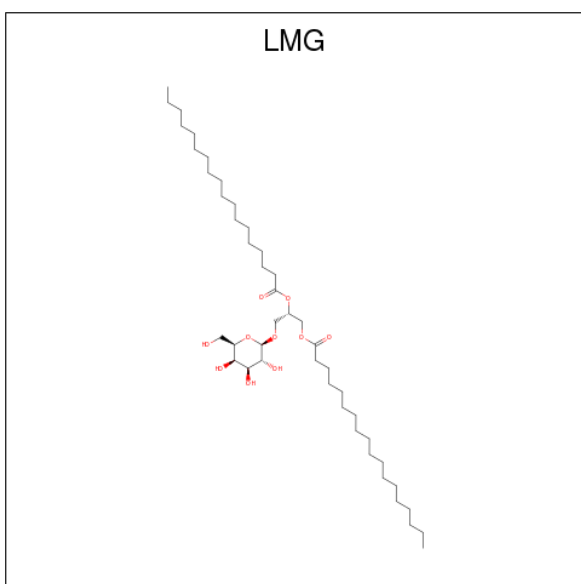
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 27 | A | 1 | Total C O 4 1 3 | 0 | 0 |
| 27 | a | 1 | Total C O 4 1 3 | 0 | 0 |

- Molecule 28 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 |
|-----|-------|----------|-------|----|---|---------|---------|
| 28 | A | 1 | Total | C | O | 0 | 0 |
| | | | 55 | 53 | 2 | | |
| 28 | a | 1 | Total | C | O | 0 | 0 |
| | | | 55 | 53 | 2 | | |
| 28 | D | 1 | Total | C | O | 0 | 0 |
| | | | 55 | 53 | 2 | | |
| 28 | d | 1 | Total | C | O | 0 | 0 |
| | | | 55 | 53 | 2 | | |

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).

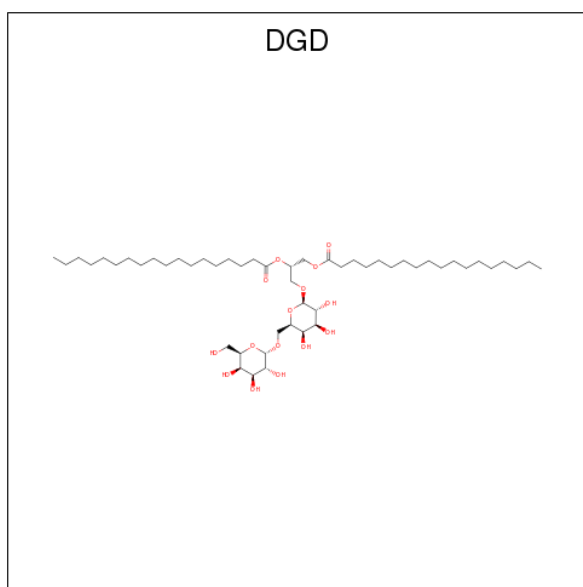


| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------------|---------|---------|
| 29 | A | 1 | Total C O 51 41 10 | 0 | 0 |
| 29 | a | 1 | Total C O 51 41 10 | 0 | 0 |
| 29 | B | 1 | Total C O 51 41 10 | 0 | 0 |
| 29 | b | 1 | Total C O 51 41 10 | 0 | 0 |
| 29 | C | 1 | Total C O 51 41 10 | 0 | 0 |
| 29 | C | 1 | Total C O 51 41 10 | 0 | 0 |
| 29 | c | 1 | Total C O 51 41 10 | 0 | 0 |
| 29 | c | 1 | Total C O 51 41 10 | 0 | 0 |
| 29 | D | 1 | Total C O 51 41 10 | 0 | 0 |
| 29 | d | 1 | Total C O 51 41 10 | 0 | 0 |
| 29 | Z | 1 | Total C O 37 27 10 | 0 | 0 |
| 29 | z | 1 | Total C O 37 27 10 | 0 | 0 |

- Molecule 30 is CALCIUM ION (three-letter code: CA) (formula: Ca).

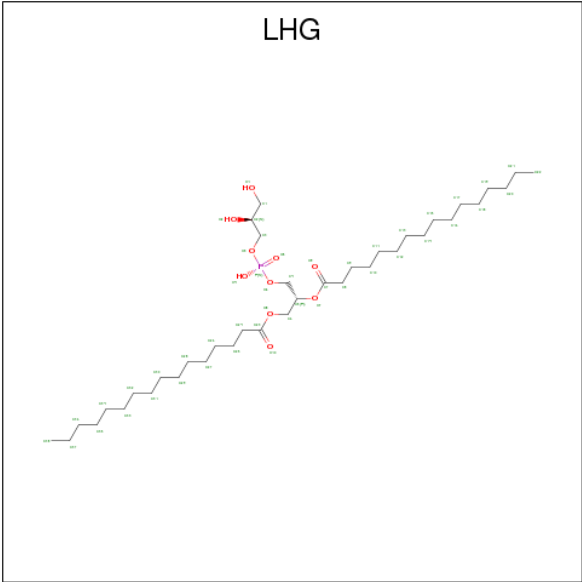
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 30 | B | 1 | Total Ca 1 1 | 0 | 0 |
| 30 | F | 1 | Total Ca 1 1 | 0 | 0 |
| 30 | o | 1 | Total Ca 1 1 | 0 | 0 |
| 30 | O | 1 | Total Ca 1 1 | 0 | 0 |
| 30 | b | 1 | Total Ca 1 1 | 0 | 0 |
| 30 | f | 1 | Total Ca 1 1 | 0 | 0 |

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 31 | C | 1 | Total | C | O | 0 | 0 |
| | | | 62 | 47 | 15 | | |
| 31 | C | 1 | Total | C | O | 0 | 0 |
| | | | 62 | 47 | 15 | | |
| 31 | C | 1 | Total | C | O | 0 | 0 |
| | | | 62 | 47 | 15 | | |
| 31 | c | 1 | Total | C | O | 0 | 0 |
| | | | 62 | 47 | 15 | | |
| 31 | c | 1 | Total | C | O | 0 | 0 |
| | | | 62 | 47 | 15 | | |
| 31 | c | 1 | Total | C | O | 0 | 0 |
| | | | 62 | 47 | 15 | | |
| 31 | D | 1 | Total | C | O | 0 | 0 |
| | | | 62 | 47 | 15 | | |
| 31 | d | 1 | Total | C | O | 0 | 0 |
| | | | 62 | 47 | 15 | | |
| 31 | H | 1 | Total | C | O | 0 | 0 |
| | | | 62 | 47 | 15 | | |
| 31 | h | 1 | Total | C | O | 0 | 0 |
| | | | 62 | 47 | 15 | | |

- Molecule 32 is 1,3-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



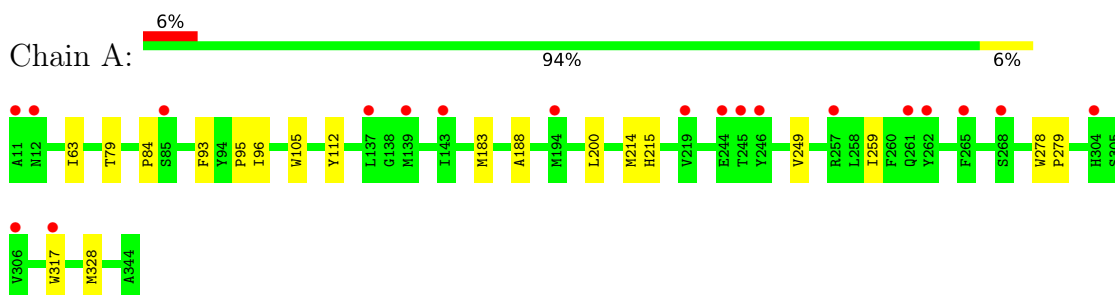
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 32 | D | 1 | Total | C | O | P | 0 | 0 |
| | | | 49 | 38 | 10 | 1 | | |
| 32 | D | 1 | Total | C | O | P | 0 | 0 |
| | | | 49 | 38 | 10 | 1 | | |
| 32 | D | 1 | Total | C | O | P | 0 | 0 |
| | | | 49 | 38 | 10 | 1 | | |
| 32 | d | 1 | Total | C | O | P | 0 | 0 |
| | | | 49 | 38 | 10 | 1 | | |
| 32 | d | 1 | Total | C | O | P | 0 | 0 |
| | | | 49 | 38 | 10 | 1 | | |
| 32 | d | 1 | Total | C | O | P | 0 | 0 |
| | | | 49 | 38 | 10 | 1 | | |
| 32 | E | 1 | Total | C | O | P | 0 | 0 |
| | | | 42 | 31 | 10 | 1 | | |
| 32 | e | 1 | Total | C | O | P | 0 | 0 |
| | | | 42 | 31 | 10 | 1 | | |
| 32 | L | 1 | Total | C | O | P | 0 | 0 |
| | | | 49 | 38 | 10 | 1 | | |
| 32 | l | 1 | Total | C | O | P | 0 | 0 |
| | | | 49 | 38 | 10 | 1 | | |

- Molecule 33 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).

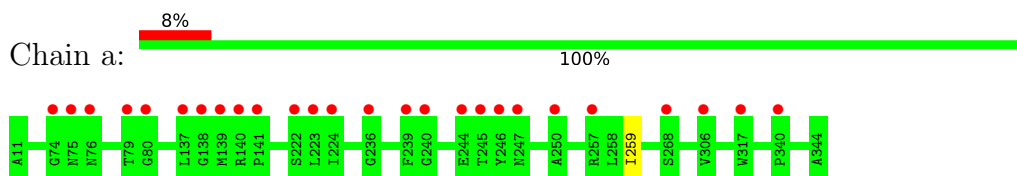
3 Residue-property plots [i](#)

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.

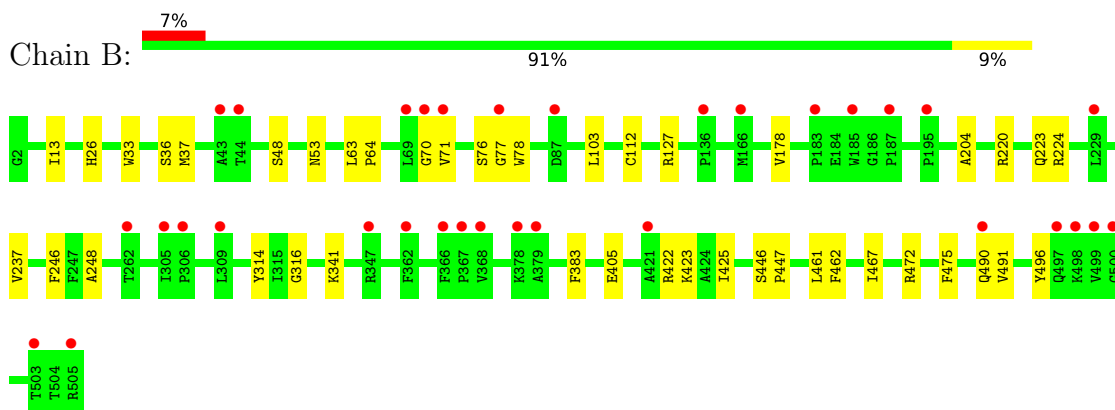
- Molecule 1: Photosystem II protein D1 1



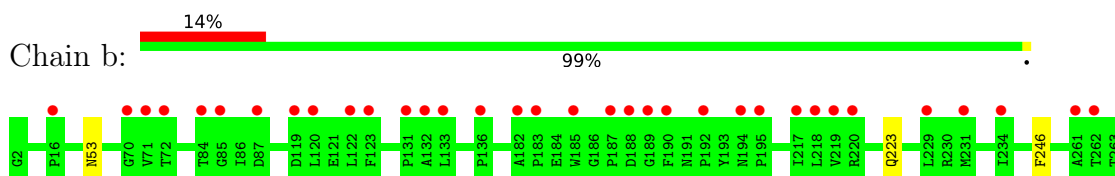
- Molecule 1: Photosystem II protein D1 1

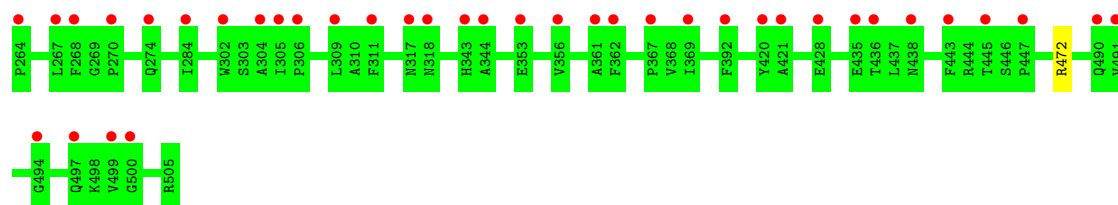


- Molecule 2: Photosystem II CP47 reaction center protein

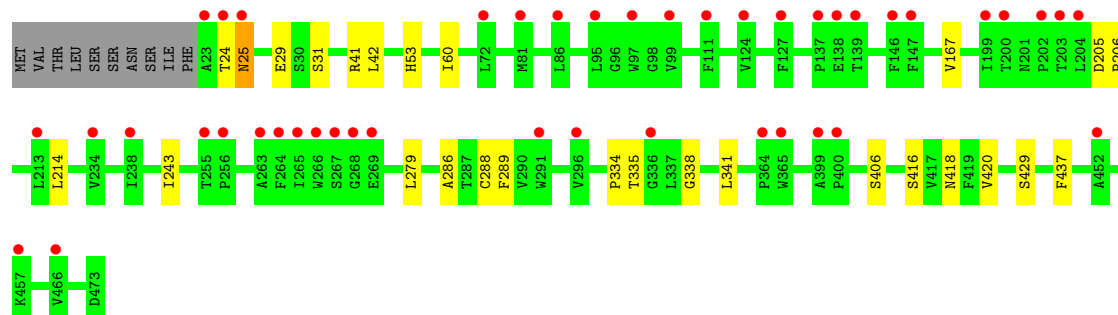


- Molecule 2: Photosystem II CP47 reaction center protein

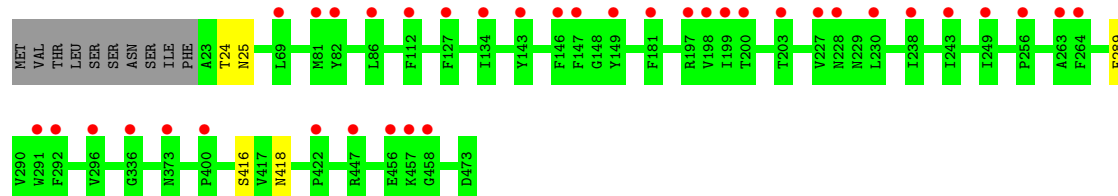




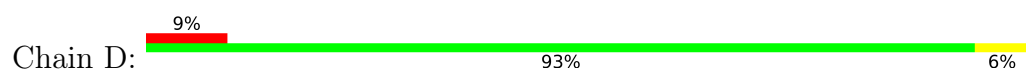
- Molecule 3: Photosystem II CP43 reaction center protein



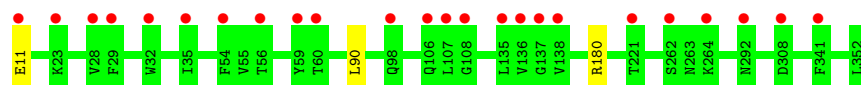
- Molecule 3: Photosystem II CP43 reaction center protein



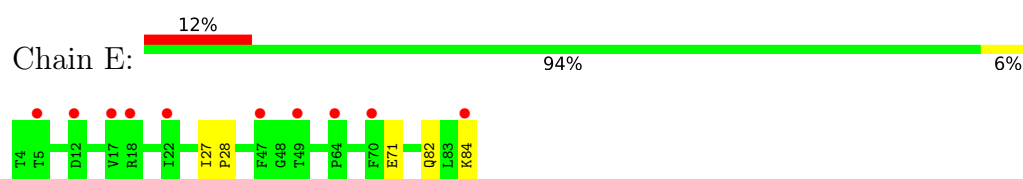
- Molecule 4: Photosystem II D2 protein



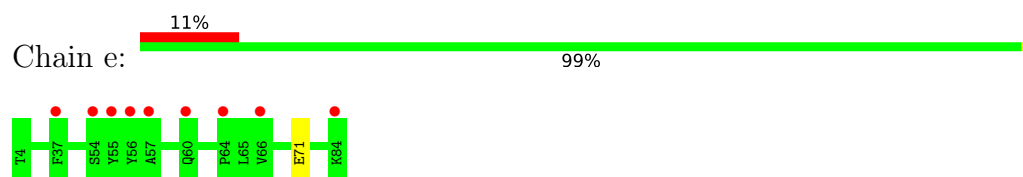
- Molecule 4: Photosystem II D2 protein



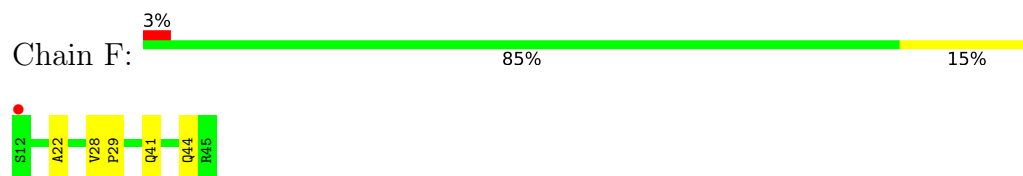
- Molecule 5: Cytochrome b559 subunit alpha



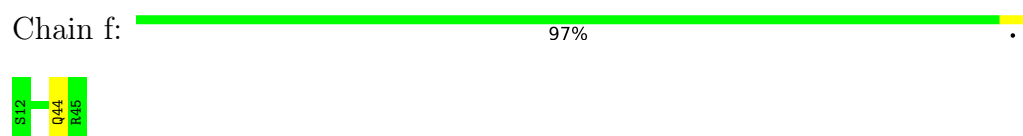
- Molecule 5: Cytochrome b559 subunit alpha



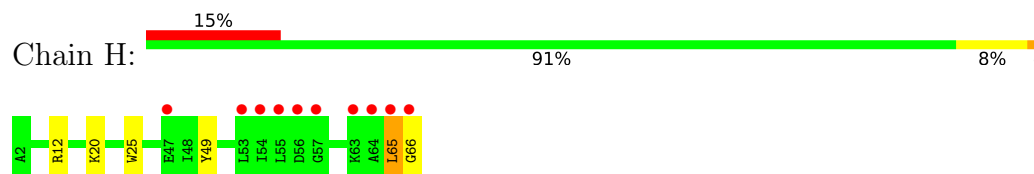
- Molecule 6: Cytochrome b559 subunit beta



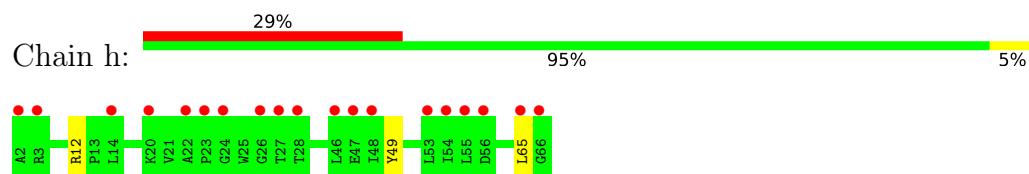
- Molecule 6: Cytochrome b559 subunit beta



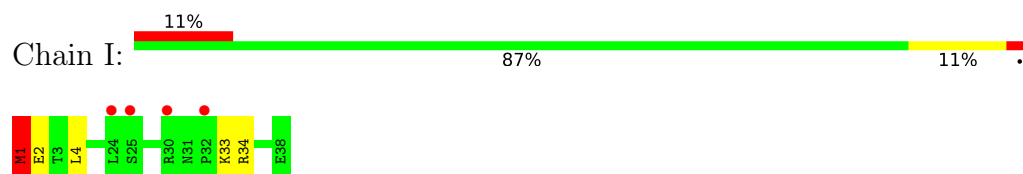
- Molecule 7: Photosystem II reaction center protein H



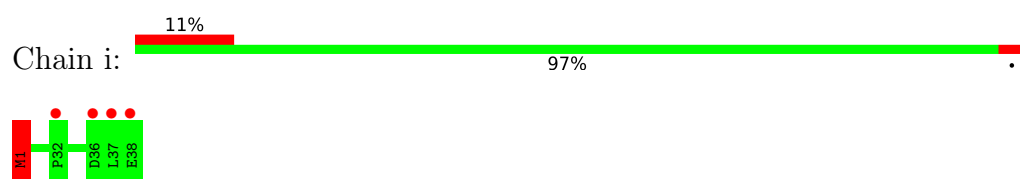
- Molecule 7: Photosystem II reaction center protein H



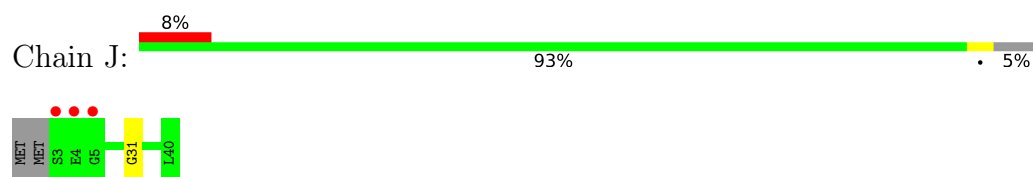
- Molecule 8: Photosystem II reaction center protein I



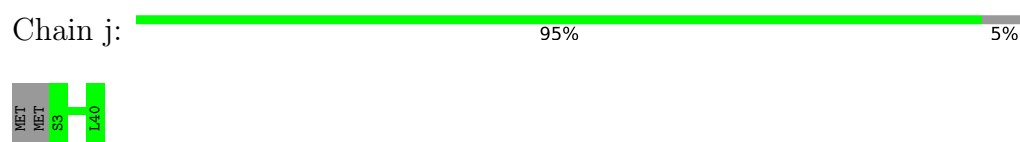
- Molecule 8: Photosystem II reaction center protein I



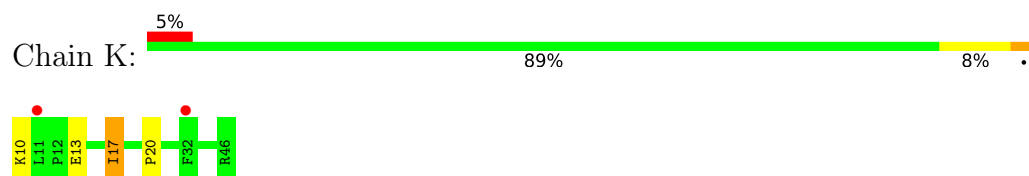
- Molecule 9: Photosystem II reaction center protein J



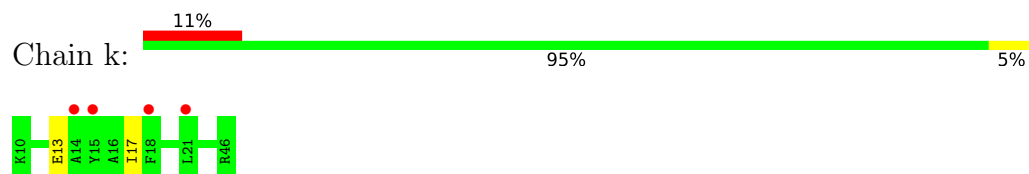
- Molecule 9: Photosystem II reaction center protein J



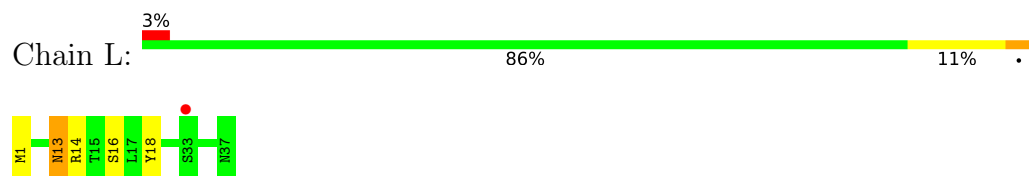
- Molecule 10: Photosystem II reaction center protein K



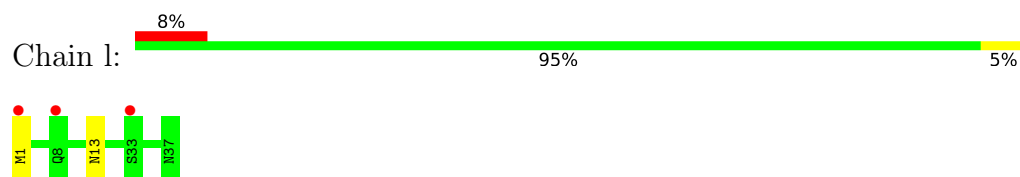
- Molecule 10: Photosystem II reaction center protein K



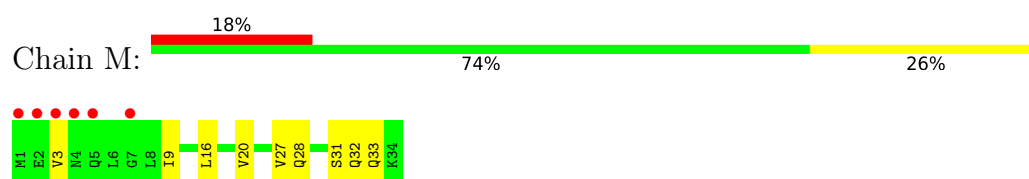
- Molecule 11: Photosystem II reaction center protein L



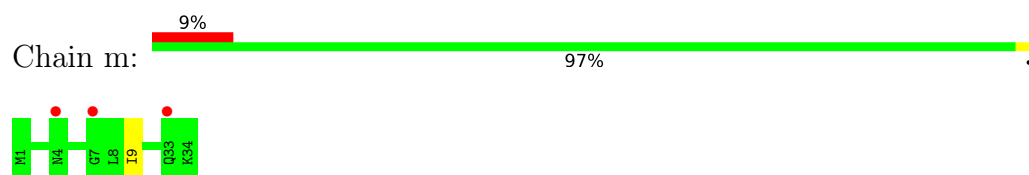
- Molecule 11: Photosystem II reaction center protein L



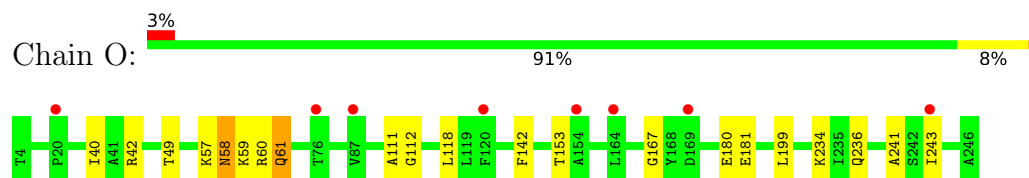
- Molecule 12: Photosystem II reaction center protein M



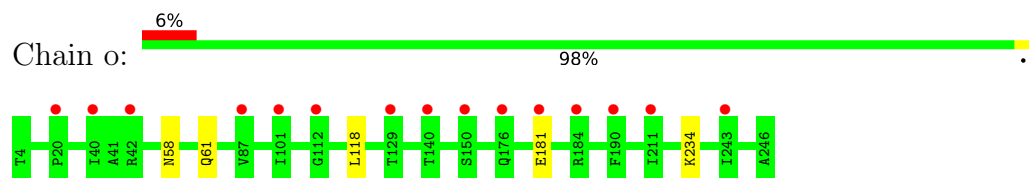
- Molecule 12: Photosystem II reaction center protein M



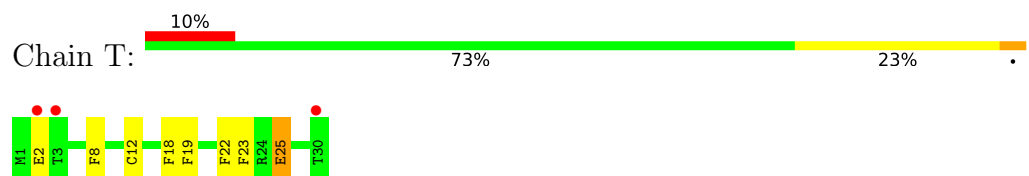
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



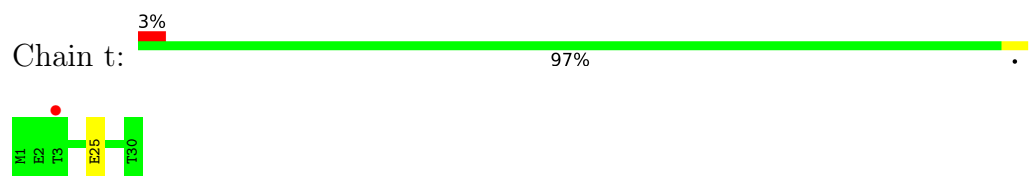
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



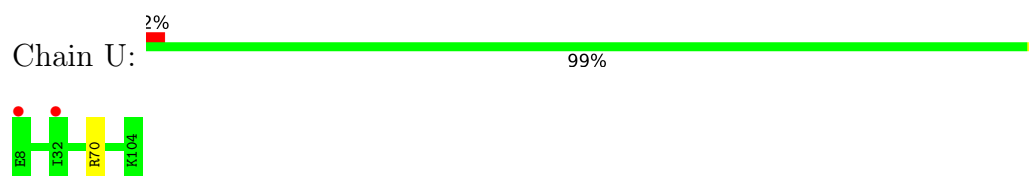
- Molecule 14: Photosystem II reaction center protein T



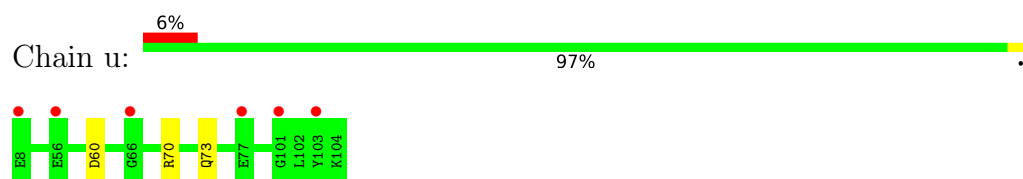
- Molecule 14: Photosystem II reaction center protein T



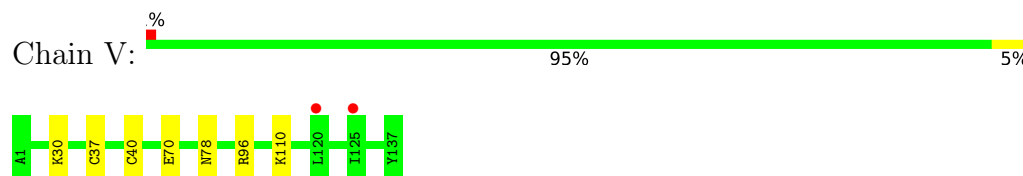
- Molecule 15: Photosystem II 12 kDa extrinsic protein



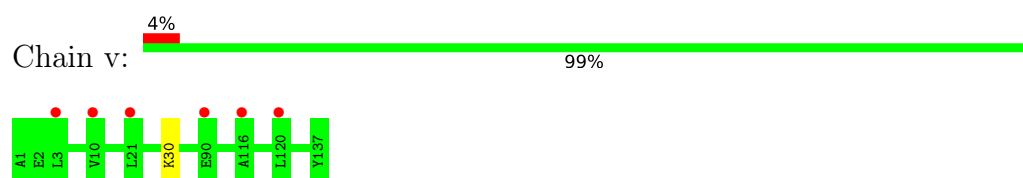
- Molecule 15: Photosystem II 12 kDa extrinsic protein



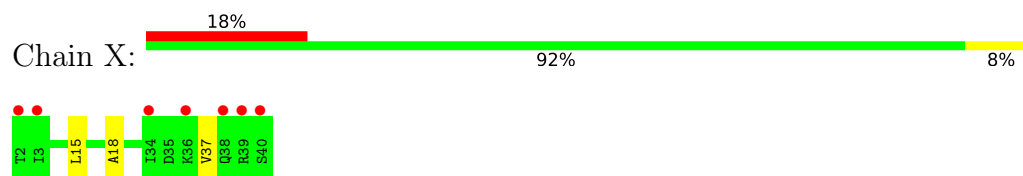
- Molecule 16: Cytochrome c-550



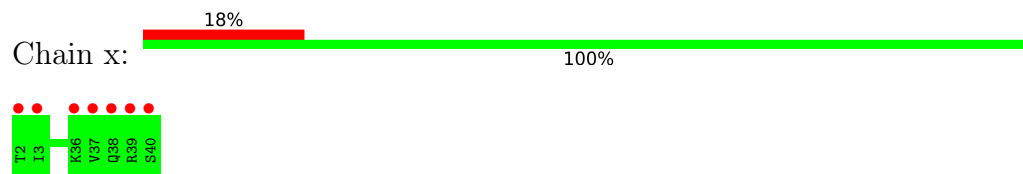
- Molecule 16: Cytochrome c-550



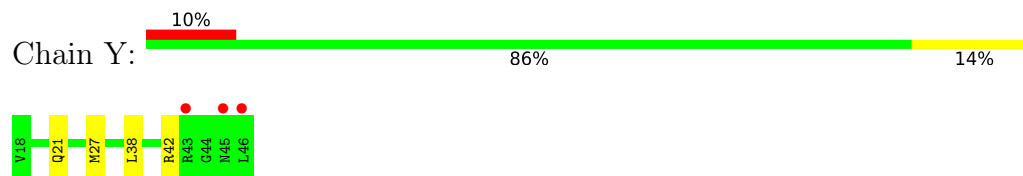
- Molecule 17: Photosystem II reaction center X protein



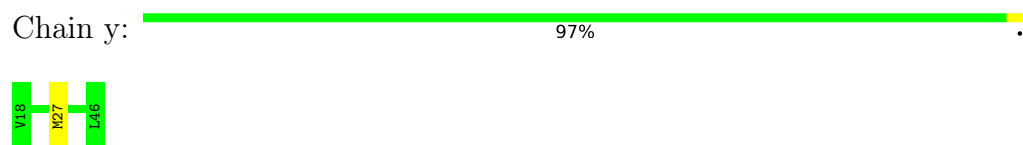
- Molecule 17: Photosystem II reaction center X protein



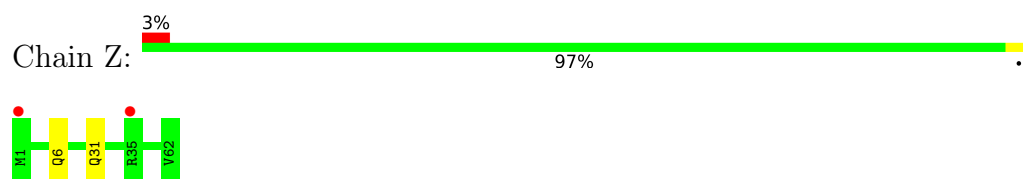
- Molecule 18: Photosystem II reaction center protein Ycf12



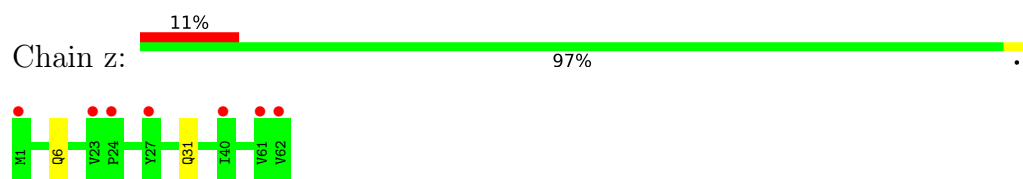
- Molecule 18: Photosystem II reaction center protein Ycf12



- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 136.61Å 228.09Å 308.68Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 102.30 – 5.50 102.29 – 5.50 | Depositor EDS |
| % Data completeness (in resolution range) | 99.9 (102.30-5.50) 100.0 (102.29-5.50) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.75 (at 5.42Å) | Xtriage |
| Refinement program | PHENIX (phenix.refine: 1.8.2_1336) | Depositor |
| R, R_{free} | 0.281 , 0.291 0.281 , 0.290 | Depositor DCC |
| R_{free} test set | 1626 reflections (5.06%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 357.8 | Xtriage |
| Anisotropy | 0.241 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.33 , 61.9 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.87 | EDS |
| Total number of atoms | 49594 | wwPDB-VP |
| Average B, all atoms (Å ²) | 32.0 | wwPDB-VP |

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

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, MG, OEX, PHO, DGD, CL, CA, CLA, PL9, FE2, BCT, HEM, SQD, 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 | 0/2705 | 0.55 | 0/3689 |
| 1 | a | 0.53 | 0/2705 | 0.55 | 0/3689 |
| 2 | B | 0.50 | 0/4109 | 0.54 | 0/5600 |
| 2 | b | 0.50 | 0/4109 | 0.54 | 0/5600 |
| 3 | C | 0.46 | 0/3599 | 0.51 | 0/4900 |
| 3 | c | 0.46 | 0/3599 | 0.51 | 0/4900 |
| 4 | D | 0.53 | 0/2821 | 0.55 | 0/3844 |
| 4 | d | 0.53 | 0/2821 | 0.55 | 0/3844 |
| 5 | E | 0.43 | 0/681 | 0.51 | 0/928 |
| 5 | e | 0.43 | 0/681 | 0.51 | 0/928 |
| 6 | F | 0.49 | 0/284 | 0.45 | 0/387 |
| 6 | f | 0.49 | 0/284 | 0.45 | 0/387 |
| 7 | H | 0.47 | 0/524 | 0.50 | 0/713 |
| 7 | h | 0.47 | 0/524 | 0.50 | 0/713 |
| 8 | I | 2.22 | 2/319 (0.6%) | 1.25 | 4/429 (0.9%) |
| 8 | i | 2.22 | 2/319 (0.6%) | 1.25 | 4/429 (0.9%) |
| 9 | J | 0.46 | 0/278 | 0.43 | 0/376 |
| 9 | j | 0.46 | 0/278 | 0.43 | 0/376 |
| 10 | K | 0.42 | 0/303 | 0.50 | 0/416 |
| 10 | k | 0.43 | 0/303 | 0.50 | 0/416 |
| 11 | L | 0.55 | 0/311 | 0.51 | 0/422 |
| 11 | l | 0.55 | 0/311 | 0.51 | 0/422 |
| 12 | M | 0.47 | 0/270 | 0.59 | 0/367 |
| 12 | m | 0.47 | 0/270 | 0.59 | 0/367 |
| 13 | O | 0.45 | 0/1896 | 0.58 | 0/2571 |
| 13 | o | 0.45 | 0/1896 | 0.58 | 0/2571 |
| 14 | T | 0.53 | 0/265 | 0.54 | 0/359 |
| 14 | t | 0.53 | 0/265 | 0.54 | 0/359 |
| 15 | U | 0.46 | 0/785 | 0.55 | 0/1064 |
| 15 | u | 0.46 | 0/785 | 0.55 | 0/1064 |
| 16 | V | 0.47 | 0/1085 | 0.53 | 0/1473 |
| 16 | v | 0.47 | 0/1085 | 0.53 | 0/1473 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 17 | X | 0.43 | 0/290 | 0.47 | 0/392 |
| 17 | x | 0.43 | 0/290 | 0.47 | 0/392 |
| 18 | Y | 0.41 | 0/216 | 0.45 | 0/289 |
| 18 | y | 0.41 | 0/216 | 0.45 | 0/289 |
| 19 | Z | 0.41 | 0/490 | 0.45 | 0/669 |
| 19 | z | 0.41 | 0/490 | 0.45 | 0/669 |
| All | All | 0.55 | 4/42462 (0.0%) | 0.55 | 8/57776 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 8 | I | 1 | 1 |
| 8 | i | 1 | 1 |
| All | All | 2 | 2 |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 8 | i | 1 | MET | N-CA | 36.97 | 2.20 | 1.46 |
| 8 | I | 1 | MET | N-CA | 36.95 | 2.20 | 1.46 |
| 8 | I | 1 | MET | CA-C | 12.27 | 1.84 | 1.52 |
| 8 | i | 1 | MET | CA-C | 12.26 | 1.84 | 1.52 |

All (8) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 8 | i | 1 | MET | N-CA-CB | -17.88 | 78.41 | 110.60 |
| 8 | I | 1 | MET | N-CA-CB | -17.86 | 78.45 | 110.60 |
| 8 | I | 1 | MET | N-CA-C | -12.99 | 75.92 | 111.00 |
| 8 | i | 1 | MET | N-CA-C | -12.98 | 75.94 | 111.00 |
| 8 | I | 1 | MET | CA-C-N | -6.32 | 103.29 | 117.20 |
| 8 | i | 1 | MET | CA-C-N | -6.30 | 103.33 | 117.20 |
| 8 | I | 1 | MET | CB-CA-C | -6.21 | 97.97 | 110.40 |
| 8 | i | 1 | MET | CB-CA-C | -6.21 | 97.97 | 110.40 |

All (2) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 8 | I | 1 | MET | CA |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 8 | i | 1 | MET | CA |

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 8 | I | 1 | MET | Mainchain |
| 8 | i | 1 | MET | Mainchain |

5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 2620 | 0 | 2517 | 16 | 0 |
| 1 | a | 2620 | 0 | 2517 | 0 | 0 |
| 2 | B | 3969 | 0 | 3828 | 47 | 0 |
| 2 | b | 3969 | 0 | 3828 | 0 | 0 |
| 3 | C | 3486 | 0 | 3407 | 20 | 0 |
| 3 | c | 3486 | 0 | 3407 | 0 | 0 |
| 4 | D | 2726 | 0 | 2627 | 21 | 0 |
| 4 | d | 2726 | 0 | 2627 | 0 | 0 |
| 5 | E | 662 | 0 | 648 | 3 | 0 |
| 5 | e | 662 | 0 | 648 | 0 | 0 |
| 6 | F | 275 | 0 | 282 | 3 | 0 |
| 6 | f | 275 | 0 | 282 | 0 | 0 |
| 7 | H | 511 | 0 | 532 | 4 | 0 |
| 7 | h | 511 | 0 | 532 | 0 | 0 |
| 8 | I | 312 | 0 | 329 | 16 | 0 |
| 8 | i | 312 | 0 | 329 | 0 | 0 |
| 9 | J | 272 | 0 | 279 | 1 | 0 |
| 9 | j | 272 | 0 | 279 | 0 | 0 |
| 10 | K | 293 | 0 | 305 | 5 | 0 |
| 10 | k | 293 | 0 | 305 | 0 | 0 |
| 11 | L | 304 | 0 | 316 | 6 | 0 |
| 11 | l | 304 | 0 | 316 | 0 | 0 |
| 12 | M | 267 | 0 | 288 | 21 | 0 |
| 12 | m | 267 | 0 | 287 | 0 | 0 |
| 13 | O | 1865 | 0 | 1838 | 21 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 13 | o | 1865 | 0 | 1838 | 0 | 0 |
| 14 | T | 256 | 0 | 262 | 12 | 0 |
| 14 | t | 256 | 0 | 262 | 0 | 0 |
| 15 | U | 774 | 0 | 773 | 0 | 0 |
| 15 | u | 774 | 0 | 773 | 0 | 7 |
| 16 | V | 1064 | 0 | 1073 | 10 | 7 |
| 16 | v | 1064 | 0 | 1073 | 0 | 0 |
| 17 | X | 287 | 0 | 317 | 3 | 0 |
| 17 | x | 287 | 0 | 317 | 0 | 0 |
| 18 | Y | 215 | 0 | 246 | 2 | 0 |
| 18 | y | 215 | 0 | 246 | 0 | 0 |
| 19 | Z | 479 | 0 | 516 | 0 | 0 |
| 19 | z | 479 | 0 | 516 | 0 | 0 |
| 20 | A | 10 | 0 | 0 | 0 | 0 |
| 20 | a | 10 | 0 | 0 | 0 | 0 |
| 21 | A | 1 | 0 | 0 | 0 | 0 |
| 21 | a | 1 | 0 | 0 | 0 | 0 |
| 22 | A | 195 | 0 | 216 | 10 | 0 |
| 22 | B | 1040 | 0 | 1152 | 32 | 0 |
| 22 | C | 845 | 0 | 936 | 29 | 0 |
| 22 | D | 195 | 0 | 216 | 8 | 0 |
| 22 | a | 195 | 0 | 216 | 0 | 0 |
| 22 | b | 1040 | 0 | 1152 | 0 | 0 |
| 22 | c | 845 | 0 | 936 | 0 | 0 |
| 22 | d | 195 | 0 | 216 | 0 | 0 |
| 23 | A | 128 | 0 | 148 | 6 | 0 |
| 23 | a | 128 | 0 | 148 | 0 | 0 |
| 24 | A | 40 | 0 | 48 | 1 | 0 |
| 24 | B | 120 | 0 | 140 | 8 | 0 |
| 24 | C | 80 | 0 | 93 | 0 | 0 |
| 24 | D | 40 | 0 | 48 | 3 | 0 |
| 24 | H | 40 | 0 | 46 | 1 | 0 |
| 24 | K | 80 | 0 | 93 | 1 | 0 |
| 24 | T | 80 | 0 | 95 | 9 | 0 |
| 24 | a | 40 | 0 | 48 | 0 | 0 |
| 24 | b | 80 | 0 | 92 | 0 | 0 |
| 24 | c | 80 | 0 | 93 | 0 | 0 |
| 24 | d | 40 | 0 | 48 | 0 | 0 |
| 24 | h | 40 | 0 | 46 | 0 | 0 |
| 24 | k | 80 | 0 | 93 | 0 | 0 |
| 24 | t | 40 | 0 | 47 | 0 | 0 |
| 25 | A | 54 | 0 | 78 | 2 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 25 | B | 54 | 0 | 78 | 4 | 0 |
| 25 | D | 43 | 0 | 53 | 0 | 0 |
| 25 | L | 54 | 0 | 34 | 5 | 0 |
| 25 | a | 54 | 0 | 78 | 0 | 0 |
| 25 | b | 108 | 0 | 112 | 0 | 0 |
| 25 | d | 43 | 0 | 53 | 0 | 0 |
| 25 | l | 108 | 0 | 59 | 0 | 0 |
| 26 | A | 2 | 0 | 0 | 0 | 0 |
| 26 | U | 1 | 0 | 0 | 0 | 0 |
| 26 | a | 2 | 0 | 0 | 0 | 0 |
| 26 | u | 1 | 0 | 0 | 0 | 0 |
| 27 | A | 4 | 0 | 0 | 0 | 0 |
| 27 | a | 4 | 0 | 0 | 0 | 0 |
| 28 | A | 55 | 0 | 80 | 8 | 0 |
| 28 | D | 55 | 0 | 80 | 0 | 0 |
| 28 | a | 55 | 0 | 80 | 0 | 0 |
| 28 | d | 55 | 0 | 80 | 0 | 0 |
| 29 | A | 51 | 0 | 72 | 3 | 0 |
| 29 | B | 51 | 0 | 72 | 3 | 0 |
| 29 | C | 102 | 0 | 144 | 1 | 0 |
| 29 | D | 51 | 0 | 72 | 2 | 0 |
| 29 | Z | 37 | 0 | 44 | 1 | 0 |
| 29 | a | 51 | 0 | 72 | 0 | 0 |
| 29 | b | 51 | 0 | 72 | 0 | 0 |
| 29 | c | 102 | 0 | 144 | 0 | 0 |
| 29 | d | 51 | 0 | 72 | 0 | 0 |
| 29 | z | 37 | 0 | 44 | 0 | 0 |
| 30 | B | 1 | 0 | 0 | 0 | 0 |
| 30 | F | 1 | 0 | 0 | 0 | 0 |
| 30 | O | 1 | 0 | 0 | 0 | 0 |
| 30 | b | 1 | 0 | 0 | 0 | 0 |
| 30 | f | 1 | 0 | 0 | 0 | 0 |
| 30 | o | 1 | 0 | 0 | 0 | 0 |
| 31 | C | 186 | 0 | 246 | 5 | 0 |
| 31 | D | 62 | 0 | 82 | 3 | 0 |
| 31 | H | 62 | 0 | 82 | 1 | 0 |
| 31 | c | 186 | 0 | 246 | 0 | 0 |
| 31 | d | 62 | 0 | 82 | 0 | 0 |
| 31 | h | 62 | 0 | 82 | 0 | 0 |
| 32 | D | 147 | 0 | 222 | 13 | 0 |
| 32 | E | 42 | 0 | 57 | 2 | 0 |
| 32 | L | 49 | 0 | 74 | 1 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 32 | d | 147 | 0 | 222 | 0 | 0 |
| 32 | e | 42 | 0 | 57 | 0 | 0 |
| 32 | l | 49 | 0 | 74 | 0 | 0 |
| 33 | F | 43 | 0 | 30 | 1 | 0 |
| 33 | V | 43 | 0 | 30 | 9 | 0 |
| 33 | f | 43 | 0 | 30 | 0 | 0 |
| 33 | v | 43 | 0 | 30 | 0 | 0 |
| 34 | J | 1 | 0 | 0 | 0 | 0 |
| 34 | j | 1 | 0 | 0 | 0 | 0 |
| All | All | 49594 | 0 | 50450 | 263 | 7 |

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 3.

All (263) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:V:37:CYS:SG | 33:V:201:HEM:HAB | 1.52 | 1.48 |
| 16:V:37:CYS:SG | 33:V:201:HEM:CAB | 2.02 | 1.47 |
| 16:V:40:CYS:SG | 33:V:201:HEM:CAC | 2.04 | 1.46 |
| 16:V:40:CYS:SG | 33:V:201:HEM:HAC | 1.57 | 1.44 |
| 8:I:1:MET:CA | 8:I:1:MET:C | 1.84 | 1.44 |
| 8:I:1:MET:HG2 | 8:I:1:MET:N | 1.37 | 1.35 |
| 8:I:1:MET:CG | 8:I:1:MET:N | 1.89 | 1.35 |
| 1:A:214:MET:HG2 | 28:A:613:PL9:H102 | 1.20 | 1.17 |
| 12:M:16:LEU:HD22 | 12:M:16:LEU:HD11 | 2.95 | 1.11 |
| 12:M:16:LEU:HD13 | 12:M:16:LEU:HD13 | 0.00 | 1.07 |
| 8:I:1:MET:CA | 8:I:1:MET:N | 2.20 | 1.04 |
| 12:M:16:LEU:CD1 | 12:M:16:LEU:HD22 | 2.70 | 0.98 |
| 10:K:17:ILE:H | 10:K:17:ILE:HD13 | 1.29 | 0.97 |
| 8:I:1:MET:HG2 | 8:I:1:MET:H1 | 0.87 | 0.97 |
| 12:M:20:VAL:CG2 | 12:M:20:VAL:HG11 | 2.72 | 0.95 |
| 32:D:409:LHG:H372 | 32:D:409:LHG:H132 | 1.48 | 0.93 |
| 2:B:76:SER:OG | 13:O:112:GLY:CA | 56.52 | 0.92 |
| 2:B:127:ARG:HG3 | 2:B:127:ARG:HH11 | 1.35 | 0.91 |
| 1:A:214:MET:HG2 | 28:A:613:PL9:C10 | 2.02 | 0.88 |
| 25:L:101:SQD:H342 | 14:T:12:CYS:HB3 | 1.90 | 0.87 |
| 11:L:14:ARG:HD3 | 25:L:101:SQD:H241 | 1.57 | 0.86 |
| 12:M:20:VAL:HG11 | 12:M:20:VAL:HG22 | 3.05 | 0.86 |
| 32:D:409:LHG:H352 | 32:D:409:LHG:H151 | 1.59 | 0.83 |
| 8:I:1:MET:CB | 8:I:1:MET:N | 2.42 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:C:509:CLA:HBB1 | 22:C:509:CLA:HMB1 | 1.63 | 0.81 |
| 8:I:1:MET:CG | 8:I:1:MET:H2 | 1.73 | 0.80 |
| 8:I:1:MET:SD | 8:I:1:MET:N | 2.43 | 0.78 |
| 2:B:76:SER:OG | 13:O:112:GLY:HA2 | 56.41 | 0.77 |
| 12:M:33:GLN:HB2 | 12:M:33:GLN:HB2 | 0.00 | 0.77 |
| 8:I:1:MET:CA | 8:I:2:GLU:N | 2.50 | 0.75 |
| 8:I:1:MET:CB | 8:I:1:MET:C | 2.56 | 0.74 |
| 12:M:20:VAL:HG11 | 12:M:20:VAL:HG21 | 2.52 | 0.73 |
| 13:O:57:LYS:O | 13:O:58:ASN:HB2 | 1.87 | 0.73 |
| 12:M:16:LEU:CD1 | 12:M:16:LEU:HD13 | 0.97 | 0.73 |
| 32:D:409:LHG:H112 | 32:D:409:LHG:H382 | 1.72 | 0.72 |
| 22:D:402:CLA:HBB1 | 22:D:402:CLA:HMB1 | 1.71 | 0.72 |
| 12:M:16:LEU:CD1 | 12:M:16:LEU:CD2 | 2.49 | 0.71 |
| 22:A:603:CLA:HBB1 | 22:A:603:CLA:HMB1 | 1.73 | 0.70 |
| 22:B:614:CLA:HBB1 | 22:B:614:CLA:HMB1 | 1.73 | 0.70 |
| 25:B:601:SQD:H252 | 24:T:101:BCR:H373 | 44.10 | 0.70 |
| 16:V:37:CYS:SG | 33:V:201:HEM:C3B | 2.85 | 0.70 |
| 22:C:508:CLA:HBB1 | 22:C:508:CLA:HMB1 | 1.75 | 0.69 |
| 1:A:214:MET:CG | 28:A:613:PL9:H102 | 2.12 | 0.69 |
| 2:B:446:SER:HB2 | 2:B:447:PRO:HD2 | 1.75 | 0.69 |
| 22:B:615:CLA:H18 | 29:B:620:LMG:H421 | 1.76 | 0.67 |
| 12:M:28:GLN:O | 12:M:31:SER:OG | 3.31 | 0.67 |
| 4:D:24:ARG:HD3 | 17:X:37:VAL:HG22 | 1.77 | 0.67 |
| 23:A:606:PHO:HBB1 | 23:A:606:PHO:HMB1 | 1.76 | 0.67 |
| 22:B:612:CLA:HMB1 | 22:B:612:CLA:HBB1 | 1.76 | 0.67 |
| 10:K:17:ILE:HD13 | 10:K:17:ILE:N | 2.08 | 0.67 |
| 22:C:506:CLA:HMC2 | 22:C:507:CLA:H102 | 1.77 | 0.66 |
| 16:V:40:CYS:SG | 33:V:201:HEM:CBC | 2.81 | 0.65 |
| 2:B:77:GLY:C | 13:O:111:ALA:HB1 | 64.18 | 0.65 |
| 8:I:1:MET:C | 8:I:1:MET:N | 2.50 | 0.65 |
| 22:B:617:CLA:HMB1 | 22:B:617:CLA:HBB1 | 1.79 | 0.65 |
| 16:V:40:CYS:SG | 33:V:201:HEM:C3C | 2.90 | 0.64 |
| 2:B:33:TRP:CD1 | 24:B:622:BCR:H381 | 2.32 | 0.64 |
| 1:A:183:MET:HA | 22:A:603:CLA:HMD2 | 1.81 | 0.63 |
| 29:Z:101:LMG:O2 | 29:Z:101:LMG:HC71 | 1.99 | 0.63 |
| 32:D:409:LHG:H112 | 32:D:409:LHG:C38 | 2.30 | 0.61 |
| 25:L:101:SQD:H45 | 14:T:23:PHE:CD1 | 2.35 | 0.61 |
| 24:D:404:BCR:H383 | 29:D:406:LMG:H172 | 1.83 | 0.60 |
| 3:C:167:VAL:HG21 | 22:C:512:CLA:HBB | 1.83 | 0.60 |
| 2:B:33:TRP:HD1 | 24:B:622:BCR:H381 | 1.66 | 0.60 |
| 32:D:409:LHG:H372 | 32:D:409:LHG:C13 | 2.29 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:76:SER:OG | 13:O:112:GLY:C | 55.95 | 0.60 |
| 22:C:510:CLA:H43 | 32:D:409:LHG:H383 | 1.84 | 0.60 |
| 23:A:605:PHO:HMB1 | 23:A:605:PHO:HBB1 | 1.84 | 0.60 |
| 22:B:606:CLA:C14 | 22:B:611:CLA:HED2 | 2.33 | 0.59 |
| 11:L:13:ASN:ND2 | 11:L:16:SER:H | 2.01 | 0.59 |
| 12:M:20:VAL:HG13 | 12:M:20:VAL:HG13 | 0.00 | 0.59 |
| 22:B:611:CLA:HBB1 | 22:B:611:CLA:HHC | 1.85 | 0.59 |
| 28:A:613:PL9:H502 | 4:D:39:PRO:HG3 | 1.85 | 0.58 |
| 2:B:76:SER:O | 13:O:111:ALA:HA | 62.72 | 0.58 |
| 2:B:462:PHE:CE1 | 22:B:614:CLA:HMB3 | 2.38 | 0.58 |
| 2:B:103:LEU:HD21 | 22:B:606:CLA:HMC3 | 1.86 | 0.57 |
| 22:B:616:CLA:H2 | 22:B:617:CLA:HBB2 | 1.87 | 0.57 |
| 12:M:28:GLN:CB | 12:M:28:GLN:HA | 2.06 | 0.57 |
| 12:M:31:SER:O | 12:M:32:GLN:HG2 | 4.82 | 0.56 |
| 2:B:76:SER:OG | 13:O:112:GLY:N | 57.94 | 0.56 |
| 2:B:224:ARG:HD3 | 7:H:25:TRP:CE2 | 2.40 | 0.56 |
| 2:B:127:ARG:NH1 | 2:B:127:ARG:HG3 | 2.12 | 0.56 |
| 2:B:224:ARG:HD3 | 7:H:25:TRP:CD2 | 2.42 | 0.55 |
| 3:C:279:LEU:HD22 | 22:C:509:CLA:HED2 | 1.89 | 0.55 |
| 2:B:70:GLY:HA2 | 2:B:178:VAL:HG21 | 1.89 | 0.55 |
| 8:I:1:MET:CE | 8:I:4:LEU:HB2 | 2.37 | 0.55 |
| 10:K:17:ILE:H | 10:K:17:ILE:CD1 | 2.00 | 0.55 |
| 2:B:26:HIS:HB2 | 22:B:613:CLA:HMB2 | 1.89 | 0.55 |
| 24:D:404:BCR:H313 | 31:D:410:DGD:HA91 | 1.89 | 0.55 |
| 16:V:37:CYS:SG | 33:V:201:HEM:CBB | 2.88 | 0.54 |
| 3:C:41:ARG:NH1 | 22:C:511:CLA:HMD1 | 2.22 | 0.54 |
| 12:M:28:GLN:HA | 12:M:28:GLN:HA | 0.00 | 0.54 |
| 22:B:614:CLA:H122 | 29:B:620:LMG:H232 | 1.88 | 0.54 |
| 22:C:501:CLA:C4D | 22:C:503:CLA:H2 | 2.38 | 0.54 |
| 7:H:65:LEU:HD12 | 7:H:66:GLY:H | 1.73 | 0.54 |
| 12:M:20:VAL:CG1 | 12:M:20:VAL:HG22 | 2.78 | 0.53 |
| 22:C:506:CLA:HBB1 | 22:C:506:CLA:HMB1 | 1.90 | 0.53 |
| 25:B:601:SQD:C25 | 24:T:101:BCR:H373 | 44.11 | 0.53 |
| 2:B:446:SER:HB2 | 2:B:447:PRO:CD | 2.38 | 0.53 |
| 22:C:513:CLA:HMB1 | 22:C:513:CLA:HBB1 | 1.91 | 0.52 |
| 4:D:123:ILE:HD11 | 31:H:102:DGD:HAE1 | 1.92 | 0.52 |
| 13:O:40:ILE:HG12 | 13:O:243:ILE:HD13 | 1.92 | 0.52 |
| 2:B:76:SER:O | 13:O:112:GLY:N | 60.38 | 0.52 |
| 22:A:603:CLA:CBF | 22:D:402:CLA:HAC2 | 2.40 | 0.52 |
| 22:C:510:CLA:C4 | 32:D:409:LHG:H383 | 2.40 | 0.52 |
| 22:C:503:CLA:HBB1 | 22:C:503:CLA:HMB1 | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:L:101:SQD:O6 | 14:T:23:PHE:CD1 | 2.92 | 0.52 |
| 1:A:84:PRO:HA | 1:A:112:TYR:CG | 2.45 | 0.52 |
| 12:M:20:VAL:CG1 | 12:M:20:VAL:CG2 | 2.55 | 0.52 |
| 2:B:248:ALA:HA | 22:B:604:CLA:H42 | 1.92 | 0.51 |
| 2:B:37:MET:CE | 24:B:622:BCR:H282 | 2.71 | 0.51 |
| 22:C:508:CLA:H92 | 32:D:409:LHG:H371 | 1.93 | 0.51 |
| 25:B:601:SQD:H252 | 24:T:101:BCR:C37 | 44.21 | 0.51 |
| 22:D:403:CLA:H192 | 17:X:15:LEU:HD11 | 1.93 | 0.51 |
| 28:A:613:PL9:H403 | 6:F:22:ALA:HB2 | 1.93 | 0.51 |
| 12:M:3:VAL:HG11 | 14:T:2:GLU:HG2 | 1.93 | 0.51 |
| 3:C:42:LEU:HD21 | 22:C:511:CLA:H2A | 1.93 | 0.51 |
| 11:L:13:ASN:C | 11:L:13:ASN:HD22 | 2.15 | 0.50 |
| 8:I:1:MET:C | 8:I:1:MET:SD | 2.90 | 0.50 |
| 2:B:112:CYS:HG | 14:T:18:PHE:HZ | 45.04 | 0.50 |
| 11:L:13:ASN:HD22 | 11:L:16:SER:H | 1.60 | 0.50 |
| 2:B:314:TYR:CE2 | 2:B:316:GLY:HA3 | 2.47 | 0.50 |
| 3:C:437:PHE:CZ | 22:C:510:CLA:HMB3 | 2.47 | 0.50 |
| 2:B:36:SER:OG | 24:B:618:BCR:H362 | 13.46 | 0.49 |
| 2:B:341:LYS:HA | 2:B:405:GLU:HG2 | 1.94 | 0.49 |
| 29:B:620:LMG:H242 | 4:D:284:ILE:HD13 | 1.94 | 0.49 |
| 22:C:501:CLA:H42 | 22:C:502:CLA:HMD1 | 1.94 | 0.49 |
| 2:B:422:ARG:O | 2:B:425:ILE:HG12 | 2.13 | 0.49 |
| 2:B:48:SER:O | 13:O:57:LYS:HE3 | 52.61 | 0.49 |
| 22:B:604:CLA:HAB | 22:B:606:CLA:H171 | 1.95 | 0.49 |
| 32:D:409:LHG:H132 | 32:D:409:LHG:C37 | 2.33 | 0.49 |
| 3:C:60:ILE:HG22 | 22:C:503:CLA:HHD | 1.95 | 0.49 |
| 2:B:36:SER:OG | 24:B:619:BCR:H362 | 2.12 | 0.49 |
| 22:A:604:CLA:HMD3 | 4:D:182:LEU:HD11 | 1.95 | 0.49 |
| 31:C:517:DGD:HB22 | 29:C:519:LMG:H302 | 1.95 | 0.49 |
| 18:Y:38:LEU:O | 18:Y:42:ARG:HD3 | 2.13 | 0.48 |
| 32:D:409:LHG:H382 | 32:D:409:LHG:C11 | 2.42 | 0.48 |
| 22:B:615:CLA:H171 | 14:T:8:PHE:CE1 | 20.74 | 0.48 |
| 2:B:462:PHE:CZ | 22:B:614:CLA:HMB3 | 2.49 | 0.48 |
| 2:B:461:LEU:HD21 | 4:D:284:ILE:HD11 | 1.96 | 0.48 |
| 13:O:49:THR:OG1 | 13:O:236:GLN:HB2 | 2.14 | 0.48 |
| 29:A:614:LMG:H291 | 3:C:214:LEU:O | 2.14 | 0.47 |
| 22:B:615:CLA:H151 | 14:T:8:PHE:HE1 | 22.71 | 0.47 |
| 3:C:25:ASN:HD21 | 3:C:31:SER:HA | 1.79 | 0.47 |
| 3:C:437:PHE:CE1 | 22:C:510:CLA:HMB3 | 2.50 | 0.47 |
| 24:K:102:BCR:H371 | 24:K:102:BCR:H24C | 1.70 | 0.47 |
| 2:B:490:GLN:HA | 2:B:496:TYR:CE2 | 2.50 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:A:606:PHO:HHD | 23:A:606:PHO:HBC2 | 1.97 | 0.47 |
| 3:C:288:CYS:SG | 31:C:516:DGD:HB32 | 2.55 | 0.47 |
| 11:L:18:TYR:OH | 25:L:101:SQD:C24 | 2.78 | 0.47 |
| 22:B:609:CLA:HMB1 | 22:B:609:CLA:HBB1 | 1.97 | 0.47 |
| 13:O:42:ARG:O | 13:O:241:ALA:HA | 2.15 | 0.47 |
| 14:T:18:PHE:HE1 | 24:T:101:BCR:H381 | 7.62 | 0.47 |
| 1:A:200:LEU:HG | 31:C:518:DGD:HAT2 | 1.97 | 0.47 |
| 2:B:127:ARG:CG | 2:B:127:ARG:HH11 | 2.18 | 0.46 |
| 5:E:27:ILE:HB | 5:E:28:PRO:HD3 | 1.98 | 0.46 |
| 24:B:618:BCR:H371 | 24:B:618:BCR:H24C | 1.83 | 0.46 |
| 11:L:14:ARG:HB3 | 14:T:25:GLU:HG2 | 1.97 | 0.46 |
| 1:A:63:ILE:HB | 3:C:335:THR:HG21 | 1.97 | 0.46 |
| 3:C:429:SER:HB3 | 31:C:517:DGD:HBT2 | 1.98 | 0.46 |
| 4:D:27:PHE:CD1 | 32:E:101:LHG:HC12 | 2.51 | 0.46 |
| 13:O:142:PHE:HB2 | 13:O:199:LEU:HB2 | 1.98 | 0.46 |
| 2:B:237:VAL:HG12 | 22:B:613:CLA:HMD1 | 1.98 | 0.46 |
| 6:F:41:GLN:OE1 | 9:J:31:GLY:HA3 | 2.16 | 0.46 |
| 8:I:1:MET:HE1 | 8:I:4:LEU:HB2 | 1.98 | 0.46 |
| 22:B:617:CLA:HED2 | 22:B:617:CLA:H43 | 1.98 | 0.45 |
| 2:B:467:ILE:HG13 | 4:D:126:MET:HE2 | 2.04 | 0.45 |
| 22:A:607:CLA:H162 | 22:A:607:CLA:H122 | 1.76 | 0.45 |
| 22:B:611:CLA:OBD | 22:B:611:CLA:H152 | 2.16 | 0.45 |
| 24:T:101:BCR:H371 | 24:T:101:BCR:H24C | 1.83 | 0.45 |
| 24:T:102:BCR:H371 | 24:T:102:BCR:H24C | 1.78 | 0.45 |
| 2:B:383:PHE:CZ | 13:O:167:GLY:HA2 | 2.51 | 0.45 |
| 8:I:1:MET:HE3 | 8:I:4:LEU:HB2 | 1.98 | 0.45 |
| 22:C:510:CLA:H192 | 22:C:510:CLA:HBC3 | 1.99 | 0.45 |
| 13:O:58:ASN:HA | 13:O:60:ARG:HH21 | 1.81 | 0.45 |
| 1:A:215:HIS:HA | 28:A:613:PL9:O1 | 2.17 | 0.44 |
| 22:B:606:CLA:H41 | 22:B:606:CLA:H62 | 1.77 | 0.44 |
| 22:A:607:CLA:H192 | 22:C:505:CLA:H142 | 2.00 | 0.44 |
| 29:A:614:LMG:H231 | 29:A:614:LMG:H201 | 1.86 | 0.44 |
| 2:B:78:TRP:N | 13:O:111:ALA:HB1 | 63.04 | 0.44 |
| 4:D:148:ALA:HB3 | 4:D:149:PRO:HD3 | 1.99 | 0.44 |
| 12:M:27:VAL:HG12 | 12:M:28:GLN:HG2 | 6.64 | 0.44 |
| 3:C:334:PRO:HA | 13:O:153:THR:OG1 | 2.17 | 0.44 |
| 22:D:403:CLA:H121 | 17:X:18:ALA:HB2 | 1.99 | 0.44 |
| 22:D:403:CLA:HBB1 | 22:D:403:CLA:HMB1 | 2.00 | 0.44 |
| 4:D:191:TRP:CE3 | 4:D:289:LEU:HD11 | 2.53 | 0.44 |
| 1:A:188:ALA:HB2 | 1:A:328:MET:HB2 | 2.00 | 0.44 |
| 5:E:82:GLN:C | 5:E:84:LYS:H | 2.21 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:A:608:BCR:H24C | 24:A:608:BCR:H371 | 1.84 | 0.44 |
| 24:B:618:BCR:C38 | 14:T:19:PHE:HZ | 34.43 | 0.44 |
| 3:C:205:ASP:HA | 3:C:206:PRO:HD3 | 1.90 | 0.43 |
| 24:D:404:BCR:HC22 | 31:D:410:DGD:HA72 | 2.00 | 0.43 |
| 22:B:616:CLA:H2 | 22:B:617:CLA:CBB | 2.48 | 0.43 |
| 22:C:505:CLA:HAA1 | 22:C:505:CLA:HBD | 1.99 | 0.43 |
| 22:C:506:CLA:H122 | 22:C:506:CLA:H162 | 1.72 | 0.43 |
| 22:A:604:CLA:HBB1 | 22:A:604:CLA:HMB1 | 2.00 | 0.43 |
| 2:B:13:ILE:HG12 | 22:B:613:CLA:HAC2 | 2.00 | 0.43 |
| 2:B:467:ILE:HG13 | 4:D:126:MET:CE | 2.48 | 0.43 |
| 24:B:622:BCR:H371 | 24:B:622:BCR:H24C | 1.89 | 0.43 |
| 4:D:85:MET:CE | 4:D:96:GLU:HG2 | 2.49 | 0.43 |
| 14:T:22:PHE:HB3 | 24:T:102:BCR:H271 | 2.00 | 0.43 |
| 13:O:58:ASN:HA | 13:O:60:ARG:NH2 | 2.33 | 0.43 |
| 29:A:614:LMG:H151 | 31:C:516:DGD:HA62 | 2.01 | 0.43 |
| 16:V:78:ASN:OD1 | 16:V:96:ARG:NH1 | 2.52 | 0.43 |
| 5:E:27:ILE:HG12 | 33:F:101:HEM:HMC3 | 2.01 | 0.43 |
| 1:A:215:HIS:ND1 | 28:A:613:PL9:O1 | 2.47 | 0.43 |
| 2:B:71:VAL:HG23 | 22:B:607:CLA:HMA2 | 2.01 | 0.43 |
| 8:I:33:LYS:HB3 | 8:I:34:ARG:H | 1.50 | 0.43 |
| 16:V:37:CYS:CB | 33:V:201:HEM:HAB | 2.43 | 0.43 |
| 3:C:53:HIS:CB | 22:C:512:CLA:HMD1 | 2.49 | 0.43 |
| 4:D:102:THR:OG1 | 31:D:410:DGD:HG31 | 2.19 | 0.43 |
| 10:K:10:LYS:N | 10:K:10:LYS:HD2 | 2.34 | 0.43 |
| 22:C:510:CLA:HBB1 | 22:C:510:CLA:HMB1 | 2.01 | 0.42 |
| 22:A:603:CLA:CAD | 22:D:402:CLA:HAC2 | 2.50 | 0.42 |
| 22:B:605:CLA:H43 | 22:B:606:CLA:H2 | 2.01 | 0.42 |
| 12:M:20:VAL:CG1 | 12:M:20:VAL:HG13 | 0.97 | 0.42 |
| 22:A:604:CLA:H142 | 29:D:406:LMG:H232 | 2.01 | 0.42 |
| 1:A:96:ILE:HG12 | 1:A:105:TRP:CE2 | 2.55 | 0.42 |
| 22:C:504:CLA:H201 | 32:D:409:LHG:H342 | 2.01 | 0.42 |
| 23:A:605:PHO:ND | 23:A:605:PHO:NC | 2.68 | 0.42 |
| 25:A:609:SQD:O10 | 32:D:409:LHG:H122 | 2.20 | 0.42 |
| 22:B:614:CLA:H162 | 22:B:614:CLA:H121 | 1.88 | 0.42 |
| 10:K:20:PRO:HB3 | 18:Y:21:GLN:HG3 | 2.01 | 0.42 |
| 4:D:272:LEU:C | 4:D:272:LEU:HD23 | 2.40 | 0.42 |
| 32:D:409:LHG:H302 | 32:D:409:LHG:H332 | 1.88 | 0.42 |
| 4:D:27:PHE:HD1 | 32:E:101:LHG:HC12 | 1.85 | 0.42 |
| 2:B:220:ARG:HG3 | 7:H:20:LYS:HD3 | 2.01 | 0.42 |
| 3:C:29:GLU:CD | 3:C:29:GLU:H | 2.22 | 0.42 |
| 24:H:101:BCR:H24C | 24:H:101:BCR:H371 | 1.81 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:B:612:CLA:H142 | 32:L:102:LHG:H361 | 2.02 | 0.42 |
| 13:O:59:LYS:HD2 | 13:O:61:GLN:CG | 2.50 | 0.42 |
| 2:B:204:ALA:CB | 22:B:603:CLA:HAB | 2.50 | 0.42 |
| 1:A:317:TRP:CZ3 | 4:D:180:ARG:HD2 | 2.55 | 0.42 |
| 4:D:185:PHE:CG | 22:D:401:CLA:HMD3 | 2.55 | 0.42 |
| 25:B:601:SQD:H252 | 24:T:101:BCR:C22 | 45.35 | 0.41 |
| 2:B:63:LEU:N | 2:B:64:PRO:HD2 | 2.35 | 0.41 |
| 22:A:603:CLA:HBD | 22:D:402:CLA:HAC2 | 2.02 | 0.41 |
| 2:B:423:LYS:HD3 | 2:B:423:LYS:HA | 1.94 | 0.41 |
| 22:B:605:CLA:H161 | 22:B:605:CLA:H141 | 1.93 | 0.41 |
| 22:C:502:CLA:H61 | 22:C:512:CLA:H42 | 2.03 | 0.41 |
| 1:A:278:TRP:HB3 | 1:A:279:PRO:CD | 2.51 | 0.41 |
| 1:A:79:THR:HG22 | 4:D:315:TYR:HB2 | 2.02 | 0.41 |
| 12:M:16:LEU:CD1 | 12:M:16:LEU:CD1 | 0.00 | 0.41 |
| 23:A:606:PHO:HMA2 | 28:A:613:PL9:C22 | 2.51 | 0.41 |
| 22:B:611:CLA:CBB | 22:B:611:CLA:HHC | 2.50 | 0.41 |
| 22:B:607:CLA:HBB1 | 22:B:607:CLA:HMB1 | 2.03 | 0.41 |
| 12:M:28:GLN:HA | 12:M:28:GLN:CA | 0.97 | 0.41 |
| 1:A:93:PHE:CD1 | 1:A:95:PRO:HD3 | 2.56 | 0.41 |
| 3:C:243:ILE:HG22 | 22:C:506:CLA:HMC1 | 2.03 | 0.41 |
| 3:C:406:SER:HA | 3:C:420:VAL:HG23 | 2.03 | 0.41 |
| 22:B:609:CLA:HMB1 | 4:D:126:MET:HB3 | 2.04 | 0.40 |
| 3:C:338:GLY:HA3 | 3:C:341:LEU:O | 2.22 | 0.40 |
| 2:B:475:PHE:CD2 | 4:D:140:PRO:HG3 | 2.56 | 0.40 |
| 14:T:18:PHE:CE1 | 24:T:101:BCR:H381 | 6.90 | 0.40 |
| 6:F:28:VAL:HB | 6:F:29:PRO:HD3 | 2.04 | 0.40 |
| 2:B:78:TRP:HD1 | 13:O:112:GLY:HA2 | 55.87 | 0.40 |
| 1:A:249:VAL:HG12 | 2:B:491:VAL:CG2 | 2.52 | 0.40 |
| 2:B:127:ARG:NH1 | 2:B:127:ARG:CG | 2.81 | 0.40 |
| 13:O:180:GLU:CD | 13:O:180:GLU:H | 2.24 | 0.40 |
| 23:A:606:PHO:ND | 23:A:606:PHO:NC | 2.70 | 0.40 |
| 3:C:286:ALA:HB2 | 22:C:502:CLA:CMD | 2.51 | 0.40 |
| 25:A:609:SQD:H291 | 22:C:508:CLA:H71 | 2.03 | 0.40 |
| 4:D:103:ARG:O | 4:D:107:LEU:HG | 2.21 | 0.40 |

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------------|--------------------------|-------------------|
| 15:u:73:GLN:OE1 | 16:V:70:GLU:CD[3_544] | 0.80 | 1.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 15:u:73:GLN:OE1 | 16:V:70:GLU:OE1[3_544] | 1.22 | 0.98 |
| 15:u:73:GLN:OE1 | 16:V:70:GLU:OE2[3_544] | 1.45 | 0.75 |
| 15:u:73:GLN:CD | 16:V:70:GLU:OE1[3_544] | 1.79 | 0.41 |
| 15:u:73:GLN:CD | 16:V:70:GLU:CD[3_544] | 1.89 | 0.31 |
| 15:u:73:GLN:OE1 | 16:V:70:GLU:CG[3_544] | 1.98 | 0.22 |
| 15:u:60:ASP:OD2 | 16:V:110:LYS:CD[3_544] | 2.18 | 0.02 |

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 1 | A | 332/334 (99%) | 328 (99%) | 3 (1%) | 1 (0%) | 43 | 81 |
| 1 | a | 332/334 (99%) | 328 (99%) | 3 (1%) | 1 (0%) | 43 | 81 |
| 2 | B | 502/504 (100%) | 497 (99%) | 5 (1%) | 0 | 100 | 100 |
| 2 | b | 502/504 (100%) | 496 (99%) | 6 (1%) | 0 | 100 | 100 |
| 3 | C | 449/461 (97%) | 440 (98%) | 8 (2%) | 1 (0%) | 49 | 84 |
| 3 | c | 449/461 (97%) | 440 (98%) | 8 (2%) | 1 (0%) | 49 | 84 |
| 4 | D | 340/342 (99%) | 332 (98%) | 8 (2%) | 0 | 100 | 100 |
| 4 | d | 340/342 (99%) | 332 (98%) | 8 (2%) | 0 | 100 | 100 |
| 5 | E | 79/81 (98%) | 78 (99%) | 1 (1%) | 0 | 100 | 100 |
| 5 | e | 79/81 (98%) | 78 (99%) | 1 (1%) | 0 | 100 | 100 |
| 6 | F | 32/34 (94%) | 32 (100%) | 0 | 0 | 100 | 100 |
| 6 | f | 32/34 (94%) | 32 (100%) | 0 | 0 | 100 | 100 |
| 7 | H | 63/65 (97%) | 58 (92%) | 5 (8%) | 0 | 100 | 100 |
| 7 | h | 63/65 (97%) | 58 (92%) | 5 (8%) | 0 | 100 | 100 |
| 8 | I | 36/38 (95%) | 34 (94%) | 2 (6%) | 0 | 100 | 100 |
| 8 | i | 36/38 (95%) | 34 (94%) | 2 (6%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 9 | J | 36/40 (90%) | 36 (100%) | 0 | 0 | 100 | 100 |
| 9 | j | 36/40 (90%) | 36 (100%) | 0 | 0 | 100 | 100 |
| 10 | K | 35/37 (95%) | 35 (100%) | 0 | 0 | 100 | 100 |
| 10 | k | 35/37 (95%) | 35 (100%) | 0 | 0 | 100 | 100 |
| 11 | L | 35/37 (95%) | 35 (100%) | 0 | 0 | 100 | 100 |
| 11 | l | 35/37 (95%) | 35 (100%) | 0 | 0 | 100 | 100 |
| 12 | M | 32/34 (94%) | 32 (100%) | 0 | 0 | 100 | 100 |
| 12 | m | 32/34 (94%) | 32 (100%) | 0 | 0 | 100 | 100 |
| 13 | O | 241/243 (99%) | 233 (97%) | 7 (3%) | 1 (0%) | 36 | 77 |
| 13 | o | 241/243 (99%) | 233 (97%) | 7 (3%) | 1 (0%) | 36 | 77 |
| 14 | T | 28/30 (93%) | 27 (96%) | 1 (4%) | 0 | 100 | 100 |
| 14 | t | 28/30 (93%) | 27 (96%) | 1 (4%) | 0 | 100 | 100 |
| 15 | U | 95/97 (98%) | 93 (98%) | 2 (2%) | 0 | 100 | 100 |
| 15 | u | 95/97 (98%) | 93 (98%) | 2 (2%) | 0 | 100 | 100 |
| 16 | V | 135/137 (98%) | 132 (98%) | 3 (2%) | 0 | 100 | 100 |
| 16 | v | 135/137 (98%) | 132 (98%) | 3 (2%) | 0 | 100 | 100 |
| 17 | X | 37/39 (95%) | 36 (97%) | 1 (3%) | 0 | 100 | 100 |
| 17 | x | 37/39 (95%) | 36 (97%) | 1 (3%) | 0 | 100 | 100 |
| 18 | Y | 27/29 (93%) | 27 (100%) | 0 | 0 | 100 | 100 |
| 18 | y | 27/29 (93%) | 27 (100%) | 0 | 0 | 100 | 100 |
| 19 | Z | 60/62 (97%) | 58 (97%) | 2 (3%) | 0 | 100 | 100 |
| 19 | z | 60/62 (97%) | 58 (97%) | 2 (3%) | 0 | 100 | 100 |
| All | All | 5188/5288 (98%) | 5085 (98%) | 97 (2%) | 6 (0%) | 53 | 88 |

All (6) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13 | O | 58 | ASN |
| 13 | o | 58 | ASN |
| 3 | C | 416 | SER |
| 3 | c | 416 | SER |
| 1 | A | 259 | ILE |
| 1 | a | 259 | ILE |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1 | A | 269/269 (100%) | 269 (100%) | 0 | 100 | 100 |
| 1 | a | 269/269 (100%) | 269 (100%) | 0 | 100 | 100 |
| 2 | B | 402/402 (100%) | 398 (99%) | 4 (1%) | 78 | 89 |
| 2 | b | 402/402 (100%) | 398 (99%) | 4 (1%) | 78 | 89 |
| 3 | C | 352/362 (97%) | 348 (99%) | 4 (1%) | 76 | 88 |
| 3 | c | 352/362 (97%) | 348 (99%) | 4 (1%) | 76 | 88 |
| 4 | D | 277/277 (100%) | 274 (99%) | 3 (1%) | 76 | 88 |
| 4 | d | 277/277 (100%) | 274 (99%) | 3 (1%) | 76 | 88 |
| 5 | E | 72/72 (100%) | 71 (99%) | 1 (1%) | 69 | 85 |
| 5 | e | 72/72 (100%) | 71 (99%) | 1 (1%) | 69 | 85 |
| 6 | F | 28/28 (100%) | 27 (96%) | 1 (4%) | 38 | 65 |
| 6 | f | 28/28 (100%) | 27 (96%) | 1 (4%) | 38 | 65 |
| 7 | H | 54/54 (100%) | 51 (94%) | 3 (6%) | 23 | 54 |
| 7 | h | 54/54 (100%) | 51 (94%) | 3 (6%) | 23 | 54 |
| 8 | I | 35/35 (100%) | 34 (97%) | 1 (3%) | 45 | 70 |
| 8 | i | 35/35 (100%) | 34 (97%) | 1 (3%) | 45 | 70 |
| 9 | J | 26/28 (93%) | 26 (100%) | 0 | 100 | 100 |
| 9 | j | 26/28 (93%) | 26 (100%) | 0 | 100 | 100 |
| 10 | K | 30/30 (100%) | 28 (93%) | 2 (7%) | 18 | 48 |
| 10 | k | 30/30 (100%) | 28 (93%) | 2 (7%) | 18 | 48 |
| 11 | L | 35/35 (100%) | 33 (94%) | 2 (6%) | 23 | 54 |
| 11 | l | 35/35 (100%) | 33 (94%) | 2 (6%) | 23 | 54 |
| 12 | M | 31/31 (100%) | 30 (97%) | 1 (3%) | 42 | 68 |
| 12 | m | 31/31 (100%) | 30 (97%) | 1 (3%) | 42 | 68 |
| 13 | O | 206/206 (100%) | 202 (98%) | 4 (2%) | 60 | 80 |
| 13 | o | 206/206 (100%) | 202 (98%) | 4 (2%) | 60 | 80 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 14 | T | 27/27 (100%) | 26 (96%) | 1 (4%) | 37 | 65 |
| 14 | t | 27/27 (100%) | 26 (96%) | 1 (4%) | 37 | 65 |
| 15 | U | 84/84 (100%) | 83 (99%) | 1 (1%) | 74 | 87 |
| 15 | u | 84/84 (100%) | 83 (99%) | 1 (1%) | 74 | 87 |
| 16 | V | 117/117 (100%) | 116 (99%) | 1 (1%) | 81 | 90 |
| 16 | v | 117/117 (100%) | 116 (99%) | 1 (1%) | 81 | 90 |
| 17 | X | 32/32 (100%) | 32 (100%) | 0 | 100 | 100 |
| 17 | x | 32/32 (100%) | 32 (100%) | 0 | 100 | 100 |
| 18 | Y | 22/22 (100%) | 21 (96%) | 1 (4%) | 30 | 60 |
| 18 | y | 22/22 (100%) | 21 (96%) | 1 (4%) | 30 | 60 |
| 19 | Z | 52/52 (100%) | 50 (96%) | 2 (4%) | 36 | 64 |
| 19 | z | 52/52 (100%) | 50 (96%) | 2 (4%) | 36 | 64 |
| All | All | 4302/4326 (99%) | 4238 (98%) | 64 (2%) | 67 | 84 |

All (64) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 53 | ASN |
| 2 | B | 223 | GLN |
| 2 | B | 246 | PHE |
| 2 | B | 472 | ARG |
| 2 | b | 53 | ASN |
| 2 | b | 223 | GLN |
| 2 | b | 246 | PHE |
| 2 | b | 472 | ARG |
| 3 | C | 24 | THR |
| 3 | C | 25 | ASN |
| 3 | C | 289 | PHE |
| 3 | C | 418 | ASN |
| 3 | c | 24 | THR |
| 3 | c | 25 | ASN |
| 3 | c | 289 | PHE |
| 3 | c | 418 | ASN |
| 4 | D | 11 | GLU |
| 4 | D | 90 | LEU |
| 4 | D | 180 | ARG |
| 4 | d | 11 | GLU |
| 4 | d | 90 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | d | 180 | ARG |
| 5 | E | 71 | GLU |
| 5 | e | 71 | GLU |
| 6 | F | 44 | GLN |
| 6 | f | 44 | GLN |
| 7 | H | 12 | ARG |
| 7 | H | 49 | TYR |
| 7 | H | 65 | LEU |
| 7 | h | 12 | ARG |
| 7 | h | 49 | TYR |
| 7 | h | 65 | LEU |
| 8 | I | 1 | MET |
| 8 | i | 1 | MET |
| 10 | K | 13 | GLU |
| 10 | K | 17 | ILE |
| 10 | k | 13 | GLU |
| 10 | k | 17 | ILE |
| 11 | L | 1 | MET |
| 11 | L | 13 | ASN |
| 11 | l | 1 | MET |
| 11 | l | 13 | ASN |
| 12 | M | 9 | ILE |
| 12 | m | 9 | ILE |
| 13 | O | 61 | GLN |
| 13 | O | 118 | LEU |
| 13 | O | 181 | GLU |
| 13 | O | 234 | LYS |
| 13 | o | 61 | GLN |
| 13 | o | 118 | LEU |
| 13 | o | 181 | GLU |
| 13 | o | 234 | LYS |
| 14 | T | 25 | GLU |
| 14 | t | 25 | GLU |
| 15 | U | 70 | ARG |
| 15 | u | 70 | ARG |
| 16 | V | 30 | LYS |
| 16 | v | 30 | LYS |
| 18 | Y | 27 | MET |
| 18 | y | 27 | MET |
| 19 | Z | 6 | GLN |
| 19 | Z | 31 | GLN |
| 19 | z | 6 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19 | z | 31 | GLN |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 261 | GLN |
| 1 | A | 315 | ASN |
| 1 | a | 261 | GLN |
| 1 | a | 315 | ASN |
| 2 | B | 53 | ASN |
| 2 | B | 223 | GLN |
| 2 | B | 281 | GLN |
| 2 | B | 331 | ASN |
| 2 | b | 53 | ASN |
| 2 | b | 223 | GLN |
| 2 | b | 281 | GLN |
| 2 | b | 331 | ASN |
| 3 | C | 25 | ASN |
| 3 | C | 373 | ASN |
| 3 | c | 25 | ASN |
| 3 | c | 373 | ASN |
| 4 | D | 83 | ASN |
| 4 | D | 332 | GLN |
| 4 | d | 83 | ASN |
| 4 | d | 332 | GLN |
| 6 | F | 44 | GLN |
| 6 | f | 44 | GLN |
| 10 | K | 40 | GLN |
| 10 | k | 40 | GLN |
| 11 | L | 13 | ASN |
| 11 | l | 13 | ASN |
| 13 | O | 82 | GLN |
| 13 | O | 124 | ASN |
| 13 | O | 147 | ASN |
| 13 | o | 82 | GLN |
| 13 | o | 124 | ASN |
| 13 | o | 147 | ASN |
| 16 | V | 34 | GLN |
| 16 | v | 34 | GLN |
| 19 | Z | 58 | ASN |
| 19 | z | 58 | ASN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 166 ligands modelled in this entry, 16 are monoatomic - leaving 150 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 | $\# Z > 2$ |
| 20 | OEX | A | 601 | 1,3 | 0,15,15 | 0.00 | - | 0,32,32 | 0.00 | - |
| 22 | CLA | A | 603 | - | 58,73,73 | 1.88 | 12 (20%) | 66,113,113 | 1.87 | 15 (22%) |
| 22 | CLA | A | 604 | - | 58,73,73 | 1.82 | 12 (20%) | 66,113,113 | 2.12 | 18 (27%) |
| 23 | PHO | A | 605 | - | 67,69,69 | 1.90 | 13 (19%) | 85,99,99 | 1.91 | 17 (20%) |
| 23 | PHO | A | 606 | - | 67,69,69 | 2.01 | 16 (23%) | 85,99,99 | 1.93 | 20 (23%) |
| 22 | CLA | A | 607 | - | 58,73,73 | 1.89 | 12 (20%) | 66,113,113 | 1.90 | 18 (27%) |
| 24 | BCR | A | 608 | - | 41,41,41 | 3.72 | 14 (34%) | 56,56,56 | 7.71 | 37 (66%) |
| 25 | SQD | A | 609 | - | 53,54,54 | 0.97 | 3 (5%) | 63,65,65 | 1.54 | 12 (19%) |
| 27 | BCT | A | 612 | 21 | 0,3,3 | 0.00 | - | 0,3,3 | 0.00 | - |
| 28 | PL9 | A | 613 | - | 55,55,55 | 0.69 | 2 (3%) | 69,69,69 | 1.53 | 14 (20%) |
| 29 | LMG | A | 614 | - | 51,51,55 | 0.94 | 2 (3%) | 59,59,63 | 0.96 | 4 (6%) |
| 25 | SQD | B | 601 | - | 53,54,54 | 1.03 | 3 (5%) | 63,65,65 | 1.25 | 7 (11%) |
| 22 | CLA | B | 602 | - | 58,73,73 | 1.99 | 14 (24%) | 66,113,113 | 1.82 | 14 (21%) |
| 22 | CLA | B | 603 | - | 58,73,73 | 1.95 | 13 (22%) | 66,113,113 | 1.73 | 15 (22%) |
| 22 | CLA | B | 604 | - | 58,73,73 | 1.90 | 13 (22%) | 66,113,113 | 2.02 | 17 (25%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 22 | CLA | B | 605 | - | 58,73,73 | 1.80 | 14 (24%) | 66,113,113 | 2.08 | 15 (22%) |
| 22 | CLA | B | 606 | - | 58,73,73 | 1.85 | 13 (22%) | 66,113,113 | 1.89 | 14 (21%) |
| 22 | CLA | B | 607 | - | 58,73,73 | 1.93 | 13 (22%) | 66,113,113 | 1.91 | 17 (25%) |
| 22 | CLA | B | 608 | - | 58,73,73 | 1.87 | 13 (22%) | 66,113,113 | 1.86 | 16 (24%) |
| 22 | CLA | B | 609 | - | 58,73,73 | 1.82 | 12 (20%) | 66,113,113 | 2.07 | 18 (27%) |
| 22 | CLA | B | 610 | - | 58,73,73 | 1.86 | 13 (22%) | 66,113,113 | 1.92 | 15 (22%) |
| 22 | CLA | B | 611 | - | 58,73,73 | 1.89 | 13 (22%) | 66,113,113 | 1.80 | 15 (22%) |
| 22 | CLA | B | 612 | - | 58,73,73 | 1.78 | 12 (20%) | 66,113,113 | 2.01 | 15 (22%) |
| 22 | CLA | B | 613 | - | 58,73,73 | 1.87 | 13 (22%) | 66,113,113 | 1.92 | 17 (25%) |
| 22 | CLA | B | 614 | - | 58,73,73 | 1.86 | 13 (22%) | 66,113,113 | 1.82 | 18 (27%) |
| 22 | CLA | B | 615 | - | 58,73,73 | 1.83 | 13 (22%) | 66,113,113 | 1.94 | 19 (28%) |
| 22 | CLA | B | 616 | - | 58,73,73 | 1.90 | 14 (24%) | 66,113,113 | 1.79 | 14 (21%) |
| 22 | CLA | B | 617 | - | 58,73,73 | 1.90 | 12 (20%) | 66,113,113 | 1.93 | 19 (28%) |
| 24 | BCR | B | 618 | - | 41,41,41 | 3.66 | 14 (34%) | 56,56,56 | 7.46 | 38 (67%) |
| 24 | BCR | B | 619 | - | 41,41,41 | 3.65 | 14 (34%) | 56,56,56 | 7.70 | 41 (73%) |
| 29 | LMG | B | 620 | - | 51,51,55 | 0.93 | 2 (3%) | 59,59,63 | 1.01 | 3 (5%) |
| 24 | BCR | B | 622 | - | 41,41,41 | 3.80 | 14 (34%) | 56,56,56 | 7.00 | 39 (69%) |
| 22 | CLA | C | 501 | - | 58,73,73 | 1.93 | 13 (22%) | 66,113,113 | 1.92 | 15 (22%) |
| 22 | CLA | C | 502 | - | 58,73,73 | 1.86 | 13 (22%) | 66,113,113 | 1.82 | 15 (22%) |
| 22 | CLA | C | 503 | - | 58,73,73 | 1.94 | 13 (22%) | 66,113,113 | 1.74 | 12 (18%) |
| 22 | CLA | C | 504 | - | 58,73,73 | 1.92 | 13 (22%) | 66,113,113 | 1.87 | 15 (22%) |
| 22 | CLA | C | 505 | - | 58,73,73 | 1.91 | 14 (24%) | 66,113,113 | 1.82 | 16 (24%) |
| 22 | CLA | C | 506 | - | 58,73,73 | 1.95 | 13 (22%) | 66,113,113 | 1.89 | 15 (22%) |
| 22 | CLA | C | 507 | - | 58,73,73 | 1.99 | 13 (22%) | 66,113,113 | 1.85 | 16 (24%) |
| 22 | CLA | C | 508 | - | 58,73,73 | 1.97 | 14 (24%) | 66,113,113 | 1.80 | 15 (22%) |
| 22 | CLA | C | 509 | - | 58,73,73 | 1.93 | 14 (24%) | 66,113,113 | 1.93 | 17 (25%) |
| 22 | CLA | C | 510 | - | 58,73,73 | 1.89 | 13 (22%) | 66,113,113 | 1.87 | 16 (24%) |
| 22 | CLA | C | 511 | 3 | 58,73,73 | 1.93 | 13 (22%) | 66,113,113 | 1.85 | 14 (21%) |
| 22 | CLA | C | 512 | - | 58,73,73 | 1.97 | 14 (24%) | 66,113,113 | 1.82 | 18 (27%) |
| 22 | CLA | C | 513 | - | 58,73,73 | 2.04 | 13 (22%) | 66,113,113 | 1.71 | 14 (21%) |
| 24 | BCR | C | 514 | - | 41,41,41 | 3.86 | 15 (36%) | 56,56,56 | 8.34 | 36 (64%) |
| 24 | BCR | C | 515 | - | 41,41,41 | 3.82 | 14 (34%) | 56,56,56 | 8.14 | 38 (67%) |
| 31 | DGD | C | 516 | - | 63,63,67 | 0.87 | 2 (3%) | 77,77,81 | 0.99 | 3 (3%) |
| 31 | DGD | C | 517 | - | 63,63,67 | 0.87 | 2 (3%) | 77,77,81 | 0.86 | 5 (6%) |
| 31 | DGD | C | 518 | - | 63,63,67 | 0.79 | 3 (4%) | 77,77,81 | 0.90 | 3 (3%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 29 | LMG | C | 519 | - | 51,51,55 | 0.93 | 2 (3%) | 59,59,63 | 1.04 | 4 (6%) |
| 29 | LMG | C | 520 | - | 51,51,55 | 1.00 | 3 (5%) | 59,59,63 | 0.99 | 2 (3%) |
| 22 | CLA | D | 401 | - | 58,73,73 | 1.90 | 15 (25%) | 66,113,113 | 1.98 | 18 (27%) |
| 22 | CLA | D | 402 | - | 58,73,73 | 1.84 | 14 (24%) | 66,113,113 | 2.14 | 16 (24%) |
| 22 | CLA | D | 403 | - | 58,73,73 | 1.93 | 14 (24%) | 66,113,113 | 1.77 | 17 (25%) |
| 24 | BCR | D | 404 | - | 41,41,41 | 3.81 | 14 (34%) | 56,56,56 | 7.70 | 40 (71%) |
| 32 | LHG | D | 405 | - | 48,48,48 | 0.86 | 2 (4%) | 51,54,54 | 1.01 | 4 (7%) |
| 29 | LMG | D | 406 | 34 | 51,51,55 | 0.86 | 2 (3%) | 59,59,63 | 0.80 | 3 (5%) |
| 32 | LHG | D | 407 | - | 48,48,48 | 0.89 | 2 (4%) | 51,54,54 | 0.84 | 2 (3%) |
| 28 | PL9 | D | 408 | - | 55,55,55 | 0.78 | 1 (1%) | 69,69,69 | 1.32 | 10 (14%) |
| 32 | LHG | D | 409 | - | 48,48,48 | 0.94 | 2 (4%) | 51,54,54 | 0.90 | 3 (5%) |
| 31 | DGD | D | 410 | - | 63,63,67 | 0.98 | 4 (6%) | 77,77,81 | 1.04 | 6 (7%) |
| 25 | SQD | D | 411 | - | 42,43,54 | 1.20 | 3 (7%) | 52,54,65 | 1.48 | 7 (13%) |
| 32 | LHG | E | 101 | - | 41,41,48 | 1.05 | 2 (4%) | 44,47,54 | 1.10 | 3 (6%) |
| 33 | HEM | F | 101 | 5,6 | 27,50,50 | 2.11 | 5 (18%) | 17,82,82 | 2.01 | 4 (23%) |
| 24 | BCR | H | 101 | - | 41,41,41 | 3.80 | 14 (34%) | 56,56,56 | 8.19 | 41 (73%) |
| 31 | DGD | H | 102 | - | 63,63,67 | 0.91 | 3 (4%) | 77,77,81 | 0.95 | 5 (6%) |
| 24 | BCR | K | 101 | - | 41,41,41 | 3.84 | 14 (34%) | 56,56,56 | 7.97 | 36 (64%) |
| 24 | BCR | K | 102 | - | 41,41,41 | 3.76 | 14 (34%) | 56,56,56 | 7.71 | 42 (75%) |
| 25 | SQD | L | 101 | - | 53,54,54 | 1.03 | 4 (7%) | 63,65,65 | 1.36 | 8 (12%) |
| 32 | LHG | L | 102 | - | 48,48,48 | 0.89 | 2 (4%) | 51,54,54 | 0.98 | 3 (5%) |
| 24 | BCR | T | 101 | - | 41,41,41 | 3.66 | 14 (34%) | 56,56,56 | 7.46 | 38 (67%) |
| 24 | BCR | T | 102 | - | 41,41,41 | 3.72 | 14 (34%) | 56,56,56 | 8.37 | 41 (73%) |
| 33 | HEM | V | 201 | 16 | 27,50,50 | 2.14 | 6 (22%) | 17,82,82 | 1.87 | 4 (23%) |
| 29 | LMG | Z | 101 | - | 37,37,55 | 1.00 | 3 (8%) | 45,45,63 | 1.29 | 4 (8%) |
| 20 | OEX | a | 601 | 1,3 | 0,15,15 | 0.00 | - | 0,32,32 | 0.00 | - |
| 22 | CLA | a | 603 | - | 58,73,73 | 1.88 | 12 (20%) | 66,113,113 | 1.87 | 15 (22%) |
| 22 | CLA | a | 604 | - | 58,73,73 | 1.82 | 12 (20%) | 66,113,113 | 2.11 | 18 (27%) |
| 23 | PHO | a | 605 | - | 67,69,69 | 1.90 | 13 (19%) | 85,99,99 | 1.92 | 17 (20%) |
| 23 | PHO | a | 606 | - | 67,69,69 | 2.00 | 16 (23%) | 85,99,99 | 1.93 | 20 (23%) |
| 22 | CLA | a | 607 | - | 58,73,73 | 1.88 | 12 (20%) | 66,113,113 | 1.90 | 17 (25%) |
| 24 | BCR | a | 608 | - | 41,41,41 | 3.71 | 14 (34%) | 56,56,56 | 7.71 | 37 (66%) |
| 25 | SQD | a | 609 | - | 53,54,54 | 0.97 | 3 (5%) | 63,65,65 | 1.55 | 12 (19%) |
| 27 | BCT | a | 612 | 21 | 0,3,3 | 0.00 | - | 0,3,3 | 0.00 | - |
| 28 | PL9 | a | 613 | - | 55,55,55 | 0.69 | 2 (3%) | 69,69,69 | 1.54 | 14 (20%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 29 | LMG | a | 614 | - | 51,51,55 | 0.94 | 2 (3%) | 59,59,63 | 0.97 | 4 (6%) |
| 25 | SQD | b | 601 | - | 53,54,54 | 1.04 | 3 (5%) | 63,65,65 | 1.25 | 7 (11%) |
| 22 | CLA | b | 602 | - | 58,73,73 | 1.99 | 13 (22%) | 66,113,113 | 1.83 | 14 (21%) |
| 22 | CLA | b | 603 | - | 58,73,73 | 1.96 | 13 (22%) | 66,113,113 | 1.73 | 15 (22%) |
| 22 | CLA | b | 604 | - | 58,73,73 | 1.90 | 13 (22%) | 66,113,113 | 2.03 | 17 (25%) |
| 22 | CLA | b | 605 | - | 58,73,73 | 1.80 | 14 (24%) | 66,113,113 | 2.07 | 15 (22%) |
| 22 | CLA | b | 606 | - | 58,73,73 | 1.84 | 12 (20%) | 66,113,113 | 1.88 | 13 (19%) |
| 22 | CLA | b | 607 | - | 58,73,73 | 1.93 | 13 (22%) | 66,113,113 | 1.91 | 17 (25%) |
| 22 | CLA | b | 608 | - | 58,73,73 | 1.87 | 13 (22%) | 66,113,113 | 1.85 | 16 (24%) |
| 22 | CLA | b | 609 | - | 58,73,73 | 1.82 | 12 (20%) | 66,113,113 | 2.07 | 19 (28%) |
| 22 | CLA | b | 610 | - | 58,73,73 | 1.86 | 13 (22%) | 66,113,113 | 1.90 | 15 (22%) |
| 22 | CLA | b | 611 | - | 58,73,73 | 1.89 | 12 (20%) | 66,113,113 | 1.80 | 15 (22%) |
| 22 | CLA | b | 612 | - | 58,73,73 | 1.78 | 12 (20%) | 66,113,113 | 2.01 | 15 (22%) |
| 22 | CLA | b | 613 | - | 58,73,73 | 1.87 | 13 (22%) | 66,113,113 | 1.92 | 17 (25%) |
| 22 | CLA | b | 614 | - | 58,73,73 | 1.86 | 13 (22%) | 66,113,113 | 1.83 | 18 (27%) |
| 22 | CLA | b | 615 | - | 58,73,73 | 1.83 | 13 (22%) | 66,113,113 | 1.94 | 19 (28%) |
| 22 | CLA | b | 616 | - | 58,73,73 | 1.90 | 14 (24%) | 66,113,113 | 1.78 | 14 (21%) |
| 22 | CLA | b | 617 | - | 58,73,73 | 1.91 | 12 (20%) | 66,113,113 | 1.94 | 19 (28%) |
| 24 | BCR | b | 618 | - | 41,41,41 | 3.65 | 14 (34%) | 56,56,56 | 7.70 | 41 (73%) |
| 29 | LMG | b | 619 | - | 51,51,55 | 0.94 | 2 (3%) | 59,59,63 | 1.01 | 3 (5%) |
| 25 | SQD | b | 621 | - | 53,54,54 | 1.07 | 4 (7%) | 63,65,65 | 1.43 | 9 (14%) |
| 24 | BCR | b | 622 | - | 41,41,41 | 3.80 | 14 (34%) | 56,56,56 | 7.00 | 39 (69%) |
| 22 | CLA | c | 501 | - | 58,73,73 | 1.92 | 13 (22%) | 66,113,113 | 1.92 | 15 (22%) |
| 22 | CLA | c | 502 | - | 58,73,73 | 1.86 | 13 (22%) | 66,113,113 | 1.83 | 15 (22%) |
| 22 | CLA | c | 503 | - | 58,73,73 | 1.93 | 13 (22%) | 66,113,113 | 1.73 | 12 (18%) |
| 22 | CLA | c | 504 | - | 58,73,73 | 1.91 | 13 (22%) | 66,113,113 | 1.87 | 15 (22%) |
| 22 | CLA | c | 505 | - | 58,73,73 | 1.92 | 14 (24%) | 66,113,113 | 1.82 | 17 (25%) |
| 22 | CLA | c | 506 | - | 58,73,73 | 1.95 | 13 (22%) | 66,113,113 | 1.89 | 15 (22%) |
| 22 | CLA | c | 507 | - | 58,73,73 | 1.99 | 13 (22%) | 66,113,113 | 1.85 | 16 (24%) |
| 22 | CLA | c | 508 | - | 58,73,73 | 1.98 | 14 (24%) | 66,113,113 | 1.80 | 15 (22%) |
| 22 | CLA | c | 509 | - | 58,73,73 | 1.94 | 14 (24%) | 66,113,113 | 1.94 | 16 (24%) |
| 22 | CLA | c | 510 | - | 58,73,73 | 1.90 | 13 (22%) | 66,113,113 | 1.88 | 16 (24%) |
| 22 | CLA | c | 511 | 3 | 58,73,73 | 1.93 | 13 (22%) | 66,113,113 | 1.85 | 14 (21%) |
| 22 | CLA | c | 512 | - | 58,73,73 | 1.98 | 14 (24%) | 66,113,113 | 1.82 | 18 (27%) |
| 22 | CLA | c | 513 | - | 58,73,73 | 2.04 | 13 (22%) | 66,113,113 | 1.71 | 14 (21%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 24 | BCR | c | 514 | - | 41,41,41 | 3.86 | 15 (36%) | 56,56,56 | 8.34 | 36 (64%) |
| 24 | BCR | c | 515 | - | 41,41,41 | 3.82 | 14 (34%) | 56,56,56 | 8.13 | 37 (66%) |
| 31 | DGD | c | 516 | - | 63,63,67 | 0.87 | 3 (4%) | 77,77,81 | 0.99 | 3 (3%) |
| 31 | DGD | c | 517 | - | 63,63,67 | 0.87 | 2 (3%) | 77,77,81 | 0.86 | 5 (6%) |
| 31 | DGD | c | 518 | - | 63,63,67 | 0.78 | 3 (4%) | 77,77,81 | 0.90 | 3 (3%) |
| 29 | LMG | c | 519 | - | 51,51,55 | 0.94 | 2 (3%) | 59,59,63 | 1.04 | 5 (8%) |
| 29 | LMG | c | 520 | - | 51,51,55 | 1.00 | 3 (5%) | 59,59,63 | 0.99 | 2 (3%) |
| 22 | CLA | d | 401 | - | 58,73,73 | 1.89 | 15 (25%) | 66,113,113 | 1.99 | 18 (27%) |
| 22 | CLA | d | 402 | - | 58,73,73 | 1.84 | 14 (24%) | 66,113,113 | 2.13 | 15 (22%) |
| 22 | CLA | d | 403 | - | 58,73,73 | 1.93 | 14 (24%) | 66,113,113 | 1.78 | 17 (25%) |
| 24 | BCR | d | 404 | - | 41,41,41 | 3.81 | 14 (34%) | 56,56,56 | 7.70 | 40 (71%) |
| 32 | LHG | d | 405 | - | 48,48,48 | 0.86 | 2 (4%) | 51,54,54 | 1.01 | 4 (7%) |
| 29 | LMG | d | 406 | 34 | 51,51,55 | 0.87 | 2 (3%) | 59,59,63 | 0.80 | 3 (5%) |
| 32 | LHG | d | 407 | - | 48,48,48 | 0.89 | 2 (4%) | 51,54,54 | 0.85 | 2 (3%) |
| 28 | PL9 | d | 408 | - | 55,55,55 | 0.78 | 1 (1%) | 69,69,69 | 1.32 | 10 (14%) |
| 32 | LHG | d | 409 | - | 48,48,48 | 0.93 | 2 (4%) | 51,54,54 | 0.90 | 3 (5%) |
| 31 | DGD | d | 410 | - | 63,63,67 | 0.99 | 4 (6%) | 77,77,81 | 1.04 | 6 (7%) |
| 25 | SQD | d | 411 | - | 42,43,54 | 1.19 | 3 (7%) | 52,54,65 | 1.48 | 7 (13%) |
| 32 | LHG | e | 101 | - | 41,41,48 | 1.05 | 2 (4%) | 44,47,54 | 1.09 | 3 (6%) |
| 33 | HEM | f | 101 | 5,6 | 27,50,50 | 2.11 | 5 (18%) | 17,82,82 | 2.00 | 4 (23%) |
| 24 | BCR | h | 101 | - | 41,41,41 | 3.80 | 14 (34%) | 56,56,56 | 8.18 | 40 (71%) |
| 31 | DGD | h | 102 | - | 63,63,67 | 0.91 | 3 (4%) | 77,77,81 | 0.95 | 5 (6%) |
| 24 | BCR | k | 101 | - | 41,41,41 | 3.84 | 14 (34%) | 56,56,56 | 7.97 | 36 (64%) |
| 24 | BCR | k | 102 | - | 41,41,41 | 3.76 | 14 (34%) | 56,56,56 | 7.71 | 42 (75%) |
| 25 | SQD | l | 101 | - | 53,54,54 | 1.03 | 4 (7%) | 63,65,65 | 1.36 | 8 (12%) |
| 25 | SQD | l | 102 | - | 53,54,54 | 1.07 | 4 (7%) | 63,65,65 | 1.43 | 9 (14%) |
| 32 | LHG | l | 103 | - | 48,48,48 | 0.89 | 2 (4%) | 51,54,54 | 0.98 | 3 (5%) |
| 24 | BCR | t | 101 | - | 41,41,41 | 3.73 | 14 (34%) | 56,56,56 | 8.36 | 42 (75%) |
| 33 | HEM | v | 201 | 16 | 27,50,50 | 2.14 | 6 (22%) | 17,82,82 | 1.87 | 4 (23%) |
| 29 | LMG | z | 101 | - | 37,37,55 | 1.00 | 3 (8%) | 45,45,63 | 1.30 | 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 |
|-----|------|-------|-----|------|-----------|--------------|---------|
| 20 | OEX | A | 601 | 1,3 | - | 0/0/68/68 | 0/0/6/6 |
| 22 | CLA | A | 603 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | A | 604 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 23 | PHO | A | 605 | - | - | 0/53/103/103 | 0/5/6/6 |
| 23 | PHO | A | 606 | - | - | 0/53/103/103 | 0/5/6/6 |
| 22 | CLA | A | 607 | - | 1/1/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | BCR | A | 608 | - | - | 0/29/63/63 | 0/2/2/2 |
| 25 | SQD | A | 609 | - | - | 0/49/69/69 | 0/1/1/1 |
| 27 | BCT | A | 612 | 21 | - | 0/0/0/0 | 0/0/0/0 |
| 28 | PL9 | A | 613 | - | - | 0/53/73/73 | 0/1/1/1 |
| 29 | LMG | A | 614 | - | - | 0/46/66/70 | 0/1/1/1 |
| 25 | SQD | B | 601 | - | - | 0/49/69/69 | 0/1/1/1 |
| 22 | CLA | B | 602 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | B | 603 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | B | 604 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | B | 605 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | B | 606 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | B | 607 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | B | 608 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | B | 609 | - | 1/1/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | B | 610 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | B | 611 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | B | 612 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | B | 613 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | B | 614 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | B | 615 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | B | 616 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | B | 617 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | BCR | B | 618 | - | - | 0/29/63/63 | 0/2/2/2 |
| 24 | BCR | B | 619 | - | - | 0/29/63/63 | 0/2/2/2 |
| 29 | LMG | B | 620 | - | - | 0/46/66/70 | 0/1/1/1 |
| 24 | BCR | B | 622 | - | - | 0/29/63/63 | 0/2/2/2 |
| 22 | CLA | C | 501 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | C | 502 | - | 1/1/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | C | 503 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | C | 504 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | C | 505 | - | 1/1/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | C | 506 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|--------------|---------|
| 22 | CLA | C | 507 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | C | 508 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | C | 509 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | C | 510 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | C | 511 | 3 | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | C | 512 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | C | 513 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | BCR | C | 514 | - | - | 0/29/63/63 | 0/2/2/2 |
| 24 | BCR | C | 515 | - | - | 0/29/63/63 | 0/2/2/2 |
| 31 | DGD | C | 516 | - | - | 0/51/91/95 | 0/2/2/2 |
| 31 | DGD | C | 517 | - | - | 0/51/91/95 | 0/2/2/2 |
| 31 | DGD | C | 518 | - | - | 0/51/91/95 | 0/2/2/2 |
| 29 | LMG | C | 519 | - | - | 0/46/66/70 | 0/1/1/1 |
| 29 | LMG | C | 520 | - | - | 0/46/66/70 | 0/1/1/1 |
| 22 | CLA | D | 401 | - | 1/1/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | D | 402 | - | 1/1/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | D | 403 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | BCR | D | 404 | - | - | 0/29/63/63 | 0/2/2/2 |
| 32 | LHG | D | 405 | - | - | 0/53/53/53 | 0/0/0/0 |
| 29 | LMG | D | 406 | 34 | - | 0/46/66/70 | 0/1/1/1 |
| 32 | LHG | D | 407 | - | - | 0/53/53/53 | 0/0/0/0 |
| 28 | PL9 | D | 408 | - | - | 0/53/73/73 | 0/1/1/1 |
| 32 | LHG | D | 409 | - | - | 0/53/53/53 | 0/0/0/0 |
| 31 | DGD | D | 410 | - | - | 0/51/91/95 | 0/2/2/2 |
| 25 | SQD | D | 411 | - | - | 0/38/58/69 | 0/1/1/1 |
| 32 | LHG | E | 101 | - | - | 0/46/46/53 | 0/0/0/0 |
| 33 | HEM | F | 101 | 5,6 | - | 0/6/54/54 | 0/0/8/8 |
| 24 | BCR | H | 101 | - | - | 0/29/63/63 | 0/2/2/2 |
| 31 | DGD | H | 102 | - | - | 0/51/91/95 | 0/2/2/2 |
| 24 | BCR | K | 101 | - | - | 0/29/63/63 | 0/2/2/2 |
| 24 | BCR | K | 102 | - | - | 0/29/63/63 | 0/2/2/2 |
| 25 | SQD | L | 101 | - | - | 0/49/69/69 | 0/1/1/1 |
| 32 | LHG | L | 102 | - | - | 0/53/53/53 | 0/0/0/0 |
| 24 | BCR | T | 101 | - | - | 0/29/63/63 | 0/2/2/2 |
| 24 | BCR | T | 102 | - | - | 0/29/63/63 | 0/2/2/2 |
| 33 | HEM | V | 201 | 16 | - | 0/6/54/54 | 0/0/8/8 |
| 29 | LMG | Z | 101 | - | - | 1/31/51/70 | 0/1/1/1 |
| 20 | OEX | a | 601 | 1,3 | - | 0/0/68/68 | 0/0/6/6 |
| 22 | CLA | a | 603 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | a | 604 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|--------------|---------|
| 23 | PHO | a | 605 | - | - | 0/53/103/103 | 0/5/6/6 |
| 23 | PHO | a | 606 | - | - | 0/53/103/103 | 0/5/6/6 |
| 22 | CLA | a | 607 | - | 1/1/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | BCR | a | 608 | - | - | 0/29/63/63 | 0/2/2/2 |
| 25 | SQD | a | 609 | - | - | 0/49/69/69 | 0/1/1/1 |
| 27 | BCT | a | 612 | 21 | - | 0/0/0/0 | 0/0/0/0 |
| 28 | PL9 | a | 613 | - | - | 0/53/73/73 | 0/1/1/1 |
| 29 | LMG | a | 614 | - | - | 0/46/66/70 | 0/1/1/1 |
| 25 | SQD | b | 601 | - | - | 0/49/69/69 | 0/1/1/1 |
| 22 | CLA | b | 602 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | b | 603 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | b | 604 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | b | 605 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | b | 606 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | b | 607 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | b | 608 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | b | 609 | - | 1/1/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | b | 610 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | b | 611 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | b | 612 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | b | 613 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | b | 614 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | b | 615 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | b | 616 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | b | 617 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | BCR | b | 618 | - | - | 0/29/63/63 | 0/2/2/2 |
| 29 | LMG | b | 619 | - | - | 0/46/66/70 | 0/1/1/1 |
| 25 | SQD | b | 621 | - | - | 0/49/69/69 | 0/1/1/1 |
| 24 | BCR | b | 622 | - | - | 0/29/63/63 | 0/2/2/2 |
| 22 | CLA | c | 501 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | c | 502 | - | 1/1/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | c | 503 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | c | 504 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | c | 505 | - | 1/1/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | c | 506 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | c | 507 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | c | 508 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|--------------|---------|
| 22 | CLA | c | 509 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | c | 510 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | c | 511 | 3 | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | c | 512 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | c | 513 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | BCR | c | 514 | - | - | 0/29/63/63 | 0/2/2/2 |
| 24 | BCR | c | 515 | - | - | 0/29/63/63 | 0/2/2/2 |
| 31 | DGD | c | 516 | - | - | 0/51/91/95 | 0/2/2/2 |
| 31 | DGD | c | 517 | - | - | 0/51/91/95 | 0/2/2/2 |
| 31 | DGD | c | 518 | - | - | 0/51/91/95 | 0/2/2/2 |
| 29 | LMG | c | 519 | - | - | 0/46/66/70 | 0/1/1/1 |
| 29 | LMG | c | 520 | - | - | 0/46/66/70 | 0/1/1/1 |
| 22 | CLA | d | 401 | - | 1/1/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | d | 402 | - | 1/1/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | d | 403 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | BCR | d | 404 | - | - | 0/29/63/63 | 0/2/2/2 |
| 32 | LHG | d | 405 | - | - | 0/53/53/53 | 0/0/0/0 |
| 29 | LMG | d | 406 | 34 | - | 0/46/66/70 | 0/1/1/1 |
| 32 | LHG | d | 407 | - | - | 0/53/53/53 | 0/0/0/0 |
| 28 | PL9 | d | 408 | - | - | 0/53/73/73 | 0/1/1/1 |
| 32 | LHG | d | 409 | - | - | 0/53/53/53 | 0/0/0/0 |
| 31 | DGD | d | 410 | - | - | 0/51/91/95 | 0/2/2/2 |
| 25 | SQD | d | 411 | - | - | 0/38/58/69 | 0/1/1/1 |
| 32 | LHG | e | 101 | - | - | 0/46/46/53 | 0/0/0/0 |
| 33 | HEM | f | 101 | 5,6 | - | 0/6/54/54 | 0/0/8/8 |
| 24 | BCR | h | 101 | - | - | 0/29/63/63 | 0/2/2/2 |
| 31 | DGD | h | 102 | - | - | 0/51/91/95 | 0/2/2/2 |
| 24 | BCR | k | 101 | - | - | 0/29/63/63 | 0/2/2/2 |
| 24 | BCR | k | 102 | - | - | 0/29/63/63 | 0/2/2/2 |
| 25 | SQD | l | 101 | - | - | 0/49/69/69 | 0/1/1/1 |
| 25 | SQD | l | 102 | - | - | 0/49/69/69 | 0/1/1/1 |
| 32 | LHG | l | 103 | - | - | 0/53/53/53 | 0/0/0/0 |
| 24 | BCR | t | 101 | - | - | 0/29/63/63 | 0/2/2/2 |
| 33 | HEM | v | 201 | 16 | - | 0/6/54/54 | 0/0/8/8 |
| 29 | LMG | z | 101 | - | - | 1/31/51/70 | 0/1/1/1 |

All (1424) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 24 | C | 514 | BCR | C8-C9 | -8.70 | 1.27 | 1.45 |
| 24 | c | 514 | BCR | C8-C9 | -8.66 | 1.27 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24 | d | 404 | BCR | C8-C9 | -8.63 | 1.27 | 1.45 |
| 24 | C | 514 | BCR | C12-C13 | -8.62 | 1.27 | 1.45 |
| 24 | K | 102 | BCR | C8-C9 | -8.61 | 1.27 | 1.45 |
| 24 | k | 102 | BCR | C8-C9 | -8.60 | 1.27 | 1.45 |
| 24 | D | 404 | BCR | C8-C9 | -8.60 | 1.27 | 1.45 |
| 24 | c | 514 | BCR | C12-C13 | -8.59 | 1.27 | 1.45 |
| 24 | h | 101 | BCR | C19-C18 | -8.57 | 1.27 | 1.45 |
| 24 | H | 101 | BCR | C19-C18 | -8.55 | 1.27 | 1.45 |
| 24 | k | 101 | BCR | C19-C18 | -8.54 | 1.27 | 1.45 |
| 24 | B | 622 | BCR | C8-C9 | -8.54 | 1.27 | 1.45 |
| 24 | b | 622 | BCR | C8-C9 | -8.53 | 1.27 | 1.45 |
| 24 | c | 515 | BCR | C8-C9 | -8.52 | 1.27 | 1.45 |
| 24 | C | 515 | BCR | C8-C9 | -8.50 | 1.27 | 1.45 |
| 24 | K | 101 | BCR | C19-C18 | -8.49 | 1.27 | 1.45 |
| 24 | K | 101 | BCR | C8-C9 | -8.48 | 1.27 | 1.45 |
| 24 | T | 102 | BCR | C8-C9 | -8.46 | 1.27 | 1.45 |
| 24 | k | 101 | BCR | C8-C9 | -8.45 | 1.27 | 1.45 |
| 24 | t | 101 | BCR | C8-C9 | -8.44 | 1.27 | 1.45 |
| 24 | b | 622 | BCR | C12-C13 | -8.42 | 1.27 | 1.45 |
| 24 | c | 515 | BCR | C19-C18 | -8.39 | 1.27 | 1.45 |
| 24 | B | 622 | BCR | C12-C13 | -8.39 | 1.27 | 1.45 |
| 24 | D | 404 | BCR | C19-C18 | -8.39 | 1.27 | 1.45 |
| 24 | C | 514 | BCR | C19-C18 | -8.38 | 1.27 | 1.45 |
| 24 | d | 404 | BCR | C19-C18 | -8.37 | 1.27 | 1.45 |
| 24 | K | 101 | BCR | C12-C13 | -8.37 | 1.27 | 1.45 |
| 24 | t | 101 | BCR | C12-C13 | -8.37 | 1.27 | 1.45 |
| 24 | c | 514 | BCR | C19-C18 | -8.36 | 1.27 | 1.45 |
| 24 | B | 618 | BCR | C8-C9 | -8.36 | 1.27 | 1.45 |
| 24 | k | 101 | BCR | C12-C13 | -8.35 | 1.27 | 1.45 |
| 24 | T | 101 | BCR | C8-C9 | -8.35 | 1.27 | 1.45 |
| 24 | C | 515 | BCR | C12-C13 | -8.35 | 1.27 | 1.45 |
| 24 | C | 515 | BCR | C19-C18 | -8.34 | 1.27 | 1.45 |
| 24 | H | 101 | BCR | C12-C13 | -8.33 | 1.27 | 1.45 |
| 24 | T | 102 | BCR | C12-C13 | -8.33 | 1.27 | 1.45 |
| 24 | H | 101 | BCR | C8-C9 | -8.32 | 1.27 | 1.45 |
| 24 | h | 101 | BCR | C8-C9 | -8.32 | 1.27 | 1.45 |
| 24 | c | 515 | BCR | C12-C13 | -8.30 | 1.27 | 1.45 |
| 24 | h | 101 | BCR | C12-C13 | -8.30 | 1.27 | 1.45 |
| 24 | B | 619 | BCR | C8-C9 | -8.29 | 1.27 | 1.45 |
| 24 | b | 618 | BCR | C8-C9 | -8.28 | 1.27 | 1.45 |
| 24 | k | 102 | BCR | C19-C18 | -8.28 | 1.27 | 1.45 |
| 24 | K | 102 | BCR | C19-C18 | -8.27 | 1.27 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24 | a | 608 | BCR | C8-C9 | -8.27 | 1.28 | 1.45 |
| 24 | A | 608 | BCR | C8-C9 | -8.25 | 1.28 | 1.45 |
| 24 | b | 622 | BCR | C19-C18 | -8.24 | 1.28 | 1.45 |
| 24 | B | 622 | BCR | C19-C18 | -8.22 | 1.28 | 1.45 |
| 24 | d | 404 | BCR | C12-C13 | -8.21 | 1.28 | 1.45 |
| 24 | B | 619 | BCR | C19-C18 | -8.20 | 1.28 | 1.45 |
| 24 | D | 404 | BCR | C12-C13 | -8.19 | 1.28 | 1.45 |
| 24 | b | 618 | BCR | C19-C18 | -8.19 | 1.28 | 1.45 |
| 24 | k | 102 | BCR | C12-C13 | -8.17 | 1.28 | 1.45 |
| 24 | B | 618 | BCR | C12-C13 | -8.17 | 1.28 | 1.45 |
| 24 | T | 101 | BCR | C12-C13 | -8.16 | 1.28 | 1.45 |
| 24 | K | 102 | BCR | C12-C13 | -8.15 | 1.28 | 1.45 |
| 24 | A | 608 | BCR | C12-C13 | -8.12 | 1.28 | 1.45 |
| 24 | a | 608 | BCR | C12-C13 | -8.10 | 1.28 | 1.45 |
| 24 | A | 608 | BCR | C19-C18 | -8.09 | 1.28 | 1.45 |
| 24 | t | 101 | BCR | C19-C18 | -8.06 | 1.28 | 1.45 |
| 24 | b | 618 | BCR | C12-C13 | -8.06 | 1.28 | 1.45 |
| 24 | a | 608 | BCR | C19-C18 | -8.04 | 1.28 | 1.45 |
| 24 | B | 619 | BCR | C12-C13 | -8.04 | 1.28 | 1.45 |
| 24 | T | 102 | BCR | C19-C18 | -8.02 | 1.28 | 1.45 |
| 24 | B | 618 | BCR | C19-C18 | -7.96 | 1.28 | 1.45 |
| 24 | T | 101 | BCR | C19-C18 | -7.91 | 1.28 | 1.45 |
| 24 | d | 404 | BCR | C20-C21 | -7.75 | 1.19 | 1.43 |
| 24 | k | 101 | BCR | C20-C21 | -7.73 | 1.20 | 1.43 |
| 24 | D | 404 | BCR | C20-C21 | -7.73 | 1.20 | 1.43 |
| 24 | K | 101 | BCR | C20-C21 | -7.72 | 1.20 | 1.43 |
| 24 | C | 514 | BCR | C20-C21 | -7.71 | 1.20 | 1.43 |
| 24 | h | 101 | BCR | C20-C21 | -7.71 | 1.20 | 1.43 |
| 24 | c | 514 | BCR | C20-C21 | -7.70 | 1.20 | 1.43 |
| 24 | H | 101 | BCR | C20-C21 | -7.70 | 1.20 | 1.43 |
| 24 | c | 514 | BCR | C16-C17 | -7.68 | 1.20 | 1.43 |
| 24 | c | 515 | BCR | C16-C17 | -7.67 | 1.20 | 1.43 |
| 24 | C | 514 | BCR | C16-C17 | -7.66 | 1.20 | 1.43 |
| 24 | K | 101 | BCR | C16-C17 | -7.66 | 1.20 | 1.43 |
| 24 | C | 515 | BCR | C16-C17 | -7.65 | 1.20 | 1.43 |
| 24 | C | 515 | BCR | C20-C21 | -7.64 | 1.20 | 1.43 |
| 24 | c | 515 | BCR | C20-C21 | -7.62 | 1.20 | 1.43 |
| 24 | k | 101 | BCR | C16-C17 | -7.62 | 1.20 | 1.43 |
| 24 | k | 102 | BCR | C20-C21 | -7.59 | 1.20 | 1.43 |
| 24 | K | 102 | BCR | C20-C21 | -7.58 | 1.20 | 1.43 |
| 24 | d | 404 | BCR | C16-C17 | -7.55 | 1.20 | 1.43 |
| 24 | D | 404 | BCR | C16-C17 | -7.54 | 1.20 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24 | H | 101 | BCR | C16-C17 | -7.54 | 1.20 | 1.43 |
| 24 | B | 622 | BCR | C16-C17 | -7.54 | 1.20 | 1.43 |
| 24 | b | 622 | BCR | C16-C17 | -7.54 | 1.20 | 1.43 |
| 24 | h | 101 | BCR | C16-C17 | -7.53 | 1.20 | 1.43 |
| 24 | b | 622 | BCR | C20-C21 | -7.53 | 1.20 | 1.43 |
| 24 | A | 608 | BCR | C20-C21 | -7.53 | 1.20 | 1.43 |
| 24 | a | 608 | BCR | C20-C21 | -7.51 | 1.20 | 1.43 |
| 24 | B | 622 | BCR | C20-C21 | -7.50 | 1.20 | 1.43 |
| 24 | t | 101 | BCR | C16-C17 | -7.49 | 1.20 | 1.43 |
| 24 | b | 618 | BCR | C20-C21 | -7.49 | 1.20 | 1.43 |
| 24 | T | 102 | BCR | C16-C17 | -7.49 | 1.20 | 1.43 |
| 24 | B | 619 | BCR | C20-C21 | -7.46 | 1.20 | 1.43 |
| 24 | A | 608 | BCR | C16-C17 | -7.46 | 1.20 | 1.43 |
| 24 | K | 102 | BCR | C16-C17 | -7.45 | 1.20 | 1.43 |
| 24 | k | 102 | BCR | C16-C17 | -7.45 | 1.20 | 1.43 |
| 24 | a | 608 | BCR | C16-C17 | -7.45 | 1.20 | 1.43 |
| 24 | t | 101 | BCR | C20-C21 | -7.43 | 1.20 | 1.43 |
| 24 | T | 102 | BCR | C20-C21 | -7.42 | 1.21 | 1.43 |
| 24 | B | 618 | BCR | C20-C21 | -7.40 | 1.21 | 1.43 |
| 24 | T | 101 | BCR | C20-C21 | -7.37 | 1.21 | 1.43 |
| 24 | T | 101 | BCR | C16-C17 | -7.31 | 1.21 | 1.43 |
| 24 | B | 618 | BCR | C16-C17 | -7.30 | 1.21 | 1.43 |
| 24 | B | 619 | BCR | C16-C17 | -7.29 | 1.21 | 1.43 |
| 24 | b | 618 | BCR | C16-C17 | -7.29 | 1.21 | 1.43 |
| 24 | c | 515 | BCR | C21-C22 | -6.38 | 1.27 | 1.35 |
| 24 | k | 101 | BCR | C21-C22 | -6.36 | 1.27 | 1.35 |
| 24 | K | 101 | BCR | C21-C22 | -6.33 | 1.27 | 1.35 |
| 24 | C | 515 | BCR | C21-C22 | -6.31 | 1.27 | 1.35 |
| 24 | D | 404 | BCR | C21-C22 | -6.27 | 1.27 | 1.35 |
| 24 | h | 101 | BCR | C21-C22 | -6.26 | 1.27 | 1.35 |
| 24 | d | 404 | BCR | C21-C22 | -6.26 | 1.27 | 1.35 |
| 24 | H | 101 | BCR | C21-C22 | -6.25 | 1.27 | 1.35 |
| 24 | B | 622 | BCR | C21-C22 | -6.25 | 1.27 | 1.35 |
| 24 | k | 102 | BCR | C21-C22 | -6.23 | 1.27 | 1.35 |
| 24 | K | 102 | BCR | C21-C22 | -6.23 | 1.27 | 1.35 |
| 24 | C | 514 | BCR | C17-C18 | -6.23 | 1.27 | 1.35 |
| 24 | c | 514 | BCR | C17-C18 | -6.21 | 1.27 | 1.35 |
| 24 | b | 622 | BCR | C21-C22 | -6.20 | 1.27 | 1.35 |
| 24 | K | 101 | BCR | C17-C18 | -6.18 | 1.27 | 1.35 |
| 24 | k | 101 | BCR | C17-C18 | -6.18 | 1.27 | 1.35 |
| 24 | B | 622 | BCR | C16-C15 | -6.17 | 1.19 | 1.35 |
| 24 | b | 622 | BCR | C16-C15 | -6.16 | 1.19 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24 | c | 514 | BCR | C16-C15 | -6.15 | 1.19 | 1.35 |
| 24 | c | 514 | BCR | C21-C22 | -6.14 | 1.27 | 1.35 |
| 24 | C | 514 | BCR | C21-C22 | -6.13 | 1.27 | 1.35 |
| 24 | B | 619 | BCR | C21-C22 | -6.12 | 1.27 | 1.35 |
| 24 | C | 514 | BCR | C16-C15 | -6.12 | 1.20 | 1.35 |
| 24 | b | 618 | BCR | C21-C22 | -6.09 | 1.27 | 1.35 |
| 24 | A | 608 | BCR | C17-C18 | -6.09 | 1.27 | 1.35 |
| 24 | a | 608 | BCR | C17-C18 | -6.07 | 1.27 | 1.35 |
| 24 | C | 515 | BCR | C16-C15 | -6.04 | 1.20 | 1.35 |
| 24 | k | 101 | BCR | C16-C15 | -6.03 | 1.20 | 1.35 |
| 24 | c | 515 | BCR | C16-C15 | -6.03 | 1.20 | 1.35 |
| 24 | K | 101 | BCR | C16-C15 | -6.02 | 1.20 | 1.35 |
| 24 | C | 515 | BCR | C17-C18 | -6.00 | 1.27 | 1.35 |
| 24 | T | 102 | BCR | C21-C22 | -5.99 | 1.27 | 1.35 |
| 24 | d | 404 | BCR | C17-C18 | -5.99 | 1.27 | 1.35 |
| 24 | t | 101 | BCR | C21-C22 | -5.99 | 1.27 | 1.35 |
| 24 | D | 404 | BCR | C17-C18 | -5.98 | 1.27 | 1.35 |
| 24 | b | 622 | BCR | C17-C18 | -5.97 | 1.27 | 1.35 |
| 24 | B | 622 | BCR | C17-C18 | -5.96 | 1.27 | 1.35 |
| 24 | a | 608 | BCR | C16-C15 | -5.94 | 1.20 | 1.35 |
| 24 | c | 515 | BCR | C17-C18 | -5.93 | 1.27 | 1.35 |
| 24 | h | 101 | BCR | C16-C15 | -5.93 | 1.20 | 1.35 |
| 24 | B | 618 | BCR | C16-C15 | -5.92 | 1.20 | 1.35 |
| 24 | H | 101 | BCR | C16-C15 | -5.91 | 1.20 | 1.35 |
| 24 | A | 608 | BCR | C16-C15 | -5.91 | 1.20 | 1.35 |
| 24 | T | 101 | BCR | C21-C22 | -5.90 | 1.28 | 1.35 |
| 24 | H | 101 | BCR | C17-C18 | -5.90 | 1.28 | 1.35 |
| 24 | T | 101 | BCR | C16-C15 | -5.90 | 1.20 | 1.35 |
| 24 | D | 404 | BCR | C16-C15 | -5.89 | 1.20 | 1.35 |
| 24 | K | 102 | BCR | C17-C18 | -5.89 | 1.28 | 1.35 |
| 24 | k | 102 | BCR | C17-C18 | -5.89 | 1.28 | 1.35 |
| 24 | d | 404 | BCR | C16-C15 | -5.89 | 1.20 | 1.35 |
| 24 | k | 102 | BCR | C16-C15 | -5.88 | 1.20 | 1.35 |
| 24 | K | 102 | BCR | C16-C15 | -5.88 | 1.20 | 1.35 |
| 24 | h | 101 | BCR | C17-C18 | -5.88 | 1.28 | 1.35 |
| 24 | T | 102 | BCR | C16-C15 | -5.88 | 1.20 | 1.35 |
| 24 | A | 608 | BCR | C21-C22 | -5.87 | 1.28 | 1.35 |
| 24 | t | 101 | BCR | C16-C15 | -5.86 | 1.20 | 1.35 |
| 24 | a | 608 | BCR | C21-C22 | -5.83 | 1.28 | 1.35 |
| 24 | B | 618 | BCR | C21-C22 | -5.82 | 1.28 | 1.35 |
| 24 | c | 514 | BCR | C11-C12 | -5.79 | 1.19 | 1.34 |
| 24 | k | 101 | BCR | C11-C12 | -5.77 | 1.19 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24 | C | 514 | BCR | C11-C12 | -5.76 | 1.19 | 1.34 |
| 24 | K | 101 | BCR | C11-C12 | -5.75 | 1.19 | 1.34 |
| 24 | a | 608 | BCR | C20-C19 | -5.75 | 1.19 | 1.34 |
| 24 | C | 515 | BCR | C20-C19 | -5.73 | 1.19 | 1.34 |
| 24 | D | 404 | BCR | C20-C19 | -5.71 | 1.20 | 1.34 |
| 24 | c | 515 | BCR | C20-C19 | -5.70 | 1.20 | 1.34 |
| 24 | A | 608 | BCR | C20-C19 | -5.70 | 1.20 | 1.34 |
| 24 | K | 101 | BCR | C20-C19 | -5.70 | 1.20 | 1.34 |
| 24 | T | 102 | BCR | C17-C18 | -5.69 | 1.28 | 1.35 |
| 24 | T | 102 | BCR | C11-C12 | -5.69 | 1.20 | 1.34 |
| 24 | t | 101 | BCR | C17-C18 | -5.68 | 1.28 | 1.35 |
| 24 | h | 101 | BCR | C20-C19 | -5.66 | 1.20 | 1.34 |
| 24 | H | 101 | BCR | C20-C19 | -5.66 | 1.20 | 1.34 |
| 24 | b | 622 | BCR | C11-C12 | -5.65 | 1.20 | 1.34 |
| 24 | t | 101 | BCR | C11-C12 | -5.65 | 1.20 | 1.34 |
| 24 | k | 101 | BCR | C20-C19 | -5.65 | 1.20 | 1.34 |
| 24 | d | 404 | BCR | C20-C19 | -5.65 | 1.20 | 1.34 |
| 24 | B | 622 | BCR | C11-C12 | -5.65 | 1.20 | 1.34 |
| 24 | c | 514 | BCR | C20-C19 | -5.65 | 1.20 | 1.34 |
| 24 | C | 514 | BCR | C20-C19 | -5.63 | 1.20 | 1.34 |
| 24 | D | 404 | BCR | C11-C12 | -5.62 | 1.20 | 1.34 |
| 24 | d | 404 | BCR | C11-C12 | -5.62 | 1.20 | 1.34 |
| 24 | B | 622 | BCR | C20-C19 | -5.57 | 1.20 | 1.34 |
| 24 | c | 515 | BCR | C11-C12 | -5.56 | 1.20 | 1.34 |
| 24 | T | 101 | BCR | C17-C18 | -5.55 | 1.28 | 1.35 |
| 24 | b | 622 | BCR | C20-C19 | -5.55 | 1.20 | 1.34 |
| 24 | h | 101 | BCR | C11-C12 | -5.54 | 1.20 | 1.34 |
| 24 | B | 618 | BCR | C17-C18 | -5.53 | 1.28 | 1.35 |
| 24 | K | 102 | BCR | C20-C19 | -5.53 | 1.20 | 1.34 |
| 24 | K | 102 | BCR | C11-C12 | -5.52 | 1.20 | 1.34 |
| 24 | C | 515 | BCR | C11-C12 | -5.52 | 1.20 | 1.34 |
| 24 | H | 101 | BCR | C11-C12 | -5.52 | 1.20 | 1.34 |
| 24 | k | 102 | BCR | C20-C19 | -5.52 | 1.20 | 1.34 |
| 24 | k | 102 | BCR | C11-C12 | -5.50 | 1.20 | 1.34 |
| 24 | B | 619 | BCR | C16-C15 | -5.49 | 1.21 | 1.35 |
| 24 | T | 102 | BCR | C20-C19 | -5.49 | 1.20 | 1.34 |
| 24 | b | 618 | BCR | C16-C15 | -5.47 | 1.21 | 1.35 |
| 24 | t | 101 | BCR | C20-C19 | -5.46 | 1.20 | 1.34 |
| 24 | C | 514 | BCR | C11-C10 | -5.45 | 1.27 | 1.43 |
| 24 | c | 514 | BCR | C11-C10 | -5.42 | 1.27 | 1.43 |
| 24 | b | 618 | BCR | C20-C19 | -5.40 | 1.20 | 1.34 |
| 24 | B | 619 | BCR | C20-C19 | -5.38 | 1.20 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24 | b | 618 | BCR | C11-C12 | -5.38 | 1.20 | 1.34 |
| 24 | B | 619 | BCR | C11-C12 | -5.37 | 1.20 | 1.34 |
| 24 | H | 101 | BCR | C11-C10 | -5.37 | 1.27 | 1.43 |
| 24 | h | 101 | BCR | C11-C10 | -5.36 | 1.27 | 1.43 |
| 24 | d | 404 | BCR | C11-C10 | -5.35 | 1.27 | 1.43 |
| 24 | D | 404 | BCR | C11-C10 | -5.35 | 1.27 | 1.43 |
| 24 | B | 618 | BCR | C11-C12 | -5.34 | 1.20 | 1.34 |
| 24 | C | 515 | BCR | C11-C10 | -5.33 | 1.27 | 1.43 |
| 24 | a | 608 | BCR | C11-C12 | -5.33 | 1.21 | 1.34 |
| 24 | b | 618 | BCR | C17-C18 | -5.33 | 1.28 | 1.35 |
| 24 | B | 619 | BCR | C17-C18 | -5.32 | 1.28 | 1.35 |
| 24 | T | 101 | BCR | C11-C12 | -5.31 | 1.21 | 1.34 |
| 24 | c | 515 | BCR | C11-C10 | -5.31 | 1.27 | 1.43 |
| 24 | A | 608 | BCR | C11-C12 | -5.30 | 1.21 | 1.34 |
| 24 | b | 622 | BCR | C11-C10 | -5.28 | 1.27 | 1.43 |
| 24 | B | 622 | BCR | C11-C10 | -5.27 | 1.27 | 1.43 |
| 24 | K | 101 | BCR | C11-C10 | -5.27 | 1.27 | 1.43 |
| 24 | C | 514 | BCR | C15-C14 | -5.27 | 1.27 | 1.43 |
| 24 | k | 101 | BCR | C11-C10 | -5.26 | 1.27 | 1.43 |
| 24 | c | 514 | BCR | C15-C14 | -5.24 | 1.27 | 1.43 |
| 24 | B | 622 | BCR | C15-C14 | -5.22 | 1.27 | 1.43 |
| 24 | A | 608 | BCR | C11-C10 | -5.22 | 1.27 | 1.43 |
| 24 | C | 515 | BCR | C15-C14 | -5.21 | 1.27 | 1.43 |
| 24 | b | 622 | BCR | C15-C14 | -5.21 | 1.27 | 1.43 |
| 24 | a | 608 | BCR | C11-C10 | -5.20 | 1.27 | 1.43 |
| 24 | H | 101 | BCR | C15-C14 | -5.20 | 1.27 | 1.43 |
| 24 | c | 515 | BCR | C15-C14 | -5.20 | 1.27 | 1.43 |
| 24 | h | 101 | BCR | C15-C14 | -5.19 | 1.27 | 1.43 |
| 24 | k | 102 | BCR | C11-C10 | -5.18 | 1.27 | 1.43 |
| 24 | K | 102 | BCR | C11-C10 | -5.18 | 1.27 | 1.43 |
| 24 | T | 102 | BCR | C11-C10 | -5.16 | 1.27 | 1.43 |
| 24 | T | 101 | BCR | C11-C10 | -5.16 | 1.27 | 1.43 |
| 24 | k | 101 | BCR | C15-C14 | -5.15 | 1.27 | 1.43 |
| 24 | K | 101 | BCR | C15-C14 | -5.15 | 1.27 | 1.43 |
| 24 | d | 404 | BCR | C15-C14 | -5.14 | 1.27 | 1.43 |
| 24 | t | 101 | BCR | C11-C10 | -5.14 | 1.27 | 1.43 |
| 24 | B | 618 | BCR | C11-C10 | -5.14 | 1.27 | 1.43 |
| 24 | D | 404 | BCR | C15-C14 | -5.14 | 1.27 | 1.43 |
| 24 | t | 101 | BCR | C15-C14 | -5.14 | 1.27 | 1.43 |
| 24 | T | 102 | BCR | C15-C14 | -5.14 | 1.27 | 1.43 |
| 24 | T | 101 | BCR | C20-C19 | -5.13 | 1.21 | 1.34 |
| 24 | k | 102 | BCR | C15-C14 | -5.10 | 1.28 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24 | B | 618 | BCR | C20-C19 | -5.09 | 1.21 | 1.34 |
| 24 | K | 102 | BCR | C15-C14 | -5.08 | 1.28 | 1.43 |
| 24 | A | 608 | BCR | C15-C14 | -5.06 | 1.28 | 1.43 |
| 24 | B | 619 | BCR | C11-C10 | -5.05 | 1.28 | 1.43 |
| 24 | b | 618 | BCR | C11-C10 | -5.04 | 1.28 | 1.43 |
| 24 | a | 608 | BCR | C15-C14 | -5.03 | 1.28 | 1.43 |
| 24 | B | 619 | BCR | C15-C14 | -4.89 | 1.28 | 1.43 |
| 24 | b | 618 | BCR | C15-C14 | -4.88 | 1.28 | 1.43 |
| 24 | B | 622 | BCR | C23-C22 | -4.86 | 1.35 | 1.45 |
| 24 | B | 618 | BCR | C15-C14 | -4.86 | 1.28 | 1.43 |
| 24 | C | 515 | BCR | C23-C22 | -4.86 | 1.35 | 1.45 |
| 24 | T | 101 | BCR | C15-C14 | -4.85 | 1.28 | 1.43 |
| 24 | b | 622 | BCR | C23-C22 | -4.85 | 1.35 | 1.45 |
| 24 | c | 515 | BCR | C23-C22 | -4.81 | 1.35 | 1.45 |
| 24 | D | 404 | BCR | C23-C22 | -4.75 | 1.35 | 1.45 |
| 24 | d | 404 | BCR | C23-C22 | -4.75 | 1.35 | 1.45 |
| 24 | K | 101 | BCR | C23-C22 | -4.71 | 1.35 | 1.45 |
| 24 | T | 101 | BCR | C23-C22 | -4.71 | 1.35 | 1.45 |
| 24 | B | 618 | BCR | C23-C22 | -4.70 | 1.35 | 1.45 |
| 24 | K | 102 | BCR | C23-C22 | -4.69 | 1.35 | 1.45 |
| 24 | k | 101 | BCR | C23-C22 | -4.69 | 1.35 | 1.45 |
| 24 | C | 514 | BCR | C23-C22 | -4.68 | 1.35 | 1.45 |
| 24 | H | 101 | BCR | C23-C22 | -4.67 | 1.35 | 1.45 |
| 24 | k | 102 | BCR | C23-C22 | -4.67 | 1.35 | 1.45 |
| 24 | c | 514 | BCR | C23-C22 | -4.66 | 1.35 | 1.45 |
| 24 | h | 101 | BCR | C23-C22 | -4.63 | 1.35 | 1.45 |
| 24 | b | 618 | BCR | C23-C22 | -4.50 | 1.36 | 1.45 |
| 24 | B | 619 | BCR | C23-C22 | -4.49 | 1.36 | 1.45 |
| 24 | T | 102 | BCR | C23-C22 | -4.43 | 1.36 | 1.45 |
| 24 | t | 101 | BCR | C23-C22 | -4.43 | 1.36 | 1.45 |
| 24 | a | 608 | BCR | C23-C22 | -4.38 | 1.36 | 1.45 |
| 23 | a | 606 | PHO | C1A-NA | -4.37 | 1.28 | 1.37 |
| 23 | A | 606 | PHO | C1A-NA | -4.34 | 1.28 | 1.37 |
| 24 | A | 608 | BCR | C23-C22 | -4.34 | 1.36 | 1.45 |
| 33 | v | 201 | HEM | C3C-C2C | -4.29 | 1.34 | 1.40 |
| 33 | V | 201 | HEM | C3C-C2C | -4.29 | 1.34 | 1.40 |
| 23 | a | 605 | PHO | C1A-NA | -4.16 | 1.28 | 1.37 |
| 23 | A | 605 | PHO | C1A-NA | -4.16 | 1.28 | 1.37 |
| 33 | f | 101 | HEM | C3C-C2C | -4.09 | 1.34 | 1.40 |
| 33 | F | 101 | HEM | C3C-C2C | -4.07 | 1.34 | 1.40 |
| 33 | f | 101 | HEM | C3B-C2B | -3.97 | 1.34 | 1.40 |
| 33 | F | 101 | HEM | C3B-C2B | -3.94 | 1.34 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 33 | v | 201 | HEM | C3B-C2B | -3.92 | 1.34 | 1.40 |
| 33 | V | 201 | HEM | C3B-C2B | -3.86 | 1.35 | 1.40 |
| 22 | b | 612 | CLA | C4A-NA | -3.82 | 1.32 | 1.38 |
| 22 | B | 612 | CLA | C4A-NA | -3.82 | 1.32 | 1.38 |
| 22 | D | 401 | CLA | C4A-NA | -3.60 | 1.32 | 1.38 |
| 22 | d | 401 | CLA | C4A-NA | -3.57 | 1.32 | 1.38 |
| 22 | a | 604 | CLA | C4A-NA | -3.32 | 1.33 | 1.38 |
| 22 | A | 604 | CLA | C4A-NA | -3.28 | 1.33 | 1.38 |
| 22 | c | 512 | CLA | C4A-NA | -3.28 | 1.33 | 1.38 |
| 22 | C | 512 | CLA | C4A-NA | -3.27 | 1.33 | 1.38 |
| 22 | c | 509 | CLA | C4A-NA | -3.13 | 1.33 | 1.38 |
| 22 | B | 611 | CLA | C4A-NA | -3.12 | 1.33 | 1.38 |
| 22 | b | 611 | CLA | C4A-NA | -3.11 | 1.33 | 1.38 |
| 22 | C | 509 | CLA | C4A-NA | -3.11 | 1.33 | 1.38 |
| 22 | c | 513 | CLA | C4A-NA | -3.09 | 1.33 | 1.38 |
| 22 | C | 513 | CLA | C4A-NA | -3.09 | 1.33 | 1.38 |
| 22 | b | 608 | CLA | C4A-NA | -3.06 | 1.33 | 1.38 |
| 22 | b | 602 | CLA | C4A-NA | -3.06 | 1.33 | 1.38 |
| 22 | B | 608 | CLA | C4A-NA | -3.06 | 1.33 | 1.38 |
| 22 | B | 602 | CLA | C4A-NA | -3.05 | 1.33 | 1.38 |
| 22 | b | 616 | CLA | C4A-NA | -3.01 | 1.33 | 1.38 |
| 22 | B | 616 | CLA | C4A-NA | -3.00 | 1.33 | 1.38 |
| 22 | b | 607 | CLA | C4A-NA | -2.95 | 1.33 | 1.38 |
| 22 | B | 607 | CLA | C4A-NA | -2.92 | 1.33 | 1.38 |
| 22 | d | 403 | CLA | C4A-NA | -2.89 | 1.33 | 1.38 |
| 22 | D | 403 | CLA | C4A-NA | -2.89 | 1.33 | 1.38 |
| 22 | A | 603 | CLA | C4A-NA | -2.87 | 1.33 | 1.38 |
| 22 | B | 604 | CLA | C4A-NA | -2.86 | 1.33 | 1.38 |
| 22 | a | 603 | CLA | C4A-NA | -2.86 | 1.33 | 1.38 |
| 22 | C | 501 | CLA | C4A-NA | -2.84 | 1.33 | 1.38 |
| 22 | D | 402 | CLA | C4A-NA | -2.84 | 1.33 | 1.38 |
| 23 | A | 606 | PHO | C3D-C4D | -2.82 | 1.34 | 1.43 |
| 22 | c | 504 | CLA | C4A-NA | -2.82 | 1.33 | 1.38 |
| 22 | d | 402 | CLA | C4A-NA | -2.82 | 1.33 | 1.38 |
| 22 | b | 604 | CLA | C4A-NA | -2.81 | 1.33 | 1.38 |
| 22 | c | 501 | CLA | C4A-NA | -2.81 | 1.33 | 1.38 |
| 22 | B | 606 | CLA | C4A-NA | -2.81 | 1.33 | 1.38 |
| 22 | b | 613 | CLA | C4A-NA | -2.79 | 1.33 | 1.38 |
| 22 | b | 606 | CLA | C4A-NA | -2.79 | 1.33 | 1.38 |
| 23 | a | 606 | PHO | C3D-C4D | -2.79 | 1.34 | 1.43 |
| 22 | c | 506 | CLA | C4A-NA | -2.79 | 1.33 | 1.38 |
| 22 | C | 504 | CLA | C4A-NA | -2.78 | 1.33 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | B | 613 | CLA | C4A-NA | -2.77 | 1.33 | 1.38 |
| 22 | c | 503 | CLA | C4A-NA | -2.76 | 1.33 | 1.38 |
| 22 | C | 506 | CLA | C4A-NA | -2.76 | 1.33 | 1.38 |
| 22 | C | 503 | CLA | C4A-NA | -2.76 | 1.33 | 1.38 |
| 22 | C | 502 | CLA | C4A-NA | -2.76 | 1.33 | 1.38 |
| 22 | b | 609 | CLA | C4A-NA | -2.76 | 1.33 | 1.38 |
| 22 | B | 609 | CLA | C4A-NA | -2.75 | 1.33 | 1.38 |
| 22 | c | 510 | CLA | C4A-NA | -2.74 | 1.34 | 1.38 |
| 22 | c | 502 | CLA | C4A-NA | -2.74 | 1.34 | 1.38 |
| 23 | a | 605 | PHO | C3D-C4D | -2.72 | 1.34 | 1.43 |
| 22 | B | 615 | CLA | C4A-NA | -2.72 | 1.34 | 1.38 |
| 23 | A | 605 | PHO | C3D-C4D | -2.71 | 1.35 | 1.43 |
| 22 | C | 510 | CLA | C4A-NA | -2.70 | 1.34 | 1.38 |
| 22 | b | 615 | CLA | C4A-NA | -2.70 | 1.34 | 1.38 |
| 22 | C | 508 | CLA | C4A-NA | -2.69 | 1.34 | 1.38 |
| 22 | c | 508 | CLA | C4A-NA | -2.67 | 1.34 | 1.38 |
| 25 | A | 609 | SQD | C6-S | -2.63 | 1.67 | 1.77 |
| 25 | a | 609 | SQD | C6-S | -2.62 | 1.67 | 1.77 |
| 22 | B | 605 | CLA | C4A-NA | -2.62 | 1.34 | 1.38 |
| 22 | b | 605 | CLA | C4A-NA | -2.61 | 1.34 | 1.38 |
| 24 | k | 102 | BCR | C24-C25 | -2.60 | 1.35 | 1.45 |
| 24 | c | 515 | BCR | C24-C25 | -2.60 | 1.35 | 1.45 |
| 24 | K | 102 | BCR | C24-C25 | -2.60 | 1.35 | 1.45 |
| 22 | c | 505 | CLA | C4A-NA | -2.60 | 1.34 | 1.38 |
| 24 | C | 515 | BCR | C24-C25 | -2.57 | 1.36 | 1.45 |
| 24 | c | 514 | BCR | C24-C25 | -2.57 | 1.36 | 1.45 |
| 24 | h | 101 | BCR | C24-C25 | -2.57 | 1.36 | 1.45 |
| 22 | C | 507 | CLA | C4A-NA | -2.56 | 1.34 | 1.38 |
| 24 | H | 101 | BCR | C24-C25 | -2.56 | 1.36 | 1.45 |
| 22 | b | 603 | CLA | C4A-NA | -2.56 | 1.34 | 1.38 |
| 24 | C | 514 | BCR | C24-C25 | -2.56 | 1.36 | 1.45 |
| 22 | C | 505 | CLA | C4A-NA | -2.56 | 1.34 | 1.38 |
| 25 | b | 601 | SQD | C6-S | -2.55 | 1.67 | 1.77 |
| 24 | k | 101 | BCR | C24-C25 | -2.54 | 1.36 | 1.45 |
| 24 | K | 101 | BCR | C24-C25 | -2.54 | 1.36 | 1.45 |
| 25 | B | 601 | SQD | C6-S | -2.53 | 1.67 | 1.77 |
| 24 | t | 101 | BCR | C24-C25 | -2.52 | 1.36 | 1.45 |
| 22 | a | 607 | CLA | C4A-NA | -2.51 | 1.34 | 1.38 |
| 25 | d | 411 | SQD | C6-S | -2.51 | 1.67 | 1.77 |
| 24 | B | 618 | BCR | C24-C25 | -2.51 | 1.36 | 1.45 |
| 24 | T | 101 | BCR | C24-C25 | -2.50 | 1.36 | 1.45 |
| 25 | D | 411 | SQD | C6-S | -2.50 | 1.67 | 1.77 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | B | 614 | CLA | C4A-NA | -2.50 | 1.34 | 1.38 |
| 24 | T | 102 | BCR | C24-C25 | -2.49 | 1.36 | 1.45 |
| 22 | c | 507 | CLA | C4A-NA | -2.48 | 1.34 | 1.38 |
| 22 | A | 607 | CLA | C4A-NA | -2.48 | 1.34 | 1.38 |
| 22 | c | 511 | CLA | C4A-NA | -2.48 | 1.34 | 1.38 |
| 24 | D | 404 | BCR | C24-C25 | -2.48 | 1.36 | 1.45 |
| 22 | B | 603 | CLA | C4A-NA | -2.47 | 1.34 | 1.38 |
| 24 | d | 404 | BCR | C24-C25 | -2.47 | 1.36 | 1.45 |
| 22 | C | 511 | CLA | C4A-NA | -2.45 | 1.34 | 1.38 |
| 22 | b | 614 | CLA | C4A-NA | -2.45 | 1.34 | 1.38 |
| 24 | a | 608 | BCR | C24-C25 | -2.45 | 1.36 | 1.45 |
| 24 | A | 608 | BCR | C24-C25 | -2.44 | 1.36 | 1.45 |
| 24 | b | 622 | BCR | C24-C25 | -2.42 | 1.36 | 1.45 |
| 22 | b | 610 | CLA | C4A-NA | -2.42 | 1.34 | 1.38 |
| 22 | B | 610 | CLA | C4A-NA | -2.42 | 1.34 | 1.38 |
| 22 | b | 617 | CLA | C4A-NA | -2.41 | 1.34 | 1.38 |
| 25 | l | 102 | SQD | C6-S | -2.40 | 1.68 | 1.77 |
| 25 | b | 621 | SQD | C6-S | -2.39 | 1.68 | 1.77 |
| 24 | B | 622 | BCR | C24-C25 | -2.39 | 1.36 | 1.45 |
| 22 | B | 617 | CLA | C4A-NA | -2.38 | 1.34 | 1.38 |
| 25 | L | 101 | SQD | C6-S | -2.32 | 1.68 | 1.77 |
| 24 | b | 618 | BCR | C24-C25 | -2.32 | 1.36 | 1.45 |
| 25 | l | 101 | SQD | C6-S | -2.31 | 1.68 | 1.77 |
| 24 | B | 619 | BCR | C24-C25 | -2.31 | 1.37 | 1.45 |
| 22 | c | 509 | CLA | C4C-NC | -2.25 | 1.34 | 1.37 |
| 22 | C | 509 | CLA | C4C-NC | -2.19 | 1.34 | 1.37 |
| 23 | a | 606 | PHO | CHB-C4A | -2.06 | 1.34 | 1.40 |
| 31 | C | 518 | DGD | O2G-C2G | -2.06 | 1.41 | 1.46 |
| 23 | A | 606 | PHO | CHB-C4A | -2.06 | 1.34 | 1.40 |
| 31 | c | 518 | DGD | O2G-C2G | -2.05 | 1.41 | 1.46 |
| 24 | c | 514 | BCR | C8-C7 | -2.03 | 1.26 | 1.33 |
| 24 | C | 514 | BCR | C8-C7 | -2.01 | 1.26 | 1.33 |
| 22 | B | 611 | CLA | C1C-C2C | 2.00 | 1.48 | 1.44 |
| 23 | A | 606 | PHO | C4C-C3C | 2.00 | 1.48 | 1.45 |
| 22 | B | 606 | CLA | CHD-C4C | 2.00 | 1.46 | 1.41 |
| 22 | B | 606 | CLA | C1C-C2C | 2.00 | 1.48 | 1.44 |
| 22 | D | 402 | CLA | C1C-C2C | 2.01 | 1.48 | 1.44 |
| 31 | c | 516 | DGD | O5D-C1E | 2.01 | 1.43 | 1.40 |
| 23 | a | 606 | PHO | C4C-C3C | 2.01 | 1.48 | 1.45 |
| 22 | d | 402 | CLA | C1C-C2C | 2.01 | 1.48 | 1.44 |
| 22 | B | 602 | CLA | C4C-C3C | 2.02 | 1.48 | 1.45 |
| 22 | b | 616 | CLA | C4C-C3C | 2.03 | 1.48 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22 | C | 504 | CLA | CHB-C4A | 2.03 | 1.35 | 1.33 |
| 22 | b | 605 | CLA | C1C-C2C | 2.03 | 1.48 | 1.44 |
| 22 | D | 402 | CLA | CHD-C4C | 2.03 | 1.47 | 1.41 |
| 22 | B | 616 | CLA | C4C-C3C | 2.03 | 1.48 | 1.45 |
| 22 | d | 402 | CLA | CHD-C4C | 2.03 | 1.47 | 1.41 |
| 22 | c | 502 | CLA | C1C-C2C | 2.04 | 1.48 | 1.44 |
| 22 | C | 502 | CLA | C1C-C2C | 2.04 | 1.48 | 1.44 |
| 22 | B | 605 | CLA | C1C-C2C | 2.05 | 1.48 | 1.44 |
| 22 | D | 401 | CLA | C1C-C2C | 2.05 | 1.48 | 1.44 |
| 31 | D | 410 | DGD | O3G-C1D | 2.05 | 1.43 | 1.40 |
| 33 | V | 201 | HEM | CMA-C3A | 2.05 | 1.55 | 1.51 |
| 22 | c | 504 | CLA | CHB-C4A | 2.05 | 1.35 | 1.33 |
| 22 | b | 606 | CLA | C1C-C2C | 2.06 | 1.48 | 1.44 |
| 22 | b | 615 | CLA | C1C-C2C | 2.06 | 1.48 | 1.44 |
| 22 | b | 610 | CLA | CHD-C4C | 2.06 | 1.47 | 1.41 |
| 22 | b | 612 | CLA | CHD-C4C | 2.06 | 1.47 | 1.41 |
| 22 | d | 401 | CLA | C1C-C2C | 2.06 | 1.48 | 1.44 |
| 22 | b | 613 | CLA | C1C-C2C | 2.07 | 1.48 | 1.44 |
| 25 | L | 101 | SQD | O6-C1 | 2.07 | 1.43 | 1.40 |
| 22 | d | 401 | CLA | C4C-C3C | 2.08 | 1.48 | 1.45 |
| 33 | v | 201 | HEM | CMA-C3A | 2.08 | 1.55 | 1.51 |
| 22 | D | 401 | CLA | CHD-C4C | 2.08 | 1.47 | 1.41 |
| 25 | b | 621 | SQD | O6-C1 | 2.08 | 1.43 | 1.40 |
| 22 | B | 613 | CLA | C1C-C2C | 2.09 | 1.48 | 1.44 |
| 22 | B | 612 | CLA | CHD-C4C | 2.09 | 1.47 | 1.41 |
| 22 | C | 502 | CLA | CHD-C4C | 2.09 | 1.47 | 1.41 |
| 22 | c | 502 | CLA | CHD-C4C | 2.10 | 1.47 | 1.41 |
| 22 | B | 615 | CLA | C1C-C2C | 2.10 | 1.48 | 1.44 |
| 22 | B | 610 | CLA | CHD-C4C | 2.10 | 1.47 | 1.41 |
| 22 | C | 505 | CLA | C4C-C3C | 2.10 | 1.48 | 1.45 |
| 22 | d | 401 | CLA | CHD-C4C | 2.10 | 1.47 | 1.41 |
| 25 | l | 102 | SQD | O6-C1 | 2.10 | 1.43 | 1.40 |
| 29 | C | 520 | LMG | O1-C1 | 2.11 | 1.43 | 1.40 |
| 22 | D | 401 | CLA | C4C-C3C | 2.12 | 1.48 | 1.45 |
| 31 | d | 410 | DGD | O3G-C1D | 2.12 | 1.43 | 1.40 |
| 22 | b | 617 | CLA | CHD-C4C | 2.12 | 1.47 | 1.41 |
| 25 | l | 101 | SQD | O6-C1 | 2.13 | 1.43 | 1.40 |
| 22 | B | 617 | CLA | CHD-C4C | 2.13 | 1.47 | 1.41 |
| 22 | b | 604 | CLA | C1C-C2C | 2.13 | 1.48 | 1.44 |
| 22 | C | 508 | CLA | C1C-C2C | 2.13 | 1.48 | 1.44 |
| 22 | B | 604 | CLA | CHD-C4C | 2.14 | 1.47 | 1.41 |
| 22 | b | 610 | CLA | CHB-C4A | 2.14 | 1.36 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 31 | D | 410 | DGD | O5D-C1E | 2.14 | 1.43 | 1.40 |
| 22 | B | 610 | CLA | CHB-C4A | 2.14 | 1.36 | 1.33 |
| 22 | c | 508 | CLA | C1C-C2C | 2.14 | 1.48 | 1.44 |
| 22 | D | 403 | CLA | C4C-C3C | 2.14 | 1.48 | 1.45 |
| 29 | c | 520 | LMG | O1-C1 | 2.15 | 1.43 | 1.40 |
| 22 | C | 509 | CLA | C4C-C3C | 2.15 | 1.48 | 1.45 |
| 22 | d | 403 | CLA | C4C-C3C | 2.16 | 1.48 | 1.45 |
| 28 | A | 613 | PL9 | C2-C3 | 2.16 | 1.40 | 1.34 |
| 22 | c | 509 | CLA | C4C-C3C | 2.16 | 1.48 | 1.45 |
| 22 | b | 608 | CLA | CHB-C4A | 2.16 | 1.36 | 1.33 |
| 22 | c | 505 | CLA | C4C-C3C | 2.16 | 1.48 | 1.45 |
| 22 | b | 604 | CLA | CHD-C4C | 2.17 | 1.47 | 1.41 |
| 22 | B | 604 | CLA | C1C-C2C | 2.17 | 1.48 | 1.44 |
| 22 | c | 512 | CLA | C4C-C3C | 2.18 | 1.48 | 1.45 |
| 22 | C | 512 | CLA | C4C-C3C | 2.18 | 1.48 | 1.45 |
| 28 | a | 613 | PL9 | C2-C3 | 2.19 | 1.40 | 1.34 |
| 22 | B | 608 | CLA | CHB-C4A | 2.20 | 1.36 | 1.33 |
| 31 | d | 410 | DGD | O5D-C1E | 2.20 | 1.44 | 1.40 |
| 29 | z | 101 | LMG | O1-C1 | 2.20 | 1.44 | 1.40 |
| 22 | c | 511 | CLA | C1C-C2C | 2.20 | 1.48 | 1.44 |
| 22 | B | 615 | CLA | CHD-C4C | 2.21 | 1.47 | 1.41 |
| 22 | A | 607 | CLA | CHD-C4C | 2.22 | 1.47 | 1.41 |
| 22 | b | 615 | CLA | CHD-C4C | 2.22 | 1.47 | 1.41 |
| 29 | Z | 101 | LMG | O1-C1 | 2.22 | 1.44 | 1.40 |
| 22 | b | 616 | CLA | C1C-C2C | 2.22 | 1.48 | 1.44 |
| 22 | B | 616 | CLA | C1C-C2C | 2.22 | 1.48 | 1.44 |
| 22 | a | 607 | CLA | CHD-C4C | 2.22 | 1.47 | 1.41 |
| 22 | C | 511 | CLA | C1C-C2C | 2.23 | 1.48 | 1.44 |
| 22 | B | 611 | CLA | CHD-C4C | 2.24 | 1.47 | 1.41 |
| 22 | b | 611 | CLA | CHD-C4C | 2.25 | 1.47 | 1.41 |
| 22 | b | 605 | CLA | CHD-C4C | 2.26 | 1.47 | 1.41 |
| 22 | b | 609 | CLA | CHD-C4C | 2.27 | 1.47 | 1.41 |
| 22 | c | 510 | CLA | C1C-C2C | 2.27 | 1.48 | 1.44 |
| 22 | b | 603 | CLA | C1C-C2C | 2.27 | 1.48 | 1.44 |
| 22 | a | 604 | CLA | CHD-C4C | 2.27 | 1.47 | 1.41 |
| 22 | C | 510 | CLA | C1C-C2C | 2.27 | 1.48 | 1.44 |
| 22 | c | 508 | CLA | C4C-C3C | 2.28 | 1.49 | 1.45 |
| 22 | B | 605 | CLA | CHD-C4C | 2.29 | 1.47 | 1.41 |
| 22 | A | 604 | CLA | CHD-C4C | 2.29 | 1.47 | 1.41 |
| 22 | B | 609 | CLA | CHD-C4C | 2.29 | 1.47 | 1.41 |
| 22 | b | 614 | CLA | C1C-C2C | 2.30 | 1.49 | 1.44 |
| 22 | B | 614 | CLA | C1C-C2C | 2.30 | 1.49 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22 | C | 508 | CLA | C4C-C3C | 2.30 | 1.49 | 1.45 |
| 22 | C | 509 | CLA | CHD-C4C | 2.30 | 1.47 | 1.41 |
| 22 | b | 607 | CLA | C1C-C2C | 2.31 | 1.49 | 1.44 |
| 22 | B | 614 | CLA | CHD-C4C | 2.31 | 1.47 | 1.41 |
| 22 | B | 607 | CLA | C1C-C2C | 2.31 | 1.49 | 1.44 |
| 22 | B | 603 | CLA | C1C-C2C | 2.32 | 1.49 | 1.44 |
| 22 | c | 508 | CLA | CHD-C4C | 2.32 | 1.47 | 1.41 |
| 22 | d | 401 | CLA | C1D-C2D | 2.32 | 1.48 | 1.42 |
| 23 | a | 606 | PHO | C3B-C4B | 2.32 | 1.48 | 1.43 |
| 22 | C | 508 | CLA | CHD-C4C | 2.33 | 1.47 | 1.41 |
| 22 | c | 505 | CLA | C1C-C2C | 2.33 | 1.49 | 1.44 |
| 22 | D | 403 | CLA | C1C-C2C | 2.33 | 1.49 | 1.44 |
| 22 | c | 506 | CLA | C1C-C2C | 2.34 | 1.49 | 1.44 |
| 22 | b | 614 | CLA | CHD-C4C | 2.34 | 1.47 | 1.41 |
| 22 | d | 403 | CLA | C1C-C2C | 2.34 | 1.49 | 1.44 |
| 22 | C | 505 | CLA | C1C-C2C | 2.34 | 1.49 | 1.44 |
| 22 | C | 506 | CLA | C1C-C2C | 2.34 | 1.49 | 1.44 |
| 22 | a | 603 | CLA | CHD-C4C | 2.34 | 1.47 | 1.41 |
| 23 | A | 606 | PHO | C3B-C4B | 2.34 | 1.48 | 1.43 |
| 22 | c | 509 | CLA | CHD-C4C | 2.35 | 1.47 | 1.41 |
| 22 | D | 401 | CLA | C1D-C2D | 2.37 | 1.48 | 1.42 |
| 22 | c | 510 | CLA | CHD-C4C | 2.37 | 1.48 | 1.41 |
| 22 | A | 603 | CLA | CHD-C4C | 2.37 | 1.48 | 1.41 |
| 22 | C | 501 | CLA | C1C-C2C | 2.38 | 1.49 | 1.44 |
| 22 | C | 513 | CLA | CHD-C4C | 2.39 | 1.48 | 1.41 |
| 22 | C | 510 | CLA | CHD-C4C | 2.39 | 1.48 | 1.41 |
| 22 | d | 402 | CLA | CHB-C4A | 2.39 | 1.36 | 1.33 |
| 22 | c | 513 | CLA | CHD-C4C | 2.39 | 1.48 | 1.41 |
| 22 | c | 501 | CLA | C1C-C2C | 2.40 | 1.49 | 1.44 |
| 22 | C | 511 | CLA | CHD-C4C | 2.40 | 1.48 | 1.41 |
| 22 | D | 402 | CLA | CHB-C4A | 2.40 | 1.36 | 1.33 |
| 22 | b | 616 | CLA | CHD-C4C | 2.41 | 1.48 | 1.41 |
| 22 | D | 403 | CLA | CHD-C4C | 2.41 | 1.48 | 1.41 |
| 22 | c | 511 | CLA | CHD-C4C | 2.42 | 1.48 | 1.41 |
| 22 | B | 607 | CLA | CHD-C4C | 2.42 | 1.48 | 1.41 |
| 22 | C | 507 | CLA | CHD-C4C | 2.42 | 1.48 | 1.41 |
| 22 | B | 605 | CLA | CHB-C4A | 2.43 | 1.36 | 1.33 |
| 22 | C | 503 | CLA | CHD-C4C | 2.44 | 1.48 | 1.41 |
| 22 | B | 616 | CLA | CHD-C4C | 2.44 | 1.48 | 1.41 |
| 22 | b | 602 | CLA | CHD-C4C | 2.44 | 1.48 | 1.41 |
| 22 | b | 603 | CLA | CHD-C4C | 2.44 | 1.48 | 1.41 |
| 22 | b | 607 | CLA | CHD-C4C | 2.44 | 1.48 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22 | c | 505 | CLA | CHD-C4C | 2.44 | 1.48 | 1.41 |
| 22 | d | 403 | CLA | CHD-C4C | 2.44 | 1.48 | 1.41 |
| 22 | c | 506 | CLA | CHD-C4C | 2.44 | 1.48 | 1.41 |
| 22 | c | 507 | CLA | CHD-C4C | 2.45 | 1.48 | 1.41 |
| 22 | B | 602 | CLA | CHD-C4C | 2.45 | 1.48 | 1.41 |
| 22 | c | 503 | CLA | CHD-C4C | 2.45 | 1.48 | 1.41 |
| 22 | B | 603 | CLA | CHD-C4C | 2.45 | 1.48 | 1.41 |
| 22 | C | 505 | CLA | CHD-C4C | 2.45 | 1.48 | 1.41 |
| 22 | b | 605 | CLA | CHB-C4A | 2.45 | 1.36 | 1.33 |
| 22 | b | 609 | CLA | C1D-C2D | 2.46 | 1.48 | 1.42 |
| 22 | B | 608 | CLA | CHD-C4C | 2.48 | 1.48 | 1.41 |
| 22 | C | 506 | CLA | CHD-C4C | 2.48 | 1.48 | 1.41 |
| 22 | B | 609 | CLA | C1D-C2D | 2.48 | 1.48 | 1.42 |
| 22 | b | 613 | CLA | CHD-C4C | 2.49 | 1.48 | 1.41 |
| 23 | A | 605 | PHO | C3D-C2D | 2.50 | 1.46 | 1.38 |
| 22 | b | 608 | CLA | CHD-C4C | 2.50 | 1.48 | 1.41 |
| 22 | a | 604 | CLA | C4B-CHC | 2.50 | 1.46 | 1.40 |
| 22 | B | 613 | CLA | CHD-C4C | 2.50 | 1.48 | 1.41 |
| 22 | A | 604 | CLA | C4B-CHC | 2.51 | 1.46 | 1.40 |
| 22 | B | 609 | CLA | C4B-CHC | 2.51 | 1.46 | 1.40 |
| 22 | b | 609 | CLA | C4B-CHC | 2.52 | 1.46 | 1.40 |
| 23 | a | 605 | PHO | C3D-C2D | 2.53 | 1.46 | 1.38 |
| 22 | C | 513 | CLA | C1C-C2C | 2.53 | 1.49 | 1.44 |
| 22 | c | 512 | CLA | C1C-C2C | 2.54 | 1.49 | 1.44 |
| 22 | A | 607 | CLA | C1D-C2D | 2.55 | 1.48 | 1.42 |
| 22 | a | 607 | CLA | C1D-C2D | 2.55 | 1.48 | 1.42 |
| 22 | C | 512 | CLA | C1C-C2C | 2.57 | 1.49 | 1.44 |
| 22 | c | 513 | CLA | C1C-C2C | 2.57 | 1.49 | 1.44 |
| 22 | C | 501 | CLA | CHD-C4C | 2.57 | 1.48 | 1.41 |
| 22 | c | 512 | CLA | CHD-C4C | 2.59 | 1.48 | 1.41 |
| 22 | C | 512 | CLA | CHD-C4C | 2.59 | 1.48 | 1.41 |
| 22 | c | 501 | CLA | CHD-C4C | 2.59 | 1.48 | 1.41 |
| 31 | h | 102 | DGD | O5D-C1E | 2.61 | 1.44 | 1.40 |
| 22 | B | 605 | CLA | C4B-CHC | 2.61 | 1.47 | 1.40 |
| 22 | b | 605 | CLA | C4B-CHC | 2.61 | 1.47 | 1.40 |
| 31 | H | 102 | DGD | O5D-C1E | 2.63 | 1.44 | 1.40 |
| 22 | C | 507 | CLA | C1C-C2C | 2.63 | 1.49 | 1.44 |
| 28 | D | 408 | PL9 | C6-C5 | 2.66 | 1.49 | 1.35 |
| 22 | C | 504 | CLA | C4B-CHC | 2.66 | 1.47 | 1.40 |
| 22 | b | 615 | CLA | C4B-CHC | 2.66 | 1.47 | 1.40 |
| 28 | d | 408 | PL9 | C6-C5 | 2.66 | 1.49 | 1.35 |
| 29 | Z | 101 | LMG | O8-C28 | 2.67 | 1.46 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22 | c | 507 | CLA | C1C-C2C | 2.68 | 1.49 | 1.44 |
| 29 | z | 101 | LMG | O8-C28 | 2.68 | 1.46 | 1.33 |
| 22 | B | 615 | CLA | C4B-CHC | 2.68 | 1.47 | 1.40 |
| 22 | c | 504 | CLA | C4B-CHC | 2.70 | 1.47 | 1.40 |
| 22 | C | 504 | CLA | CHD-C4C | 2.70 | 1.48 | 1.41 |
| 22 | B | 602 | CLA | C1C-C2C | 2.71 | 1.49 | 1.44 |
| 22 | b | 602 | CLA | C1C-C2C | 2.71 | 1.49 | 1.44 |
| 22 | B | 606 | CLA | C1D-C2D | 2.71 | 1.48 | 1.42 |
| 22 | b | 608 | CLA | C4B-CHC | 2.72 | 1.47 | 1.40 |
| 28 | a | 613 | PL9 | C6-C5 | 2.72 | 1.49 | 1.35 |
| 28 | A | 613 | PL9 | C6-C5 | 2.72 | 1.49 | 1.35 |
| 22 | B | 608 | CLA | C4B-CHC | 2.72 | 1.47 | 1.40 |
| 22 | b | 606 | CLA | C1D-C2D | 2.72 | 1.48 | 1.42 |
| 22 | c | 504 | CLA | CHD-C4C | 2.75 | 1.49 | 1.41 |
| 22 | C | 510 | CLA | C4B-CHC | 2.76 | 1.47 | 1.40 |
| 22 | a | 603 | CLA | C1D-C2D | 2.78 | 1.49 | 1.42 |
| 22 | c | 510 | CLA | C4B-CHC | 2.78 | 1.47 | 1.40 |
| 22 | B | 604 | CLA | C4B-CHC | 2.78 | 1.47 | 1.40 |
| 22 | c | 503 | CLA | C1C-C2C | 2.79 | 1.49 | 1.44 |
| 23 | a | 606 | PHO | C3D-C2D | 2.79 | 1.46 | 1.38 |
| 22 | b | 614 | CLA | C1D-C2D | 2.79 | 1.49 | 1.42 |
| 22 | b | 604 | CLA | C4B-CHC | 2.79 | 1.47 | 1.40 |
| 22 | B | 614 | CLA | C1D-C2D | 2.79 | 1.49 | 1.42 |
| 23 | A | 606 | PHO | C3D-C2D | 2.81 | 1.46 | 1.38 |
| 22 | C | 509 | CLA | C4B-CHC | 2.81 | 1.47 | 1.40 |
| 22 | c | 511 | CLA | C1D-C2D | 2.82 | 1.49 | 1.42 |
| 22 | C | 503 | CLA | C1C-C2C | 2.82 | 1.50 | 1.44 |
| 22 | D | 401 | CLA | CHB-C4A | 2.82 | 1.36 | 1.33 |
| 22 | c | 509 | CLA | C4B-CHC | 2.83 | 1.47 | 1.40 |
| 23 | A | 605 | PHO | CHC-C4B | 2.83 | 1.47 | 1.40 |
| 23 | A | 606 | PHO | CHD-C4C | 2.84 | 1.47 | 1.40 |
| 22 | A | 603 | CLA | C1D-C2D | 2.84 | 1.49 | 1.42 |
| 22 | A | 604 | CLA | C1B-CHB | 2.84 | 1.47 | 1.40 |
| 22 | D | 402 | CLA | C1B-CHB | 2.84 | 1.47 | 1.40 |
| 22 | B | 617 | CLA | C1D-C2D | 2.84 | 1.49 | 1.42 |
| 22 | d | 401 | CLA | CHB-C4A | 2.84 | 1.36 | 1.33 |
| 22 | C | 502 | CLA | C1D-C2D | 2.84 | 1.49 | 1.42 |
| 23 | a | 605 | PHO | CHC-C4B | 2.84 | 1.47 | 1.40 |
| 22 | B | 611 | CLA | C1D-C2D | 2.85 | 1.49 | 1.42 |
| 22 | b | 616 | CLA | C4B-CHC | 2.85 | 1.47 | 1.40 |
| 23 | a | 606 | PHO | CHD-C4C | 2.85 | 1.47 | 1.40 |
| 22 | d | 402 | CLA | C1B-CHB | 2.85 | 1.47 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22 | B | 616 | CLA | C4B-CHC | 2.85 | 1.47 | 1.40 |
| 22 | c | 502 | CLA | C1D-C2D | 2.85 | 1.49 | 1.42 |
| 22 | C | 511 | CLA | C1D-C2D | 2.85 | 1.49 | 1.42 |
| 22 | B | 612 | CLA | C4B-CHC | 2.85 | 1.47 | 1.40 |
| 22 | b | 611 | CLA | C1D-C2D | 2.86 | 1.49 | 1.42 |
| 22 | a | 604 | CLA | C1B-CHB | 2.87 | 1.47 | 1.40 |
| 22 | d | 403 | CLA | C1D-C2D | 2.87 | 1.49 | 1.42 |
| 22 | c | 505 | CLA | C1D-C2D | 2.88 | 1.49 | 1.42 |
| 22 | b | 617 | CLA | C1D-C2D | 2.88 | 1.49 | 1.42 |
| 22 | D | 402 | CLA | C4B-CHC | 2.89 | 1.47 | 1.40 |
| 22 | b | 612 | CLA | C4B-CHC | 2.89 | 1.47 | 1.40 |
| 22 | D | 403 | CLA | C1D-C2D | 2.89 | 1.49 | 1.42 |
| 22 | b | 606 | CLA | C4B-CHC | 2.89 | 1.47 | 1.40 |
| 22 | d | 402 | CLA | C4B-CHC | 2.90 | 1.47 | 1.40 |
| 22 | B | 606 | CLA | C4B-CHC | 2.90 | 1.47 | 1.40 |
| 22 | C | 505 | CLA | C1D-C2D | 2.90 | 1.49 | 1.42 |
| 22 | b | 617 | CLA | C4B-CHC | 2.91 | 1.47 | 1.40 |
| 22 | b | 612 | CLA | C1D-C2D | 2.91 | 1.49 | 1.42 |
| 22 | D | 401 | CLA | C1B-CHB | 2.92 | 1.47 | 1.40 |
| 22 | b | 604 | CLA | C1D-C2D | 2.92 | 1.49 | 1.42 |
| 23 | A | 605 | PHO | OBD-CAD | 2.92 | 1.27 | 1.22 |
| 22 | c | 502 | CLA | C4B-CHC | 2.92 | 1.47 | 1.40 |
| 23 | a | 605 | PHO | OBD-CAD | 2.93 | 1.27 | 1.22 |
| 22 | c | 511 | CLA | C4B-CHC | 2.93 | 1.47 | 1.40 |
| 22 | B | 612 | CLA | C1D-C2D | 2.93 | 1.49 | 1.42 |
| 22 | d | 401 | CLA | C1B-CHB | 2.94 | 1.47 | 1.40 |
| 22 | B | 604 | CLA | C1D-C2D | 2.94 | 1.49 | 1.42 |
| 22 | B | 613 | CLA | C1D-C2D | 2.94 | 1.49 | 1.42 |
| 22 | b | 613 | CLA | C1D-C2D | 2.94 | 1.49 | 1.42 |
| 22 | C | 502 | CLA | C4B-CHC | 2.95 | 1.48 | 1.40 |
| 22 | b | 610 | CLA | C4B-CHC | 2.95 | 1.48 | 1.40 |
| 22 | B | 614 | CLA | C4B-CHC | 2.95 | 1.48 | 1.40 |
| 22 | b | 614 | CLA | C4B-CHC | 2.95 | 1.48 | 1.40 |
| 22 | C | 511 | CLA | C4B-CHC | 2.96 | 1.48 | 1.40 |
| 22 | B | 617 | CLA | C4B-CHC | 2.96 | 1.48 | 1.40 |
| 22 | B | 610 | CLA | C4B-CHC | 2.96 | 1.48 | 1.40 |
| 22 | c | 512 | CLA | C1D-C2D | 2.96 | 1.49 | 1.42 |
| 22 | B | 616 | CLA | C1D-C2D | 2.96 | 1.49 | 1.42 |
| 22 | d | 401 | CLA | C4B-CHC | 2.97 | 1.48 | 1.40 |
| 22 | D | 401 | CLA | C4B-CHC | 2.97 | 1.48 | 1.40 |
| 22 | C | 512 | CLA | C1D-C2D | 2.97 | 1.49 | 1.42 |
| 22 | C | 508 | CLA | C1D-C2D | 2.97 | 1.49 | 1.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22 | B | 609 | CLA | C1B-CHB | 2.98 | 1.48 | 1.40 |
| 22 | B | 615 | CLA | C1D-C2D | 2.99 | 1.49 | 1.42 |
| 22 | b | 616 | CLA | C1D-C2D | 2.99 | 1.49 | 1.42 |
| 23 | A | 605 | PHO | CHD-C4C | 2.99 | 1.47 | 1.40 |
| 22 | b | 609 | CLA | C1B-CHB | 3.00 | 1.48 | 1.40 |
| 22 | c | 508 | CLA | C1D-C2D | 3.00 | 1.49 | 1.42 |
| 22 | b | 605 | CLA | C1D-C2D | 3.01 | 1.49 | 1.42 |
| 22 | B | 605 | CLA | C1D-C2D | 3.02 | 1.49 | 1.42 |
| 22 | b | 615 | CLA | C1D-C2D | 3.02 | 1.49 | 1.42 |
| 23 | a | 605 | PHO | CHD-C4C | 3.03 | 1.47 | 1.40 |
| 22 | c | 508 | CLA | C4B-CHC | 3.03 | 1.48 | 1.40 |
| 22 | C | 508 | CLA | C4B-CHC | 3.03 | 1.48 | 1.40 |
| 22 | B | 613 | CLA | C4B-CHC | 3.03 | 1.48 | 1.40 |
| 22 | A | 603 | CLA | C4B-CHC | 3.04 | 1.48 | 1.40 |
| 22 | D | 403 | CLA | C4B-CHC | 3.04 | 1.48 | 1.40 |
| 22 | c | 512 | CLA | C4B-CHC | 3.04 | 1.48 | 1.40 |
| 22 | b | 613 | CLA | C4B-CHC | 3.05 | 1.48 | 1.40 |
| 22 | B | 607 | CLA | C4B-CHC | 3.05 | 1.48 | 1.40 |
| 22 | c | 507 | CLA | C1D-C2D | 3.05 | 1.49 | 1.42 |
| 22 | C | 507 | CLA | C1D-C2D | 3.05 | 1.49 | 1.42 |
| 22 | d | 403 | CLA | C4B-CHC | 3.05 | 1.48 | 1.40 |
| 22 | c | 509 | CLA | C1D-C2D | 3.05 | 1.49 | 1.42 |
| 22 | a | 603 | CLA | C4B-CHC | 3.06 | 1.48 | 1.40 |
| 22 | B | 611 | CLA | C4B-CHC | 3.06 | 1.48 | 1.40 |
| 22 | C | 506 | CLA | C4B-CHC | 3.06 | 1.48 | 1.40 |
| 22 | b | 607 | CLA | C4B-CHC | 3.07 | 1.48 | 1.40 |
| 22 | b | 612 | CLA | C1B-CHB | 3.07 | 1.48 | 1.40 |
| 22 | C | 512 | CLA | C4B-CHC | 3.07 | 1.48 | 1.40 |
| 22 | c | 506 | CLA | C4B-CHC | 3.07 | 1.48 | 1.40 |
| 22 | B | 612 | CLA | C1B-CHB | 3.07 | 1.48 | 1.40 |
| 22 | B | 610 | CLA | C1D-C2D | 3.08 | 1.49 | 1.42 |
| 32 | d | 405 | LHG | O7-C7 | 3.08 | 1.43 | 1.34 |
| 22 | b | 611 | CLA | C4B-CHC | 3.09 | 1.48 | 1.40 |
| 22 | C | 509 | CLA | C1D-C2D | 3.09 | 1.49 | 1.42 |
| 22 | C | 510 | CLA | C1D-C2D | 3.10 | 1.49 | 1.42 |
| 22 | b | 608 | CLA | C1D-C2D | 3.10 | 1.49 | 1.42 |
| 32 | D | 405 | LHG | O7-C7 | 3.10 | 1.43 | 1.34 |
| 22 | B | 608 | CLA | C1D-C2D | 3.11 | 1.49 | 1.42 |
| 22 | d | 402 | CLA | C1D-C2D | 3.11 | 1.49 | 1.42 |
| 22 | c | 504 | CLA | C1D-C2D | 3.11 | 1.49 | 1.42 |
| 22 | A | 607 | CLA | C4B-CHC | 3.12 | 1.48 | 1.40 |
| 22 | b | 610 | CLA | C1D-C2D | 3.13 | 1.49 | 1.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22 | b | 602 | CLA | C1B-CHB | 3.13 | 1.48 | 1.40 |
| 22 | C | 504 | CLA | C1D-C2D | 3.13 | 1.49 | 1.42 |
| 22 | a | 607 | CLA | C4B-CHC | 3.13 | 1.48 | 1.40 |
| 22 | a | 604 | CLA | C1D-C2D | 3.14 | 1.49 | 1.42 |
| 22 | B | 605 | CLA | C3D-C2D | 3.14 | 1.46 | 1.39 |
| 22 | c | 510 | CLA | C1D-C2D | 3.14 | 1.49 | 1.42 |
| 22 | b | 605 | CLA | C3D-C2D | 3.14 | 1.46 | 1.39 |
| 22 | B | 602 | CLA | C1B-CHB | 3.15 | 1.48 | 1.40 |
| 22 | D | 402 | CLA | C1D-C2D | 3.15 | 1.49 | 1.42 |
| 22 | C | 507 | CLA | C4B-CHC | 3.15 | 1.48 | 1.40 |
| 22 | c | 507 | CLA | C4B-CHC | 3.16 | 1.48 | 1.40 |
| 22 | A | 604 | CLA | C1D-C2D | 3.16 | 1.49 | 1.42 |
| 22 | C | 509 | CLA | C1B-CHB | 3.16 | 1.48 | 1.40 |
| 22 | c | 509 | CLA | C1B-CHB | 3.17 | 1.48 | 1.40 |
| 22 | c | 503 | CLA | C1D-C2D | 3.17 | 1.49 | 1.42 |
| 22 | c | 501 | CLA | C4B-CHC | 3.17 | 1.48 | 1.40 |
| 22 | D | 401 | CLA | C3D-C2D | 3.17 | 1.46 | 1.39 |
| 22 | d | 401 | CLA | C3D-C2D | 3.17 | 1.46 | 1.39 |
| 22 | C | 506 | CLA | C1D-C2D | 3.19 | 1.50 | 1.42 |
| 22 | c | 503 | CLA | C1B-CHB | 3.19 | 1.48 | 1.40 |
| 22 | c | 506 | CLA | C1D-C2D | 3.19 | 1.50 | 1.42 |
| 22 | C | 503 | CLA | C1D-C2D | 3.20 | 1.50 | 1.42 |
| 22 | b | 611 | CLA | C1B-CHB | 3.20 | 1.48 | 1.40 |
| 22 | B | 611 | CLA | C1B-CHB | 3.20 | 1.48 | 1.40 |
| 22 | B | 603 | CLA | C4B-CHC | 3.20 | 1.48 | 1.40 |
| 22 | c | 502 | CLA | C1B-CHB | 3.21 | 1.48 | 1.40 |
| 22 | b | 617 | CLA | C1B-CHB | 3.21 | 1.48 | 1.40 |
| 22 | b | 603 | CLA | C4B-CHC | 3.21 | 1.48 | 1.40 |
| 22 | C | 501 | CLA | C4B-CHC | 3.21 | 1.48 | 1.40 |
| 22 | B | 617 | CLA | C1B-CHB | 3.21 | 1.48 | 1.40 |
| 22 | C | 503 | CLA | C1B-CHB | 3.21 | 1.48 | 1.40 |
| 22 | A | 603 | CLA | C1B-CHB | 3.21 | 1.48 | 1.40 |
| 22 | C | 502 | CLA | C1B-CHB | 3.21 | 1.48 | 1.40 |
| 22 | C | 505 | CLA | C4B-CHC | 3.22 | 1.48 | 1.40 |
| 22 | a | 603 | CLA | C1B-CHB | 3.22 | 1.48 | 1.40 |
| 22 | c | 505 | CLA | C4B-CHC | 3.23 | 1.48 | 1.40 |
| 22 | B | 616 | CLA | C1B-CHB | 3.24 | 1.48 | 1.40 |
| 22 | b | 602 | CLA | C3D-C2D | 3.24 | 1.46 | 1.39 |
| 22 | c | 513 | CLA | C1D-C2D | 3.24 | 1.50 | 1.42 |
| 22 | b | 616 | CLA | C1B-CHB | 3.24 | 1.48 | 1.40 |
| 22 | C | 513 | CLA | C1D-C2D | 3.24 | 1.50 | 1.42 |
| 22 | B | 602 | CLA | C3D-C2D | 3.25 | 1.46 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22 | C | 501 | CLA | C1B-CHB | 3.25 | 1.48 | 1.40 |
| 22 | c | 503 | CLA | C4B-CHC | 3.26 | 1.48 | 1.40 |
| 22 | B | 603 | CLA | C1D-C2D | 3.27 | 1.50 | 1.42 |
| 22 | c | 501 | CLA | C1D-C2D | 3.27 | 1.50 | 1.42 |
| 22 | C | 503 | CLA | C4B-CHC | 3.28 | 1.48 | 1.40 |
| 22 | c | 501 | CLA | C1B-CHB | 3.28 | 1.48 | 1.40 |
| 22 | C | 501 | CLA | C1D-C2D | 3.29 | 1.50 | 1.42 |
| 31 | C | 518 | DGD | O2G-C1B | 3.30 | 1.43 | 1.34 |
| 22 | b | 603 | CLA | C1D-C2D | 3.31 | 1.50 | 1.42 |
| 22 | c | 503 | CLA | C3D-C2D | 3.31 | 1.46 | 1.39 |
| 23 | A | 606 | PHO | CHC-C4B | 3.31 | 1.48 | 1.40 |
| 22 | B | 613 | CLA | C1B-CHB | 3.31 | 1.48 | 1.40 |
| 31 | c | 518 | DGD | O2G-C1B | 3.31 | 1.43 | 1.34 |
| 22 | c | 513 | CLA | C4B-CHC | 3.32 | 1.49 | 1.40 |
| 22 | b | 610 | CLA | C1B-CHB | 3.32 | 1.49 | 1.40 |
| 22 | C | 513 | CLA | C4B-CHC | 3.32 | 1.49 | 1.40 |
| 22 | B | 612 | CLA | C3D-C2D | 3.33 | 1.46 | 1.39 |
| 22 | b | 613 | CLA | C1B-CHB | 3.33 | 1.49 | 1.40 |
| 22 | B | 608 | CLA | O2A-CGA | 3.33 | 1.43 | 1.33 |
| 22 | B | 610 | CLA | C1B-CHB | 3.33 | 1.49 | 1.40 |
| 22 | b | 608 | CLA | O2A-CGA | 3.34 | 1.43 | 1.33 |
| 22 | B | 607 | CLA | C1D-C2D | 3.34 | 1.50 | 1.42 |
| 22 | b | 612 | CLA | C3D-C2D | 3.34 | 1.46 | 1.39 |
| 22 | b | 607 | CLA | C3D-C2D | 3.34 | 1.46 | 1.39 |
| 22 | C | 503 | CLA | C3D-C2D | 3.35 | 1.46 | 1.39 |
| 23 | a | 606 | PHO | CHC-C4B | 3.35 | 1.48 | 1.40 |
| 22 | b | 607 | CLA | C1D-C2D | 3.35 | 1.50 | 1.42 |
| 22 | B | 604 | CLA | C1B-CHB | 3.36 | 1.49 | 1.40 |
| 22 | b | 605 | CLA | C1B-CHB | 3.36 | 1.49 | 1.40 |
| 22 | B | 607 | CLA | C3D-C2D | 3.38 | 1.46 | 1.39 |
| 22 | b | 604 | CLA | C1B-CHB | 3.38 | 1.49 | 1.40 |
| 22 | B | 605 | CLA | C1B-CHB | 3.39 | 1.49 | 1.40 |
| 22 | B | 613 | CLA | C3D-C2D | 3.41 | 1.46 | 1.39 |
| 22 | a | 607 | CLA | C3D-C2D | 3.42 | 1.46 | 1.39 |
| 22 | B | 602 | CLA | C1D-C2D | 3.43 | 1.50 | 1.42 |
| 22 | b | 602 | CLA | C1D-C2D | 3.43 | 1.50 | 1.42 |
| 22 | C | 509 | CLA | C3D-C2D | 3.43 | 1.46 | 1.39 |
| 22 | c | 505 | CLA | C1B-CHB | 3.44 | 1.49 | 1.40 |
| 22 | C | 506 | CLA | C3D-C2D | 3.44 | 1.46 | 1.39 |
| 22 | c | 506 | CLA | C3D-C2D | 3.45 | 1.46 | 1.39 |
| 22 | b | 613 | CLA | C3D-C2D | 3.45 | 1.46 | 1.39 |
| 22 | c | 509 | CLA | C3D-C2D | 3.45 | 1.46 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22 | B | 607 | CLA | C1B-CHB | 3.45 | 1.49 | 1.40 |
| 22 | A | 607 | CLA | C3D-C2D | 3.45 | 1.46 | 1.39 |
| 22 | A | 603 | CLA | C3D-C2D | 3.45 | 1.46 | 1.39 |
| 22 | b | 602 | CLA | C4B-CHC | 3.46 | 1.49 | 1.40 |
| 22 | C | 507 | CLA | C1B-CHB | 3.46 | 1.49 | 1.40 |
| 22 | C | 502 | CLA | C3D-C2D | 3.47 | 1.46 | 1.39 |
| 22 | a | 607 | CLA | C1B-CHB | 3.47 | 1.49 | 1.40 |
| 22 | c | 507 | CLA | C1B-CHB | 3.47 | 1.49 | 1.40 |
| 22 | C | 508 | CLA | C1B-CHB | 3.47 | 1.49 | 1.40 |
| 22 | c | 508 | CLA | C1B-CHB | 3.47 | 1.49 | 1.40 |
| 22 | C | 504 | CLA | C1B-CHB | 3.47 | 1.49 | 1.40 |
| 22 | b | 608 | CLA | C3D-C2D | 3.48 | 1.46 | 1.39 |
| 22 | b | 607 | CLA | C1B-CHB | 3.48 | 1.49 | 1.40 |
| 22 | b | 615 | CLA | C3D-C2D | 3.48 | 1.46 | 1.39 |
| 22 | b | 615 | CLA | C1B-CHB | 3.48 | 1.49 | 1.40 |
| 22 | A | 607 | CLA | C1B-CHB | 3.48 | 1.49 | 1.40 |
| 22 | B | 602 | CLA | C4B-CHC | 3.48 | 1.49 | 1.40 |
| 22 | c | 507 | CLA | C3D-C2D | 3.48 | 1.46 | 1.39 |
| 22 | C | 505 | CLA | C3D-C2D | 3.48 | 1.46 | 1.39 |
| 22 | C | 512 | CLA | C1B-CHB | 3.48 | 1.49 | 1.40 |
| 22 | c | 502 | CLA | C3D-C2D | 3.48 | 1.46 | 1.39 |
| 22 | C | 507 | CLA | C3D-C2D | 3.49 | 1.46 | 1.39 |
| 22 | B | 615 | CLA | C3D-C2D | 3.49 | 1.46 | 1.39 |
| 22 | b | 603 | CLA | O2A-CGA | 3.49 | 1.43 | 1.33 |
| 22 | C | 505 | CLA | C1B-CHB | 3.49 | 1.49 | 1.40 |
| 22 | c | 504 | CLA | C1B-CHB | 3.49 | 1.49 | 1.40 |
| 22 | b | 612 | CLA | O2A-CGA | 3.49 | 1.43 | 1.33 |
| 22 | a | 603 | CLA | C3D-C2D | 3.49 | 1.46 | 1.39 |
| 22 | B | 603 | CLA | O2A-CGA | 3.49 | 1.43 | 1.33 |
| 22 | B | 608 | CLA | C3D-C2D | 3.49 | 1.46 | 1.39 |
| 22 | c | 505 | CLA | C3D-C2D | 3.50 | 1.46 | 1.39 |
| 22 | B | 615 | CLA | C1B-CHB | 3.50 | 1.49 | 1.40 |
| 22 | B | 612 | CLA | O2A-CGA | 3.50 | 1.43 | 1.33 |
| 22 | C | 513 | CLA | C1B-CHB | 3.50 | 1.49 | 1.40 |
| 22 | c | 512 | CLA | C1B-CHB | 3.50 | 1.49 | 1.40 |
| 22 | c | 513 | CLA | C1B-CHB | 3.51 | 1.49 | 1.40 |
| 22 | C | 510 | CLA | C3D-C2D | 3.51 | 1.46 | 1.39 |
| 22 | c | 510 | CLA | C3D-C2D | 3.51 | 1.46 | 1.39 |
| 22 | c | 511 | CLA | C1B-CHB | 3.52 | 1.49 | 1.40 |
| 22 | b | 603 | CLA | C1B-CHB | 3.53 | 1.49 | 1.40 |
| 22 | C | 511 | CLA | C1B-CHB | 3.54 | 1.49 | 1.40 |
| 22 | B | 614 | CLA | C1B-CHB | 3.54 | 1.49 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22 | B | 603 | CLA | C1B-CHB | 3.54 | 1.49 | 1.40 |
| 22 | b | 606 | CLA | C1B-CHB | 3.55 | 1.49 | 1.40 |
| 22 | C | 506 | CLA | C1B-CHB | 3.55 | 1.49 | 1.40 |
| 22 | C | 510 | CLA | C1B-CHB | 3.55 | 1.49 | 1.40 |
| 22 | a | 603 | CLA | O2A-CGA | 3.55 | 1.43 | 1.33 |
| 22 | B | 606 | CLA | C3D-C2D | 3.55 | 1.46 | 1.39 |
| 22 | c | 510 | CLA | C1B-CHB | 3.56 | 1.49 | 1.40 |
| 22 | B | 606 | CLA | C1B-CHB | 3.56 | 1.49 | 1.40 |
| 22 | b | 614 | CLA | C1B-CHB | 3.56 | 1.49 | 1.40 |
| 22 | c | 506 | CLA | C1B-CHB | 3.57 | 1.49 | 1.40 |
| 22 | d | 403 | CLA | C3D-C2D | 3.57 | 1.46 | 1.39 |
| 22 | A | 603 | CLA | O2A-CGA | 3.58 | 1.43 | 1.33 |
| 22 | b | 616 | CLA | C3D-C2D | 3.58 | 1.46 | 1.39 |
| 22 | b | 606 | CLA | C3D-C2D | 3.58 | 1.46 | 1.39 |
| 22 | B | 616 | CLA | C3D-C2D | 3.58 | 1.46 | 1.39 |
| 22 | b | 610 | CLA | C3D-C2D | 3.58 | 1.46 | 1.39 |
| 22 | b | 608 | CLA | C1B-CHB | 3.59 | 1.49 | 1.40 |
| 22 | D | 403 | CLA | C3D-C2D | 3.59 | 1.46 | 1.39 |
| 22 | B | 608 | CLA | C1B-CHB | 3.60 | 1.49 | 1.40 |
| 22 | d | 403 | CLA | C1B-CHB | 3.60 | 1.49 | 1.40 |
| 22 | b | 609 | CLA | C3D-C2D | 3.61 | 1.46 | 1.39 |
| 22 | B | 609 | CLA | C3D-C2D | 3.62 | 1.46 | 1.39 |
| 22 | B | 610 | CLA | C3D-C2D | 3.62 | 1.46 | 1.39 |
| 23 | a | 606 | PHO | OBD-CAD | 3.62 | 1.28 | 1.22 |
| 22 | D | 403 | CLA | C1B-CHB | 3.62 | 1.49 | 1.40 |
| 22 | B | 605 | CLA | OBD-CAD | 3.63 | 1.27 | 1.22 |
| 23 | A | 606 | PHO | OBD-CAD | 3.65 | 1.28 | 1.22 |
| 31 | C | 517 | DGD | O2G-C1B | 3.65 | 1.44 | 1.34 |
| 22 | A | 604 | CLA | C3D-C2D | 3.66 | 1.47 | 1.39 |
| 31 | c | 517 | DGD | O2G-C1B | 3.67 | 1.44 | 1.34 |
| 22 | d | 402 | CLA | C3D-C2D | 3.67 | 1.47 | 1.39 |
| 22 | b | 614 | CLA | C3D-C2D | 3.68 | 1.47 | 1.39 |
| 22 | B | 614 | CLA | C3D-C2D | 3.68 | 1.47 | 1.39 |
| 22 | D | 402 | CLA | C3D-C2D | 3.68 | 1.47 | 1.39 |
| 22 | b | 605 | CLA | OBD-CAD | 3.68 | 1.27 | 1.22 |
| 22 | c | 501 | CLA | C3D-C2D | 3.69 | 1.47 | 1.39 |
| 22 | a | 604 | CLA | C3D-C2D | 3.69 | 1.47 | 1.39 |
| 32 | D | 407 | LHG | O7-C7 | 3.70 | 1.45 | 1.34 |
| 23 | A | 605 | PHO | CHD-C1D | 3.70 | 1.45 | 1.38 |
| 23 | a | 605 | PHO | CHD-C1D | 3.70 | 1.45 | 1.38 |
| 22 | C | 501 | CLA | C3D-C2D | 3.70 | 1.47 | 1.39 |
| 32 | d | 407 | LHG | O7-C7 | 3.71 | 1.45 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22 | c | 512 | CLA | C3D-C2D | 3.72 | 1.47 | 1.39 |
| 22 | b | 611 | CLA | C3D-C2D | 3.72 | 1.47 | 1.39 |
| 22 | B | 611 | CLA | C3D-C2D | 3.72 | 1.47 | 1.39 |
| 22 | C | 503 | CLA | OBD-CAD | 3.73 | 1.27 | 1.22 |
| 22 | b | 613 | CLA | O2A-CGA | 3.73 | 1.44 | 1.33 |
| 32 | L | 102 | LHG | O7-C7 | 3.73 | 1.45 | 1.34 |
| 32 | l | 103 | LHG | O7-C7 | 3.74 | 1.45 | 1.34 |
| 22 | c | 503 | CLA | OBD-CAD | 3.74 | 1.27 | 1.22 |
| 29 | D | 406 | LMG | O8-C28 | 3.74 | 1.44 | 1.33 |
| 22 | b | 614 | CLA | O2A-CGA | 3.74 | 1.44 | 1.33 |
| 29 | d | 406 | LMG | O8-C28 | 3.74 | 1.44 | 1.33 |
| 33 | f | 101 | HEM | C3C-CAC | 3.74 | 1.55 | 1.47 |
| 22 | B | 613 | CLA | O2A-CGA | 3.75 | 1.44 | 1.33 |
| 22 | C | 512 | CLA | C3D-C2D | 3.75 | 1.47 | 1.39 |
| 22 | C | 504 | CLA | C3D-C2D | 3.75 | 1.47 | 1.39 |
| 22 | B | 614 | CLA | O2A-CGA | 3.76 | 1.44 | 1.33 |
| 22 | B | 606 | CLA | O2A-CGA | 3.76 | 1.44 | 1.33 |
| 23 | a | 606 | PHO | O2A-CGA | 3.77 | 1.44 | 1.33 |
| 23 | A | 606 | PHO | O2A-CGA | 3.77 | 1.44 | 1.33 |
| 33 | F | 101 | HEM | C3C-CAC | 3.77 | 1.55 | 1.47 |
| 22 | c | 511 | CLA | C3D-C2D | 3.77 | 1.47 | 1.39 |
| 31 | h | 102 | DGD | O2G-C1B | 3.78 | 1.45 | 1.34 |
| 22 | b | 606 | CLA | O2A-CGA | 3.78 | 1.44 | 1.33 |
| 31 | H | 102 | DGD | O2G-C1B | 3.78 | 1.45 | 1.34 |
| 22 | c | 504 | CLA | C3D-C2D | 3.78 | 1.47 | 1.39 |
| 22 | b | 604 | CLA | C3D-C2D | 3.79 | 1.47 | 1.39 |
| 22 | C | 511 | CLA | C3D-C2D | 3.80 | 1.47 | 1.39 |
| 22 | B | 604 | CLA | C3D-C2D | 3.80 | 1.47 | 1.39 |
| 22 | C | 513 | CLA | C3D-C2D | 3.81 | 1.47 | 1.39 |
| 22 | b | 617 | CLA | C3D-C2D | 3.81 | 1.47 | 1.39 |
| 22 | A | 604 | CLA | O2A-CGA | 3.82 | 1.44 | 1.33 |
| 22 | c | 513 | CLA | C3D-C2D | 3.82 | 1.47 | 1.39 |
| 22 | B | 617 | CLA | C3D-C2D | 3.82 | 1.47 | 1.39 |
| 22 | b | 605 | CLA | O2A-CGA | 3.82 | 1.44 | 1.33 |
| 32 | d | 409 | LHG | O7-C7 | 3.83 | 1.45 | 1.34 |
| 32 | D | 409 | LHG | O7-C7 | 3.83 | 1.45 | 1.34 |
| 22 | B | 605 | CLA | O2A-CGA | 3.83 | 1.44 | 1.33 |
| 29 | d | 406 | LMG | O7-C10 | 3.84 | 1.45 | 1.34 |
| 29 | B | 620 | LMG | O7-C10 | 3.85 | 1.45 | 1.34 |
| 29 | D | 406 | LMG | O7-C10 | 3.85 | 1.45 | 1.34 |
| 22 | b | 603 | CLA | C3D-C2D | 3.87 | 1.47 | 1.39 |
| 31 | C | 516 | DGD | O2G-C1B | 3.87 | 1.45 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22 | a | 604 | CLA | O2A-CGA | 3.87 | 1.44 | 1.33 |
| 29 | b | 619 | LMG | O7-C10 | 3.88 | 1.45 | 1.34 |
| 22 | b | 611 | CLA | O2A-CGA | 3.89 | 1.44 | 1.33 |
| 31 | c | 516 | DGD | O2G-C1B | 3.89 | 1.45 | 1.34 |
| 22 | C | 505 | CLA | O2A-CGA | 3.89 | 1.44 | 1.33 |
| 33 | F | 101 | HEM | C3B-CAB | 3.89 | 1.55 | 1.47 |
| 22 | B | 603 | CLA | C3D-C2D | 3.90 | 1.47 | 1.39 |
| 22 | B | 611 | CLA | O2A-CGA | 3.91 | 1.44 | 1.33 |
| 33 | f | 101 | HEM | C3B-CAB | 3.91 | 1.55 | 1.47 |
| 22 | c | 505 | CLA | O2A-CGA | 3.91 | 1.44 | 1.33 |
| 31 | C | 516 | DGD | O1G-C1A | 3.91 | 1.44 | 1.33 |
| 22 | C | 508 | CLA | C3D-C2D | 3.92 | 1.47 | 1.39 |
| 31 | c | 516 | DGD | O1G-C1A | 3.94 | 1.44 | 1.33 |
| 22 | B | 609 | CLA | O2A-CGA | 3.95 | 1.44 | 1.33 |
| 23 | A | 605 | PHO | O2A-CGA | 3.96 | 1.44 | 1.33 |
| 22 | b | 609 | CLA | O2A-CGA | 3.96 | 1.44 | 1.33 |
| 31 | c | 518 | DGD | O1G-C1A | 3.96 | 1.44 | 1.33 |
| 31 | C | 518 | DGD | O1G-C1A | 3.97 | 1.44 | 1.33 |
| 22 | c | 508 | CLA | C3D-C2D | 3.98 | 1.47 | 1.39 |
| 23 | a | 605 | PHO | O2A-CGA | 3.98 | 1.44 | 1.33 |
| 32 | D | 407 | LHG | O8-C23 | 3.98 | 1.44 | 1.33 |
| 22 | d | 402 | CLA | O2A-CGA | 3.98 | 1.44 | 1.33 |
| 22 | B | 612 | CLA | OBD-CAD | 3.99 | 1.28 | 1.22 |
| 22 | D | 402 | CLA | O2A-CGA | 3.99 | 1.44 | 1.33 |
| 22 | C | 510 | CLA | O2A-CGA | 3.99 | 1.44 | 1.33 |
| 32 | d | 407 | LHG | O8-C23 | 4.00 | 1.44 | 1.33 |
| 22 | b | 612 | CLA | OBD-CAD | 4.00 | 1.28 | 1.22 |
| 22 | d | 402 | CLA | CHC-C1C | 4.00 | 1.46 | 1.35 |
| 31 | H | 102 | DGD | O1G-C1A | 4.01 | 1.45 | 1.33 |
| 22 | D | 402 | CLA | CHC-C1C | 4.01 | 1.46 | 1.35 |
| 32 | D | 405 | LHG | O8-C23 | 4.01 | 1.45 | 1.33 |
| 22 | c | 510 | CLA | O2A-CGA | 4.01 | 1.45 | 1.33 |
| 22 | B | 604 | CLA | O2A-CGA | 4.01 | 1.45 | 1.33 |
| 22 | B | 609 | CLA | CHC-C1C | 4.01 | 1.46 | 1.35 |
| 32 | d | 405 | LHG | O8-C23 | 4.02 | 1.45 | 1.33 |
| 22 | d | 401 | CLA | CHC-C1C | 4.02 | 1.46 | 1.35 |
| 22 | c | 504 | CLA | O2A-CGA | 4.03 | 1.45 | 1.33 |
| 31 | h | 102 | DGD | O1G-C1A | 4.03 | 1.45 | 1.33 |
| 22 | D | 401 | CLA | CHC-C1C | 4.03 | 1.46 | 1.35 |
| 25 | a | 609 | SQD | O48-C23 | 4.03 | 1.45 | 1.33 |
| 25 | a | 609 | SQD | O47-C7 | 4.04 | 1.45 | 1.34 |
| 22 | b | 609 | CLA | CHC-C1C | 4.04 | 1.46 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 25 | A | 609 | SQD | O47-C7 | 4.04 | 1.46 | 1.34 |
| 22 | c | 508 | CLA | O2A-CGA | 4.04 | 1.45 | 1.33 |
| 33 | v | 201 | HEM | C3C-CAC | 4.04 | 1.55 | 1.47 |
| 22 | b | 614 | CLA | OBD-CAD | 4.05 | 1.28 | 1.22 |
| 22 | C | 504 | CLA | O2A-CGA | 4.05 | 1.45 | 1.33 |
| 33 | V | 201 | HEM | C3C-CAC | 4.05 | 1.55 | 1.47 |
| 25 | A | 609 | SQD | O48-C23 | 4.05 | 1.45 | 1.33 |
| 22 | B | 614 | CLA | OBD-CAD | 4.05 | 1.28 | 1.22 |
| 22 | C | 508 | CLA | O2A-CGA | 4.06 | 1.45 | 1.33 |
| 22 | b | 604 | CLA | O2A-CGA | 4.06 | 1.45 | 1.33 |
| 32 | l | 103 | LHG | O8-C23 | 4.06 | 1.45 | 1.33 |
| 32 | L | 102 | LHG | O8-C23 | 4.07 | 1.45 | 1.33 |
| 22 | B | 615 | CLA | O2A-CGA | 4.08 | 1.45 | 1.33 |
| 22 | c | 501 | CLA | O2A-CGA | 4.09 | 1.45 | 1.33 |
| 22 | B | 607 | CLA | O2A-CGA | 4.10 | 1.45 | 1.33 |
| 22 | c | 502 | CLA | O2A-CGA | 4.10 | 1.45 | 1.33 |
| 22 | d | 402 | CLA | O2D-CGD | 4.10 | 1.43 | 1.33 |
| 22 | b | 615 | CLA | O2A-CGA | 4.10 | 1.45 | 1.33 |
| 22 | b | 607 | CLA | O2A-CGA | 4.10 | 1.45 | 1.33 |
| 22 | C | 501 | CLA | O2A-CGA | 4.10 | 1.45 | 1.33 |
| 22 | B | 605 | CLA | CHC-C1C | 4.11 | 1.47 | 1.35 |
| 22 | b | 612 | CLA | CHC-C1C | 4.11 | 1.47 | 1.35 |
| 22 | B | 612 | CLA | CHC-C1C | 4.12 | 1.47 | 1.35 |
| 22 | B | 610 | CLA | O2A-CGA | 4.12 | 1.45 | 1.33 |
| 22 | a | 604 | CLA | CHC-C1C | 4.12 | 1.47 | 1.35 |
| 29 | C | 519 | LMG | O7-C10 | 4.12 | 1.46 | 1.34 |
| 22 | b | 605 | CLA | CHC-C1C | 4.12 | 1.47 | 1.35 |
| 22 | C | 502 | CLA | O2A-CGA | 4.12 | 1.45 | 1.33 |
| 31 | c | 517 | DGD | O1G-C1A | 4.13 | 1.45 | 1.33 |
| 22 | A | 604 | CLA | CHC-C1C | 4.13 | 1.47 | 1.35 |
| 31 | C | 517 | DGD | O1G-C1A | 4.13 | 1.45 | 1.33 |
| 22 | c | 512 | CLA | OBD-CAD | 4.13 | 1.28 | 1.22 |
| 22 | D | 402 | CLA | O2D-CGD | 4.13 | 1.43 | 1.33 |
| 32 | e | 101 | LHG | O7-C7 | 4.14 | 1.46 | 1.34 |
| 33 | V | 201 | HEM | C3B-CAB | 4.14 | 1.56 | 1.47 |
| 22 | c | 510 | CLA | CHC-C1C | 4.14 | 1.47 | 1.35 |
| 25 | l | 101 | SQD | O48-C23 | 4.14 | 1.45 | 1.33 |
| 29 | a | 614 | LMG | O7-C10 | 4.14 | 1.46 | 1.34 |
| 22 | b | 610 | CLA | O2A-CGA | 4.14 | 1.45 | 1.33 |
| 22 | C | 510 | CLA | CHC-C1C | 4.15 | 1.47 | 1.35 |
| 29 | A | 614 | LMG | O7-C10 | 4.15 | 1.46 | 1.34 |
| 32 | E | 101 | LHG | O7-C7 | 4.15 | 1.46 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22 | B | 615 | CLA | OBD-CAD | 4.15 | 1.28 | 1.22 |
| 29 | c | 519 | LMG | O7-C10 | 4.15 | 1.46 | 1.34 |
| 25 | L | 101 | SQD | O48-C23 | 4.16 | 1.45 | 1.33 |
| 22 | B | 609 | CLA | OBD-CAD | 4.16 | 1.28 | 1.22 |
| 22 | C | 512 | CLA | OBD-CAD | 4.16 | 1.28 | 1.22 |
| 32 | D | 409 | LHG | O8-C23 | 4.16 | 1.45 | 1.33 |
| 32 | d | 409 | LHG | O8-C23 | 4.16 | 1.45 | 1.33 |
| 22 | C | 511 | CLA | O2A-CGA | 4.16 | 1.45 | 1.33 |
| 22 | B | 616 | CLA | O2A-CGA | 4.17 | 1.45 | 1.33 |
| 22 | b | 608 | CLA | OBD-CAD | 4.17 | 1.28 | 1.22 |
| 22 | D | 403 | CLA | O2A-CGA | 4.17 | 1.45 | 1.33 |
| 33 | v | 201 | HEM | C3B-CAB | 4.17 | 1.56 | 1.47 |
| 29 | Z | 101 | LMG | O7-C10 | 4.17 | 1.46 | 1.34 |
| 22 | B | 608 | CLA | OBD-CAD | 4.18 | 1.28 | 1.22 |
| 25 | B | 601 | SQD | O47-C7 | 4.18 | 1.46 | 1.34 |
| 25 | b | 601 | SQD | O47-C7 | 4.18 | 1.46 | 1.34 |
| 22 | c | 511 | CLA | O2A-CGA | 4.18 | 1.45 | 1.33 |
| 22 | b | 616 | CLA | O2A-CGA | 4.18 | 1.45 | 1.33 |
| 22 | b | 609 | CLA | OBD-CAD | 4.19 | 1.28 | 1.22 |
| 29 | z | 101 | LMG | O7-C10 | 4.19 | 1.46 | 1.34 |
| 22 | d | 403 | CLA | O2A-CGA | 4.19 | 1.45 | 1.33 |
| 22 | C | 513 | CLA | O2A-CGA | 4.20 | 1.45 | 1.33 |
| 22 | b | 615 | CLA | OBD-CAD | 4.20 | 1.28 | 1.22 |
| 22 | A | 607 | CLA | O2A-CGA | 4.20 | 1.45 | 1.33 |
| 22 | c | 503 | CLA | O2A-CGA | 4.21 | 1.45 | 1.33 |
| 22 | c | 513 | CLA | O2A-CGA | 4.21 | 1.45 | 1.33 |
| 22 | B | 606 | CLA | OBD-CAD | 4.21 | 1.28 | 1.22 |
| 22 | C | 503 | CLA | O2A-CGA | 4.23 | 1.45 | 1.33 |
| 22 | A | 607 | CLA | O2D-CGD | 4.23 | 1.43 | 1.33 |
| 22 | a | 607 | CLA | O2A-CGA | 4.23 | 1.45 | 1.33 |
| 22 | a | 607 | CLA | O2D-CGD | 4.23 | 1.43 | 1.33 |
| 22 | b | 606 | CLA | OBD-CAD | 4.25 | 1.28 | 1.22 |
| 22 | C | 512 | CLA | O2A-CGA | 4.25 | 1.45 | 1.33 |
| 22 | d | 401 | CLA | O2A-CGA | 4.25 | 1.45 | 1.33 |
| 25 | L | 101 | SQD | O47-C7 | 4.26 | 1.46 | 1.34 |
| 29 | a | 614 | LMG | O8-C28 | 4.26 | 1.45 | 1.33 |
| 22 | B | 604 | CLA | CHC-C1C | 4.27 | 1.47 | 1.35 |
| 22 | c | 507 | CLA | O2A-CGA | 4.27 | 1.45 | 1.33 |
| 29 | A | 614 | LMG | O8-C28 | 4.27 | 1.45 | 1.33 |
| 22 | C | 507 | CLA | O2A-CGA | 4.27 | 1.45 | 1.33 |
| 25 | l | 101 | SQD | O47-C7 | 4.28 | 1.46 | 1.34 |
| 22 | B | 617 | CLA | O2A-CGA | 4.28 | 1.45 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22 | c | 509 | CLA | O2A-CGA | 4.29 | 1.45 | 1.33 |
| 22 | B | 613 | CLA | OBD-CAD | 4.29 | 1.28 | 1.22 |
| 22 | c | 512 | CLA | O2A-CGA | 4.29 | 1.45 | 1.33 |
| 29 | C | 519 | LMG | O8-C28 | 4.29 | 1.45 | 1.33 |
| 22 | c | 504 | CLA | CHC-C1C | 4.30 | 1.47 | 1.35 |
| 25 | b | 621 | SQD | O47-C7 | 4.30 | 1.46 | 1.34 |
| 22 | D | 403 | CLA | OBD-CAD | 4.30 | 1.28 | 1.22 |
| 22 | b | 617 | CLA | O2A-CGA | 4.30 | 1.45 | 1.33 |
| 22 | C | 509 | CLA | O2A-CGA | 4.30 | 1.45 | 1.33 |
| 22 | C | 504 | CLA | CHC-C1C | 4.31 | 1.47 | 1.35 |
| 29 | c | 519 | LMG | O8-C28 | 4.31 | 1.45 | 1.33 |
| 22 | D | 401 | CLA | O2A-CGA | 4.31 | 1.45 | 1.33 |
| 25 | l | 102 | SQD | O47-C7 | 4.32 | 1.46 | 1.34 |
| 22 | b | 604 | CLA | CHC-C1C | 4.32 | 1.47 | 1.35 |
| 22 | b | 603 | CLA | O2D-CGD | 4.32 | 1.44 | 1.33 |
| 22 | B | 611 | CLA | OBD-CAD | 4.32 | 1.28 | 1.22 |
| 22 | B | 616 | CLA | OBD-CAD | 4.32 | 1.28 | 1.22 |
| 23 | A | 605 | PHO | CHC-C1C | 4.33 | 1.47 | 1.38 |
| 22 | b | 608 | CLA | CHC-C1C | 4.33 | 1.47 | 1.35 |
| 22 | b | 613 | CLA | OBD-CAD | 4.33 | 1.28 | 1.22 |
| 22 | d | 403 | CLA | OBD-CAD | 4.33 | 1.28 | 1.22 |
| 22 | c | 508 | CLA | OBD-CAD | 4.33 | 1.28 | 1.22 |
| 22 | B | 605 | CLA | O2D-CGD | 4.34 | 1.44 | 1.33 |
| 22 | c | 506 | CLA | OBD-CAD | 4.34 | 1.28 | 1.22 |
| 22 | b | 605 | CLA | O2D-CGD | 4.34 | 1.44 | 1.33 |
| 22 | b | 611 | CLA | OBD-CAD | 4.34 | 1.28 | 1.22 |
| 22 | B | 603 | CLA | O2D-CGD | 4.34 | 1.44 | 1.33 |
| 22 | C | 505 | CLA | OBD-CAD | 4.35 | 1.28 | 1.22 |
| 22 | C | 506 | CLA | O2A-CGA | 4.36 | 1.46 | 1.33 |
| 31 | d | 410 | DGD | O2G-C1B | 4.36 | 1.46 | 1.34 |
| 22 | C | 508 | CLA | OBD-CAD | 4.37 | 1.28 | 1.22 |
| 22 | B | 608 | CLA | CHC-C1C | 4.37 | 1.47 | 1.35 |
| 22 | C | 507 | CLA | OBD-CAD | 4.37 | 1.28 | 1.22 |
| 22 | b | 616 | CLA | OBD-CAD | 4.37 | 1.28 | 1.22 |
| 29 | c | 520 | LMG | O8-C28 | 4.37 | 1.46 | 1.33 |
| 25 | d | 411 | SQD | O47-C7 | 4.38 | 1.46 | 1.34 |
| 22 | B | 610 | CLA | OBD-CAD | 4.38 | 1.28 | 1.22 |
| 22 | c | 509 | CLA | CHC-C1C | 4.38 | 1.47 | 1.35 |
| 22 | C | 506 | CLA | OBD-CAD | 4.38 | 1.28 | 1.22 |
| 31 | D | 410 | DGD | O2G-C1B | 4.38 | 1.46 | 1.34 |
| 25 | D | 411 | SQD | O47-C7 | 4.38 | 1.47 | 1.34 |
| 23 | a | 605 | PHO | CHC-C1C | 4.38 | 1.47 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22 | C | 509 | CLA | CHC-C1C | 4.38 | 1.47 | 1.35 |
| 22 | C | 511 | CLA | CHC-C1C | 4.39 | 1.47 | 1.35 |
| 22 | c | 506 | CLA | O2A-CGA | 4.39 | 1.46 | 1.33 |
| 22 | B | 610 | CLA | O2D-CGD | 4.39 | 1.44 | 1.33 |
| 22 | c | 507 | CLA | OBD-CAD | 4.40 | 1.28 | 1.22 |
| 22 | a | 603 | CLA | CHC-C1C | 4.40 | 1.47 | 1.35 |
| 22 | C | 502 | CLA | OBD-CAD | 4.40 | 1.28 | 1.22 |
| 22 | B | 612 | CLA | C3B-C2B | 4.40 | 1.46 | 1.40 |
| 22 | C | 501 | CLA | OBD-CAD | 4.40 | 1.28 | 1.22 |
| 22 | b | 612 | CLA | O2D-CGD | 4.40 | 1.44 | 1.33 |
| 22 | c | 505 | CLA | OBD-CAD | 4.40 | 1.28 | 1.22 |
| 22 | A | 603 | CLA | CHC-C1C | 4.40 | 1.47 | 1.35 |
| 22 | B | 612 | CLA | O2D-CGD | 4.40 | 1.44 | 1.33 |
| 22 | b | 610 | CLA | O2D-CGD | 4.41 | 1.44 | 1.33 |
| 22 | B | 610 | CLA | CHC-C1C | 4.41 | 1.47 | 1.35 |
| 23 | A | 606 | PHO | CHD-C1D | 4.41 | 1.47 | 1.38 |
| 29 | C | 520 | LMG | O8-C28 | 4.41 | 1.46 | 1.33 |
| 22 | c | 511 | CLA | CHC-C1C | 4.41 | 1.47 | 1.35 |
| 22 | b | 616 | CLA | CHC-C1C | 4.41 | 1.47 | 1.35 |
| 29 | c | 520 | LMG | O7-C10 | 4.42 | 1.47 | 1.34 |
| 29 | C | 520 | LMG | O7-C10 | 4.42 | 1.47 | 1.34 |
| 23 | a | 606 | PHO | CHD-C1D | 4.42 | 1.47 | 1.38 |
| 22 | B | 616 | CLA | CHC-C1C | 4.42 | 1.48 | 1.35 |
| 22 | B | 617 | CLA | CHC-C1C | 4.43 | 1.48 | 1.35 |
| 22 | b | 610 | CLA | CHC-C1C | 4.43 | 1.48 | 1.35 |
| 22 | c | 504 | CLA | OBD-CAD | 4.43 | 1.28 | 1.22 |
| 22 | c | 501 | CLA | OBD-CAD | 4.43 | 1.28 | 1.22 |
| 22 | B | 614 | CLA | O2D-CGD | 4.43 | 1.44 | 1.33 |
| 22 | b | 610 | CLA | OBD-CAD | 4.44 | 1.28 | 1.22 |
| 22 | b | 602 | CLA | OBD-CAD | 4.44 | 1.28 | 1.22 |
| 22 | b | 612 | CLA | C3B-C2B | 4.44 | 1.46 | 1.40 |
| 22 | b | 617 | CLA | CHC-C1C | 4.45 | 1.48 | 1.35 |
| 22 | b | 614 | CLA | O2D-CGD | 4.45 | 1.44 | 1.33 |
| 22 | B | 602 | CLA | OBD-CAD | 4.45 | 1.28 | 1.22 |
| 22 | B | 615 | CLA | CHC-C1C | 4.45 | 1.48 | 1.35 |
| 22 | b | 606 | CLA | C3B-C2B | 4.46 | 1.46 | 1.40 |
| 25 | b | 621 | SQD | O48-C23 | 4.46 | 1.46 | 1.33 |
| 22 | b | 615 | CLA | CHC-C1C | 4.46 | 1.48 | 1.35 |
| 22 | A | 604 | CLA | OBD-CAD | 4.47 | 1.28 | 1.22 |
| 22 | c | 502 | CLA | OBD-CAD | 4.47 | 1.28 | 1.22 |
| 22 | b | 611 | CLA | O2D-CGD | 4.47 | 1.44 | 1.33 |
| 23 | A | 605 | PHO | O2D-CGD | 4.47 | 1.44 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22 | B | 611 | CLA | O2D-CGD | 4.47 | 1.44 | 1.33 |
| 22 | D | 403 | CLA | CHC-C1C | 4.48 | 1.48 | 1.35 |
| 25 | l | 102 | SQD | O48-C23 | 4.48 | 1.46 | 1.33 |
| 22 | C | 504 | CLA | OBD-CAD | 4.48 | 1.28 | 1.22 |
| 22 | C | 508 | CLA | CHC-C1C | 4.49 | 1.48 | 1.35 |
| 22 | b | 614 | CLA | CHC-C1C | 4.49 | 1.48 | 1.35 |
| 23 | a | 605 | PHO | O2D-CGD | 4.49 | 1.44 | 1.33 |
| 22 | c | 508 | CLA | CHC-C1C | 4.49 | 1.48 | 1.35 |
| 22 | B | 606 | CLA | C3B-C2B | 4.49 | 1.46 | 1.40 |
| 22 | a | 607 | CLA | CHC-C1C | 4.49 | 1.48 | 1.35 |
| 22 | b | 615 | CLA | C3B-C2B | 4.50 | 1.46 | 1.40 |
| 22 | C | 501 | CLA | O2D-CGD | 4.50 | 1.44 | 1.33 |
| 22 | c | 501 | CLA | O2D-CGD | 4.51 | 1.44 | 1.33 |
| 32 | E | 101 | LHG | O8-C23 | 4.51 | 1.46 | 1.33 |
| 22 | b | 611 | CLA | CHC-C1C | 4.51 | 1.48 | 1.35 |
| 22 | c | 505 | CLA | CHC-C1C | 4.51 | 1.48 | 1.35 |
| 22 | d | 403 | CLA | CHC-C1C | 4.52 | 1.48 | 1.35 |
| 22 | B | 611 | CLA | CHC-C1C | 4.52 | 1.48 | 1.35 |
| 22 | B | 614 | CLA | CHC-C1C | 4.52 | 1.48 | 1.35 |
| 25 | B | 601 | SQD | O48-C23 | 4.52 | 1.46 | 1.33 |
| 22 | A | 607 | CLA | CHC-C1C | 4.53 | 1.48 | 1.35 |
| 22 | a | 604 | CLA | OBD-CAD | 4.53 | 1.28 | 1.22 |
| 22 | B | 607 | CLA | CHC-C1C | 4.53 | 1.48 | 1.35 |
| 32 | e | 101 | LHG | O8-C23 | 4.53 | 1.46 | 1.33 |
| 25 | b | 601 | SQD | O48-C23 | 4.54 | 1.46 | 1.33 |
| 31 | d | 410 | DGD | O1G-C1A | 4.54 | 1.46 | 1.33 |
| 22 | d | 401 | CLA | O2D-CGD | 4.54 | 1.44 | 1.33 |
| 22 | C | 505 | CLA | CHC-C1C | 4.54 | 1.48 | 1.35 |
| 22 | B | 607 | CLA | OBD-CAD | 4.54 | 1.28 | 1.22 |
| 22 | a | 604 | CLA | O2D-CGD | 4.55 | 1.44 | 1.33 |
| 25 | d | 411 | SQD | O48-C23 | 4.55 | 1.46 | 1.33 |
| 22 | B | 615 | CLA | C3B-C2B | 4.55 | 1.46 | 1.40 |
| 31 | D | 410 | DGD | O1G-C1A | 4.56 | 1.46 | 1.33 |
| 22 | b | 607 | CLA | CHC-C1C | 4.56 | 1.48 | 1.35 |
| 22 | C | 506 | CLA | CHC-C1C | 4.56 | 1.48 | 1.35 |
| 22 | d | 403 | CLA | O2D-CGD | 4.56 | 1.44 | 1.33 |
| 22 | c | 506 | CLA | CHC-C1C | 4.57 | 1.48 | 1.35 |
| 22 | C | 513 | CLA | OBD-CAD | 4.57 | 1.28 | 1.22 |
| 22 | b | 606 | CLA | CHC-C1C | 4.58 | 1.48 | 1.35 |
| 22 | D | 403 | CLA | O2D-CGD | 4.58 | 1.44 | 1.33 |
| 22 | b | 607 | CLA | OBD-CAD | 4.58 | 1.28 | 1.22 |
| 22 | B | 606 | CLA | CHC-C1C | 4.59 | 1.48 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22 | D | 401 | CLA | O2D-CGD | 4.59 | 1.44 | 1.33 |
| 22 | C | 504 | CLA | O2D-CGD | 4.59 | 1.44 | 1.33 |
| 22 | A | 604 | CLA | O2D-CGD | 4.59 | 1.44 | 1.33 |
| 22 | c | 507 | CLA | CHC-C1C | 4.59 | 1.48 | 1.35 |
| 22 | c | 501 | CLA | CHC-C1C | 4.59 | 1.48 | 1.35 |
| 29 | B | 620 | LMG | O8-C28 | 4.59 | 1.46 | 1.33 |
| 22 | c | 504 | CLA | O2D-CGD | 4.59 | 1.44 | 1.33 |
| 25 | D | 411 | SQD | O48-C23 | 4.60 | 1.46 | 1.33 |
| 22 | C | 501 | CLA | CHC-C1C | 4.60 | 1.48 | 1.35 |
| 22 | C | 507 | CLA | CHC-C1C | 4.60 | 1.48 | 1.35 |
| 22 | c | 513 | CLA | OBD-CAD | 4.60 | 1.28 | 1.22 |
| 22 | C | 511 | CLA | OBD-CAD | 4.61 | 1.28 | 1.22 |
| 22 | c | 511 | CLA | OBD-CAD | 4.61 | 1.28 | 1.22 |
| 22 | B | 602 | CLA | CHC-C1C | 4.61 | 1.48 | 1.35 |
| 29 | b | 619 | LMG | O8-C28 | 4.62 | 1.46 | 1.33 |
| 22 | b | 603 | CLA | OBD-CAD | 4.62 | 1.28 | 1.22 |
| 22 | B | 603 | CLA | OBD-CAD | 4.62 | 1.28 | 1.22 |
| 22 | B | 604 | CLA | OBD-CAD | 4.63 | 1.28 | 1.22 |
| 22 | B | 605 | CLA | C3B-C2B | 4.63 | 1.46 | 1.40 |
| 22 | b | 615 | CLA | O2D-CGD | 4.63 | 1.44 | 1.33 |
| 22 | B | 615 | CLA | O2D-CGD | 4.64 | 1.44 | 1.33 |
| 22 | b | 602 | CLA | CHC-C1C | 4.64 | 1.48 | 1.35 |
| 22 | b | 608 | CLA | O2D-CGD | 4.65 | 1.44 | 1.33 |
| 22 | B | 608 | CLA | O2D-CGD | 4.65 | 1.44 | 1.33 |
| 22 | c | 503 | CLA | O2D-CGD | 4.65 | 1.44 | 1.33 |
| 22 | C | 503 | CLA | CHC-C1C | 4.65 | 1.48 | 1.35 |
| 22 | C | 503 | CLA | O2D-CGD | 4.65 | 1.44 | 1.33 |
| 22 | c | 503 | CLA | CHC-C1C | 4.65 | 1.48 | 1.35 |
| 23 | a | 606 | PHO | CHC-C1C | 4.65 | 1.47 | 1.38 |
| 22 | C | 513 | CLA | CHC-C1C | 4.66 | 1.48 | 1.35 |
| 22 | c | 513 | CLA | CHC-C1C | 4.66 | 1.48 | 1.35 |
| 22 | C | 512 | CLA | CHC-C1C | 4.66 | 1.48 | 1.35 |
| 23 | A | 606 | PHO | CHC-C1C | 4.66 | 1.47 | 1.38 |
| 22 | d | 401 | CLA | OBD-CAD | 4.66 | 1.29 | 1.22 |
| 22 | b | 613 | CLA | O2D-CGD | 4.67 | 1.44 | 1.33 |
| 22 | A | 603 | CLA | OBD-CAD | 4.67 | 1.29 | 1.22 |
| 22 | D | 401 | CLA | OBD-CAD | 4.68 | 1.29 | 1.22 |
| 22 | b | 604 | CLA | OBD-CAD | 4.68 | 1.29 | 1.22 |
| 22 | B | 613 | CLA | O2D-CGD | 4.68 | 1.44 | 1.33 |
| 22 | c | 512 | CLA | CHC-C1C | 4.68 | 1.48 | 1.35 |
| 22 | b | 605 | CLA | C3B-C2B | 4.68 | 1.46 | 1.40 |
| 22 | b | 612 | CLA | C3C-C2C | 4.69 | 1.46 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22 | b | 617 | CLA | OBD-CAD | 4.69 | 1.29 | 1.22 |
| 22 | B | 612 | CLA | C3C-C2C | 4.69 | 1.46 | 1.36 |
| 22 | c | 502 | CLA | C3B-C2B | 4.70 | 1.46 | 1.40 |
| 22 | B | 617 | CLA | OBD-CAD | 4.70 | 1.29 | 1.22 |
| 22 | c | 502 | CLA | CHC-C1C | 4.71 | 1.48 | 1.35 |
| 22 | C | 502 | CLA | CHC-C1C | 4.71 | 1.48 | 1.35 |
| 22 | D | 402 | CLA | OBD-CAD | 4.71 | 1.29 | 1.22 |
| 22 | b | 604 | CLA | O2D-CGD | 4.72 | 1.45 | 1.33 |
| 22 | b | 613 | CLA | CHC-C1C | 4.72 | 1.48 | 1.35 |
| 22 | b | 616 | CLA | O2D-CGD | 4.72 | 1.45 | 1.33 |
| 22 | b | 610 | CLA | C3B-C2B | 4.72 | 1.46 | 1.40 |
| 22 | B | 613 | CLA | CHC-C1C | 4.72 | 1.48 | 1.35 |
| 22 | C | 502 | CLA | C3B-C2B | 4.72 | 1.46 | 1.40 |
| 22 | b | 617 | CLA | O2D-CGD | 4.72 | 1.45 | 1.33 |
| 22 | a | 603 | CLA | O2D-CGD | 4.72 | 1.45 | 1.33 |
| 22 | A | 603 | CLA | O2D-CGD | 4.73 | 1.45 | 1.33 |
| 22 | B | 617 | CLA | O2D-CGD | 4.73 | 1.45 | 1.33 |
| 22 | B | 604 | CLA | O2D-CGD | 4.73 | 1.45 | 1.33 |
| 22 | a | 603 | CLA | OBD-CAD | 4.74 | 1.29 | 1.22 |
| 22 | B | 604 | CLA | C3C-C2C | 4.74 | 1.46 | 1.36 |
| 22 | b | 604 | CLA | C3C-C2C | 4.74 | 1.46 | 1.36 |
| 22 | b | 606 | CLA | O2D-CGD | 4.74 | 1.45 | 1.33 |
| 22 | B | 616 | CLA | O2D-CGD | 4.74 | 1.45 | 1.33 |
| 22 | B | 606 | CLA | O2D-CGD | 4.74 | 1.45 | 1.33 |
| 22 | a | 604 | CLA | C3C-C2C | 4.75 | 1.46 | 1.36 |
| 22 | d | 402 | CLA | OBD-CAD | 4.76 | 1.29 | 1.22 |
| 22 | C | 510 | CLA | O2D-CGD | 4.76 | 1.45 | 1.33 |
| 22 | c | 510 | CLA | O2D-CGD | 4.77 | 1.45 | 1.33 |
| 22 | B | 603 | CLA | CHC-C1C | 4.78 | 1.49 | 1.35 |
| 22 | B | 611 | CLA | C3B-C2B | 4.78 | 1.47 | 1.40 |
| 22 | B | 610 | CLA | C3B-C2B | 4.78 | 1.47 | 1.40 |
| 22 | A | 604 | CLA | C3C-C2C | 4.79 | 1.47 | 1.36 |
| 22 | a | 604 | CLA | C3B-C2B | 4.79 | 1.47 | 1.40 |
| 22 | B | 616 | CLA | C3B-C2B | 4.80 | 1.47 | 1.40 |
| 22 | b | 603 | CLA | CHC-C1C | 4.80 | 1.49 | 1.35 |
| 22 | C | 510 | CLA | OBD-CAD | 4.80 | 1.29 | 1.22 |
| 22 | b | 607 | CLA | O2D-CGD | 4.81 | 1.45 | 1.33 |
| 22 | B | 613 | CLA | C3C-C2C | 4.81 | 1.47 | 1.36 |
| 22 | b | 611 | CLA | C3B-C2B | 4.81 | 1.47 | 1.40 |
| 22 | C | 505 | CLA | O2D-CGD | 4.81 | 1.45 | 1.33 |
| 23 | a | 606 | PHO | O2D-CGD | 4.81 | 1.45 | 1.33 |
| 22 | B | 602 | CLA | O2A-CGA | 4.82 | 1.47 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22 | D | 402 | CLA | C3B-C2B | 4.82 | 1.47 | 1.40 |
| 22 | b | 616 | CLA | C3B-C2B | 4.82 | 1.47 | 1.40 |
| 22 | b | 602 | CLA | O2A-CGA | 4.82 | 1.47 | 1.33 |
| 22 | d | 402 | CLA | C3B-C2B | 4.82 | 1.47 | 1.40 |
| 23 | A | 606 | PHO | O2D-CGD | 4.83 | 1.45 | 1.33 |
| 22 | c | 502 | CLA | O2D-CGD | 4.83 | 1.45 | 1.33 |
| 22 | b | 613 | CLA | C3C-C2C | 4.83 | 1.47 | 1.36 |
| 22 | c | 505 | CLA | O2D-CGD | 4.85 | 1.45 | 1.33 |
| 22 | A | 604 | CLA | C3B-C2B | 4.85 | 1.47 | 1.40 |
| 22 | B | 607 | CLA | O2D-CGD | 4.85 | 1.45 | 1.33 |
| 22 | c | 510 | CLA | OBD-CAD | 4.85 | 1.29 | 1.22 |
| 22 | C | 509 | CLA | C3B-C2B | 4.86 | 1.47 | 1.40 |
| 22 | C | 502 | CLA | O2D-CGD | 4.86 | 1.45 | 1.33 |
| 22 | a | 607 | CLA | OBD-CAD | 4.86 | 1.29 | 1.22 |
| 22 | C | 502 | CLA | C3C-C2C | 4.87 | 1.47 | 1.36 |
| 22 | b | 605 | CLA | C3C-C2C | 4.87 | 1.47 | 1.36 |
| 22 | B | 615 | CLA | C3C-C2C | 4.87 | 1.47 | 1.36 |
| 23 | A | 606 | PHO | C3C-C2C | 4.87 | 1.47 | 1.36 |
| 22 | c | 502 | CLA | C3C-C2C | 4.88 | 1.47 | 1.36 |
| 22 | D | 401 | CLA | C3C-C2C | 4.89 | 1.47 | 1.36 |
| 22 | b | 615 | CLA | C3C-C2C | 4.89 | 1.47 | 1.36 |
| 22 | B | 614 | CLA | C3B-C2B | 4.89 | 1.47 | 1.40 |
| 22 | d | 401 | CLA | C3C-C2C | 4.89 | 1.47 | 1.36 |
| 22 | b | 609 | CLA | O2D-CGD | 4.89 | 1.45 | 1.33 |
| 22 | c | 512 | CLA | O2D-CGD | 4.89 | 1.45 | 1.33 |
| 23 | a | 606 | PHO | C3C-C2C | 4.90 | 1.47 | 1.36 |
| 22 | A | 607 | CLA | OBD-CAD | 4.90 | 1.29 | 1.22 |
| 22 | c | 504 | CLA | C3C-C2C | 4.90 | 1.47 | 1.36 |
| 22 | B | 605 | CLA | C3C-C2C | 4.91 | 1.47 | 1.36 |
| 22 | C | 512 | CLA | O2D-CGD | 4.91 | 1.45 | 1.33 |
| 22 | B | 609 | CLA | O2D-CGD | 4.91 | 1.45 | 1.33 |
| 22 | b | 614 | CLA | C3B-C2B | 4.91 | 1.47 | 1.40 |
| 22 | c | 501 | CLA | C3C-C2C | 4.91 | 1.47 | 1.36 |
| 22 | c | 511 | CLA | C3B-C2B | 4.91 | 1.47 | 1.40 |
| 22 | D | 402 | CLA | C3C-C2C | 4.91 | 1.47 | 1.36 |
| 22 | C | 507 | CLA | O2D-CGD | 4.92 | 1.45 | 1.33 |
| 22 | d | 402 | CLA | C3C-C2C | 4.93 | 1.47 | 1.36 |
| 22 | B | 617 | CLA | C3C-C2C | 4.94 | 1.47 | 1.36 |
| 22 | C | 511 | CLA | C3B-C2B | 4.94 | 1.47 | 1.40 |
| 22 | C | 508 | CLA | O2D-CGD | 4.94 | 1.45 | 1.33 |
| 22 | c | 509 | CLA | OBD-CAD | 4.94 | 1.29 | 1.22 |
| 22 | C | 504 | CLA | C3C-C2C | 4.94 | 1.47 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22 | B | 610 | CLA | C3C-C2C | 4.94 | 1.47 | 1.36 |
| 22 | b | 610 | CLA | C3C-C2C | 4.94 | 1.47 | 1.36 |
| 22 | C | 501 | CLA | C3C-C2C | 4.95 | 1.47 | 1.36 |
| 22 | C | 509 | CLA | OBD-CAD | 4.95 | 1.29 | 1.22 |
| 33 | v | 201 | HEM | C3D-C2D | 4.95 | 1.52 | 1.37 |
| 22 | B | 614 | CLA | C3C-C2C | 4.96 | 1.47 | 1.36 |
| 22 | C | 509 | CLA | C3C-C2C | 4.96 | 1.47 | 1.36 |
| 22 | b | 617 | CLA | C3C-C2C | 4.97 | 1.47 | 1.36 |
| 22 | c | 508 | CLA | O2D-CGD | 4.97 | 1.45 | 1.33 |
| 22 | C | 506 | CLA | O2D-CGD | 4.97 | 1.45 | 1.33 |
| 22 | c | 511 | CLA | O2D-CGD | 4.97 | 1.45 | 1.33 |
| 22 | c | 507 | CLA | O2D-CGD | 4.97 | 1.45 | 1.33 |
| 22 | c | 509 | CLA | C3B-C2B | 4.97 | 1.47 | 1.40 |
| 33 | V | 201 | HEM | C3D-C2D | 4.98 | 1.52 | 1.37 |
| 22 | C | 511 | CLA | O2D-CGD | 4.98 | 1.45 | 1.33 |
| 22 | b | 602 | CLA | C3B-C2B | 4.99 | 1.47 | 1.40 |
| 22 | B | 608 | CLA | C3B-C2B | 4.99 | 1.47 | 1.40 |
| 22 | C | 509 | CLA | O2D-CGD | 4.99 | 1.45 | 1.33 |
| 22 | c | 506 | CLA | O2D-CGD | 4.99 | 1.45 | 1.33 |
| 22 | c | 509 | CLA | C3C-C2C | 4.99 | 1.47 | 1.36 |
| 22 | b | 614 | CLA | C3C-C2C | 4.99 | 1.47 | 1.36 |
| 22 | b | 608 | CLA | C3C-C2C | 4.99 | 1.47 | 1.36 |
| 22 | b | 608 | CLA | C3B-C2B | 4.99 | 1.47 | 1.40 |
| 23 | A | 605 | PHO | C3C-C2C | 5.00 | 1.47 | 1.36 |
| 22 | c | 513 | CLA | O2D-CGD | 5.00 | 1.45 | 1.33 |
| 22 | c | 509 | CLA | O2D-CGD | 5.00 | 1.45 | 1.33 |
| 22 | c | 511 | CLA | C3C-C2C | 5.01 | 1.47 | 1.36 |
| 22 | C | 510 | CLA | C3B-C2B | 5.01 | 1.47 | 1.40 |
| 23 | a | 605 | PHO | C3C-C2C | 5.01 | 1.47 | 1.36 |
| 22 | B | 602 | CLA | C3B-C2B | 5.02 | 1.47 | 1.40 |
| 22 | B | 608 | CLA | C3C-C2C | 5.02 | 1.47 | 1.36 |
| 22 | b | 604 | CLA | C3B-C2B | 5.02 | 1.47 | 1.40 |
| 22 | C | 513 | CLA | O2D-CGD | 5.03 | 1.45 | 1.33 |
| 22 | c | 506 | CLA | C3C-C2C | 5.03 | 1.47 | 1.36 |
| 22 | c | 510 | CLA | C3B-C2B | 5.03 | 1.47 | 1.40 |
| 22 | B | 604 | CLA | C3B-C2B | 5.04 | 1.47 | 1.40 |
| 22 | B | 609 | CLA | C3B-C2B | 5.04 | 1.47 | 1.40 |
| 22 | C | 511 | CLA | C3C-C2C | 5.04 | 1.47 | 1.36 |
| 22 | a | 607 | CLA | C3C-C2C | 5.05 | 1.47 | 1.36 |
| 22 | b | 609 | CLA | C3B-C2B | 5.06 | 1.47 | 1.40 |
| 22 | C | 506 | CLA | C3C-C2C | 5.06 | 1.47 | 1.36 |
| 22 | C | 510 | CLA | C3C-C2C | 5.06 | 1.47 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22 | c | 510 | CLA | C3C-C2C | 5.06 | 1.47 | 1.36 |
| 22 | B | 609 | CLA | C3C-C2C | 5.06 | 1.47 | 1.36 |
| 22 | C | 506 | CLA | C3B-C2B | 5.06 | 1.47 | 1.40 |
| 22 | c | 506 | CLA | C3B-C2B | 5.06 | 1.47 | 1.40 |
| 22 | b | 609 | CLA | C3C-C2C | 5.07 | 1.47 | 1.36 |
| 22 | a | 603 | CLA | C3B-C2B | 5.07 | 1.47 | 1.40 |
| 22 | A | 607 | CLA | C3C-C2C | 5.08 | 1.47 | 1.36 |
| 22 | A | 603 | CLA | C3B-C2B | 5.09 | 1.47 | 1.40 |
| 22 | b | 607 | CLA | C3B-C2B | 5.10 | 1.47 | 1.40 |
| 22 | D | 403 | CLA | C3C-C2C | 5.11 | 1.47 | 1.36 |
| 22 | C | 505 | CLA | C3C-C2C | 5.11 | 1.47 | 1.36 |
| 22 | c | 505 | CLA | C3C-C2C | 5.11 | 1.47 | 1.36 |
| 22 | a | 607 | CLA | C3B-C2B | 5.11 | 1.47 | 1.40 |
| 22 | d | 403 | CLA | C3C-C2C | 5.11 | 1.47 | 1.36 |
| 23 | a | 606 | PHO | CHB-C1B | 5.11 | 1.48 | 1.38 |
| 23 | A | 606 | PHO | CHB-C1B | 5.12 | 1.48 | 1.38 |
| 22 | A | 607 | CLA | C3B-C2B | 5.13 | 1.47 | 1.40 |
| 22 | B | 607 | CLA | C3B-C2B | 5.13 | 1.47 | 1.40 |
| 22 | b | 602 | CLA | O2D-CGD | 5.13 | 1.46 | 1.33 |
| 22 | b | 611 | CLA | C3C-C2C | 5.13 | 1.47 | 1.36 |
| 22 | B | 602 | CLA | O2D-CGD | 5.14 | 1.46 | 1.33 |
| 22 | d | 401 | CLA | C3B-C2B | 5.15 | 1.47 | 1.40 |
| 22 | b | 606 | CLA | C3C-C2C | 5.15 | 1.47 | 1.36 |
| 22 | b | 607 | CLA | C3C-C2C | 5.16 | 1.47 | 1.36 |
| 22 | a | 603 | CLA | C3C-C2C | 5.16 | 1.47 | 1.36 |
| 22 | B | 611 | CLA | C3C-C2C | 5.17 | 1.47 | 1.36 |
| 22 | b | 613 | CLA | C3B-C2B | 5.17 | 1.47 | 1.40 |
| 22 | d | 403 | CLA | C3B-C2B | 5.18 | 1.47 | 1.40 |
| 22 | D | 401 | CLA | C3B-C2B | 5.19 | 1.47 | 1.40 |
| 22 | C | 505 | CLA | C3B-C2B | 5.19 | 1.47 | 1.40 |
| 22 | B | 606 | CLA | C3C-C2C | 5.19 | 1.47 | 1.36 |
| 22 | B | 607 | CLA | C3C-C2C | 5.19 | 1.47 | 1.36 |
| 22 | B | 602 | CLA | C3C-C2C | 5.22 | 1.47 | 1.36 |
| 22 | B | 613 | CLA | C3B-C2B | 5.22 | 1.47 | 1.40 |
| 22 | c | 505 | CLA | C3B-C2B | 5.22 | 1.47 | 1.40 |
| 22 | C | 507 | CLA | C3C-C2C | 5.22 | 1.47 | 1.36 |
| 22 | A | 603 | CLA | C3C-C2C | 5.22 | 1.47 | 1.36 |
| 22 | D | 403 | CLA | C3B-C2B | 5.23 | 1.47 | 1.40 |
| 22 | b | 602 | CLA | C3C-C2C | 5.23 | 1.47 | 1.36 |
| 22 | C | 504 | CLA | C3B-C2B | 5.25 | 1.47 | 1.40 |
| 22 | B | 616 | CLA | C3C-C2C | 5.25 | 1.47 | 1.36 |
| 22 | c | 507 | CLA | C3C-C2C | 5.25 | 1.48 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22 | b | 616 | CLA | C3C-C2C | 5.25 | 1.48 | 1.36 |
| 33 | f | 101 | HEM | C3D-C2D | 5.27 | 1.53 | 1.37 |
| 33 | F | 101 | HEM | C3D-C2D | 5.28 | 1.53 | 1.37 |
| 22 | c | 503 | CLA | C3C-C2C | 5.28 | 1.48 | 1.36 |
| 22 | c | 504 | CLA | C3B-C2B | 5.28 | 1.47 | 1.40 |
| 22 | C | 512 | CLA | C3B-C2B | 5.30 | 1.47 | 1.40 |
| 23 | a | 605 | PHO | C3B-C2B | 5.32 | 1.47 | 1.37 |
| 22 | C | 503 | CLA | C3C-C2C | 5.33 | 1.48 | 1.36 |
| 23 | A | 605 | PHO | C3B-C2B | 5.35 | 1.47 | 1.37 |
| 23 | a | 605 | PHO | CHB-C1B | 5.35 | 1.49 | 1.38 |
| 22 | c | 512 | CLA | C3B-C2B | 5.35 | 1.47 | 1.40 |
| 23 | A | 605 | PHO | CHB-C1B | 5.36 | 1.49 | 1.38 |
| 22 | c | 513 | CLA | C3C-C2C | 5.36 | 1.48 | 1.36 |
| 22 | C | 501 | CLA | C3B-C2B | 5.36 | 1.47 | 1.40 |
| 22 | c | 501 | CLA | C3B-C2B | 5.37 | 1.47 | 1.40 |
| 22 | C | 512 | CLA | C3C-C2C | 5.38 | 1.48 | 1.36 |
| 22 | B | 603 | CLA | C3C-C2C | 5.40 | 1.48 | 1.36 |
| 22 | C | 513 | CLA | C3C-C2C | 5.40 | 1.48 | 1.36 |
| 22 | c | 512 | CLA | C3C-C2C | 5.40 | 1.48 | 1.36 |
| 22 | b | 603 | CLA | C3C-C2C | 5.44 | 1.48 | 1.36 |
| 22 | C | 508 | CLA | C3C-C2C | 5.44 | 1.48 | 1.36 |
| 22 | c | 508 | CLA | C3C-C2C | 5.49 | 1.48 | 1.36 |
| 22 | C | 508 | CLA | C3B-C2B | 5.51 | 1.48 | 1.40 |
| 22 | C | 503 | CLA | C3B-C2B | 5.52 | 1.48 | 1.40 |
| 22 | c | 503 | CLA | C3B-C2B | 5.53 | 1.48 | 1.40 |
| 22 | B | 617 | CLA | C3B-C2B | 5.54 | 1.48 | 1.40 |
| 22 | c | 508 | CLA | C3B-C2B | 5.56 | 1.48 | 1.40 |
| 22 | b | 617 | CLA | C3B-C2B | 5.60 | 1.48 | 1.40 |
| 23 | a | 606 | PHO | C3B-C2B | 5.63 | 1.48 | 1.37 |
| 23 | A | 606 | PHO | C3B-C2B | 5.64 | 1.48 | 1.37 |
| 22 | B | 603 | CLA | C3B-C2B | 5.66 | 1.48 | 1.40 |
| 22 | b | 603 | CLA | C3B-C2B | 5.67 | 1.48 | 1.40 |
| 22 | C | 513 | CLA | C3B-C2B | 5.80 | 1.48 | 1.40 |
| 22 | c | 513 | CLA | C3B-C2B | 5.82 | 1.48 | 1.40 |
| 22 | c | 507 | CLA | C3B-C2B | 6.06 | 1.48 | 1.40 |
| 22 | C | 507 | CLA | C3B-C2B | 6.06 | 1.48 | 1.40 |

All (2310) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 24 | T | 102 | BCR | C36-C18-C17 | -10.60 | 108.08 | 122.92 |
| 24 | t | 101 | BCR | C36-C18-C17 | -10.59 | 108.09 | 122.92 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24 | a | 608 | BCR | C37-C22-C21 | -9.76 | 109.26 | 122.92 |
| 24 | A | 608 | BCR | C37-C22-C21 | -9.72 | 109.31 | 122.92 |
| 24 | D | 404 | BCR | C30-C25-C26 | -9.10 | 109.80 | 122.59 |
| 24 | d | 404 | BCR | C30-C25-C26 | -9.09 | 109.82 | 122.59 |
| 24 | B | 619 | BCR | C36-C18-C19 | -8.70 | 104.24 | 118.10 |
| 24 | b | 618 | BCR | C36-C18-C19 | -8.69 | 104.25 | 118.10 |
| 24 | B | 618 | BCR | C36-C18-C17 | -8.69 | 110.75 | 122.92 |
| 24 | T | 101 | BCR | C36-C18-C17 | -8.68 | 110.77 | 122.92 |
| 24 | k | 101 | BCR | C33-C5-C4 | -8.63 | 97.25 | 113.56 |
| 24 | K | 101 | BCR | C33-C5-C4 | -8.61 | 97.27 | 113.56 |
| 22 | D | 402 | CLA | C1C-NC-C4C | -8.48 | 102.27 | 107.05 |
| 22 | d | 402 | CLA | C1C-NC-C4C | -8.46 | 102.29 | 107.05 |
| 24 | A | 608 | BCR | C36-C18-C17 | -8.24 | 111.38 | 122.92 |
| 24 | a | 608 | BCR | C36-C18-C17 | -8.21 | 111.43 | 122.92 |
| 22 | B | 605 | CLA | C1C-NC-C4C | -8.20 | 102.43 | 107.05 |
| 22 | b | 605 | CLA | C1C-NC-C4C | -8.12 | 102.48 | 107.05 |
| 22 | b | 612 | CLA | C1C-NC-C4C | -7.97 | 102.56 | 107.05 |
| 22 | B | 612 | CLA | C1C-NC-C4C | -7.96 | 102.57 | 107.05 |
| 24 | a | 608 | BCR | C35-C13-C14 | -7.83 | 111.95 | 122.92 |
| 24 | A | 608 | BCR | C35-C13-C14 | -7.83 | 111.95 | 122.92 |
| 24 | T | 101 | BCR | C35-C13-C12 | -7.62 | 105.96 | 118.10 |
| 24 | B | 618 | BCR | C35-C13-C12 | -7.60 | 105.99 | 118.10 |
| 22 | d | 401 | CLA | C1C-NC-C4C | -7.59 | 102.77 | 107.05 |
| 22 | D | 401 | CLA | C1C-NC-C4C | -7.56 | 102.79 | 107.05 |
| 24 | C | 514 | BCR | C38-C26-C27 | -7.53 | 99.32 | 113.56 |
| 24 | H | 101 | BCR | C37-C22-C21 | -7.51 | 112.40 | 122.92 |
| 24 | c | 514 | BCR | C38-C26-C27 | -7.50 | 99.37 | 113.56 |
| 22 | a | 604 | CLA | C1C-NC-C4C | -7.49 | 102.83 | 107.05 |
| 24 | h | 101 | BCR | C37-C22-C21 | -7.46 | 112.47 | 122.92 |
| 22 | A | 604 | CLA | C1C-NC-C4C | -7.45 | 102.86 | 107.05 |
| 22 | B | 609 | CLA | C1C-NC-C4C | -7.39 | 102.89 | 107.05 |
| 22 | b | 609 | CLA | C1C-NC-C4C | -7.28 | 102.95 | 107.05 |
| 24 | B | 618 | BCR | C36-C18-C19 | -7.25 | 106.56 | 118.10 |
| 24 | K | 101 | BCR | C37-C22-C21 | -7.24 | 112.78 | 122.92 |
| 24 | T | 101 | BCR | C36-C18-C19 | -7.24 | 106.57 | 118.10 |
| 24 | b | 618 | BCR | C30-C25-C26 | -7.23 | 112.43 | 122.59 |
| 24 | B | 619 | BCR | C30-C25-C26 | -7.23 | 112.43 | 122.59 |
| 24 | k | 101 | BCR | C37-C22-C21 | -7.19 | 112.85 | 122.92 |
| 24 | B | 622 | BCR | C36-C18-C17 | -7.12 | 112.95 | 122.92 |
| 24 | b | 622 | BCR | C36-C18-C17 | -7.12 | 112.95 | 122.92 |
| 24 | a | 608 | BCR | C38-C26-C27 | -6.93 | 100.45 | 113.56 |
| 24 | A | 608 | BCR | C38-C26-C27 | -6.92 | 100.48 | 113.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24 | c | 514 | BCR | C36-C18-C17 | -6.83 | 113.36 | 122.92 |
| 24 | C | 514 | BCR | C36-C18-C17 | -6.81 | 113.38 | 122.92 |
| 24 | H | 101 | BCR | C36-C18-C19 | -6.79 | 107.29 | 118.10 |
| 24 | h | 101 | BCR | C36-C18-C19 | -6.78 | 107.29 | 118.10 |
| 24 | K | 101 | BCR | C36-C18-C19 | -6.78 | 107.29 | 118.10 |
| 22 | b | 617 | CLA | C1C-NC-C4C | -6.76 | 103.25 | 107.05 |
| 24 | k | 101 | BCR | C36-C18-C19 | -6.71 | 107.41 | 118.10 |
| 22 | b | 604 | CLA | C1C-NC-C4C | -6.68 | 103.29 | 107.05 |
| 22 | B | 617 | CLA | C1C-NC-C4C | -6.63 | 103.31 | 107.05 |
| 24 | B | 618 | BCR | C34-C9-C10 | -6.59 | 113.69 | 122.92 |
| 24 | k | 102 | BCR | C36-C18-C19 | -6.58 | 107.62 | 118.10 |
| 24 | T | 101 | BCR | C34-C9-C10 | -6.57 | 113.71 | 122.92 |
| 22 | B | 610 | CLA | C1C-NC-C4C | -6.57 | 103.35 | 107.05 |
| 22 | B | 604 | CLA | C1C-NC-C4C | -6.55 | 103.36 | 107.05 |
| 24 | K | 102 | BCR | C36-C18-C19 | -6.54 | 107.68 | 118.10 |
| 22 | B | 606 | CLA | C1C-NC-C4C | -6.52 | 103.38 | 107.05 |
| 24 | K | 102 | BCR | C37-C22-C21 | -6.49 | 113.83 | 122.92 |
| 22 | b | 606 | CLA | C1C-NC-C4C | -6.48 | 103.40 | 107.05 |
| 24 | k | 102 | BCR | C37-C22-C21 | -6.48 | 113.85 | 122.92 |
| 22 | b | 610 | CLA | C1C-NC-C4C | -6.41 | 103.44 | 107.05 |
| 22 | B | 613 | CLA | C1C-NC-C4C | -6.39 | 103.45 | 107.05 |
| 22 | a | 603 | CLA | C1C-NC-C4C | -6.38 | 103.46 | 107.05 |
| 22 | b | 613 | CLA | C1C-NC-C4C | -6.36 | 103.47 | 107.05 |
| 22 | A | 603 | CLA | C1C-NC-C4C | -6.34 | 103.48 | 107.05 |
| 33 | F | 101 | HEM | CBD-CAD-C3D | -6.24 | 100.56 | 112.47 |
| 33 | f | 101 | HEM | CBD-CAD-C3D | -6.22 | 100.60 | 112.47 |
| 24 | k | 101 | BCR | C36-C18-C17 | -6.20 | 114.24 | 122.92 |
| 24 | K | 101 | BCR | C36-C18-C17 | -6.16 | 114.29 | 122.92 |
| 22 | C | 506 | CLA | C1C-NC-C4C | -6.09 | 103.62 | 107.05 |
| 22 | c | 510 | CLA | C1C-NC-C4C | -6.08 | 103.63 | 107.05 |
| 22 | c | 506 | CLA | C1C-NC-C4C | -6.07 | 103.63 | 107.05 |
| 22 | C | 510 | CLA | C1C-NC-C4C | -6.03 | 103.65 | 107.05 |
| 22 | a | 607 | CLA | C1C-NC-C4C | -5.97 | 103.69 | 107.05 |
| 24 | H | 101 | BCR | C34-C9-C10 | -5.96 | 114.58 | 122.92 |
| 24 | K | 102 | BCR | C36-C18-C17 | -5.95 | 114.59 | 122.92 |
| 22 | C | 505 | CLA | C1C-NC-C4C | -5.94 | 103.71 | 107.05 |
| 24 | b | 618 | BCR | C38-C26-C27 | -5.94 | 102.34 | 113.56 |
| 22 | c | 505 | CLA | C1C-NC-C4C | -5.93 | 103.71 | 107.05 |
| 22 | A | 607 | CLA | C1C-NC-C4C | -5.93 | 103.71 | 107.05 |
| 24 | B | 619 | BCR | C38-C26-C27 | -5.93 | 102.35 | 113.56 |
| 24 | h | 101 | BCR | C34-C9-C10 | -5.93 | 114.62 | 122.92 |
| 22 | C | 509 | CLA | C1C-NC-C4C | -5.93 | 103.71 | 107.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | c | 509 | CLA | C1C-NC-C4C | -5.92 | 103.71 | 107.05 |
| 24 | k | 102 | BCR | C36-C18-C17 | -5.91 | 114.65 | 122.92 |
| 22 | b | 614 | CLA | C1C-NC-C4C | -5.90 | 103.73 | 107.05 |
| 24 | h | 101 | BCR | C33-C5-C4 | -5.89 | 102.42 | 113.56 |
| 24 | H | 101 | BCR | C33-C5-C4 | -5.88 | 102.44 | 113.56 |
| 24 | H | 101 | BCR | C30-C25-C26 | -5.85 | 114.37 | 122.59 |
| 24 | B | 619 | BCR | C37-C22-C21 | -5.85 | 114.73 | 122.92 |
| 22 | B | 614 | CLA | C1C-NC-C4C | -5.85 | 103.75 | 107.05 |
| 24 | b | 618 | BCR | C37-C22-C21 | -5.84 | 114.74 | 122.92 |
| 24 | b | 618 | BCR | C36-C18-C17 | -5.83 | 114.75 | 122.92 |
| 24 | B | 619 | BCR | C36-C18-C17 | -5.82 | 114.77 | 122.92 |
| 24 | h | 101 | BCR | C30-C25-C26 | -5.81 | 114.43 | 122.59 |
| 24 | B | 619 | BCR | C35-C13-C14 | -5.80 | 114.80 | 122.92 |
| 22 | c | 502 | CLA | C1C-NC-C4C | -5.80 | 103.78 | 107.05 |
| 24 | b | 618 | BCR | C35-C13-C14 | -5.79 | 114.82 | 122.92 |
| 22 | C | 502 | CLA | C1C-NC-C4C | -5.76 | 103.80 | 107.05 |
| 22 | B | 616 | CLA | C1C-NC-C4C | -5.74 | 103.82 | 107.05 |
| 24 | k | 101 | BCR | C30-C25-C26 | -5.70 | 114.57 | 122.59 |
| 24 | K | 101 | BCR | C30-C25-C26 | -5.69 | 114.59 | 122.59 |
| 24 | B | 618 | BCR | C38-C26-C27 | -5.69 | 102.81 | 113.56 |
| 22 | b | 616 | CLA | C1C-NC-C4C | -5.68 | 103.85 | 107.05 |
| 24 | T | 101 | BCR | C38-C26-C27 | -5.66 | 102.86 | 113.56 |
| 22 | b | 615 | CLA | C1C-NC-C4C | -5.59 | 103.90 | 107.05 |
| 22 | B | 615 | CLA | C1C-NC-C4C | -5.59 | 103.90 | 107.05 |
| 24 | t | 101 | BCR | C33-C5-C4 | -5.49 | 103.19 | 113.56 |
| 24 | T | 102 | BCR | C33-C5-C4 | -5.47 | 103.22 | 113.56 |
| 24 | D | 404 | BCR | C36-C18-C17 | -5.42 | 115.33 | 122.92 |
| 22 | B | 608 | CLA | C1C-NC-C4C | -5.42 | 104.00 | 107.05 |
| 24 | d | 404 | BCR | C36-C18-C17 | -5.40 | 115.36 | 122.92 |
| 22 | b | 607 | CLA | C1C-NC-C4C | -5.37 | 104.02 | 107.05 |
| 22 | c | 511 | CLA | C1C-NC-C4C | -5.36 | 104.03 | 107.05 |
| 22 | B | 607 | CLA | C1C-NC-C4C | -5.36 | 104.03 | 107.05 |
| 22 | C | 511 | CLA | C1C-NC-C4C | -5.33 | 104.05 | 107.05 |
| 24 | a | 608 | BCR | C30-C25-C26 | -5.31 | 115.13 | 122.59 |
| 24 | A | 608 | BCR | C30-C25-C26 | -5.31 | 115.13 | 122.59 |
| 22 | b | 608 | CLA | C1C-NC-C4C | -5.30 | 104.07 | 107.05 |
| 24 | C | 515 | BCR | C37-C22-C21 | -5.27 | 115.54 | 122.92 |
| 22 | c | 501 | CLA | C1C-NC-C4C | -5.25 | 104.09 | 107.05 |
| 24 | K | 102 | BCR | C35-C13-C14 | -5.24 | 115.59 | 122.92 |
| 22 | b | 611 | CLA | C1C-NC-C4C | -5.24 | 104.10 | 107.05 |
| 22 | C | 501 | CLA | C1C-NC-C4C | -5.22 | 104.11 | 107.05 |
| 22 | B | 611 | CLA | C1C-NC-C4C | -5.22 | 104.11 | 107.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24 | k | 102 | BCR | C35-C13-C14 | -5.22 | 115.61 | 122.92 |
| 24 | H | 101 | BCR | C35-C13-C12 | -5.21 | 109.81 | 118.10 |
| 24 | h | 101 | BCR | C35-C13-C12 | -5.20 | 109.82 | 118.10 |
| 24 | t | 101 | BCR | C37-C22-C23 | -5.19 | 109.83 | 118.10 |
| 24 | c | 515 | BCR | C37-C22-C21 | -5.18 | 115.67 | 122.92 |
| 24 | C | 515 | BCR | C35-C13-C12 | -5.16 | 109.88 | 118.10 |
| 24 | D | 404 | BCR | C34-C9-C10 | -5.16 | 115.70 | 122.92 |
| 24 | d | 404 | BCR | C39-C30-C29 | -5.15 | 88.70 | 108.78 |
| 24 | D | 404 | BCR | C39-C30-C29 | -5.15 | 88.71 | 108.78 |
| 24 | c | 515 | BCR | C35-C13-C12 | -5.15 | 109.90 | 118.10 |
| 24 | T | 102 | BCR | C37-C22-C23 | -5.14 | 109.90 | 118.10 |
| 24 | d | 404 | BCR | C34-C9-C10 | -5.14 | 115.72 | 122.92 |
| 24 | k | 101 | BCR | C34-C9-C10 | -5.13 | 115.74 | 122.92 |
| 24 | K | 101 | BCR | C34-C9-C10 | -5.12 | 115.75 | 122.92 |
| 22 | d | 402 | CLA | C1C-C2C-C3C | -5.08 | 101.49 | 106.93 |
| 22 | D | 402 | CLA | C1C-C2C-C3C | -5.08 | 101.49 | 106.93 |
| 24 | c | 514 | BCR | C33-C5-C4 | -5.07 | 103.97 | 113.56 |
| 24 | C | 514 | BCR | C33-C5-C4 | -5.06 | 103.99 | 113.56 |
| 24 | c | 515 | BCR | C38-C26-C27 | -5.04 | 104.03 | 113.56 |
| 24 | C | 515 | BCR | C38-C26-C27 | -5.04 | 104.04 | 113.56 |
| 33 | V | 201 | HEM | CBD-CAD-C3D | -5.04 | 102.86 | 112.47 |
| 33 | v | 201 | HEM | CBD-CAD-C3D | -5.03 | 102.87 | 112.47 |
| 23 | a | 605 | PHO | C3D-C2D-C1D | -5.00 | 98.37 | 105.85 |
| 24 | B | 622 | BCR | C33-C5-C4 | -4.96 | 104.18 | 113.56 |
| 24 | b | 622 | BCR | C33-C5-C4 | -4.96 | 104.19 | 113.56 |
| 24 | C | 515 | BCR | C36-C18-C19 | -4.96 | 110.20 | 118.10 |
| 23 | A | 605 | PHO | C3D-C2D-C1D | -4.95 | 98.43 | 105.85 |
| 24 | B | 622 | BCR | C38-C26-C27 | -4.95 | 104.20 | 113.56 |
| 24 | k | 101 | BCR | C35-C13-C14 | -4.94 | 116.00 | 122.92 |
| 24 | K | 101 | BCR | C35-C13-C14 | -4.94 | 116.01 | 122.92 |
| 24 | b | 622 | BCR | C38-C26-C27 | -4.93 | 104.24 | 113.56 |
| 24 | c | 515 | BCR | C36-C18-C19 | -4.93 | 110.25 | 118.10 |
| 22 | c | 503 | CLA | C1C-NC-C4C | -4.92 | 104.28 | 107.05 |
| 22 | C | 503 | CLA | C1C-NC-C4C | -4.90 | 104.29 | 107.05 |
| 24 | c | 515 | BCR | C36-C18-C17 | -4.90 | 116.06 | 122.92 |
| 22 | c | 504 | CLA | C1C-NC-C4C | -4.88 | 104.30 | 107.05 |
| 24 | C | 515 | BCR | C36-C18-C17 | -4.86 | 116.12 | 122.92 |
| 22 | C | 504 | CLA | C1C-NC-C4C | -4.82 | 104.34 | 107.05 |
| 22 | A | 604 | CLA | C1C-C2C-C3C | -4.81 | 101.78 | 106.93 |
| 22 | a | 604 | CLA | C1C-C2C-C3C | -4.79 | 101.81 | 106.93 |
| 23 | A | 606 | PHO | C3D-C2D-C1D | -4.77 | 98.71 | 105.85 |
| 22 | C | 507 | CLA | C1C-NC-C4C | -4.77 | 104.36 | 107.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24 | B | 619 | BCR | C33-C5-C4 | -4.75 | 104.58 | 113.56 |
| 24 | a | 608 | BCR | C36-C18-C19 | -4.74 | 110.54 | 118.10 |
| 22 | c | 507 | CLA | C1C-NC-C4C | -4.74 | 104.38 | 107.05 |
| 24 | A | 608 | BCR | C36-C18-C19 | -4.74 | 110.55 | 118.10 |
| 23 | a | 606 | PHO | C3D-C2D-C1D | -4.73 | 98.76 | 105.85 |
| 24 | b | 618 | BCR | C33-C5-C4 | -4.73 | 104.62 | 113.56 |
| 24 | D | 404 | BCR | C33-C5-C4 | -4.70 | 104.68 | 113.56 |
| 22 | c | 508 | CLA | C1C-NC-C4C | -4.69 | 104.41 | 107.05 |
| 24 | d | 404 | BCR | C33-C5-C4 | -4.65 | 104.78 | 113.56 |
| 24 | k | 102 | BCR | C35-C13-C12 | -4.64 | 110.70 | 118.10 |
| 24 | K | 102 | BCR | C35-C13-C12 | -4.64 | 110.71 | 118.10 |
| 22 | C | 508 | CLA | C1C-NC-C4C | -4.63 | 104.44 | 107.05 |
| 22 | b | 602 | CLA | C1C-NC-C4C | -4.61 | 104.45 | 107.05 |
| 22 | b | 604 | CLA | C1C-C2C-C3C | -4.59 | 102.01 | 106.93 |
| 24 | C | 515 | BCR | C35-C13-C14 | -4.59 | 116.50 | 122.92 |
| 24 | c | 515 | BCR | C35-C13-C14 | -4.58 | 116.51 | 122.92 |
| 22 | B | 604 | CLA | C1C-C2C-C3C | -4.58 | 102.03 | 106.93 |
| 24 | c | 514 | BCR | C35-C13-C12 | -4.56 | 110.83 | 118.10 |
| 24 | C | 514 | BCR | C35-C13-C12 | -4.56 | 110.84 | 118.10 |
| 22 | B | 603 | CLA | C1C-NC-C4C | -4.52 | 104.50 | 107.05 |
| 22 | B | 605 | CLA | C1C-C2C-C3C | -4.51 | 102.11 | 106.93 |
| 22 | b | 605 | CLA | C1C-C2C-C3C | -4.50 | 102.11 | 106.93 |
| 24 | T | 102 | BCR | C34-C9-C8 | -4.48 | 110.96 | 118.10 |
| 24 | t | 101 | BCR | C34-C9-C8 | -4.47 | 110.98 | 118.10 |
| 22 | c | 512 | CLA | C1C-NC-C4C | -4.46 | 104.54 | 107.05 |
| 22 | b | 603 | CLA | C1C-NC-C4C | -4.45 | 104.54 | 107.05 |
| 22 | B | 602 | CLA | C1C-NC-C4C | -4.45 | 104.54 | 107.05 |
| 24 | d | 404 | BCR | C35-C13-C12 | -4.45 | 111.02 | 118.10 |
| 24 | b | 622 | BCR | C35-C13-C14 | -4.44 | 116.70 | 122.92 |
| 24 | D | 404 | BCR | C35-C13-C12 | -4.43 | 111.03 | 118.10 |
| 22 | C | 504 | CLA | C1C-C2C-C3C | -4.43 | 102.18 | 106.93 |
| 23 | A | 606 | PHO | C4C-C3C-C2C | -4.43 | 101.87 | 106.80 |
| 24 | B | 622 | BCR | C35-C13-C14 | -4.42 | 116.73 | 122.92 |
| 23 | a | 606 | PHO | C4C-C3C-C2C | -4.42 | 101.88 | 106.80 |
| 24 | H | 101 | BCR | C35-C13-C14 | -4.42 | 116.73 | 122.92 |
| 24 | h | 101 | BCR | C35-C13-C14 | -4.42 | 116.73 | 122.92 |
| 24 | T | 101 | BCR | C37-C22-C23 | -4.42 | 111.06 | 118.10 |
| 22 | d | 403 | CLA | C1C-NC-C4C | -4.42 | 104.56 | 107.05 |
| 24 | d | 404 | BCR | C36-C18-C19 | -4.39 | 111.10 | 118.10 |
| 22 | D | 403 | CLA | C1C-NC-C4C | -4.39 | 104.58 | 107.05 |
| 24 | B | 618 | BCR | C37-C22-C23 | -4.39 | 111.11 | 118.10 |
| 22 | c | 504 | CLA | C1C-C2C-C3C | -4.38 | 102.24 | 106.93 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24 | D | 404 | BCR | C36-C18-C19 | -4.37 | 111.13 | 118.10 |
| 24 | c | 514 | BCR | C30-C25-C26 | -4.37 | 116.45 | 122.59 |
| 24 | K | 101 | BCR | C1-C6-C5 | -4.36 | 116.46 | 122.59 |
| 22 | C | 512 | CLA | C1C-NC-C4C | -4.36 | 104.59 | 107.05 |
| 24 | k | 101 | BCR | C1-C6-C5 | -4.36 | 116.47 | 122.59 |
| 24 | d | 404 | BCR | C38-C26-C27 | -4.35 | 105.33 | 113.56 |
| 24 | D | 404 | BCR | C38-C26-C27 | -4.35 | 105.34 | 113.56 |
| 24 | C | 514 | BCR | C30-C25-C26 | -4.34 | 116.49 | 122.59 |
| 22 | c | 501 | CLA | O2D-CGD-O1D | -4.33 | 115.22 | 123.82 |
| 22 | C | 501 | CLA | O2D-CGD-O1D | -4.33 | 115.23 | 123.82 |
| 24 | T | 101 | BCR | C30-C25-C26 | -4.32 | 116.51 | 122.59 |
| 22 | B | 609 | CLA | C1C-C2C-C3C | -4.32 | 102.30 | 106.93 |
| 22 | b | 609 | CLA | C1C-C2C-C3C | -4.31 | 102.32 | 106.93 |
| 24 | B | 618 | BCR | C30-C25-C26 | -4.30 | 116.55 | 122.59 |
| 24 | K | 101 | BCR | C38-C26-C27 | -4.23 | 105.56 | 113.56 |
| 24 | k | 101 | BCR | C38-C26-C27 | -4.23 | 105.57 | 113.56 |
| 22 | c | 509 | CLA | C1C-C2C-C3C | -4.21 | 102.42 | 106.93 |
| 22 | A | 607 | CLA | C1C-C2C-C3C | -4.20 | 102.43 | 106.93 |
| 22 | a | 607 | CLA | C1C-C2C-C3C | -4.19 | 102.44 | 106.93 |
| 22 | B | 608 | CLA | C1C-C2C-C3C | -4.19 | 102.45 | 106.93 |
| 24 | T | 102 | BCR | C30-C25-C26 | -4.18 | 116.71 | 122.59 |
| 24 | t | 101 | BCR | C30-C25-C26 | -4.18 | 116.72 | 122.59 |
| 24 | C | 515 | BCR | C33-C5-C4 | -4.18 | 105.67 | 113.56 |
| 24 | c | 515 | BCR | C33-C5-C4 | -4.17 | 105.67 | 113.56 |
| 22 | C | 509 | CLA | C1C-C2C-C3C | -4.16 | 102.47 | 106.93 |
| 22 | b | 614 | CLA | C1C-C2C-C3C | -4.16 | 102.48 | 106.93 |
| 22 | b | 607 | CLA | O2D-CGD-O1D | -4.16 | 115.56 | 123.82 |
| 23 | a | 605 | PHO | C4C-C3C-C2C | -4.16 | 102.17 | 106.80 |
| 22 | B | 614 | CLA | C1C-C2C-C3C | -4.16 | 102.48 | 106.93 |
| 22 | B | 607 | CLA | O2D-CGD-O1D | -4.15 | 115.58 | 123.82 |
| 24 | T | 102 | BCR | C35-C13-C14 | -4.15 | 117.11 | 122.92 |
| 24 | T | 101 | BCR | C35-C13-C14 | -4.15 | 117.11 | 122.92 |
| 24 | c | 514 | BCR | C36-C18-C19 | -4.15 | 111.49 | 118.10 |
| 24 | B | 618 | BCR | C35-C13-C14 | -4.14 | 117.13 | 122.92 |
| 24 | C | 514 | BCR | C36-C18-C19 | -4.14 | 111.51 | 118.10 |
| 23 | A | 605 | PHO | C4C-C3C-C2C | -4.13 | 102.20 | 106.80 |
| 22 | b | 608 | CLA | C1C-C2C-C3C | -4.13 | 102.51 | 106.93 |
| 24 | t | 101 | BCR | C35-C13-C14 | -4.12 | 117.14 | 122.92 |
| 22 | c | 501 | CLA | C1C-C2C-C3C | -4.07 | 102.57 | 106.93 |
| 24 | h | 101 | BCR | C38-C26-C27 | -4.07 | 105.87 | 113.56 |
| 22 | C | 501 | CLA | C1C-C2C-C3C | -4.06 | 102.58 | 106.93 |
| 24 | H | 101 | BCR | C38-C26-C27 | -4.06 | 105.88 | 113.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24 | b | 618 | BCR | C35-C13-C12 | -4.06 | 111.64 | 118.10 |
| 24 | b | 622 | BCR | C30-C25-C26 | -4.05 | 116.89 | 122.59 |
| 24 | B | 619 | BCR | C35-C13-C12 | -4.04 | 111.67 | 118.10 |
| 22 | c | 507 | CLA | C1C-C2C-C3C | -4.02 | 102.62 | 106.93 |
| 22 | C | 507 | CLA | C1C-C2C-C3C | -4.01 | 102.64 | 106.93 |
| 24 | h | 101 | BCR | C36-C18-C17 | -4.01 | 117.31 | 122.92 |
| 24 | H | 101 | BCR | C36-C18-C17 | -4.00 | 117.31 | 122.92 |
| 24 | B | 622 | BCR | C30-C25-C26 | -4.00 | 116.96 | 122.59 |
| 24 | T | 102 | BCR | C37-C22-C21 | -3.99 | 117.34 | 122.92 |
| 24 | t | 101 | BCR | C37-C22-C21 | -3.97 | 117.36 | 122.92 |
| 24 | C | 515 | BCR | C31-C1-C2 | -3.97 | 93.32 | 108.78 |
| 24 | c | 515 | BCR | C31-C1-C2 | -3.97 | 93.32 | 108.78 |
| 24 | k | 102 | BCR | C38-C26-C27 | -3.94 | 106.10 | 113.56 |
| 24 | c | 514 | BCR | C32-C1-C2 | -3.94 | 93.42 | 108.78 |
| 24 | B | 619 | BCR | C40-C30-C29 | -3.94 | 93.43 | 108.78 |
| 24 | K | 102 | BCR | C38-C26-C27 | -3.94 | 106.12 | 113.56 |
| 24 | k | 102 | BCR | C30-C25-C26 | -3.94 | 117.06 | 122.59 |
| 24 | b | 618 | BCR | C40-C30-C29 | -3.94 | 93.44 | 108.78 |
| 24 | C | 514 | BCR | C32-C1-C2 | -3.93 | 93.45 | 108.78 |
| 24 | K | 102 | BCR | C30-C25-C26 | -3.91 | 117.09 | 122.59 |
| 22 | d | 403 | CLA | C1C-C2C-C3C | -3.91 | 102.74 | 106.93 |
| 22 | C | 503 | CLA | C1C-C2C-C3C | -3.90 | 102.76 | 106.93 |
| 22 | b | 602 | CLA | C1C-C2C-C3C | -3.89 | 102.76 | 106.93 |
| 22 | D | 403 | CLA | C1C-C2C-C3C | -3.89 | 102.77 | 106.93 |
| 22 | B | 607 | CLA | C1C-C2C-C3C | -3.88 | 102.77 | 106.93 |
| 22 | B | 602 | CLA | C1C-C2C-C3C | -3.87 | 102.78 | 106.93 |
| 22 | C | 506 | CLA | C1C-C2C-C3C | -3.86 | 102.80 | 106.93 |
| 22 | c | 503 | CLA | C1C-C2C-C3C | -3.86 | 102.80 | 106.93 |
| 22 | c | 510 | CLA | C1C-C2C-C3C | -3.85 | 102.81 | 106.93 |
| 22 | b | 607 | CLA | C1C-C2C-C3C | -3.85 | 102.81 | 106.93 |
| 24 | d | 404 | BCR | C37-C22-C21 | -3.83 | 117.56 | 122.92 |
| 22 | c | 513 | CLA | C1C-C2C-C3C | -3.82 | 102.84 | 106.93 |
| 22 | C | 513 | CLA | C1C-C2C-C3C | -3.81 | 102.85 | 106.93 |
| 22 | C | 511 | CLA | C1C-C2C-C3C | -3.81 | 102.85 | 106.93 |
| 22 | C | 510 | CLA | C1C-C2C-C3C | -3.80 | 102.86 | 106.93 |
| 22 | c | 506 | CLA | C1C-C2C-C3C | -3.80 | 102.87 | 106.93 |
| 24 | D | 404 | BCR | C37-C22-C21 | -3.79 | 117.61 | 122.92 |
| 22 | b | 610 | CLA | C1C-C2C-C3C | -3.79 | 102.87 | 106.93 |
| 22 | B | 610 | CLA | C1C-C2C-C3C | -3.78 | 102.88 | 106.93 |
| 22 | c | 511 | CLA | C1C-C2C-C3C | -3.78 | 102.88 | 106.93 |
| 24 | K | 102 | BCR | C33-C5-C4 | -3.75 | 106.47 | 113.56 |
| 22 | c | 508 | CLA | C1C-C2C-C3C | -3.75 | 102.91 | 106.93 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | b | 615 | CLA | C1C-C2C-C3C | -3.75 | 102.92 | 106.93 |
| 24 | k | 102 | BCR | C33-C5-C4 | -3.74 | 106.49 | 113.56 |
| 22 | B | 615 | CLA | C1C-C2C-C3C | -3.74 | 102.92 | 106.93 |
| 22 | C | 513 | CLA | C1C-NC-C4C | -3.72 | 104.95 | 107.05 |
| 22 | A | 603 | CLA | C1C-C2C-C3C | -3.72 | 102.94 | 106.93 |
| 24 | c | 514 | BCR | C37-C22-C21 | -3.71 | 117.73 | 122.92 |
| 22 | C | 508 | CLA | C1C-C2C-C3C | -3.70 | 102.97 | 106.93 |
| 22 | a | 603 | CLA | C1C-C2C-C3C | -3.70 | 102.97 | 106.93 |
| 24 | C | 514 | BCR | C37-C22-C21 | -3.70 | 117.75 | 122.92 |
| 24 | d | 404 | BCR | C35-C13-C14 | -3.69 | 117.75 | 122.92 |
| 24 | D | 404 | BCR | C35-C13-C14 | -3.68 | 117.76 | 122.92 |
| 22 | B | 616 | CLA | C1C-C2C-C3C | -3.66 | 103.01 | 106.93 |
| 22 | c | 513 | CLA | C1C-NC-C4C | -3.66 | 104.99 | 107.05 |
| 22 | b | 616 | CLA | C1C-C2C-C3C | -3.63 | 103.04 | 106.93 |
| 22 | C | 512 | CLA | C1C-C2C-C3C | -3.58 | 103.09 | 106.93 |
| 22 | c | 512 | CLA | C1C-C2C-C3C | -3.58 | 103.09 | 106.93 |
| 22 | B | 612 | CLA | C1C-C2C-C3C | -3.56 | 103.12 | 106.93 |
| 24 | a | 608 | BCR | C35-C13-C12 | -3.55 | 112.45 | 118.10 |
| 24 | A | 608 | BCR | C35-C13-C12 | -3.54 | 112.46 | 118.10 |
| 22 | b | 612 | CLA | C1C-C2C-C3C | -3.53 | 103.15 | 106.93 |
| 22 | C | 505 | CLA | C1C-C2C-C3C | -3.53 | 103.15 | 106.93 |
| 24 | a | 608 | BCR | C33-C5-C4 | -3.53 | 106.89 | 113.56 |
| 22 | b | 603 | CLA | C1C-C2C-C3C | -3.53 | 103.15 | 106.93 |
| 22 | c | 505 | CLA | C1C-C2C-C3C | -3.52 | 103.16 | 106.93 |
| 24 | A | 608 | BCR | C33-C5-C4 | -3.52 | 106.91 | 113.56 |
| 22 | C | 502 | CLA | C1C-C2C-C3C | -3.52 | 103.17 | 106.93 |
| 24 | D | 404 | BCR | C32-C1-C2 | -3.51 | 95.11 | 108.78 |
| 24 | b | 618 | BCR | C37-C22-C23 | -3.50 | 112.53 | 118.10 |
| 24 | d | 404 | BCR | C32-C1-C2 | -3.50 | 95.15 | 108.78 |
| 22 | c | 502 | CLA | C1C-C2C-C3C | -3.49 | 103.19 | 106.93 |
| 22 | B | 603 | CLA | C1C-C2C-C3C | -3.49 | 103.20 | 106.93 |
| 24 | D | 404 | BCR | C1-C6-C5 | -3.49 | 117.69 | 122.59 |
| 24 | B | 619 | BCR | C37-C22-C23 | -3.48 | 112.56 | 118.10 |
| 22 | B | 611 | CLA | C1C-C2C-C3C | -3.47 | 103.22 | 106.93 |
| 24 | d | 404 | BCR | C1-C6-C5 | -3.47 | 117.72 | 122.59 |
| 22 | B | 604 | CLA | O2D-CGD-O1D | -3.47 | 116.94 | 123.82 |
| 22 | b | 611 | CLA | C1C-C2C-C3C | -3.46 | 103.22 | 106.93 |
| 22 | b | 617 | CLA | C4C-C3C-C2C | -3.45 | 101.78 | 106.90 |
| 22 | b | 606 | CLA | C1C-C2C-C3C | -3.44 | 103.25 | 106.93 |
| 22 | B | 617 | CLA | C4C-C3C-C2C | -3.44 | 101.80 | 106.90 |
| 24 | A | 608 | BCR | C34-C9-C8 | -3.43 | 112.64 | 118.10 |
| 24 | T | 102 | BCR | C36-C18-C19 | -3.42 | 112.64 | 118.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | B | 606 | CLA | C1C-C2C-C3C | -3.41 | 103.28 | 106.93 |
| 23 | a | 605 | PHO | C4D-ND-C1D | -3.40 | 100.83 | 106.98 |
| 22 | b | 604 | CLA | O2D-CGD-O1D | -3.40 | 117.07 | 123.82 |
| 22 | B | 606 | CLA | C4C-C3C-C2C | -3.40 | 101.86 | 106.90 |
| 23 | A | 605 | PHO | C4D-ND-C1D | -3.39 | 100.86 | 106.98 |
| 24 | a | 608 | BCR | C34-C9-C8 | -3.39 | 112.70 | 118.10 |
| 24 | t | 101 | BCR | C36-C18-C19 | -3.38 | 112.71 | 118.10 |
| 22 | d | 401 | CLA | C1C-C2C-C3C | -3.37 | 103.32 | 106.93 |
| 22 | b | 606 | CLA | C4C-C3C-C2C | -3.36 | 101.92 | 106.90 |
| 24 | T | 102 | BCR | C35-C13-C12 | -3.36 | 112.75 | 118.10 |
| 22 | D | 401 | CLA | C1C-C2C-C3C | -3.36 | 103.34 | 106.93 |
| 24 | t | 101 | BCR | C35-C13-C12 | -3.35 | 112.76 | 118.10 |
| 22 | d | 401 | CLA | C4C-C3C-C2C | -3.34 | 101.94 | 106.90 |
| 22 | D | 401 | CLA | C4C-C3C-C2C | -3.33 | 101.96 | 106.90 |
| 22 | b | 615 | CLA | O2D-CGD-O1D | -3.30 | 117.27 | 123.82 |
| 22 | B | 611 | CLA | C4C-C3C-C2C | -3.29 | 102.02 | 106.90 |
| 25 | A | 609 | SQD | C1-C2-C3 | -3.28 | 103.11 | 109.98 |
| 22 | D | 402 | CLA | CBC-CAC-C3C | -3.28 | 103.29 | 112.42 |
| 25 | a | 609 | SQD | C1-C2-C3 | -3.28 | 103.12 | 109.98 |
| 22 | b | 611 | CLA | C4C-C3C-C2C | -3.27 | 102.05 | 106.90 |
| 22 | B | 615 | CLA | O2D-CGD-O1D | -3.27 | 117.33 | 123.82 |
| 22 | d | 402 | CLA | CBC-CAC-C3C | -3.26 | 103.34 | 112.42 |
| 22 | D | 401 | CLA | O2D-CGD-O1D | -3.25 | 117.36 | 123.82 |
| 31 | C | 518 | DGD | O3G-C3G-C2G | -3.25 | 103.25 | 110.99 |
| 22 | B | 613 | CLA | C1C-C2C-C3C | -3.24 | 103.46 | 106.93 |
| 22 | d | 401 | CLA | O2D-CGD-O1D | -3.23 | 117.40 | 123.82 |
| 31 | c | 518 | DGD | O3G-C3G-C2G | -3.23 | 103.30 | 110.99 |
| 22 | b | 613 | CLA | C1C-C2C-C3C | -3.23 | 103.47 | 106.93 |
| 22 | b | 616 | CLA | C4C-C3C-C2C | -3.21 | 102.14 | 106.90 |
| 22 | B | 616 | CLA | C4C-C3C-C2C | -3.21 | 102.14 | 106.90 |
| 24 | B | 619 | BCR | C34-C9-C10 | -3.20 | 118.44 | 122.92 |
| 33 | v | 201 | HEM | C1D-C2D-C3D | -3.19 | 104.78 | 107.00 |
| 22 | C | 508 | CLA | C4C-C3C-C2C | -3.19 | 102.18 | 106.90 |
| 22 | c | 508 | CLA | C4C-C3C-C2C | -3.18 | 102.19 | 106.90 |
| 24 | b | 618 | BCR | C34-C9-C10 | -3.18 | 118.47 | 122.92 |
| 24 | B | 619 | BCR | C34-C9-C8 | -3.18 | 113.04 | 118.10 |
| 24 | b | 618 | BCR | C34-C9-C8 | -3.17 | 113.04 | 118.10 |
| 22 | B | 612 | CLA | C4C-C3C-C2C | -3.17 | 102.20 | 106.90 |
| 22 | b | 612 | CLA | C4C-C3C-C2C | -3.17 | 102.21 | 106.90 |
| 23 | A | 606 | PHO | C4D-ND-C1D | -3.15 | 101.29 | 106.98 |
| 33 | V | 201 | HEM | C1D-C2D-C3D | -3.15 | 104.81 | 107.00 |
| 24 | B | 622 | BCR | C34-C9-C8 | -3.14 | 113.10 | 118.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | c | 513 | CLA | O2D-CGD-O1D | -3.13 | 117.61 | 123.82 |
| 22 | C | 507 | CLA | CBC-CAC-C3C | -3.13 | 103.71 | 112.42 |
| 24 | B | 622 | BCR | C36-C18-C19 | -3.13 | 113.11 | 118.10 |
| 24 | b | 622 | BCR | C36-C18-C19 | -3.13 | 113.12 | 118.10 |
| 22 | c | 507 | CLA | CBC-CAC-C3C | -3.13 | 103.72 | 112.42 |
| 23 | a | 606 | PHO | C4D-ND-C1D | -3.13 | 101.34 | 106.98 |
| 24 | b | 622 | BCR | C34-C9-C8 | -3.12 | 113.13 | 118.10 |
| 22 | B | 607 | CLA | O1D-CGD-CBD | -3.12 | 118.80 | 124.58 |
| 22 | b | 607 | CLA | O1D-CGD-CBD | -3.11 | 118.81 | 124.58 |
| 32 | D | 405 | LHG | O8-C23-O10 | -3.11 | 116.00 | 123.58 |
| 22 | b | 613 | CLA | C4C-C3C-C2C | -3.10 | 102.30 | 106.90 |
| 32 | d | 405 | LHG | O8-C23-O10 | -3.10 | 116.02 | 123.58 |
| 22 | C | 513 | CLA | O2D-CGD-O1D | -3.10 | 117.67 | 123.82 |
| 22 | c | 502 | CLA | C4C-C3C-C2C | -3.09 | 102.32 | 106.90 |
| 22 | B | 613 | CLA | C4C-C3C-C2C | -3.08 | 102.33 | 106.90 |
| 22 | b | 608 | CLA | CBC-CAC-C3C | -3.08 | 103.85 | 112.42 |
| 22 | B | 608 | CLA | CBC-CAC-C3C | -3.08 | 103.86 | 112.42 |
| 23 | a | 605 | PHO | C1C-C2C-C3C | -3.06 | 102.95 | 106.50 |
| 22 | C | 502 | CLA | C4C-C3C-C2C | -3.05 | 102.37 | 106.90 |
| 24 | K | 102 | BCR | C34-C9-C10 | -3.04 | 118.66 | 122.92 |
| 23 | A | 605 | PHO | C1C-C2C-C3C | -3.04 | 102.98 | 106.50 |
| 22 | c | 511 | CLA | C4C-C3C-C2C | -3.03 | 102.40 | 106.90 |
| 22 | c | 506 | CLA | C4C-C3C-C2C | -3.03 | 102.41 | 106.90 |
| 22 | C | 511 | CLA | C4C-C3C-C2C | -3.03 | 102.41 | 106.90 |
| 22 | C | 506 | CLA | C4C-C3C-C2C | -3.02 | 102.42 | 106.90 |
| 22 | B | 610 | CLA | C4C-C3C-C2C | -3.02 | 102.43 | 106.90 |
| 24 | k | 102 | BCR | C34-C9-C10 | -3.02 | 118.70 | 122.92 |
| 24 | c | 515 | BCR | C30-C25-C26 | -3.01 | 118.36 | 122.59 |
| 24 | C | 515 | BCR | C30-C25-C26 | -3.00 | 118.37 | 122.59 |
| 25 | A | 609 | SQD | C45-O47-C7 | -3.00 | 110.80 | 117.88 |
| 22 | b | 610 | CLA | C4C-C3C-C2C | -2.99 | 102.47 | 106.90 |
| 25 | a | 609 | SQD | C45-O47-C7 | -2.99 | 110.82 | 117.88 |
| 24 | B | 622 | BCR | C37-C22-C21 | -2.98 | 118.74 | 122.92 |
| 22 | B | 617 | CLA | O2D-CGD-O1D | -2.98 | 117.90 | 123.82 |
| 22 | b | 617 | CLA | O2D-CGD-O1D | -2.97 | 117.92 | 123.82 |
| 31 | h | 102 | DGD | O1G-C1A-O1A | -2.97 | 116.33 | 123.58 |
| 24 | B | 622 | BCR | C35-C13-C12 | -2.96 | 113.38 | 118.10 |
| 24 | b | 622 | BCR | C37-C22-C21 | -2.96 | 118.78 | 122.92 |
| 24 | C | 515 | BCR | C34-C9-C8 | -2.96 | 113.38 | 118.10 |
| 22 | B | 603 | CLA | C4C-C3C-C2C | -2.96 | 102.52 | 106.90 |
| 24 | c | 515 | BCR | C34-C9-C8 | -2.95 | 113.39 | 118.10 |
| 31 | H | 102 | DGD | O1G-C1A-O1A | -2.95 | 116.38 | 123.58 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24 | b | 622 | BCR | C35-C13-C12 | -2.95 | 113.40 | 118.10 |
| 24 | A | 608 | BCR | C34-C9-C10 | -2.95 | 118.80 | 122.92 |
| 22 | b | 603 | CLA | C4C-C3C-C2C | -2.95 | 102.53 | 106.90 |
| 24 | a | 608 | BCR | C34-C9-C10 | -2.94 | 118.80 | 122.92 |
| 22 | B | 615 | CLA | C4C-C3C-C2C | -2.94 | 102.55 | 106.90 |
| 22 | C | 513 | CLA | C4C-C3C-C2C | -2.94 | 102.55 | 106.90 |
| 22 | c | 512 | CLA | C4C-C3C-C2C | -2.93 | 102.55 | 106.90 |
| 22 | c | 505 | CLA | C4C-C3C-C2C | -2.93 | 102.55 | 106.90 |
| 22 | b | 615 | CLA | C4C-C3C-C2C | -2.93 | 102.56 | 106.90 |
| 24 | b | 618 | BCR | C1-C6-C5 | -2.93 | 118.48 | 122.59 |
| 22 | C | 505 | CLA | C4C-C3C-C2C | -2.92 | 102.58 | 106.90 |
| 24 | B | 619 | BCR | C1-C6-C5 | -2.92 | 118.49 | 122.59 |
| 22 | C | 512 | CLA | C4C-C3C-C2C | -2.91 | 102.58 | 106.90 |
| 22 | b | 617 | CLA | C1C-C2C-C3C | -2.89 | 103.83 | 106.93 |
| 22 | b | 615 | CLA | CBC-CAC-C3C | -2.89 | 104.37 | 112.42 |
| 22 | B | 615 | CLA | CBC-CAC-C3C | -2.89 | 104.37 | 112.42 |
| 22 | c | 513 | CLA | C4C-C3C-C2C | -2.89 | 102.61 | 106.90 |
| 24 | T | 101 | BCR | C37-C22-C21 | -2.89 | 118.88 | 122.92 |
| 22 | B | 609 | CLA | O2D-CGD-O1D | -2.89 | 118.09 | 123.82 |
| 22 | d | 403 | CLA | C4C-C3C-C2C | -2.88 | 102.63 | 106.90 |
| 24 | B | 618 | BCR | C37-C22-C21 | -2.88 | 118.89 | 122.92 |
| 22 | B | 617 | CLA | C1C-C2C-C3C | -2.88 | 103.85 | 106.93 |
| 22 | b | 609 | CLA | O1D-CGD-CBD | -2.87 | 119.25 | 124.58 |
| 22 | b | 609 | CLA | O2D-CGD-O1D | -2.87 | 118.13 | 123.82 |
| 22 | D | 403 | CLA | C4C-C3C-C2C | -2.86 | 102.66 | 106.90 |
| 22 | c | 503 | CLA | C4C-C3C-C2C | -2.86 | 102.67 | 106.90 |
| 22 | c | 504 | CLA | O2D-CGD-O1D | -2.85 | 118.16 | 123.82 |
| 22 | A | 603 | CLA | C4C-C3C-C2C | -2.85 | 102.67 | 106.90 |
| 24 | h | 101 | BCR | C39-C30-C29 | -2.85 | 97.68 | 108.78 |
| 22 | C | 503 | CLA | C4C-C3C-C2C | -2.85 | 102.68 | 106.90 |
| 24 | H | 101 | BCR | C39-C30-C29 | -2.85 | 97.69 | 108.78 |
| 22 | c | 509 | CLA | C4C-C3C-C2C | -2.84 | 102.69 | 106.90 |
| 22 | C | 504 | CLA | O2D-CGD-O1D | -2.84 | 118.19 | 123.82 |
| 22 | C | 509 | CLA | C4C-C3C-C2C | -2.84 | 102.69 | 106.90 |
| 22 | B | 611 | CLA | O2D-CGD-O1D | -2.84 | 118.19 | 123.82 |
| 22 | B | 609 | CLA | O1D-CGD-CBD | -2.83 | 119.33 | 124.58 |
| 22 | b | 607 | CLA | C4C-C3C-C2C | -2.82 | 102.71 | 106.90 |
| 22 | a | 603 | CLA | C4C-C3C-C2C | -2.82 | 102.71 | 106.90 |
| 22 | b | 611 | CLA | O2D-CGD-O1D | -2.82 | 118.22 | 123.82 |
| 22 | c | 506 | CLA | O2D-CGD-O1D | -2.82 | 118.22 | 123.82 |
| 22 | C | 507 | CLA | O1D-CGD-CBD | -2.81 | 119.36 | 124.58 |
| 24 | C | 514 | BCR | C39-C30-C29 | -2.81 | 97.83 | 108.78 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24 | K | 102 | BCR | C31-C1-C2 | -2.81 | 97.84 | 108.78 |
| 28 | A | 613 | PL9 | C32-C33-C34 | -2.81 | 120.71 | 127.66 |
| 24 | c | 514 | BCR | C39-C30-C29 | -2.81 | 97.85 | 108.78 |
| 24 | k | 102 | BCR | C31-C1-C2 | -2.80 | 97.85 | 108.78 |
| 22 | b | 609 | CLA | C4C-C3C-C2C | -2.80 | 102.74 | 106.90 |
| 25 | l | 101 | SQD | C1-O5-C5 | -2.80 | 108.18 | 113.71 |
| 24 | H | 101 | BCR | C32-C1-C31 | -2.80 | 100.06 | 108.52 |
| 28 | a | 613 | PL9 | C32-C33-C34 | -2.80 | 120.73 | 127.66 |
| 24 | h | 101 | BCR | C32-C1-C31 | -2.80 | 100.07 | 108.52 |
| 24 | k | 101 | BCR | C35-C13-C12 | -2.80 | 113.65 | 118.10 |
| 22 | B | 609 | CLA | C4C-C3C-C2C | -2.79 | 102.76 | 106.90 |
| 22 | B | 607 | CLA | C4C-C3C-C2C | -2.79 | 102.76 | 106.90 |
| 22 | B | 605 | CLA | C4C-C3C-C2C | -2.79 | 102.76 | 106.90 |
| 22 | c | 507 | CLA | O1D-CGD-CBD | -2.79 | 119.41 | 124.58 |
| 22 | C | 506 | CLA | O2D-CGD-O1D | -2.79 | 118.28 | 123.82 |
| 24 | K | 101 | BCR | C35-C13-C12 | -2.78 | 113.68 | 118.10 |
| 25 | L | 101 | SQD | C1-O5-C5 | -2.77 | 108.26 | 113.71 |
| 25 | a | 609 | SQD | C44-O6-C1 | -2.76 | 108.25 | 113.80 |
| 22 | B | 603 | CLA | O2D-CGD-O1D | -2.76 | 118.33 | 123.82 |
| 25 | A | 609 | SQD | C44-O6-C1 | -2.76 | 108.25 | 113.80 |
| 22 | C | 510 | CLA | C4C-C3C-C2C | -2.76 | 102.80 | 106.90 |
| 22 | C | 510 | CLA | CHD-C4C-C3C | -2.75 | 120.82 | 124.88 |
| 22 | b | 605 | CLA | C4C-C3C-C2C | -2.75 | 102.82 | 106.90 |
| 22 | b | 614 | CLA | C4C-C3C-C2C | -2.75 | 102.83 | 106.90 |
| 24 | B | 622 | BCR | C1-C6-C5 | -2.74 | 118.74 | 122.59 |
| 22 | C | 502 | CLA | O2D-CGD-O1D | -2.74 | 118.38 | 123.82 |
| 22 | B | 602 | CLA | C4C-C3C-C2C | -2.74 | 102.84 | 106.90 |
| 22 | b | 603 | CLA | O2D-CGD-O1D | -2.73 | 118.40 | 123.82 |
| 22 | c | 502 | CLA | O2D-CGD-O1D | -2.73 | 118.40 | 123.82 |
| 22 | c | 510 | CLA | CHD-C4C-C3C | -2.73 | 120.86 | 124.88 |
| 22 | c | 510 | CLA | C4C-C3C-C2C | -2.72 | 102.86 | 106.90 |
| 22 | b | 602 | CLA | C4C-C3C-C2C | -2.72 | 102.87 | 106.90 |
| 23 | a | 606 | PHO | C1-C2-C3 | -2.72 | 120.95 | 125.96 |
| 24 | b | 622 | BCR | C1-C6-C5 | -2.72 | 118.77 | 122.59 |
| 23 | A | 606 | PHO | C1-C2-C3 | -2.72 | 120.95 | 125.96 |
| 22 | B | 614 | CLA | C4C-C3C-C2C | -2.71 | 102.88 | 106.90 |
| 24 | k | 102 | BCR | C37-C22-C23 | -2.71 | 113.78 | 118.10 |
| 24 | K | 102 | BCR | C37-C22-C23 | -2.70 | 113.79 | 118.10 |
| 31 | C | 516 | DGD | O3G-C3G-C2G | -2.69 | 104.59 | 110.99 |
| 22 | B | 617 | CLA | O1D-CGD-CBD | -2.69 | 119.59 | 124.58 |
| 22 | B | 608 | CLA | C1-C2-C3 | -2.68 | 121.02 | 125.96 |
| 31 | c | 516 | DGD | O3G-C3G-C2G | -2.68 | 104.61 | 110.99 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | b | 617 | CLA | O1D-CGD-CBD | -2.68 | 119.61 | 124.58 |
| 24 | k | 101 | BCR | C39-C30-C29 | -2.68 | 98.34 | 108.78 |
| 24 | K | 101 | BCR | C39-C30-C29 | -2.68 | 98.35 | 108.78 |
| 22 | a | 604 | CLA | CBC-CAC-C3C | -2.67 | 104.97 | 112.42 |
| 22 | b | 608 | CLA | C1-C2-C3 | -2.67 | 121.03 | 125.96 |
| 24 | B | 618 | BCR | C39-C30-C29 | -2.66 | 98.40 | 108.78 |
| 24 | T | 101 | BCR | C39-C30-C29 | -2.66 | 98.42 | 108.78 |
| 22 | A | 604 | CLA | CBC-CAC-C3C | -2.66 | 105.02 | 112.42 |
| 22 | B | 612 | CLA | CHD-C4C-C3C | -2.66 | 120.96 | 124.88 |
| 22 | b | 612 | CLA | CHD-C4C-C3C | -2.65 | 120.97 | 124.88 |
| 22 | A | 607 | CLA | C4C-C3C-C2C | -2.64 | 102.98 | 106.90 |
| 22 | C | 511 | CLA | O2D-CGD-O1D | -2.63 | 118.59 | 123.82 |
| 22 | B | 612 | CLA | C1-C2-C3 | -2.63 | 121.11 | 125.96 |
| 22 | a | 607 | CLA | C4C-C3C-C2C | -2.63 | 103.00 | 106.90 |
| 22 | b | 612 | CLA | C1-C2-C3 | -2.63 | 121.11 | 125.96 |
| 22 | c | 511 | CLA | O2D-CGD-O1D | -2.63 | 118.61 | 123.82 |
| 22 | b | 602 | CLA | O1D-CGD-CBD | -2.61 | 119.75 | 124.58 |
| 22 | b | 604 | CLA | C4C-C3C-C2C | -2.60 | 103.05 | 106.90 |
| 22 | B | 602 | CLA | O1D-CGD-CBD | -2.60 | 119.77 | 124.58 |
| 22 | b | 608 | CLA | C4C-C3C-C2C | -2.59 | 103.05 | 106.90 |
| 22 | B | 610 | CLA | O2D-CGD-O1D | -2.59 | 118.69 | 123.82 |
| 22 | b | 614 | CLA | CHD-C4C-C3C | -2.59 | 121.06 | 124.88 |
| 22 | B | 608 | CLA | C4C-C3C-C2C | -2.58 | 103.07 | 106.90 |
| 22 | b | 610 | CLA | O2D-CGD-O1D | -2.58 | 118.70 | 123.82 |
| 22 | B | 612 | CLA | O2D-CGD-O1D | -2.58 | 118.70 | 123.82 |
| 22 | B | 604 | CLA | C4C-C3C-C2C | -2.58 | 103.08 | 106.90 |
| 22 | b | 612 | CLA | O2D-CGD-O1D | -2.58 | 118.71 | 123.82 |
| 22 | d | 401 | CLA | CHD-C4C-C3C | -2.57 | 121.08 | 124.88 |
| 22 | C | 507 | CLA | C4C-C3C-C2C | -2.57 | 103.09 | 106.90 |
| 22 | c | 507 | CLA | C4C-C3C-C2C | -2.56 | 103.10 | 106.90 |
| 24 | k | 102 | BCR | C34-C9-C8 | -2.56 | 114.02 | 118.10 |
| 22 | d | 403 | CLA | O2D-CGD-O1D | -2.56 | 118.74 | 123.82 |
| 22 | B | 614 | CLA | CHD-C4C-C3C | -2.56 | 121.10 | 124.88 |
| 24 | h | 101 | BCR | C29-C28-C27 | -2.56 | 105.51 | 111.36 |
| 22 | D | 401 | CLA | CHD-C4C-C3C | -2.55 | 121.11 | 124.88 |
| 22 | D | 403 | CLA | O2D-CGD-O1D | -2.54 | 118.77 | 123.82 |
| 22 | C | 512 | CLA | O2D-CGD-O1D | -2.54 | 118.77 | 123.82 |
| 24 | K | 102 | BCR | C34-C9-C8 | -2.54 | 114.05 | 118.10 |
| 22 | c | 509 | CLA | O2D-CGD-O1D | -2.54 | 118.78 | 123.82 |
| 22 | a | 603 | CLA | O2D-CGD-O1D | -2.54 | 118.79 | 123.82 |
| 22 | A | 603 | CLA | O2D-CGD-O1D | -2.53 | 118.79 | 123.82 |
| 24 | H | 101 | BCR | C29-C28-C27 | -2.53 | 105.56 | 111.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 33 | F | 101 | HEM | C1D-C2D-C3D | -2.53 | 105.24 | 107.00 |
| 22 | C | 509 | CLA | O2D-CGD-O1D | -2.52 | 118.82 | 123.82 |
| 24 | B | 622 | BCR | C37-C22-C23 | -2.52 | 114.08 | 118.10 |
| 29 | D | 406 | LMG | O8-C28-O10 | -2.52 | 117.44 | 123.58 |
| 25 | a | 609 | SQD | C1-O5-C5 | -2.52 | 108.75 | 113.71 |
| 29 | d | 406 | LMG | O8-C28-O10 | -2.52 | 117.44 | 123.58 |
| 22 | c | 512 | CLA | O2D-CGD-O1D | -2.51 | 118.83 | 123.82 |
| 22 | C | 501 | CLA | CBC-CAC-C3C | -2.51 | 105.43 | 112.42 |
| 22 | c | 501 | CLA | CBC-CAC-C3C | -2.51 | 105.43 | 112.42 |
| 24 | b | 622 | BCR | C37-C22-C23 | -2.50 | 114.11 | 118.10 |
| 28 | A | 613 | PL9 | C37-C38-C39 | -2.49 | 121.49 | 127.66 |
| 24 | C | 515 | BCR | C1-C6-C5 | -2.49 | 119.09 | 122.59 |
| 25 | A | 609 | SQD | C1-O5-C5 | -2.49 | 108.80 | 113.71 |
| 33 | f | 101 | HEM | C1D-C2D-C3D | -2.48 | 105.27 | 107.00 |
| 24 | c | 515 | BCR | C1-C6-C5 | -2.48 | 119.10 | 122.59 |
| 28 | a | 613 | PL9 | C37-C38-C39 | -2.48 | 121.52 | 127.66 |
| 22 | b | 606 | CLA | O2A-CGA-O1A | -2.48 | 117.53 | 123.58 |
| 24 | t | 101 | BCR | C40-C30-C39 | -2.47 | 101.07 | 108.52 |
| 22 | B | 606 | CLA | O2A-CGA-O1A | -2.46 | 117.57 | 123.58 |
| 24 | T | 102 | BCR | C40-C30-C39 | -2.46 | 101.09 | 108.52 |
| 31 | c | 517 | DGD | O2G-C1B-O1B | -2.46 | 117.62 | 123.69 |
| 31 | C | 517 | DGD | O2G-C1B-O1B | -2.46 | 117.62 | 123.69 |
| 22 | B | 602 | CLA | O2D-CGD-O1D | -2.45 | 118.95 | 123.82 |
| 22 | C | 501 | CLA | C4C-C3C-C2C | -2.45 | 103.26 | 106.90 |
| 24 | B | 618 | BCR | C1-C6-C5 | -2.45 | 119.14 | 122.59 |
| 22 | B | 614 | CLA | O2D-CGD-O1D | -2.45 | 118.95 | 123.82 |
| 22 | b | 614 | CLA | O2D-CGD-O1D | -2.45 | 118.96 | 123.82 |
| 24 | T | 101 | BCR | C1-C6-C5 | -2.45 | 119.15 | 122.59 |
| 24 | B | 618 | BCR | C33-C5-C4 | -2.45 | 108.94 | 113.56 |
| 24 | t | 101 | BCR | C1-C6-C5 | -2.44 | 119.16 | 122.59 |
| 24 | T | 101 | BCR | C33-C5-C4 | -2.44 | 108.95 | 113.56 |
| 22 | c | 501 | CLA | C4C-C3C-C2C | -2.43 | 103.29 | 106.90 |
| 24 | T | 102 | BCR | C1-C6-C5 | -2.43 | 119.17 | 122.59 |
| 22 | b | 602 | CLA | O2D-CGD-O1D | -2.43 | 118.99 | 123.82 |
| 22 | d | 402 | CLA | CHD-C4C-C3C | -2.42 | 121.31 | 124.88 |
| 22 | D | 402 | CLA | CHD-C4C-C3C | -2.42 | 121.31 | 124.88 |
| 22 | b | 604 | CLA | O2A-CGA-O1A | -2.42 | 117.67 | 123.58 |
| 22 | B | 604 | CLA | O2A-CGA-O1A | -2.41 | 117.69 | 123.58 |
| 22 | d | 402 | CLA | CHC-C1C-C2C | -2.40 | 120.06 | 126.75 |
| 22 | A | 604 | CLA | O2D-CGD-O1D | -2.40 | 119.06 | 123.82 |
| 22 | a | 604 | CLA | O2D-CGD-O1D | -2.39 | 119.07 | 123.82 |
| 22 | D | 402 | CLA | CHC-C1C-C2C | -2.39 | 120.09 | 126.75 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 33 | F | 101 | HEM | CBA-CAA-C2A | -2.38 | 107.93 | 112.48 |
| 33 | f | 101 | HEM | CBA-CAA-C2A | -2.38 | 107.94 | 112.48 |
| 22 | c | 510 | CLA | O1D-CGD-CBD | -2.38 | 120.17 | 124.58 |
| 22 | C | 512 | CLA | C1-C2-C3 | -2.37 | 121.58 | 125.96 |
| 24 | T | 102 | BCR | C32-C1-C2 | -2.36 | 99.57 | 108.78 |
| 23 | A | 606 | PHO | O2D-CGD-O1D | -2.36 | 119.14 | 123.82 |
| 24 | t | 101 | BCR | C32-C1-C2 | -2.36 | 99.60 | 108.78 |
| 22 | A | 604 | CLA | C4C-C3C-C2C | -2.35 | 103.41 | 106.90 |
| 22 | C | 510 | CLA | O1D-CGD-CBD | -2.35 | 120.22 | 124.58 |
| 22 | B | 614 | CLA | CBC-CAC-C3C | -2.34 | 105.89 | 112.42 |
| 22 | b | 614 | CLA | CBC-CAC-C3C | -2.34 | 105.89 | 112.42 |
| 24 | K | 102 | BCR | C1-C6-C5 | -2.34 | 119.30 | 122.59 |
| 22 | a | 604 | CLA | C4C-C3C-C2C | -2.34 | 103.43 | 106.90 |
| 22 | c | 512 | CLA | C1-C2-C3 | -2.34 | 121.64 | 125.96 |
| 23 | a | 606 | PHO | O2D-CGD-O1D | -2.34 | 119.18 | 123.82 |
| 24 | k | 102 | BCR | C1-C6-C5 | -2.34 | 119.31 | 122.59 |
| 22 | B | 612 | CLA | CBC-CAC-C3C | -2.32 | 105.97 | 112.42 |
| 22 | c | 512 | CLA | O1D-CGD-CBD | -2.32 | 120.28 | 124.58 |
| 22 | c | 504 | CLA | C4C-C3C-C2C | -2.32 | 103.47 | 106.90 |
| 29 | c | 519 | LMG | O8-C28-O10 | -2.32 | 117.93 | 123.58 |
| 22 | C | 504 | CLA | C4C-C3C-C2C | -2.31 | 103.47 | 106.90 |
| 29 | B | 620 | LMG | O7-C10-O9 | -2.31 | 117.99 | 123.69 |
| 22 | D | 402 | CLA | C4C-C3C-C2C | -2.31 | 103.48 | 106.90 |
| 22 | d | 402 | CLA | C4C-C3C-C2C | -2.31 | 103.48 | 106.90 |
| 29 | C | 519 | LMG | O8-C28-O10 | -2.30 | 117.96 | 123.58 |
| 22 | b | 612 | CLA | CBC-CAC-C3C | -2.30 | 106.02 | 112.42 |
| 28 | d | 408 | PL9 | C7-C8-C9 | -2.30 | 122.90 | 126.79 |
| 22 | C | 512 | CLA | O1D-CGD-CBD | -2.30 | 120.32 | 124.58 |
| 29 | c | 519 | LMG | O1-C7-C8 | -2.29 | 105.53 | 110.99 |
| 29 | C | 519 | LMG | O1-C7-C8 | -2.29 | 105.53 | 110.99 |
| 25 | d | 411 | SQD | O48-C23-O10 | -2.29 | 117.99 | 123.58 |
| 28 | D | 408 | PL9 | C7-C8-C9 | -2.29 | 122.91 | 126.79 |
| 22 | C | 510 | CLA | O2D-CGD-O1D | -2.29 | 119.27 | 123.82 |
| 23 | A | 606 | PHO | CHD-C1D-ND | -2.29 | 119.80 | 124.63 |
| 23 | A | 605 | PHO | O1D-CGD-CBD | -2.29 | 120.34 | 124.58 |
| 32 | E | 101 | LHG | O8-C23-O10 | -2.29 | 118.00 | 123.58 |
| 23 | a | 606 | PHO | C1C-C2C-C3C | -2.28 | 103.85 | 106.50 |
| 29 | b | 619 | LMG | O7-C10-O9 | -2.28 | 118.05 | 123.69 |
| 25 | D | 411 | SQD | O48-C23-O10 | -2.28 | 118.01 | 123.58 |
| 23 | a | 606 | PHO | CHD-C1D-ND | -2.28 | 119.82 | 124.63 |
| 24 | b | 618 | BCR | C29-C28-C27 | -2.28 | 106.14 | 111.36 |
| 25 | A | 609 | SQD | O48-C23-O10 | -2.27 | 118.03 | 123.58 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | C | 506 | CLA | O1D-CGD-CBD | -2.27 | 120.36 | 124.58 |
| 23 | a | 605 | PHO | O1D-CGD-CBD | -2.27 | 120.37 | 124.58 |
| 32 | e | 101 | LHG | O8-C23-O10 | -2.26 | 118.06 | 123.58 |
| 24 | A | 608 | BCR | C37-C22-C23 | -2.26 | 114.49 | 118.10 |
| 24 | D | 404 | BCR | C37-C22-C23 | -2.26 | 114.49 | 118.10 |
| 25 | a | 609 | SQD | O48-C23-O10 | -2.26 | 118.06 | 123.58 |
| 24 | B | 619 | BCR | C29-C28-C27 | -2.26 | 106.19 | 111.36 |
| 22 | c | 502 | CLA | CHD-C4C-C3C | -2.25 | 121.56 | 124.88 |
| 22 | c | 510 | CLA | O2D-CGD-O1D | -2.25 | 119.35 | 123.82 |
| 23 | A | 606 | PHO | C1C-C2C-C3C | -2.25 | 103.89 | 106.50 |
| 22 | B | 610 | CLA | C1-C2-C3 | -2.25 | 121.81 | 125.96 |
| 22 | b | 607 | CLA | C1-C2-C3 | -2.25 | 121.81 | 125.96 |
| 24 | a | 608 | BCR | C37-C22-C23 | -2.24 | 114.52 | 118.10 |
| 23 | a | 605 | PHO | CHD-C1D-ND | -2.24 | 119.90 | 124.63 |
| 22 | c | 506 | CLA | O1D-CGD-CBD | -2.24 | 120.42 | 124.58 |
| 22 | C | 502 | CLA | CHD-C4C-C3C | -2.24 | 121.57 | 124.88 |
| 22 | B | 607 | CLA | C1-C2-C3 | -2.24 | 121.83 | 125.96 |
| 23 | A | 605 | PHO | CHD-C1D-ND | -2.24 | 119.91 | 124.63 |
| 24 | d | 404 | BCR | C37-C22-C23 | -2.23 | 114.55 | 118.10 |
| 22 | b | 604 | CLA | O1D-CGD-CBD | -2.23 | 120.45 | 124.58 |
| 22 | b | 606 | CLA | O2D-CGD-O1D | -2.23 | 119.40 | 123.82 |
| 22 | B | 606 | CLA | O2D-CGD-O1D | -2.23 | 119.41 | 123.82 |
| 22 | b | 613 | CLA | O2D-CGD-O1D | -2.22 | 119.41 | 123.82 |
| 22 | B | 617 | CLA | CHD-C4C-C3C | -2.22 | 121.60 | 124.88 |
| 22 | b | 610 | CLA | C1-C2-C3 | -2.22 | 121.87 | 125.96 |
| 25 | b | 601 | SQD | C5-C6-S | -2.22 | 111.25 | 114.34 |
| 22 | B | 613 | CLA | O2D-CGD-O1D | -2.22 | 119.42 | 123.82 |
| 25 | B | 601 | SQD | C5-C6-S | -2.22 | 111.25 | 114.34 |
| 22 | B | 616 | CLA | O2D-CGD-O1D | -2.21 | 119.43 | 123.82 |
| 24 | t | 101 | BCR | C38-C26-C27 | -2.21 | 109.39 | 113.56 |
| 22 | b | 608 | CLA | O1D-CGD-CBD | -2.21 | 120.49 | 124.58 |
| 22 | b | 616 | CLA | O2D-CGD-O1D | -2.21 | 119.44 | 123.82 |
| 22 | b | 609 | CLA | O2A-CGA-O1A | -2.21 | 118.20 | 123.58 |
| 22 | b | 617 | CLA | CHD-C4C-C3C | -2.21 | 121.62 | 124.88 |
| 22 | c | 509 | CLA | O2A-CGA-O1A | -2.20 | 118.20 | 123.58 |
| 24 | a | 608 | BCR | C28-C27-C26 | -2.20 | 110.13 | 113.99 |
| 24 | c | 515 | BCR | C37-C22-C23 | -2.20 | 114.60 | 118.10 |
| 28 | d | 408 | PL9 | C27-C28-C29 | -2.20 | 122.22 | 127.66 |
| 24 | c | 514 | BCR | C40-C30-C29 | -2.20 | 100.22 | 108.78 |
| 31 | D | 410 | DGD | O2G-C1B-O1B | -2.20 | 118.27 | 123.69 |
| 22 | C | 509 | CLA | O2A-CGA-O1A | -2.19 | 118.23 | 123.58 |
| 23 | a | 606 | PHO | O1D-CGD-CBD | -2.19 | 120.52 | 124.58 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24 | C | 515 | BCR | C37-C22-C23 | -2.19 | 114.61 | 118.10 |
| 31 | d | 410 | DGD | O2G-C1B-O1B | -2.19 | 118.28 | 123.69 |
| 24 | C | 514 | BCR | C40-C30-C29 | -2.19 | 100.25 | 108.78 |
| 28 | D | 408 | PL9 | C27-C28-C29 | -2.19 | 122.24 | 127.66 |
| 24 | A | 608 | BCR | C28-C27-C26 | -2.19 | 110.16 | 113.99 |
| 22 | B | 617 | CLA | O2A-CGA-O1A | -2.19 | 118.25 | 123.58 |
| 22 | B | 609 | CLA | O2A-CGA-O1A | -2.19 | 118.25 | 123.58 |
| 22 | b | 606 | CLA | CHD-C4C-C3C | -2.19 | 121.66 | 124.88 |
| 29 | Z | 101 | LMG | O7-C10-O9 | -2.18 | 118.30 | 123.69 |
| 29 | z | 101 | LMG | O7-C10-O9 | -2.18 | 118.30 | 123.69 |
| 22 | B | 608 | CLA | O1D-CGD-CBD | -2.18 | 120.53 | 124.58 |
| 22 | B | 604 | CLA | O1D-CGD-CBD | -2.18 | 120.53 | 124.58 |
| 23 | A | 606 | PHO | O1D-CGD-CBD | -2.18 | 120.54 | 124.58 |
| 22 | b | 617 | CLA | O2A-CGA-O1A | -2.18 | 118.27 | 123.58 |
| 22 | B | 611 | CLA | O2A-CGA-O1A | -2.18 | 118.27 | 123.58 |
| 31 | c | 518 | DGD | O1G-C1A-O1A | -2.18 | 118.27 | 123.58 |
| 22 | b | 614 | CLA | O2A-CGA-O1A | -2.17 | 118.28 | 123.58 |
| 22 | b | 609 | CLA | C11-C12-C13 | -2.17 | 108.60 | 115.73 |
| 22 | b | 605 | CLA | O2A-CGA-O1A | -2.17 | 118.28 | 123.58 |
| 22 | B | 606 | CLA | CHD-C4C-C3C | -2.17 | 121.68 | 124.88 |
| 22 | B | 614 | CLA | O2A-CGA-O1A | -2.17 | 118.29 | 123.58 |
| 22 | B | 609 | CLA | C11-C12-C13 | -2.17 | 108.62 | 115.73 |
| 24 | T | 102 | BCR | C38-C26-C27 | -2.17 | 109.47 | 113.56 |
| 22 | b | 611 | CLA | O2A-CGA-O1A | -2.17 | 118.30 | 123.58 |
| 22 | B | 605 | CLA | O2A-CGA-O1A | -2.17 | 118.30 | 123.58 |
| 22 | B | 603 | CLA | C1-C2-C3 | -2.16 | 121.97 | 125.96 |
| 31 | C | 518 | DGD | O1G-C1A-O1A | -2.16 | 118.31 | 123.58 |
| 22 | b | 605 | CLA | O2D-CGD-O1D | -2.16 | 119.53 | 123.82 |
| 25 | a | 609 | SQD | C5-C6-S | -2.16 | 111.33 | 114.34 |
| 22 | b | 603 | CLA | C1-C2-C3 | -2.16 | 121.98 | 125.96 |
| 33 | V | 201 | HEM | CMA-C3A-C4A | -2.16 | 125.15 | 128.46 |
| 22 | B | 605 | CLA | O2D-CGD-O1D | -2.15 | 119.55 | 123.82 |
| 22 | b | 615 | CLA | O2A-CGA-O1A | -2.15 | 118.33 | 123.58 |
| 33 | v | 201 | HEM | CMA-C3A-C4A | -2.14 | 125.18 | 128.46 |
| 23 | a | 605 | PHO | C1C-NC-C4C | -2.13 | 102.37 | 106.51 |
| 22 | A | 604 | CLA | O1D-CGD-CBD | -2.13 | 120.63 | 124.58 |
| 22 | C | 505 | CLA | O1D-CGD-CBD | -2.13 | 120.64 | 124.58 |
| 22 | a | 604 | CLA | O1D-CGD-CBD | -2.13 | 120.64 | 124.58 |
| 22 | c | 505 | CLA | O1D-CGD-CBD | -2.13 | 120.64 | 124.58 |
| 22 | C | 508 | CLA | O1D-CGD-CBD | -2.13 | 120.64 | 124.58 |
| 22 | B | 615 | CLA | O2A-CGA-O1A | -2.12 | 118.39 | 123.58 |
| 22 | b | 617 | CLA | CBC-CAC-C3C | -2.12 | 106.51 | 112.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | b | 604 | CLA | CHD-C4C-C3C | -2.12 | 121.75 | 124.88 |
| 25 | A | 609 | SQD | C5-C6-S | -2.12 | 111.39 | 114.34 |
| 22 | D | 401 | CLA | CAA-CBA-CGA | -2.12 | 107.03 | 113.35 |
| 22 | B | 604 | CLA | CHD-C4C-C3C | -2.11 | 121.76 | 124.88 |
| 22 | c | 508 | CLA | O1D-CGD-CBD | -2.11 | 120.66 | 124.58 |
| 23 | A | 605 | PHO | C1C-NC-C4C | -2.11 | 102.41 | 106.51 |
| 22 | B | 615 | CLA | O1D-CGD-CBD | -2.11 | 120.67 | 124.58 |
| 22 | b | 609 | CLA | CHC-C1C-C2C | -2.11 | 120.88 | 126.75 |
| 22 | d | 401 | CLA | CAA-CBA-CGA | -2.11 | 107.06 | 113.35 |
| 22 | b | 610 | CLA | CBC-CAC-C3C | -2.11 | 106.56 | 112.42 |
| 33 | f | 101 | HEM | CMA-C3A-C4A | -2.11 | 125.23 | 128.46 |
| 22 | B | 610 | CLA | CBC-CAC-C3C | -2.10 | 106.57 | 112.42 |
| 22 | b | 615 | CLA | O1D-CGD-CBD | -2.10 | 120.68 | 124.58 |
| 22 | A | 607 | CLA | O2D-CGD-O1D | -2.10 | 119.65 | 123.82 |
| 22 | B | 617 | CLA | CBC-CAC-C3C | -2.10 | 106.58 | 112.42 |
| 22 | D | 402 | CLA | O2D-CGD-O1D | -2.10 | 119.66 | 123.82 |
| 22 | B | 609 | CLA | CHC-C1C-C2C | -2.09 | 120.92 | 126.75 |
| 25 | l | 102 | SQD | O5-C1-C2 | -2.09 | 105.86 | 110.34 |
| 31 | c | 516 | DGD | C3G-C2G-C1G | -2.09 | 107.15 | 111.86 |
| 22 | a | 607 | CLA | O2D-CGD-O1D | -2.08 | 119.69 | 123.82 |
| 22 | d | 402 | CLA | O2D-CGD-O1D | -2.08 | 119.69 | 123.82 |
| 25 | l | 102 | SQD | O47-C7-O49 | -2.08 | 118.56 | 123.69 |
| 31 | C | 516 | DGD | C3G-C2G-C1G | -2.07 | 107.18 | 111.86 |
| 25 | b | 621 | SQD | O5-C1-C2 | -2.07 | 105.89 | 110.34 |
| 33 | F | 101 | HEM | CMA-C3A-C4A | -2.07 | 125.28 | 128.46 |
| 22 | A | 604 | CLA | CHC-C1C-C2C | -2.07 | 120.99 | 126.75 |
| 22 | C | 508 | CLA | O2D-CGD-O1D | -2.07 | 119.72 | 123.82 |
| 22 | c | 508 | CLA | O2D-CGD-O1D | -2.06 | 119.73 | 123.82 |
| 32 | L | 102 | LHG | C6-C5-C4 | -2.06 | 107.20 | 111.86 |
| 25 | b | 621 | SQD | O47-C7-O49 | -2.06 | 118.61 | 123.69 |
| 22 | c | 505 | CLA | O2D-CGD-O1D | -2.06 | 119.74 | 123.82 |
| 22 | D | 401 | CLA | O2A-CGA-O1A | -2.05 | 118.57 | 123.58 |
| 22 | B | 604 | CLA | CBC-CAC-C3C | -2.05 | 106.71 | 112.42 |
| 24 | h | 101 | BCR | C40-C30-C29 | -2.05 | 100.78 | 108.78 |
| 28 | d | 408 | PL9 | C7-C3-C2 | -2.05 | 120.56 | 123.27 |
| 31 | H | 102 | DGD | O3G-C3G-C2G | -2.05 | 106.11 | 110.99 |
| 24 | H | 101 | BCR | C40-C30-C29 | -2.05 | 100.78 | 108.78 |
| 22 | D | 403 | CLA | CBC-CAC-C3C | -2.05 | 106.71 | 112.42 |
| 22 | a | 604 | CLA | CHC-C1C-C2C | -2.05 | 121.04 | 126.75 |
| 22 | b | 604 | CLA | CBC-CAC-C3C | -2.05 | 106.72 | 112.42 |
| 22 | C | 505 | CLA | O2D-CGD-O1D | -2.05 | 119.75 | 123.82 |
| 31 | h | 102 | DGD | O3G-C3G-C2G | -2.05 | 106.11 | 110.99 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | b | 613 | CLA | O1D-CGD-CBD | -2.05 | 120.78 | 124.58 |
| 31 | c | 517 | DGD | O1G-C1A-O1A | -2.05 | 118.59 | 123.58 |
| 28 | D | 408 | PL9 | C7-C3-C2 | -2.05 | 120.57 | 123.27 |
| 24 | K | 102 | BCR | C29-C28-C27 | -2.04 | 106.69 | 111.36 |
| 32 | l | 103 | LHG | C6-C5-C4 | -2.04 | 107.25 | 111.86 |
| 22 | C | 504 | CLA | C7-C6-C5 | -2.04 | 107.62 | 113.17 |
| 22 | d | 403 | CLA | CBC-CAC-C3C | -2.04 | 106.75 | 112.42 |
| 22 | B | 607 | CLA | O2A-CGA-O1A | -2.04 | 118.61 | 123.58 |
| 24 | k | 102 | BCR | C29-C28-C27 | -2.04 | 106.70 | 111.36 |
| 22 | B | 613 | CLA | O1D-CGD-CBD | -2.04 | 120.81 | 124.58 |
| 22 | c | 505 | CLA | CHD-C4C-C3C | -2.03 | 121.88 | 124.88 |
| 22 | c | 509 | CLA | CHC-C1C-C2C | -2.03 | 121.08 | 126.75 |
| 22 | d | 403 | CLA | O1D-CGD-CBD | -2.03 | 120.81 | 124.58 |
| 22 | b | 607 | CLA | O2A-CGA-O1A | -2.03 | 118.62 | 123.58 |
| 22 | C | 510 | CLA | O2A-CGA-O1A | -2.03 | 118.62 | 123.58 |
| 22 | A | 603 | CLA | CHC-C1C-C2C | -2.03 | 121.09 | 126.75 |
| 31 | C | 517 | DGD | O1G-C1A-O1A | -2.03 | 118.63 | 123.58 |
| 22 | c | 504 | CLA | C7-C6-C5 | -2.03 | 107.65 | 113.17 |
| 22 | d | 401 | CLA | O2A-CGA-O1A | -2.03 | 118.63 | 123.58 |
| 22 | C | 509 | CLA | CHC-C1C-C2C | -2.02 | 121.11 | 126.75 |
| 22 | c | 510 | CLA | O2A-CGA-O1A | -2.02 | 118.64 | 123.58 |
| 29 | a | 614 | LMG | C7-O1-C1 | -2.02 | 109.74 | 113.80 |
| 22 | a | 603 | CLA | CHC-C1C-C2C | -2.02 | 121.12 | 126.75 |
| 22 | D | 403 | CLA | O1D-CGD-CBD | -2.02 | 120.83 | 124.58 |
| 29 | c | 519 | LMG | C8-O7-C10 | -2.02 | 113.10 | 117.88 |
| 31 | c | 517 | DGD | C2G-O2G-C1B | -2.02 | 113.10 | 117.88 |
| 22 | C | 509 | CLA | O1D-CGD-CBD | -2.02 | 120.83 | 124.58 |
| 25 | A | 609 | SQD | O5-C1-C2 | -2.02 | 106.01 | 110.34 |
| 29 | A | 614 | LMG | C7-O1-C1 | -2.02 | 109.75 | 113.80 |
| 25 | a | 609 | SQD | O5-C1-C2 | -2.02 | 106.02 | 110.34 |
| 31 | C | 517 | DGD | C2G-O2G-C1B | -2.01 | 113.12 | 117.88 |
| 24 | H | 101 | BCR | C1-C6-C5 | -2.01 | 119.76 | 122.59 |
| 22 | B | 614 | CLA | C1-C2-C3 | -2.01 | 122.25 | 125.96 |
| 22 | A | 607 | CLA | O1D-CGD-CBD | -2.01 | 120.85 | 124.58 |
| 22 | b | 609 | CLA | C11-C10-C8 | -2.00 | 109.16 | 115.73 |
| 22 | b | 614 | CLA | C1-C2-C3 | -2.00 | 122.27 | 125.96 |
| 24 | C | 515 | BCR | C4-C5-C6 | 2.00 | 125.68 | 122.74 |
| 24 | B | 622 | BCR | C2-C3-C4 | 2.00 | 115.95 | 111.36 |
| 24 | K | 102 | BCR | C30-C25-C24 | 2.00 | 121.36 | 115.73 |
| 22 | d | 403 | CLA | C1-O2A-CGA | 2.00 | 121.39 | 116.77 |
| 24 | b | 622 | BCR | C2-C3-C4 | 2.01 | 115.96 | 111.36 |
| 24 | k | 102 | BCR | C30-C25-C24 | 2.01 | 121.37 | 115.73 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 22 | b | 608 | CLA | CHB-C4A-NA | 2.01 | 127.29 | 124.51 |
| 24 | t | 101 | BCR | C1-C6-C7 | 2.01 | 121.37 | 115.73 |
| 22 | B | 608 | CLA | CHB-C4A-NA | 2.01 | 127.30 | 124.51 |
| 25 | l | 101 | SQD | C4-C3-C2 | 2.01 | 114.36 | 110.83 |
| 22 | C | 505 | CLA | O2A-CGA-CBA | 2.02 | 117.75 | 111.92 |
| 29 | z | 101 | LMG | C9-O8-C28 | 2.02 | 122.27 | 117.14 |
| 24 | t | 101 | BCR | C40-C30-C25 | 2.02 | 113.58 | 110.31 |
| 22 | C | 509 | CLA | C4-C3-C5 | 2.02 | 118.77 | 115.29 |
| 22 | B | 609 | CLA | C4A-NA-C1A | 2.02 | 108.93 | 106.32 |
| 22 | b | 616 | CLA | CMC-C2C-C1C | 2.02 | 128.15 | 125.05 |
| 22 | D | 403 | CLA | C1-O2A-CGA | 2.02 | 121.43 | 116.77 |
| 22 | D | 402 | CLA | C4A-NA-C1A | 2.02 | 108.93 | 106.32 |
| 22 | c | 509 | CLA | C4-C3-C5 | 2.03 | 118.78 | 115.29 |
| 28 | A | 613 | PL9 | C2-C1-C6 | 2.03 | 121.28 | 118.02 |
| 28 | d | 408 | PL9 | C51-C49-C50 | 2.03 | 119.16 | 114.59 |
| 22 | b | 607 | CLA | CMC-C2C-C1C | 2.03 | 128.16 | 125.05 |
| 29 | Z | 101 | LMG | C9-O8-C28 | 2.03 | 122.30 | 117.14 |
| 28 | a | 613 | PL9 | C2-C1-C6 | 2.03 | 121.28 | 118.02 |
| 24 | a | 608 | BCR | C2-C1-C6 | 2.03 | 113.65 | 110.48 |
| 25 | L | 101 | SQD | C4-C3-C2 | 2.03 | 114.39 | 110.83 |
| 24 | T | 102 | BCR | C40-C30-C25 | 2.03 | 113.60 | 110.31 |
| 28 | D | 408 | PL9 | C51-C49-C50 | 2.03 | 119.17 | 114.59 |
| 22 | c | 502 | CLA | O2A-CGA-CBA | 2.03 | 117.79 | 111.92 |
| 22 | b | 610 | CLA | CMC-C2C-C1C | 2.03 | 128.16 | 125.05 |
| 22 | c | 505 | CLA | O2A-CGA-CBA | 2.03 | 117.80 | 111.92 |
| 25 | l | 101 | SQD | O9-S-C6 | 2.03 | 109.36 | 106.94 |
| 22 | B | 609 | CLA | CMC-C2C-C1C | 2.04 | 128.17 | 125.05 |
| 28 | a | 613 | PL9 | C51-C49-C50 | 2.04 | 119.19 | 114.59 |
| 22 | B | 617 | CLA | C4-C3-C5 | 2.04 | 118.81 | 115.29 |
| 22 | B | 610 | CLA | CMC-C2C-C1C | 2.04 | 128.18 | 125.05 |
| 22 | B | 607 | CLA | CMC-C2C-C1C | 2.04 | 128.18 | 125.05 |
| 22 | B | 616 | CLA | CMC-C2C-C1C | 2.04 | 128.18 | 125.05 |
| 22 | B | 606 | CLA | CMC-C2C-C1C | 2.04 | 128.18 | 125.05 |
| 22 | b | 609 | CLA | C4A-NA-C1A | 2.05 | 108.96 | 106.32 |
| 22 | C | 502 | CLA | O2A-CGA-CBA | 2.05 | 117.83 | 111.92 |
| 25 | L | 101 | SQD | O9-S-C6 | 2.05 | 109.37 | 106.94 |
| 24 | A | 608 | BCR | C2-C1-C6 | 2.05 | 113.68 | 110.48 |
| 28 | A | 613 | PL9 | C51-C49-C50 | 2.05 | 119.21 | 114.59 |
| 22 | b | 617 | CLA | C4-C3-C5 | 2.05 | 118.83 | 115.29 |
| 22 | b | 609 | CLA | CMC-C2C-C1C | 2.06 | 128.20 | 125.05 |
| 22 | C | 508 | CLA | O2A-CGA-CBA | 2.06 | 117.88 | 111.92 |
| 22 | a | 607 | CLA | CHB-C4A-NA | 2.06 | 127.36 | 124.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 22 | C | 503 | CLA | CED-O2D-CGD | 2.06 | 120.72 | 115.97 |
| 25 | D | 411 | SQD | C3-C4-C5 | 2.06 | 113.93 | 110.24 |
| 22 | c | 511 | CLA | CMC-C2C-C1C | 2.06 | 128.21 | 125.05 |
| 22 | B | 613 | CLA | C1D-CHD-C4C | 2.07 | 125.31 | 122.48 |
| 22 | A | 607 | CLA | CHB-C4A-NA | 2.07 | 127.37 | 124.51 |
| 22 | c | 503 | CLA | CED-O2D-CGD | 2.07 | 120.74 | 115.97 |
| 24 | C | 514 | BCR | C2-C3-C4 | 2.07 | 116.11 | 111.36 |
| 24 | c | 514 | BCR | C2-C3-C4 | 2.08 | 116.12 | 111.36 |
| 22 | c | 508 | CLA | O2A-CGA-CBA | 2.08 | 117.92 | 111.92 |
| 32 | l | 103 | LHG | O8-C23-C24 | 2.08 | 117.93 | 111.92 |
| 32 | L | 102 | LHG | O8-C23-C24 | 2.08 | 117.93 | 111.92 |
| 22 | C | 512 | CLA | CMC-C2C-C1C | 2.08 | 128.24 | 125.05 |
| 22 | b | 607 | CLA | CMB-C2B-C3B | 2.08 | 128.67 | 124.88 |
| 32 | D | 405 | LHG | O4-P-O5 | 2.08 | 122.72 | 112.14 |
| 32 | d | 405 | LHG | O4-P-O5 | 2.09 | 122.74 | 112.14 |
| 22 | B | 607 | CLA | CMB-C2B-C3B | 2.09 | 128.68 | 124.88 |
| 25 | d | 411 | SQD | C3-C4-C5 | 2.09 | 113.97 | 110.24 |
| 24 | d | 404 | BCR | C24-C25-C26 | 2.09 | 126.53 | 121.54 |
| 22 | d | 403 | CLA | O2A-CGA-CBA | 2.09 | 117.97 | 111.92 |
| 24 | D | 404 | BCR | C24-C25-C26 | 2.09 | 126.53 | 121.54 |
| 22 | C | 511 | CLA | CMC-C2C-C1C | 2.10 | 128.26 | 125.05 |
| 22 | b | 613 | CLA | C1D-CHD-C4C | 2.10 | 125.35 | 122.48 |
| 22 | D | 403 | CLA | O2A-CGA-CBA | 2.10 | 118.00 | 111.92 |
| 22 | c | 512 | CLA | CMC-C2C-C1C | 2.11 | 128.28 | 125.05 |
| 22 | C | 508 | CLA | CAC-C3C-C4C | 2.11 | 127.73 | 124.82 |
| 29 | d | 406 | LMG | O8-C28-C29 | 2.11 | 118.01 | 111.92 |
| 29 | D | 406 | LMG | O8-C28-C29 | 2.11 | 118.02 | 111.92 |
| 22 | c | 501 | CLA | C4-C3-C5 | 2.11 | 118.94 | 115.29 |
| 22 | c | 511 | CLA | CED-O2D-CGD | 2.12 | 120.85 | 115.97 |
| 22 | C | 511 | CLA | CED-O2D-CGD | 2.12 | 120.85 | 115.97 |
| 22 | b | 605 | CLA | CMC-C2C-C1C | 2.12 | 128.30 | 125.05 |
| 22 | C | 501 | CLA | C4-C3-C5 | 2.12 | 118.94 | 115.29 |
| 22 | B | 611 | CLA | CAC-C3C-C4C | 2.12 | 127.75 | 124.82 |
| 22 | b | 611 | CLA | CAC-C3C-C4C | 2.12 | 127.75 | 124.82 |
| 32 | d | 409 | LHG | O4-P-O5 | 2.13 | 122.95 | 112.14 |
| 24 | B | 619 | BCR | C28-C29-C30 | 2.13 | 122.15 | 114.58 |
| 24 | b | 618 | BCR | C28-C29-C30 | 2.13 | 122.15 | 114.58 |
| 22 | b | 615 | CLA | CED-O2D-CGD | 2.13 | 120.88 | 115.97 |
| 24 | t | 101 | BCR | C3-C2-C1 | 2.13 | 122.16 | 114.58 |
| 24 | T | 102 | BCR | C3-C2-C1 | 2.14 | 122.17 | 114.58 |
| 32 | D | 409 | LHG | O4-P-O5 | 2.14 | 123.00 | 112.14 |
| 22 | B | 615 | CLA | CED-O2D-CGD | 2.14 | 120.89 | 115.97 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 22 | c | 507 | CLA | CED-O2D-CGD | 2.14 | 120.91 | 115.97 |
| 22 | b | 605 | CLA | CAC-C3C-C4C | 2.14 | 127.77 | 124.82 |
| 24 | k | 102 | BCR | C1-C6-C7 | 2.15 | 121.77 | 115.73 |
| 22 | B | 615 | CLA | O2A-CGA-CBA | 2.15 | 118.13 | 111.92 |
| 31 | h | 102 | DGD | O6E-C5E-C6E | 2.15 | 111.83 | 106.43 |
| 22 | a | 604 | CLA | CED-O2D-CGD | 2.15 | 120.93 | 115.97 |
| 22 | B | 603 | CLA | O2A-CGA-CBA | 2.15 | 118.14 | 111.92 |
| 31 | C | 517 | DGD | O1G-C1A-C2A | 2.15 | 118.15 | 111.92 |
| 24 | K | 102 | BCR | C1-C6-C7 | 2.15 | 121.78 | 115.73 |
| 24 | D | 404 | BCR | C38-C26-C25 | 2.15 | 126.92 | 124.51 |
| 32 | D | 407 | LHG | O7-C7-C8 | 2.15 | 116.09 | 111.55 |
| 22 | B | 617 | CLA | CED-O2D-CGD | 2.16 | 120.94 | 115.97 |
| 31 | H | 102 | DGD | O6E-C5E-C6E | 2.16 | 111.85 | 106.43 |
| 33 | V | 201 | HEM | C4C-C3C-C2C | 2.16 | 108.40 | 106.90 |
| 22 | B | 605 | CLA | CMC-C2C-C1C | 2.16 | 128.35 | 125.05 |
| 22 | C | 507 | CLA | C1-O2A-CGA | 2.16 | 121.75 | 116.77 |
| 22 | c | 508 | CLA | CAC-C3C-C4C | 2.16 | 127.80 | 124.82 |
| 31 | c | 517 | DGD | O1G-C1A-C2A | 2.16 | 118.17 | 111.92 |
| 32 | d | 407 | LHG | O7-C7-C8 | 2.16 | 116.11 | 111.55 |
| 22 | b | 603 | CLA | O2A-CGA-CBA | 2.16 | 118.17 | 111.92 |
| 22 | A | 604 | CLA | CED-O2D-CGD | 2.16 | 120.95 | 115.97 |
| 22 | C | 507 | CLA | CED-O2D-CGD | 2.16 | 120.95 | 115.97 |
| 24 | d | 404 | BCR | C38-C26-C25 | 2.16 | 126.93 | 124.51 |
| 22 | b | 617 | CLA | CED-O2D-CGD | 2.17 | 120.96 | 115.97 |
| 22 | b | 615 | CLA | O2A-CGA-CBA | 2.17 | 118.18 | 111.92 |
| 22 | c | 507 | CLA | C1-O2A-CGA | 2.17 | 121.76 | 116.77 |
| 22 | d | 401 | CLA | CED-O2D-CGD | 2.17 | 120.96 | 115.97 |
| 22 | D | 401 | CLA | CED-O2D-CGD | 2.17 | 120.97 | 115.97 |
| 22 | B | 614 | CLA | C1D-CHD-C4C | 2.17 | 125.45 | 122.48 |
| 22 | B | 614 | CLA | CMC-C2C-C1C | 2.17 | 128.38 | 125.05 |
| 22 | B | 605 | CLA | CAC-C3C-C4C | 2.18 | 127.82 | 124.82 |
| 22 | B | 616 | CLA | CED-O2D-CGD | 2.18 | 120.99 | 115.97 |
| 33 | v | 201 | HEM | C4C-C3C-C2C | 2.18 | 108.42 | 106.90 |
| 22 | b | 614 | CLA | C1D-CHD-C4C | 2.18 | 125.47 | 122.48 |
| 22 | b | 616 | CLA | CED-O2D-CGD | 2.18 | 121.00 | 115.97 |
| 22 | B | 609 | CLA | C4-C3-C5 | 2.18 | 119.06 | 115.29 |
| 22 | c | 506 | CLA | O2A-CGA-CBA | 2.18 | 118.24 | 111.92 |
| 28 | D | 408 | PL9 | C2-C1-C6 | 2.19 | 121.54 | 118.02 |
| 22 | b | 609 | CLA | C4-C3-C5 | 2.19 | 119.07 | 115.29 |
| 22 | a | 603 | CLA | C4-C3-C5 | 2.20 | 119.08 | 115.29 |
| 22 | C | 506 | CLA | O2A-CGA-CBA | 2.20 | 118.27 | 111.92 |
| 22 | b | 602 | CLA | C1-O2A-CGA | 2.20 | 121.83 | 116.77 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 22 | b | 614 | CLA | CMC-C2C-C1C | 2.20 | 128.42 | 125.05 |
| 22 | B | 602 | CLA | C1-O2A-CGA | 2.20 | 121.85 | 116.77 |
| 22 | C | 509 | CLA | C1-O2A-CGA | 2.21 | 121.86 | 116.77 |
| 23 | a | 606 | PHO | CMB-C2B-C1B | 2.21 | 128.47 | 125.05 |
| 22 | c | 509 | CLA | C1-O2A-CGA | 2.21 | 121.86 | 116.77 |
| 22 | a | 603 | CLA | CMC-C2C-C1C | 2.21 | 128.44 | 125.05 |
| 28 | d | 408 | PL9 | C2-C1-C6 | 2.21 | 121.58 | 118.02 |
| 28 | D | 408 | PL9 | C10-C9-C11 | 2.21 | 119.11 | 115.29 |
| 28 | d | 408 | PL9 | C10-C9-C11 | 2.22 | 119.12 | 115.29 |
| 22 | c | 502 | CLA | CMB-C2B-C3B | 2.23 | 128.93 | 124.88 |
| 29 | D | 406 | LMG | O7-C10-C11 | 2.23 | 116.26 | 111.55 |
| 22 | B | 606 | CLA | CED-O2D-CGD | 2.23 | 121.12 | 115.97 |
| 22 | C | 512 | CLA | CAC-C3C-C4C | 2.23 | 127.90 | 124.82 |
| 22 | b | 606 | CLA | CED-O2D-CGD | 2.24 | 121.12 | 115.97 |
| 29 | d | 406 | LMG | O7-C10-C11 | 2.24 | 116.27 | 111.55 |
| 22 | B | 603 | CLA | CED-O2D-CGD | 2.24 | 121.14 | 115.97 |
| 23 | A | 605 | PHO | CMB-C2B-C1B | 2.24 | 128.52 | 125.05 |
| 23 | A | 606 | PHO | CMB-C2B-C1B | 2.24 | 128.52 | 125.05 |
| 22 | b | 603 | CLA | CED-O2D-CGD | 2.24 | 121.14 | 115.97 |
| 22 | A | 603 | CLA | CMC-C2C-C1C | 2.25 | 128.49 | 125.05 |
| 22 | A | 603 | CLA | C4-C3-C5 | 2.25 | 119.16 | 115.29 |
| 22 | c | 513 | CLA | CAC-C3C-C4C | 2.25 | 127.92 | 124.82 |
| 22 | c | 512 | CLA | CAC-C3C-C4C | 2.26 | 127.93 | 124.82 |
| 22 | C | 502 | CLA | CMB-C2B-C3B | 2.26 | 129.00 | 124.88 |
| 22 | b | 604 | CLA | O2A-CGA-CBA | 2.26 | 118.46 | 111.92 |
| 25 | b | 601 | SQD | C3-C4-C5 | 2.26 | 114.29 | 110.24 |
| 22 | c | 505 | CLA | C1-O2A-CGA | 2.26 | 121.99 | 116.77 |
| 23 | a | 605 | PHO | CMB-C2B-C1B | 2.26 | 128.56 | 125.05 |
| 24 | C | 515 | BCR | C27-C26-C25 | 2.26 | 126.06 | 122.74 |
| 22 | c | 511 | CLA | CAC-C3C-C4C | 2.26 | 127.94 | 124.82 |
| 22 | C | 511 | CLA | CAC-C3C-C4C | 2.27 | 127.94 | 124.82 |
| 22 | C | 505 | CLA | C1-O2A-CGA | 2.27 | 121.99 | 116.77 |
| 24 | c | 515 | BCR | C27-C26-C25 | 2.27 | 126.07 | 122.74 |
| 28 | d | 408 | PL9 | C35-C34-C36 | 2.27 | 119.21 | 115.29 |
| 22 | c | 509 | CLA | CMB-C2B-C3B | 2.27 | 129.02 | 124.88 |
| 22 | B | 604 | CLA | O2A-CGA-CBA | 2.27 | 118.50 | 111.92 |
| 22 | C | 509 | CLA | CMB-C2B-C3B | 2.28 | 129.03 | 124.88 |
| 25 | B | 601 | SQD | C3-C4-C5 | 2.28 | 114.32 | 110.24 |
| 22 | b | 607 | CLA | C1-O2A-CGA | 2.28 | 122.02 | 116.77 |
| 22 | c | 510 | CLA | CAC-C3C-C4C | 2.28 | 127.96 | 124.82 |
| 22 | A | 603 | CLA | O2A-CGA-CBA | 2.28 | 118.51 | 111.92 |
| 22 | a | 604 | CLA | C1-O2A-CGA | 2.28 | 122.03 | 116.77 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 28 | D | 408 | PL9 | C35-C34-C36 | 2.28 | 119.23 | 115.29 |
| 32 | d | 409 | LHG | O8-C23-C24 | 2.29 | 118.53 | 111.92 |
| 22 | b | 611 | CLA | CMB-C2B-C3B | 2.29 | 129.05 | 124.88 |
| 32 | D | 409 | LHG | O8-C23-C24 | 2.29 | 118.54 | 111.92 |
| 22 | a | 603 | CLA | O2A-CGA-CBA | 2.29 | 118.54 | 111.92 |
| 22 | C | 513 | CLA | CAC-C3C-C4C | 2.29 | 127.98 | 124.82 |
| 22 | B | 607 | CLA | C1-O2A-CGA | 2.29 | 122.05 | 116.77 |
| 22 | B | 613 | CLA | O2A-CGA-CBA | 2.29 | 118.55 | 111.92 |
| 24 | K | 101 | BCR | C30-C25-C24 | 2.30 | 122.18 | 115.73 |
| 22 | C | 510 | CLA | CAC-C3C-C4C | 2.30 | 127.99 | 124.82 |
| 22 | B | 608 | CLA | C1-O2A-CGA | 2.30 | 122.07 | 116.77 |
| 24 | b | 622 | BCR | C32-C1-C6 | 2.30 | 114.04 | 110.31 |
| 28 | A | 613 | PL9 | C45-C44-C46 | 2.30 | 119.26 | 115.29 |
| 22 | b | 610 | CLA | CED-O2D-CGD | 2.30 | 121.28 | 115.97 |
| 22 | B | 610 | CLA | CED-O2D-CGD | 2.31 | 121.28 | 115.97 |
| 22 | b | 613 | CLA | O2A-CGA-CBA | 2.31 | 118.59 | 111.92 |
| 22 | c | 501 | CLA | CMB-C2B-C3B | 2.31 | 129.08 | 124.88 |
| 22 | A | 604 | CLA | C1-O2A-CGA | 2.31 | 122.09 | 116.77 |
| 24 | k | 101 | BCR | C30-C25-C24 | 2.31 | 122.22 | 115.73 |
| 24 | b | 618 | BCR | C4-C5-C6 | 2.31 | 126.13 | 122.74 |
| 22 | C | 501 | CLA | CMB-C2B-C3B | 2.31 | 129.09 | 124.88 |
| 28 | a | 613 | PL9 | C45-C44-C46 | 2.31 | 119.28 | 115.29 |
| 22 | b | 616 | CLA | C1-O2A-CGA | 2.32 | 122.10 | 116.77 |
| 22 | B | 611 | CLA | CMB-C2B-C3B | 2.32 | 129.10 | 124.88 |
| 22 | D | 401 | CLA | O2A-CGA-CBA | 2.32 | 118.63 | 111.92 |
| 24 | K | 102 | BCR | C4-C5-C6 | 2.32 | 126.15 | 122.74 |
| 22 | b | 608 | CLA | C1-O2A-CGA | 2.32 | 122.11 | 116.77 |
| 24 | B | 619 | BCR | C4-C5-C6 | 2.33 | 126.15 | 122.74 |
| 31 | D | 410 | DGD | O6E-C5E-C6E | 2.33 | 112.28 | 106.43 |
| 22 | d | 401 | CLA | O2A-CGA-CBA | 2.33 | 118.65 | 111.92 |
| 24 | k | 102 | BCR | C4-C5-C6 | 2.33 | 126.16 | 122.74 |
| 22 | b | 616 | CLA | CMB-C2B-C3B | 2.33 | 129.12 | 124.88 |
| 31 | d | 410 | DGD | O6E-C5E-C6E | 2.33 | 112.29 | 106.43 |
| 22 | D | 402 | CLA | CMC-C2C-C1C | 2.33 | 128.62 | 125.05 |
| 22 | B | 615 | CLA | CMC-C2C-C1C | 2.33 | 128.62 | 125.05 |
| 24 | B | 622 | BCR | C32-C1-C6 | 2.33 | 114.09 | 110.31 |
| 22 | B | 616 | CLA | C1-O2A-CGA | 2.33 | 122.15 | 116.77 |
| 22 | c | 504 | CLA | CMC-C2C-C1C | 2.33 | 128.63 | 125.05 |
| 22 | B | 615 | CLA | CMB-C2B-C3B | 2.34 | 129.13 | 124.88 |
| 22 | B | 616 | CLA | CMB-C2B-C3B | 2.34 | 129.14 | 124.88 |
| 22 | c | 506 | CLA | CMC-C2C-C1C | 2.34 | 128.63 | 125.05 |
| 22 | d | 402 | CLA | CMC-C2C-C1C | 2.34 | 128.64 | 125.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 22 | B | 608 | CLA | CMB-C2B-C3B | 2.34 | 129.15 | 124.88 |
| 22 | b | 611 | CLA | CHB-C4A-NA | 2.35 | 127.76 | 124.51 |
| 22 | B | 611 | CLA | CHB-C4A-NA | 2.35 | 127.76 | 124.51 |
| 22 | b | 615 | CLA | CMB-C2B-C3B | 2.35 | 129.16 | 124.88 |
| 22 | c | 508 | CLA | C1D-CHD-C4C | 2.35 | 125.70 | 122.48 |
| 22 | b | 610 | CLA | CMB-C2B-C3B | 2.35 | 129.17 | 124.88 |
| 22 | c | 513 | CLA | C4-C3-C5 | 2.36 | 119.35 | 115.29 |
| 22 | B | 602 | CLA | CMB-C2B-C3B | 2.36 | 129.17 | 124.88 |
| 24 | H | 101 | BCR | C28-C29-C30 | 2.36 | 122.97 | 114.58 |
| 22 | b | 615 | CLA | CMC-C2C-C1C | 2.36 | 128.67 | 125.05 |
| 22 | C | 506 | CLA | CMC-C2C-C1C | 2.36 | 128.67 | 125.05 |
| 22 | c | 505 | CLA | CED-O2D-CGD | 2.36 | 121.41 | 115.97 |
| 22 | B | 612 | CLA | CMB-C2B-C3B | 2.36 | 129.18 | 124.88 |
| 22 | C | 505 | CLA | CED-O2D-CGD | 2.36 | 121.42 | 115.97 |
| 24 | h | 101 | BCR | C28-C29-C30 | 2.37 | 122.99 | 114.58 |
| 22 | b | 602 | CLA | CMB-C2B-C3B | 2.37 | 129.19 | 124.88 |
| 22 | c | 507 | CLA | O2A-CGA-CBA | 2.37 | 118.77 | 111.92 |
| 22 | C | 507 | CLA | O2A-CGA-CBA | 2.37 | 118.77 | 111.92 |
| 22 | b | 608 | CLA | CMB-C2B-C3B | 2.37 | 129.20 | 124.88 |
| 22 | C | 513 | CLA | C4-C3-C5 | 2.37 | 119.38 | 115.29 |
| 22 | C | 508 | CLA | C1D-CHD-C4C | 2.38 | 125.73 | 122.48 |
| 22 | B | 603 | CLA | C1-O2A-CGA | 2.38 | 122.25 | 116.77 |
| 24 | K | 101 | BCR | C28-C27-C26 | 2.38 | 118.17 | 113.99 |
| 22 | C | 504 | CLA | CMC-C2C-C1C | 2.38 | 128.69 | 125.05 |
| 22 | B | 610 | CLA | CMB-C2B-C3B | 2.38 | 129.21 | 124.88 |
| 24 | b | 622 | BCR | C1-C6-C7 | 2.38 | 122.42 | 115.73 |
| 24 | B | 622 | BCR | C1-C6-C7 | 2.38 | 122.42 | 115.73 |
| 24 | k | 101 | BCR | C28-C27-C26 | 2.38 | 118.17 | 113.99 |
| 22 | b | 603 | CLA | C1-O2A-CGA | 2.38 | 122.25 | 116.77 |
| 24 | b | 622 | BCR | C40-C30-C25 | 2.38 | 114.17 | 110.31 |
| 24 | B | 622 | BCR | C40-C30-C25 | 2.38 | 114.17 | 110.31 |
| 22 | a | 607 | CLA | CAC-C3C-C4C | 2.39 | 128.11 | 124.82 |
| 24 | t | 101 | BCR | C31-C1-C6 | 2.39 | 114.18 | 110.31 |
| 22 | c | 506 | CLA | CAC-C3C-C4C | 2.39 | 128.12 | 124.82 |
| 23 | a | 606 | PHO | CED-O2D-CGD | 2.39 | 121.48 | 115.97 |
| 31 | d | 410 | DGD | O6D-C5D-C6D | 2.40 | 111.43 | 106.64 |
| 22 | b | 612 | CLA | CMB-C2B-C3B | 2.40 | 129.25 | 124.88 |
| 22 | B | 605 | CLA | O2A-CGA-CBA | 2.40 | 118.86 | 111.92 |
| 29 | A | 614 | LMG | O1-C1-C2 | 2.40 | 112.12 | 108.24 |
| 22 | C | 510 | CLA | O2A-CGA-CBA | 2.40 | 118.86 | 111.92 |
| 22 | c | 512 | CLA | CED-O2D-CGD | 2.40 | 121.50 | 115.97 |
| 23 | A | 606 | PHO | CED-O2D-CGD | 2.40 | 121.51 | 115.97 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 22 | a | 607 | CLA | C1-O2A-CGA | 2.41 | 122.31 | 116.77 |
| 22 | c | 507 | CLA | CMC-C2C-C1C | 2.41 | 128.74 | 125.05 |
| 22 | b | 605 | CLA | O2A-CGA-CBA | 2.41 | 118.88 | 111.92 |
| 22 | A | 607 | CLA | C1-O2A-CGA | 2.41 | 122.32 | 116.77 |
| 25 | A | 609 | SQD | O48-C23-C24 | 2.41 | 118.88 | 111.92 |
| 22 | C | 512 | CLA | CED-O2D-CGD | 2.41 | 121.52 | 115.97 |
| 22 | c | 510 | CLA | O2A-CGA-CBA | 2.41 | 118.88 | 111.92 |
| 25 | a | 609 | SQD | O48-C23-C24 | 2.41 | 118.89 | 111.92 |
| 22 | A | 607 | CLA | O2A-CGA-CBA | 2.43 | 118.93 | 111.92 |
| 29 | a | 614 | LMG | O1-C1-C2 | 2.43 | 112.16 | 108.24 |
| 22 | C | 507 | CLA | CMC-C2C-C1C | 2.43 | 128.77 | 125.05 |
| 22 | A | 607 | CLA | CAC-C3C-C4C | 2.43 | 128.17 | 124.82 |
| 22 | C | 506 | CLA | CAC-C3C-C4C | 2.43 | 128.17 | 124.82 |
| 22 | C | 502 | CLA | CMC-C2C-C1C | 2.43 | 128.77 | 125.05 |
| 22 | C | 509 | CLA | CAC-C3C-C4C | 2.43 | 128.17 | 124.82 |
| 24 | C | 514 | BCR | C3-C4-C5 | 2.43 | 118.26 | 113.99 |
| 24 | T | 102 | BCR | C31-C1-C6 | 2.43 | 114.25 | 110.31 |
| 31 | D | 410 | DGD | O6D-C5D-C6D | 2.43 | 111.50 | 106.64 |
| 23 | a | 606 | PHO | C4D-C3D-CAD | 2.43 | 109.81 | 105.39 |
| 24 | H | 101 | BCR | C30-C25-C24 | 2.43 | 122.57 | 115.73 |
| 22 | c | 512 | CLA | C1-O2A-CGA | 2.43 | 122.38 | 116.77 |
| 24 | h | 101 | BCR | C30-C25-C24 | 2.43 | 122.57 | 115.73 |
| 22 | d | 403 | CLA | C4-C3-C5 | 2.44 | 119.49 | 115.29 |
| 24 | T | 101 | BCR | C2-C3-C4 | 2.44 | 116.95 | 111.36 |
| 24 | c | 514 | BCR | C3-C4-C5 | 2.44 | 118.27 | 113.99 |
| 23 | A | 606 | PHO | C4D-C3D-CAD | 2.44 | 109.82 | 105.39 |
| 22 | a | 607 | CLA | O2A-CGA-CBA | 2.44 | 118.97 | 111.92 |
| 22 | c | 502 | CLA | CMC-C2C-C1C | 2.44 | 128.79 | 125.05 |
| 24 | b | 622 | BCR | C38-C26-C25 | 2.45 | 127.25 | 124.51 |
| 28 | A | 613 | PL9 | C10-C9-C11 | 2.45 | 119.52 | 115.29 |
| 24 | B | 618 | BCR | C2-C3-C4 | 2.45 | 116.99 | 111.36 |
| 22 | B | 611 | CLA | C4-C3-C5 | 2.46 | 119.52 | 115.29 |
| 32 | D | 407 | LHG | O8-C23-C24 | 2.46 | 119.03 | 111.92 |
| 32 | d | 407 | LHG | O8-C23-C24 | 2.46 | 119.03 | 111.92 |
| 22 | b | 611 | CLA | C4-C3-C5 | 2.46 | 119.54 | 115.29 |
| 22 | D | 403 | CLA | C4-C3-C5 | 2.46 | 119.54 | 115.29 |
| 22 | c | 509 | CLA | CAC-C3C-C4C | 2.47 | 128.22 | 124.82 |
| 28 | a | 613 | PL9 | C10-C9-C11 | 2.47 | 119.55 | 115.29 |
| 22 | c | 503 | CLA | CMC-C2C-C1C | 2.47 | 128.84 | 125.05 |
| 22 | D | 403 | CLA | CAC-C3C-C4C | 2.47 | 128.23 | 124.82 |
| 24 | H | 101 | BCR | C39-C30-C25 | 2.48 | 114.33 | 110.31 |
| 22 | A | 607 | CLA | CMB-C2B-C3B | 2.48 | 129.40 | 124.88 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 22 | b | 609 | CLA | CAC-C3C-C4C | 2.48 | 128.24 | 124.82 |
| 22 | B | 614 | CLA | C4-C3-C5 | 2.48 | 119.57 | 115.29 |
| 22 | C | 506 | CLA | CMB-C2B-C3B | 2.48 | 129.40 | 124.88 |
| 22 | c | 506 | CLA | CMB-C2B-C3B | 2.48 | 129.40 | 124.88 |
| 24 | h | 101 | BCR | C39-C30-C25 | 2.49 | 114.34 | 110.31 |
| 29 | A | 614 | LMG | O8-C28-C29 | 2.49 | 119.11 | 111.92 |
| 22 | C | 512 | CLA | C1-O2A-CGA | 2.49 | 122.50 | 116.77 |
| 22 | C | 503 | CLA | CMC-C2C-C1C | 2.50 | 128.88 | 125.05 |
| 22 | d | 401 | CLA | C4A-NA-C1A | 2.50 | 109.54 | 106.32 |
| 22 | B | 617 | CLA | C1-O2A-CGA | 2.50 | 122.52 | 116.77 |
| 22 | A | 607 | CLA | CMC-C2C-C1C | 2.50 | 128.88 | 125.05 |
| 22 | a | 607 | CLA | CMB-C2B-C3B | 2.50 | 129.43 | 124.88 |
| 24 | B | 622 | BCR | C38-C26-C25 | 2.50 | 127.31 | 124.51 |
| 22 | B | 613 | CLA | CMC-C2C-C1C | 2.50 | 128.88 | 125.05 |
| 29 | a | 614 | LMG | O8-C28-C29 | 2.50 | 119.15 | 111.92 |
| 22 | b | 617 | CLA | C1-O2A-CGA | 2.50 | 122.53 | 116.77 |
| 24 | b | 622 | BCR | C3-C4-C5 | 2.50 | 118.38 | 113.99 |
| 24 | B | 622 | BCR | C3-C4-C5 | 2.50 | 118.38 | 113.99 |
| 22 | b | 614 | CLA | C4-C3-C5 | 2.50 | 119.61 | 115.29 |
| 22 | a | 607 | CLA | CMC-C2C-C1C | 2.50 | 128.89 | 125.05 |
| 22 | B | 614 | CLA | O2A-CGA-CBA | 2.50 | 119.16 | 111.92 |
| 22 | d | 403 | CLA | CAC-C3C-C4C | 2.51 | 128.28 | 124.82 |
| 22 | d | 401 | CLA | CMC-C2C-C1C | 2.51 | 128.89 | 125.05 |
| 22 | b | 614 | CLA | O2A-CGA-CBA | 2.51 | 119.17 | 111.92 |
| 22 | A | 603 | CLA | C4A-NA-C1A | 2.51 | 109.56 | 106.32 |
| 23 | A | 605 | PHO | C4D-C3D-CAD | 2.51 | 109.95 | 105.39 |
| 22 | B | 609 | CLA | CAC-C3C-C4C | 2.52 | 128.29 | 124.82 |
| 24 | d | 404 | BCR | C30-C25-C24 | 2.52 | 122.80 | 115.73 |
| 22 | D | 401 | CLA | CMC-C2C-C1C | 2.52 | 128.91 | 125.05 |
| 22 | a | 607 | CLA | CED-O2D-CGD | 2.52 | 121.77 | 115.97 |
| 24 | D | 404 | BCR | C30-C25-C24 | 2.52 | 122.80 | 115.73 |
| 32 | d | 405 | LHG | O7-C7-C8 | 2.52 | 116.87 | 111.55 |
| 22 | A | 607 | CLA | CED-O2D-CGD | 2.53 | 121.79 | 115.97 |
| 22 | C | 501 | CLA | CAC-C3C-C4C | 2.53 | 128.31 | 124.82 |
| 22 | b | 612 | CLA | CAC-C3C-C4C | 2.53 | 128.31 | 124.82 |
| 24 | T | 101 | BCR | C4-C5-C6 | 2.54 | 126.46 | 122.74 |
| 22 | B | 616 | CLA | C4-C3-C5 | 2.54 | 119.66 | 115.29 |
| 31 | d | 410 | DGD | O5D-C1E-C2E | 2.54 | 112.34 | 108.24 |
| 22 | b | 616 | CLA | C4-C3-C5 | 2.54 | 119.67 | 115.29 |
| 22 | c | 501 | CLA | CMC-C2C-C1C | 2.54 | 128.94 | 125.05 |
| 25 | B | 601 | SQD | O8-S-C6 | 2.54 | 109.78 | 105.74 |
| 24 | a | 608 | BCR | C29-C30-C25 | 2.54 | 114.45 | 110.48 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 22 | C | 502 | CLA | C4-C3-C5 | 2.54 | 119.67 | 115.29 |
| 22 | c | 501 | CLA | CAC-C3C-C4C | 2.54 | 128.33 | 124.82 |
| 24 | B | 618 | BCR | C4-C5-C6 | 2.54 | 126.47 | 122.74 |
| 24 | k | 102 | BCR | C33-C5-C6 | 2.55 | 127.36 | 124.51 |
| 22 | C | 511 | CLA | C4-C3-C5 | 2.55 | 119.68 | 115.29 |
| 32 | D | 405 | LHG | O7-C7-C8 | 2.55 | 116.92 | 111.55 |
| 22 | D | 403 | CLA | CED-O2D-CGD | 2.55 | 121.84 | 115.97 |
| 22 | D | 403 | CLA | CMB-C2B-C3B | 2.55 | 129.52 | 124.88 |
| 22 | d | 403 | CLA | CMB-C2B-C3B | 2.55 | 129.52 | 124.88 |
| 22 | a | 603 | CLA | C4A-NA-C1A | 2.55 | 109.61 | 106.32 |
| 22 | c | 502 | CLA | C4-C3-C5 | 2.55 | 119.68 | 115.29 |
| 23 | a | 605 | PHO | C4D-C3D-CAD | 2.55 | 110.02 | 105.39 |
| 22 | b | 614 | CLA | CMB-C2B-C3B | 2.55 | 129.52 | 124.88 |
| 25 | b | 601 | SQD | O8-S-C6 | 2.55 | 109.81 | 105.74 |
| 22 | D | 401 | CLA | C4A-NA-C1A | 2.55 | 109.61 | 106.32 |
| 22 | b | 613 | CLA | CMC-C2C-C1C | 2.55 | 128.96 | 125.05 |
| 28 | D | 408 | PL9 | C7-C3-C4 | 2.56 | 118.95 | 116.88 |
| 24 | A | 608 | BCR | C29-C30-C25 | 2.56 | 114.48 | 110.48 |
| 22 | c | 511 | CLA | C4-C3-C5 | 2.56 | 119.70 | 115.29 |
| 22 | B | 612 | CLA | CAC-C3C-C4C | 2.56 | 128.35 | 124.82 |
| 22 | d | 403 | CLA | CED-O2D-CGD | 2.56 | 121.87 | 115.97 |
| 31 | D | 410 | DGD | O5D-C1E-C2E | 2.56 | 112.38 | 108.24 |
| 22 | B | 615 | CLA | C1-O2A-CGA | 2.56 | 122.67 | 116.77 |
| 22 | c | 513 | CLA | O2A-CGA-CBA | 2.56 | 119.33 | 111.92 |
| 24 | c | 514 | BCR | C39-C30-C25 | 2.57 | 114.47 | 110.31 |
| 28 | d | 408 | PL9 | C7-C3-C4 | 2.57 | 118.96 | 116.88 |
| 22 | B | 614 | CLA | CMB-C2B-C3B | 2.57 | 129.55 | 124.88 |
| 22 | C | 513 | CLA | O2A-CGA-CBA | 2.57 | 119.34 | 111.92 |
| 22 | b | 615 | CLA | C1-O2A-CGA | 2.57 | 122.68 | 116.77 |
| 22 | B | 607 | CLA | O2A-CGA-CBA | 2.57 | 119.34 | 111.92 |
| 22 | b | 607 | CLA | O2A-CGA-CBA | 2.57 | 119.34 | 111.92 |
| 22 | D | 401 | CLA | CAC-C3C-C4C | 2.57 | 128.36 | 124.82 |
| 24 | c | 515 | BCR | C23-C24-C25 | 2.57 | 134.45 | 127.25 |
| 24 | K | 102 | BCR | C33-C5-C6 | 2.57 | 127.39 | 124.51 |
| 24 | K | 102 | BCR | C29-C30-C25 | 2.58 | 114.51 | 110.48 |
| 22 | C | 501 | CLA | CMC-C2C-C1C | 2.58 | 129.00 | 125.05 |
| 22 | c | 503 | CLA | C4-C3-C5 | 2.58 | 119.74 | 115.29 |
| 22 | a | 603 | CLA | CAC-C3C-C4C | 2.58 | 128.38 | 124.82 |
| 24 | C | 514 | BCR | C39-C30-C25 | 2.59 | 114.50 | 110.31 |
| 22 | C | 503 | CLA | C4-C3-C5 | 2.59 | 119.76 | 115.29 |
| 24 | C | 515 | BCR | C23-C24-C25 | 2.59 | 134.51 | 127.25 |
| 22 | D | 401 | CLA | C4-C3-C5 | 2.59 | 119.76 | 115.29 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 24 | b | 622 | BCR | C23-C24-C25 | 2.60 | 134.53 | 127.25 |
| 22 | c | 512 | CLA | O2A-CGA-CBA | 2.60 | 119.45 | 111.92 |
| 24 | B | 622 | BCR | C23-C24-C25 | 2.60 | 134.54 | 127.25 |
| 24 | k | 102 | BCR | C29-C30-C25 | 2.62 | 114.57 | 110.48 |
| 22 | d | 402 | CLA | CAC-C3C-C4C | 2.62 | 128.43 | 124.82 |
| 22 | D | 402 | CLA | CAC-C3C-C4C | 2.62 | 128.43 | 124.82 |
| 22 | d | 401 | CLA | CAC-C3C-C4C | 2.62 | 128.43 | 124.82 |
| 24 | d | 404 | BCR | C2-C1-C6 | 2.62 | 114.58 | 110.48 |
| 22 | A | 603 | CLA | CAC-C3C-C4C | 2.62 | 128.44 | 124.82 |
| 22 | C | 513 | CLA | CMC-C2C-C1C | 2.62 | 129.07 | 125.05 |
| 22 | C | 510 | CLA | CMC-C2C-C1C | 2.62 | 129.07 | 125.05 |
| 22 | d | 401 | CLA | C4-C3-C5 | 2.63 | 119.82 | 115.29 |
| 22 | b | 614 | CLA | O2D-CGD-CBD | 2.63 | 115.94 | 111.28 |
| 22 | c | 513 | CLA | CMC-C2C-C1C | 2.63 | 129.08 | 125.05 |
| 22 | C | 512 | CLA | O2A-CGA-CBA | 2.63 | 119.53 | 111.92 |
| 22 | B | 614 | CLA | O2D-CGD-CBD | 2.63 | 115.95 | 111.28 |
| 28 | A | 613 | PL9 | C40-C39-C41 | 2.64 | 119.84 | 115.29 |
| 22 | C | 509 | CLA | O2A-CGA-CBA | 2.65 | 119.58 | 111.92 |
| 25 | b | 621 | SQD | C4-C3-C2 | 2.65 | 115.48 | 110.83 |
| 22 | c | 509 | CLA | O2A-CGA-CBA | 2.65 | 119.59 | 111.92 |
| 22 | c | 510 | CLA | CMC-C2C-C1C | 2.66 | 129.13 | 125.05 |
| 24 | D | 404 | BCR | C2-C1-C6 | 2.66 | 114.64 | 110.48 |
| 28 | a | 613 | PL9 | C40-C39-C41 | 2.66 | 119.88 | 115.29 |
| 22 | c | 508 | CLA | C4-C3-C5 | 2.67 | 119.89 | 115.29 |
| 25 | l | 102 | SQD | C4-C3-C2 | 2.67 | 115.51 | 110.83 |
| 22 | B | 602 | CLA | C3B-C4B-NB | 2.67 | 112.66 | 109.21 |
| 24 | B | 619 | BCR | C1-C6-C7 | 2.67 | 123.24 | 115.73 |
| 25 | l | 101 | SQD | O8-S-C6 | 2.67 | 110.00 | 105.74 |
| 25 | b | 621 | SQD | O9-S-C6 | 2.68 | 110.12 | 106.94 |
| 22 | B | 605 | CLA | C4-C3-C5 | 2.68 | 119.91 | 115.29 |
| 29 | C | 520 | LMG | O8-C28-C29 | 2.68 | 119.66 | 111.92 |
| 29 | c | 520 | LMG | O8-C28-C29 | 2.68 | 119.67 | 111.92 |
| 25 | L | 101 | SQD | O8-S-C6 | 2.68 | 110.01 | 105.74 |
| 22 | C | 508 | CLA | C4-C3-C5 | 2.68 | 119.92 | 115.29 |
| 24 | B | 622 | BCR | C29-C30-C25 | 2.69 | 114.68 | 110.48 |
| 24 | b | 618 | BCR | C1-C6-C7 | 2.69 | 123.28 | 115.73 |
| 25 | l | 102 | SQD | O9-S-C6 | 2.69 | 110.13 | 106.94 |
| 28 | A | 613 | PL9 | C35-C34-C36 | 2.69 | 119.92 | 115.29 |
| 22 | B | 613 | CLA | CED-O2D-CGD | 2.69 | 122.17 | 115.97 |
| 22 | C | 505 | CLA | CMB-C2B-C3B | 2.69 | 129.79 | 124.88 |
| 22 | c | 505 | CLA | CMB-C2B-C3B | 2.70 | 129.80 | 124.88 |
| 22 | c | 506 | CLA | C3B-C4B-NB | 2.70 | 112.70 | 109.21 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 24 | b | 622 | BCR | C29-C30-C25 | 2.70 | 114.70 | 110.48 |
| 22 | b | 602 | CLA | C3B-C4B-NB | 2.70 | 112.70 | 109.21 |
| 28 | a | 613 | PL9 | C35-C34-C36 | 2.71 | 119.95 | 115.29 |
| 22 | b | 613 | CLA | CED-O2D-CGD | 2.71 | 122.21 | 115.97 |
| 22 | C | 506 | CLA | C3B-C4B-NB | 2.71 | 112.72 | 109.21 |
| 22 | C | 513 | CLA | C3B-C4B-NB | 2.71 | 112.72 | 109.21 |
| 22 | b | 605 | CLA | C4-C3-C5 | 2.71 | 119.97 | 115.29 |
| 22 | C | 501 | CLA | C1-O2A-CGA | 2.72 | 123.05 | 116.77 |
| 22 | b | 606 | CLA | C3B-C4B-NB | 2.73 | 112.74 | 109.21 |
| 22 | c | 513 | CLA | C3B-C4B-NB | 2.73 | 112.74 | 109.21 |
| 22 | C | 508 | CLA | CMB-C2B-C3B | 2.73 | 129.86 | 124.88 |
| 22 | d | 402 | CLA | CMB-C2B-C3B | 2.74 | 129.86 | 124.88 |
| 22 | c | 501 | CLA | C1-O2A-CGA | 2.74 | 123.08 | 116.77 |
| 22 | c | 508 | CLA | CMB-C2B-C3B | 2.75 | 129.88 | 124.88 |
| 22 | c | 503 | CLA | C3B-C4B-NB | 2.76 | 112.78 | 109.21 |
| 22 | D | 402 | CLA | CMB-C2B-C3B | 2.77 | 129.91 | 124.88 |
| 22 | B | 608 | CLA | C4-C3-C5 | 2.77 | 120.06 | 115.29 |
| 22 | c | 510 | CLA | CMB-C2B-C3B | 2.77 | 129.93 | 124.88 |
| 24 | T | 101 | BCR | C39-C30-C25 | 2.78 | 114.81 | 110.31 |
| 22 | d | 402 | CLA | C4-C3-C5 | 2.78 | 120.08 | 115.29 |
| 22 | b | 608 | CLA | C4-C3-C5 | 2.78 | 120.08 | 115.29 |
| 22 | B | 606 | CLA | C3B-C4B-NB | 2.78 | 112.80 | 109.21 |
| 22 | C | 510 | CLA | CMB-C2B-C3B | 2.78 | 129.94 | 124.88 |
| 22 | c | 505 | CLA | CAC-C3C-C4C | 2.78 | 128.66 | 124.82 |
| 22 | C | 505 | CLA | CAC-C3C-C4C | 2.78 | 128.66 | 124.82 |
| 28 | a | 613 | PL9 | C15-C14-C16 | 2.79 | 120.09 | 115.29 |
| 22 | c | 504 | CLA | CAC-C3C-C4C | 2.79 | 128.66 | 124.82 |
| 31 | C | 518 | DGD | O1G-C1A-C2A | 2.79 | 119.98 | 111.92 |
| 22 | c | 512 | CLA | C3B-C4B-NB | 2.79 | 112.81 | 109.21 |
| 28 | A | 613 | PL9 | C25-C24-C26 | 2.79 | 120.10 | 115.29 |
| 31 | c | 518 | DGD | O1G-C1A-C2A | 2.79 | 119.99 | 111.92 |
| 22 | C | 503 | CLA | C3B-C4B-NB | 2.79 | 112.82 | 109.21 |
| 28 | A | 613 | PL9 | C15-C14-C16 | 2.79 | 120.11 | 115.29 |
| 22 | c | 507 | CLA | CMB-C2B-C3B | 2.79 | 129.97 | 124.88 |
| 22 | D | 402 | CLA | C4-C3-C5 | 2.80 | 120.11 | 115.29 |
| 31 | D | 410 | DGD | O1G-C1A-C2A | 2.80 | 120.01 | 111.92 |
| 22 | C | 504 | CLA | CAC-C3C-C4C | 2.80 | 128.68 | 124.82 |
| 31 | d | 410 | DGD | O1G-C1A-C2A | 2.80 | 120.01 | 111.92 |
| 22 | b | 602 | CLA | CMC-C2C-C1C | 2.80 | 129.34 | 125.05 |
| 22 | C | 512 | CLA | C3B-C4B-NB | 2.81 | 112.84 | 109.21 |
| 22 | C | 507 | CLA | CMB-C2B-C3B | 2.81 | 130.00 | 124.88 |
| 22 | c | 504 | CLA | C1-O2A-CGA | 2.81 | 123.25 | 116.77 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 22 | B | 602 | CLA | CMC-C2C-C1C | 2.82 | 129.37 | 125.05 |
| 22 | C | 504 | CLA | C1-O2A-CGA | 2.82 | 123.26 | 116.77 |
| 24 | T | 102 | BCR | C39-C30-C25 | 2.82 | 114.87 | 110.31 |
| 22 | b | 607 | CLA | C4-C3-C5 | 2.82 | 120.14 | 115.29 |
| 22 | B | 608 | CLA | O2D-CGD-CBD | 2.82 | 116.28 | 111.28 |
| 28 | a | 613 | PL9 | C25-C24-C26 | 2.82 | 120.15 | 115.29 |
| 28 | A | 613 | PL9 | C53-C6-C1 | 2.82 | 120.83 | 114.87 |
| 22 | B | 607 | CLA | C4-C3-C5 | 2.83 | 120.17 | 115.29 |
| 22 | b | 608 | CLA | O2D-CGD-CBD | 2.83 | 116.30 | 111.28 |
| 28 | a | 613 | PL9 | C53-C6-C1 | 2.83 | 120.85 | 114.87 |
| 24 | B | 618 | BCR | C39-C30-C25 | 2.84 | 114.91 | 110.31 |
| 22 | b | 617 | CLA | CMB-C2B-C3B | 2.84 | 130.06 | 124.88 |
| 22 | c | 512 | CLA | CMB-C2B-C3B | 2.84 | 130.06 | 124.88 |
| 22 | b | 617 | CLA | O2A-CGA-CBA | 2.85 | 120.15 | 111.92 |
| 22 | B | 617 | CLA | CMB-C2B-C3B | 2.85 | 130.07 | 124.88 |
| 28 | a | 613 | PL9 | C30-C29-C31 | 2.85 | 120.20 | 115.29 |
| 24 | t | 101 | BCR | C39-C30-C25 | 2.85 | 114.93 | 110.31 |
| 22 | C | 507 | CLA | C3B-C4B-NB | 2.86 | 112.91 | 109.21 |
| 22 | C | 512 | CLA | CMB-C2B-C3B | 2.86 | 130.09 | 124.88 |
| 22 | B | 615 | CLA | CAC-C3C-C4C | 2.86 | 128.77 | 124.82 |
| 22 | b | 615 | CLA | CAC-C3C-C4C | 2.86 | 128.77 | 124.82 |
| 24 | a | 608 | BCR | C8-C7-C6 | 2.86 | 135.27 | 127.25 |
| 22 | c | 505 | CLA | C3B-C4B-NB | 2.87 | 112.92 | 109.21 |
| 23 | A | 605 | PHO | CAC-C3C-C4C | 2.87 | 128.28 | 125.19 |
| 22 | B | 617 | CLA | O2A-CGA-CBA | 2.88 | 120.24 | 111.92 |
| 22 | b | 611 | CLA | O2A-CGA-CBA | 2.88 | 120.24 | 111.92 |
| 22 | c | 507 | CLA | C3B-C4B-NB | 2.88 | 112.93 | 109.21 |
| 28 | A | 613 | PL9 | C30-C29-C31 | 2.88 | 120.25 | 115.29 |
| 22 | B | 611 | CLA | O2A-CGA-CBA | 2.88 | 120.25 | 111.92 |
| 24 | A | 608 | BCR | C8-C7-C6 | 2.89 | 135.34 | 127.25 |
| 22 | C | 505 | CLA | C3B-C4B-NB | 2.89 | 112.95 | 109.21 |
| 23 | a | 605 | PHO | CAC-C3C-C4C | 2.89 | 128.30 | 125.19 |
| 28 | D | 408 | PL9 | C53-C6-C1 | 2.90 | 120.98 | 114.87 |
| 22 | b | 609 | CLA | O2A-CGA-CBA | 2.90 | 120.30 | 111.92 |
| 24 | h | 101 | BCR | C4-C5-C6 | 2.90 | 127.00 | 122.74 |
| 22 | B | 609 | CLA | O2A-CGA-CBA | 2.91 | 120.33 | 111.92 |
| 22 | B | 603 | CLA | C4A-NA-C1A | 2.91 | 110.08 | 106.32 |
| 28 | d | 408 | PL9 | C53-C6-C1 | 2.91 | 121.02 | 114.87 |
| 24 | a | 608 | BCR | C31-C1-C6 | 2.92 | 115.04 | 110.31 |
| 22 | b | 604 | CLA | CMB-C2B-C3B | 2.92 | 130.19 | 124.88 |
| 28 | A | 613 | PL9 | C7-C3-C4 | 2.92 | 119.25 | 116.88 |
| 24 | k | 102 | BCR | C40-C30-C25 | 2.92 | 115.05 | 110.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 22 | B | 604 | CLA | C4-C3-C5 | 2.93 | 120.34 | 115.29 |
| 22 | B | 613 | CLA | C3B-C4B-NB | 2.93 | 113.00 | 109.21 |
| 24 | K | 102 | BCR | C40-C30-C25 | 2.93 | 115.06 | 110.31 |
| 24 | A | 608 | BCR | C31-C1-C6 | 2.93 | 115.06 | 110.31 |
| 24 | H | 101 | BCR | C4-C5-C6 | 2.93 | 127.04 | 122.74 |
| 29 | b | 619 | LMG | O8-C28-C29 | 2.93 | 120.40 | 111.92 |
| 22 | c | 504 | CLA | C4-C3-C5 | 2.94 | 120.35 | 115.29 |
| 22 | B | 604 | CLA | CMB-C2B-C3B | 2.94 | 130.23 | 124.88 |
| 22 | b | 613 | CLA | C3B-C4B-NB | 2.94 | 113.01 | 109.21 |
| 25 | b | 621 | SQD | O48-C23-C24 | 2.94 | 120.42 | 111.92 |
| 22 | C | 504 | CLA | C4-C3-C5 | 2.95 | 120.37 | 115.29 |
| 22 | b | 604 | CLA | C4-C3-C5 | 2.95 | 120.37 | 115.29 |
| 22 | c | 505 | CLA | CMC-C2C-C1C | 2.95 | 129.57 | 125.05 |
| 25 | L | 101 | SQD | O48-C23-C24 | 2.95 | 120.46 | 111.92 |
| 22 | C | 505 | CLA | CMC-C2C-C1C | 2.95 | 129.58 | 125.05 |
| 25 | l | 102 | SQD | O48-C23-C24 | 2.95 | 120.46 | 111.92 |
| 29 | B | 620 | LMG | O8-C28-C29 | 2.96 | 120.47 | 111.92 |
| 25 | l | 101 | SQD | O48-C23-C24 | 2.96 | 120.47 | 111.92 |
| 22 | b | 603 | CLA | C4A-NA-C1A | 2.96 | 110.14 | 106.32 |
| 31 | h | 102 | DGD | O2G-C1B-C2B | 2.98 | 117.82 | 111.55 |
| 31 | H | 102 | DGD | O2G-C1B-C2B | 2.98 | 117.84 | 111.55 |
| 22 | a | 604 | CLA | C4A-NA-C1A | 2.98 | 110.17 | 106.32 |
| 22 | C | 513 | CLA | CMB-C2B-C3B | 2.99 | 130.33 | 124.88 |
| 22 | b | 612 | CLA | CMC-C2C-C1C | 2.99 | 129.64 | 125.05 |
| 22 | c | 507 | CLA | C4-C3-C5 | 2.99 | 120.45 | 115.29 |
| 28 | a | 613 | PL9 | C7-C3-C4 | 3.00 | 119.31 | 116.88 |
| 22 | A | 604 | CLA | C4A-NA-C1A | 3.00 | 110.19 | 106.32 |
| 24 | A | 608 | BCR | C33-C5-C6 | 3.00 | 127.86 | 124.51 |
| 22 | C | 507 | CLA | C4-C3-C5 | 3.00 | 120.47 | 115.29 |
| 24 | k | 102 | BCR | C27-C26-C25 | 3.01 | 127.15 | 122.74 |
| 22 | B | 603 | CLA | C3B-C4B-NB | 3.01 | 113.10 | 109.21 |
| 24 | K | 102 | BCR | C27-C26-C25 | 3.01 | 127.16 | 122.74 |
| 22 | C | 506 | CLA | C4-C3-C5 | 3.01 | 120.48 | 115.29 |
| 22 | b | 604 | CLA | C4A-NA-C1A | 3.01 | 110.21 | 106.32 |
| 22 | B | 612 | CLA | CMC-C2C-C1C | 3.02 | 129.67 | 125.05 |
| 22 | c | 506 | CLA | C4-C3-C5 | 3.02 | 120.49 | 115.29 |
| 24 | t | 101 | BCR | C30-C25-C24 | 3.02 | 124.22 | 115.73 |
| 24 | T | 102 | BCR | C30-C25-C24 | 3.02 | 124.22 | 115.73 |
| 25 | B | 601 | SQD | O6-C1-C2 | 3.02 | 113.13 | 108.24 |
| 22 | c | 501 | CLA | C3B-C4B-NB | 3.02 | 113.12 | 109.21 |
| 22 | c | 513 | CLA | CMB-C2B-C3B | 3.02 | 130.39 | 124.88 |
| 22 | a | 604 | CLA | C4-C3-C5 | 3.03 | 120.51 | 115.29 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 25 | b | 601 | SQD | O6-C1-C2 | 3.03 | 113.14 | 108.24 |
| 22 | a | 604 | CLA | CMC-C2C-C1C | 3.03 | 129.69 | 125.05 |
| 22 | A | 604 | CLA | C4-C3-C5 | 3.03 | 120.52 | 115.29 |
| 24 | a | 608 | BCR | C33-C5-C6 | 3.04 | 127.91 | 124.51 |
| 22 | B | 604 | CLA | C4A-NA-C1A | 3.04 | 110.24 | 106.32 |
| 22 | C | 501 | CLA | C3B-C4B-NB | 3.04 | 113.14 | 109.21 |
| 22 | b | 603 | CLA | C3B-C4B-NB | 3.05 | 113.15 | 109.21 |
| 22 | B | 603 | CLA | C4-C3-C5 | 3.05 | 120.56 | 115.29 |
| 22 | A | 604 | CLA | CMC-C2C-C1C | 3.05 | 129.73 | 125.05 |
| 22 | b | 608 | CLA | C4A-NA-C1A | 3.06 | 110.27 | 106.32 |
| 22 | b | 603 | CLA | CMB-C2B-C3B | 3.06 | 130.45 | 124.88 |
| 22 | B | 603 | CLA | CMB-C2B-C3B | 3.06 | 130.45 | 124.88 |
| 22 | C | 502 | CLA | C4A-NA-C1A | 3.06 | 110.27 | 106.32 |
| 22 | b | 610 | CLA | CAC-C3C-C4C | 3.07 | 129.05 | 124.82 |
| 22 | a | 604 | CLA | CAC-C3C-C4C | 3.07 | 129.05 | 124.82 |
| 24 | D | 404 | BCR | C3-C2-C1 | 3.07 | 125.48 | 114.58 |
| 22 | a | 603 | CLA | O2D-CGD-CBD | 3.07 | 116.72 | 111.28 |
| 22 | C | 504 | CLA | CMB-C2B-C3B | 3.07 | 130.47 | 124.88 |
| 22 | c | 504 | CLA | CMB-C2B-C3B | 3.08 | 130.48 | 124.88 |
| 22 | b | 603 | CLA | C4-C3-C5 | 3.08 | 120.59 | 115.29 |
| 22 | A | 603 | CLA | O2D-CGD-CBD | 3.08 | 116.74 | 111.28 |
| 22 | c | 502 | CLA | C4A-NA-C1A | 3.08 | 110.29 | 106.32 |
| 23 | A | 606 | PHO | C4-C3-C5 | 3.08 | 120.60 | 115.29 |
| 24 | d | 404 | BCR | C3-C2-C1 | 3.08 | 125.54 | 114.58 |
| 22 | B | 610 | CLA | CAC-C3C-C4C | 3.08 | 129.07 | 124.82 |
| 22 | B | 608 | CLA | C4A-NA-C1A | 3.09 | 110.31 | 106.32 |
| 22 | B | 615 | CLA | C4A-NA-C1A | 3.10 | 110.32 | 106.32 |
| 22 | A | 604 | CLA | CAC-C3C-C4C | 3.11 | 129.10 | 124.82 |
| 22 | B | 608 | CLA | CED-O2D-CGD | 3.11 | 123.14 | 115.97 |
| 25 | d | 411 | SQD | O9-S-C6 | 3.11 | 110.63 | 106.94 |
| 25 | D | 411 | SQD | O9-S-C6 | 3.11 | 110.64 | 106.94 |
| 22 | b | 615 | CLA | C4A-NA-C1A | 3.11 | 110.33 | 106.32 |
| 22 | b | 608 | CLA | CED-O2D-CGD | 3.11 | 123.14 | 115.97 |
| 22 | b | 616 | CLA | O2D-CGD-CBD | 3.11 | 116.80 | 111.28 |
| 22 | b | 606 | CLA | C4A-NA-C1A | 3.11 | 110.34 | 106.32 |
| 22 | a | 607 | CLA | C4A-NA-C1A | 3.11 | 110.34 | 106.32 |
| 22 | A | 607 | CLA | C4A-NA-C1A | 3.12 | 110.34 | 106.32 |
| 23 | a | 606 | PHO | C4-C3-C5 | 3.12 | 120.66 | 115.29 |
| 31 | H | 102 | DGD | O1G-C1A-C2A | 3.12 | 120.95 | 111.92 |
| 31 | h | 102 | DGD | O1G-C1A-C2A | 3.13 | 120.97 | 111.92 |
| 22 | B | 617 | CLA | CAC-C3C-C4C | 3.14 | 129.15 | 124.82 |
| 22 | B | 606 | CLA | C4A-NA-C1A | 3.14 | 110.37 | 106.32 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 22 | C | 502 | CLA | CAC-C3C-C4C | 3.14 | 129.16 | 124.82 |
| 22 | B | 616 | CLA | O2D-CGD-CBD | 3.14 | 116.86 | 111.28 |
| 22 | b | 617 | CLA | CAC-C3C-C4C | 3.15 | 129.16 | 124.82 |
| 22 | b | 613 | CLA | C4-C3-C5 | 3.15 | 120.72 | 115.29 |
| 22 | c | 502 | CLA | CAC-C3C-C4C | 3.15 | 129.17 | 124.82 |
| 24 | a | 608 | BCR | C40-C30-C25 | 3.15 | 115.42 | 110.31 |
| 32 | l | 103 | LHG | O7-C7-C8 | 3.16 | 118.20 | 111.55 |
| 32 | L | 102 | LHG | O7-C7-C8 | 3.16 | 118.21 | 111.55 |
| 22 | B | 607 | CLA | C3B-C4B-NB | 3.16 | 113.30 | 109.21 |
| 29 | C | 519 | LMG | O8-C28-C29 | 3.16 | 121.07 | 111.92 |
| 24 | A | 608 | BCR | C40-C30-C25 | 3.16 | 115.44 | 110.31 |
| 25 | d | 411 | SQD | O7-S-C6 | 3.17 | 110.70 | 106.94 |
| 29 | c | 519 | LMG | O8-C28-C29 | 3.17 | 121.09 | 111.92 |
| 25 | D | 411 | SQD | O7-S-C6 | 3.18 | 110.72 | 106.94 |
| 22 | B | 613 | CLA | C4-C3-C5 | 3.18 | 120.77 | 115.29 |
| 22 | b | 607 | CLA | C3B-C4B-NB | 3.18 | 113.32 | 109.21 |
| 23 | A | 606 | PHO | C2C-C1C-NC | 3.18 | 114.61 | 109.79 |
| 24 | b | 618 | BCR | C38-C26-C25 | 3.18 | 128.07 | 124.51 |
| 25 | b | 601 | SQD | O48-C23-C24 | 3.18 | 121.12 | 111.92 |
| 24 | B | 619 | BCR | C38-C26-C25 | 3.19 | 128.08 | 124.51 |
| 25 | D | 411 | SQD | O48-C23-C24 | 3.19 | 121.14 | 111.92 |
| 25 | B | 601 | SQD | O48-C23-C24 | 3.19 | 121.15 | 111.92 |
| 23 | a | 606 | PHO | C2C-C1C-NC | 3.19 | 114.63 | 109.79 |
| 24 | B | 618 | BCR | C32-C1-C6 | 3.20 | 115.50 | 110.31 |
| 22 | B | 613 | CLA | CMB-C2B-C3B | 3.20 | 130.71 | 124.88 |
| 25 | d | 411 | SQD | O48-C23-C24 | 3.20 | 121.18 | 111.92 |
| 22 | c | 512 | CLA | C4-C3-C5 | 3.21 | 120.82 | 115.29 |
| 22 | D | 401 | CLA | O2D-CGD-CBD | 3.21 | 116.98 | 111.28 |
| 22 | d | 401 | CLA | O2D-CGD-CBD | 3.21 | 116.98 | 111.28 |
| 22 | b | 613 | CLA | CMB-C2B-C3B | 3.21 | 130.73 | 124.88 |
| 32 | d | 409 | LHG | O7-C7-C8 | 3.21 | 118.32 | 111.55 |
| 22 | D | 403 | CLA | O2D-CGD-CBD | 3.22 | 116.99 | 111.28 |
| 24 | a | 608 | BCR | C30-C25-C24 | 3.22 | 124.78 | 115.73 |
| 24 | T | 101 | BCR | C32-C1-C6 | 3.22 | 115.53 | 110.31 |
| 32 | e | 101 | LHG | O8-C23-C24 | 3.22 | 121.23 | 111.92 |
| 22 | b | 602 | CLA | O2A-CGA-CBA | 3.22 | 121.23 | 111.92 |
| 22 | C | 504 | CLA | C3C-C4C-NC | 3.22 | 114.42 | 110.43 |
| 22 | C | 512 | CLA | C4-C3-C5 | 3.23 | 120.86 | 115.29 |
| 22 | c | 502 | CLA | C3B-C4B-NB | 3.23 | 113.38 | 109.21 |
| 22 | c | 504 | CLA | C3C-C4C-NC | 3.23 | 114.42 | 110.43 |
| 22 | b | 609 | CLA | CMB-C2B-C3B | 3.23 | 130.76 | 124.88 |
| 22 | B | 609 | CLA | CMB-C2B-C3B | 3.23 | 130.76 | 124.88 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 22 | B | 602 | CLA | O2A-CGA-CBA | 3.23 | 121.27 | 111.92 |
| 22 | C | 502 | CLA | C3B-C4B-NB | 3.24 | 113.39 | 109.21 |
| 22 | B | 604 | CLA | CMC-C2C-C1C | 3.24 | 130.01 | 125.05 |
| 24 | A | 608 | BCR | C30-C25-C24 | 3.24 | 124.83 | 115.73 |
| 32 | E | 101 | LHG | O8-C23-C24 | 3.24 | 121.28 | 111.92 |
| 32 | D | 409 | LHG | O7-C7-C8 | 3.24 | 118.38 | 111.55 |
| 22 | b | 617 | CLA | C4A-NA-C1A | 3.24 | 110.50 | 106.32 |
| 24 | k | 102 | BCR | C31-C1-C6 | 3.24 | 115.56 | 110.31 |
| 22 | d | 403 | CLA | O2D-CGD-CBD | 3.25 | 117.04 | 111.28 |
| 24 | K | 102 | BCR | C31-C1-C6 | 3.25 | 115.57 | 110.31 |
| 22 | b | 617 | CLA | C3B-C4B-NB | 3.26 | 113.42 | 109.21 |
| 22 | B | 617 | CLA | C4A-NA-C1A | 3.26 | 110.52 | 106.32 |
| 22 | b | 604 | CLA | CMC-C2C-C1C | 3.29 | 130.10 | 125.05 |
| 22 | b | 613 | CLA | CAC-C3C-C4C | 3.30 | 129.37 | 124.82 |
| 24 | h | 101 | BCR | C27-C26-C25 | 3.30 | 127.58 | 122.74 |
| 22 | B | 617 | CLA | C3B-C4B-NB | 3.31 | 113.49 | 109.21 |
| 22 | B | 613 | CLA | CAC-C3C-C4C | 3.31 | 129.39 | 124.82 |
| 22 | b | 611 | CLA | C4A-NA-C1A | 3.32 | 110.60 | 106.32 |
| 24 | H | 101 | BCR | C27-C26-C25 | 3.32 | 127.61 | 122.74 |
| 22 | B | 611 | CLA | C4A-NA-C1A | 3.33 | 110.61 | 106.32 |
| 24 | k | 101 | BCR | C2-C1-C6 | 3.33 | 115.68 | 110.48 |
| 29 | A | 614 | LMG | O7-C10-C11 | 3.33 | 118.58 | 111.55 |
| 24 | K | 101 | BCR | C2-C1-C6 | 3.34 | 115.69 | 110.48 |
| 22 | B | 615 | CLA | C4-C3-C5 | 3.34 | 121.05 | 115.29 |
| 29 | a | 614 | LMG | O7-C10-C11 | 3.34 | 118.59 | 111.55 |
| 22 | b | 615 | CLA | C4-C3-C5 | 3.34 | 121.06 | 115.29 |
| 25 | A | 609 | SQD | O8-S-C6 | 3.35 | 111.07 | 105.74 |
| 24 | c | 515 | BCR | C40-C30-C25 | 3.35 | 115.74 | 110.31 |
| 24 | C | 515 | BCR | C40-C30-C25 | 3.36 | 115.76 | 110.31 |
| 22 | B | 612 | CLA | C3B-C4B-NB | 3.36 | 113.56 | 109.21 |
| 23 | A | 605 | PHO | C2B-C1B-NB | 3.36 | 114.89 | 109.79 |
| 23 | a | 605 | PHO | C2B-C1B-NB | 3.37 | 114.90 | 109.79 |
| 25 | a | 609 | SQD | O8-S-C6 | 3.37 | 111.12 | 105.74 |
| 22 | b | 607 | CLA | C4A-NA-C1A | 3.38 | 110.69 | 106.32 |
| 22 | B | 605 | CLA | CED-O2D-CGD | 3.38 | 123.77 | 115.97 |
| 22 | b | 605 | CLA | CED-O2D-CGD | 3.39 | 123.78 | 115.97 |
| 22 | C | 501 | CLA | C4A-NA-C1A | 3.39 | 110.69 | 106.32 |
| 22 | c | 508 | CLA | C4A-NA-C1A | 3.39 | 110.70 | 106.32 |
| 25 | B | 601 | SQD | O9-S-C6 | 3.40 | 110.98 | 106.94 |
| 22 | c | 503 | CLA | C4A-NA-C1A | 3.40 | 110.71 | 106.32 |
| 22 | c | 501 | CLA | C4A-NA-C1A | 3.40 | 110.71 | 106.32 |
| 24 | t | 101 | BCR | C4-C5-C6 | 3.40 | 127.73 | 122.74 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 24 | d | 404 | BCR | C27-C26-C25 | 3.40 | 127.74 | 122.74 |
| 24 | D | 404 | BCR | C27-C26-C25 | 3.41 | 127.74 | 122.74 |
| 24 | t | 101 | BCR | C27-C26-C25 | 3.41 | 127.75 | 122.74 |
| 22 | B | 616 | CLA | C3B-C4B-NB | 3.41 | 113.62 | 109.21 |
| 24 | T | 102 | BCR | C27-C26-C25 | 3.41 | 127.75 | 122.74 |
| 25 | b | 601 | SQD | O9-S-C6 | 3.41 | 111.00 | 106.94 |
| 23 | A | 606 | PHO | C4A-NA-C1A | 3.42 | 110.92 | 108.16 |
| 22 | C | 503 | CLA | C4A-NA-C1A | 3.42 | 110.73 | 106.32 |
| 22 | B | 607 | CLA | C4A-NA-C1A | 3.42 | 110.73 | 106.32 |
| 24 | T | 102 | BCR | C4-C5-C6 | 3.42 | 127.76 | 122.74 |
| 22 | C | 508 | CLA | C4A-NA-C1A | 3.43 | 110.74 | 106.32 |
| 25 | b | 601 | SQD | O47-C7-C8 | 3.43 | 118.79 | 111.55 |
| 22 | b | 614 | CLA | C4A-NA-C1A | 3.44 | 110.75 | 106.32 |
| 22 | D | 401 | CLA | CMB-C2B-C3B | 3.44 | 131.14 | 124.88 |
| 22 | d | 401 | CLA | CMB-C2B-C3B | 3.44 | 131.14 | 124.88 |
| 25 | B | 601 | SQD | O47-C7-C8 | 3.44 | 118.80 | 111.55 |
| 22 | B | 614 | CLA | C4A-NA-C1A | 3.45 | 110.78 | 106.32 |
| 22 | b | 612 | CLA | C3B-C4B-NB | 3.45 | 113.68 | 109.21 |
| 23 | a | 606 | PHO | C4A-NA-C1A | 3.46 | 110.96 | 108.16 |
| 22 | B | 611 | CLA | C3B-C4B-NB | 3.46 | 113.69 | 109.21 |
| 22 | A | 607 | CLA | C4-C3-C5 | 3.46 | 121.26 | 115.29 |
| 22 | b | 611 | CLA | C3B-C4B-NB | 3.47 | 113.69 | 109.21 |
| 22 | b | 616 | CLA | C3B-C4B-NB | 3.47 | 113.70 | 109.21 |
| 22 | a | 607 | CLA | C4-C3-C5 | 3.48 | 121.29 | 115.29 |
| 22 | b | 612 | CLA | C4A-NA-C1A | 3.49 | 110.82 | 106.32 |
| 22 | B | 614 | CLA | C3B-C4B-NB | 3.50 | 113.74 | 109.21 |
| 22 | C | 512 | CLA | C4A-NA-C1A | 3.50 | 110.84 | 106.32 |
| 24 | h | 101 | BCR | C23-C24-C25 | 3.50 | 137.06 | 127.25 |
| 22 | b | 614 | CLA | C3B-C4B-NB | 3.50 | 113.74 | 109.21 |
| 24 | H | 101 | BCR | C23-C24-C25 | 3.51 | 137.07 | 127.25 |
| 22 | B | 612 | CLA | C4A-NA-C1A | 3.51 | 110.85 | 106.32 |
| 22 | b | 610 | CLA | C4A-NA-C1A | 3.51 | 110.85 | 106.32 |
| 22 | b | 615 | CLA | C3B-C4B-NB | 3.52 | 113.76 | 109.21 |
| 22 | c | 512 | CLA | C4A-NA-C1A | 3.52 | 110.86 | 106.32 |
| 24 | K | 102 | BCR | C24-C23-C22 | 3.52 | 131.50 | 126.21 |
| 24 | k | 102 | BCR | C24-C23-C22 | 3.52 | 131.50 | 126.21 |
| 22 | D | 403 | CLA | C3B-C4B-NB | 3.53 | 113.77 | 109.21 |
| 22 | B | 615 | CLA | C3B-C4B-NB | 3.53 | 113.77 | 109.21 |
| 24 | K | 101 | BCR | C27-C26-C25 | 3.54 | 127.93 | 122.74 |
| 22 | b | 610 | CLA | C3B-C4B-NB | 3.54 | 113.78 | 109.21 |
| 22 | d | 403 | CLA | C3B-C4B-NB | 3.54 | 113.79 | 109.21 |
| 22 | B | 610 | CLA | C4A-NA-C1A | 3.54 | 110.89 | 106.32 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 22 | B | 610 | CLA | C3B-C4B-NB | 3.55 | 113.79 | 109.21 |
| 28 | A | 613 | PL9 | C20-C19-C21 | 3.55 | 121.41 | 115.29 |
| 22 | c | 511 | CLA | C1-O2A-CGA | 3.55 | 124.95 | 116.77 |
| 24 | k | 101 | BCR | C27-C26-C25 | 3.55 | 127.95 | 122.74 |
| 22 | A | 604 | CLA | CMB-C2B-C3B | 3.56 | 131.36 | 124.88 |
| 22 | D | 403 | CLA | C4A-NA-C1A | 3.56 | 110.92 | 106.32 |
| 22 | a | 604 | CLA | CMB-C2B-C3B | 3.56 | 131.37 | 124.88 |
| 22 | c | 503 | CLA | CMB-C2B-C3B | 3.57 | 131.39 | 124.88 |
| 28 | a | 613 | PL9 | C20-C19-C21 | 3.57 | 121.45 | 115.29 |
| 22 | D | 401 | CLA | C3B-C4B-NB | 3.58 | 113.83 | 109.21 |
| 22 | C | 508 | CLA | C3B-C4B-NB | 3.58 | 113.83 | 109.21 |
| 22 | c | 510 | CLA | C4A-NA-C1A | 3.58 | 110.94 | 106.32 |
| 24 | k | 102 | BCR | C2-C1-C6 | 3.58 | 116.07 | 110.48 |
| 22 | c | 505 | CLA | C4A-NA-C1A | 3.58 | 110.94 | 106.32 |
| 22 | d | 401 | CLA | C3B-C4B-NB | 3.58 | 113.84 | 109.21 |
| 22 | C | 511 | CLA | C1-O2A-CGA | 3.58 | 125.03 | 116.77 |
| 22 | b | 608 | CLA | C3C-C4C-NC | 3.58 | 114.86 | 110.43 |
| 22 | C | 510 | CLA | C4A-NA-C1A | 3.59 | 110.95 | 106.32 |
| 22 | d | 403 | CLA | C4A-NA-C1A | 3.59 | 110.95 | 106.32 |
| 22 | c | 508 | CLA | C3B-C4B-NB | 3.59 | 113.85 | 109.21 |
| 22 | C | 501 | CLA | C3C-C4C-NC | 3.59 | 114.88 | 110.43 |
| 24 | K | 102 | BCR | C2-C1-C6 | 3.60 | 116.11 | 110.48 |
| 24 | T | 101 | BCR | C27-C26-C25 | 3.60 | 128.03 | 122.74 |
| 22 | c | 511 | CLA | C3B-C4B-NB | 3.61 | 113.87 | 109.21 |
| 22 | C | 504 | CLA | C3B-C4B-NB | 3.61 | 113.87 | 109.21 |
| 24 | B | 618 | BCR | C27-C26-C25 | 3.61 | 128.04 | 122.74 |
| 32 | D | 405 | LHG | O8-C23-C24 | 3.61 | 122.36 | 111.92 |
| 22 | B | 605 | CLA | O2D-CGD-CBD | 3.61 | 117.68 | 111.28 |
| 32 | d | 405 | LHG | O8-C23-C24 | 3.61 | 122.36 | 111.92 |
| 22 | c | 501 | CLA | C3C-C4C-NC | 3.61 | 114.90 | 110.43 |
| 22 | C | 503 | CLA | CMB-C2B-C3B | 3.62 | 131.47 | 124.88 |
| 22 | b | 605 | CLA | O2D-CGD-CBD | 3.62 | 117.71 | 111.28 |
| 22 | C | 509 | CLA | C3B-C4B-NB | 3.63 | 113.90 | 109.21 |
| 22 | B | 608 | CLA | C3C-C4C-NC | 3.63 | 114.92 | 110.43 |
| 23 | A | 606 | PHO | C3C-C4C-NC | 3.63 | 116.00 | 110.24 |
| 22 | B | 611 | CLA | O2D-CGD-CBD | 3.63 | 117.72 | 111.28 |
| 23 | a | 606 | PHO | C3C-C4C-NC | 3.63 | 116.00 | 110.24 |
| 22 | C | 505 | CLA | C4A-NA-C1A | 3.63 | 111.01 | 106.32 |
| 22 | c | 509 | CLA | C3B-C4B-NB | 3.64 | 113.92 | 109.21 |
| 24 | k | 102 | BCR | C32-C1-C6 | 3.64 | 116.21 | 110.31 |
| 22 | b | 611 | CLA | O2D-CGD-CBD | 3.64 | 117.74 | 111.28 |
| 22 | B | 613 | CLA | C4A-NA-C1A | 3.64 | 111.02 | 106.32 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 22 | C | 511 | CLA | C3B-C4B-NB | 3.65 | 113.93 | 109.21 |
| 28 | d | 408 | PL9 | C40-C39-C41 | 3.65 | 121.58 | 115.29 |
| 22 | B | 605 | CLA | C3B-C4B-NB | 3.65 | 113.93 | 109.21 |
| 22 | C | 506 | CLA | C4A-NA-C1A | 3.65 | 111.03 | 106.32 |
| 25 | l | 101 | SQD | O7-S-C6 | 3.66 | 111.29 | 106.94 |
| 29 | Z | 101 | LMG | O1-C1-C2 | 3.67 | 114.17 | 108.24 |
| 24 | K | 102 | BCR | C32-C1-C6 | 3.67 | 116.25 | 110.31 |
| 22 | b | 605 | CLA | C3B-C4B-NB | 3.67 | 113.95 | 109.21 |
| 22 | c | 504 | CLA | C3B-C4B-NB | 3.67 | 113.96 | 109.21 |
| 22 | c | 506 | CLA | C4A-NA-C1A | 3.68 | 111.06 | 106.32 |
| 22 | b | 613 | CLA | C4A-NA-C1A | 3.68 | 111.06 | 106.32 |
| 23 | A | 606 | PHO | C2B-C1B-NB | 3.68 | 115.37 | 109.79 |
| 24 | H | 101 | BCR | C24-C23-C22 | 3.68 | 131.74 | 126.21 |
| 23 | a | 606 | PHO | C2B-C1B-NB | 3.68 | 115.37 | 109.79 |
| 28 | D | 408 | PL9 | C40-C39-C41 | 3.69 | 121.64 | 115.29 |
| 25 | L | 101 | SQD | O7-S-C6 | 3.69 | 111.33 | 106.94 |
| 22 | C | 507 | CLA | C3C-C4C-NC | 3.70 | 115.00 | 110.43 |
| 29 | z | 101 | LMG | O1-C1-C2 | 3.70 | 114.22 | 108.24 |
| 24 | h | 101 | BCR | C24-C23-C22 | 3.70 | 131.77 | 126.21 |
| 24 | C | 515 | BCR | C33-C5-C6 | 3.70 | 128.66 | 124.51 |
| 22 | b | 607 | CLA | O2D-CGD-CBD | 3.71 | 117.85 | 111.28 |
| 24 | c | 515 | BCR | C33-C5-C6 | 3.71 | 128.66 | 124.51 |
| 22 | B | 607 | CLA | O2D-CGD-CBD | 3.71 | 117.86 | 111.28 |
| 22 | a | 607 | CLA | C3B-C4B-NB | 3.73 | 114.03 | 109.21 |
| 23 | A | 605 | PHO | C4A-NA-C1A | 3.73 | 111.18 | 108.16 |
| 22 | D | 402 | CLA | C3B-C4B-NB | 3.73 | 114.03 | 109.21 |
| 24 | T | 101 | BCR | C8-C7-C6 | 3.73 | 137.71 | 127.25 |
| 22 | A | 607 | CLA | C3B-C4B-NB | 3.74 | 114.04 | 109.21 |
| 23 | a | 606 | PHO | C2D-C1D-ND | 3.74 | 115.46 | 109.79 |
| 22 | c | 509 | CLA | C4A-NA-C1A | 3.75 | 111.15 | 106.32 |
| 22 | d | 402 | CLA | C3B-C4B-NB | 3.75 | 114.06 | 109.21 |
| 24 | c | 515 | BCR | C2-C1-C6 | 3.75 | 116.35 | 110.48 |
| 22 | c | 507 | CLA | C3C-C4C-NC | 3.76 | 115.08 | 110.43 |
| 22 | C | 504 | CLA | C4A-NA-C1A | 3.76 | 111.17 | 106.32 |
| 24 | B | 618 | BCR | C8-C7-C6 | 3.76 | 137.77 | 127.25 |
| 31 | c | 517 | DGD | O2G-C1B-C2B | 3.76 | 119.47 | 111.55 |
| 22 | C | 509 | CLA | C4A-NA-C1A | 3.76 | 111.17 | 106.32 |
| 23 | A | 606 | PHO | C2D-C1D-ND | 3.76 | 115.50 | 109.79 |
| 22 | D | 403 | CLA | C3C-C4C-NC | 3.77 | 115.09 | 110.43 |
| 24 | C | 515 | BCR | C2-C1-C6 | 3.77 | 116.38 | 110.48 |
| 25 | b | 621 | SQD | C3-C4-C5 | 3.78 | 117.01 | 110.24 |
| 31 | C | 517 | DGD | O2G-C1B-C2B | 3.78 | 119.52 | 111.55 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 25 | l | 102 | SQD | C3-C4-C5 | 3.78 | 117.01 | 110.24 |
| 22 | c | 510 | CLA | O2D-CGD-CBD | 3.78 | 117.99 | 111.28 |
| 22 | c | 504 | CLA | C4A-NA-C1A | 3.79 | 111.20 | 106.32 |
| 23 | a | 605 | PHO | C4A-NA-C1A | 3.79 | 111.22 | 108.16 |
| 25 | L | 101 | SQD | O47-C7-C8 | 3.79 | 119.54 | 111.55 |
| 22 | C | 503 | CLA | O2D-CGD-CBD | 3.79 | 118.00 | 111.28 |
| 22 | C | 510 | CLA | O2D-CGD-CBD | 3.80 | 118.01 | 111.28 |
| 25 | d | 411 | SQD | O47-C7-C8 | 3.80 | 119.55 | 111.55 |
| 22 | c | 513 | CLA | C4A-NA-C1A | 3.80 | 111.22 | 106.32 |
| 25 | D | 411 | SQD | O47-C7-C8 | 3.80 | 119.56 | 111.55 |
| 22 | d | 403 | CLA | C3C-C4C-NC | 3.80 | 115.13 | 110.43 |
| 25 | l | 101 | SQD | O47-C7-C8 | 3.80 | 119.57 | 111.55 |
| 22 | b | 606 | CLA | C4-C3-C5 | 3.81 | 121.86 | 115.29 |
| 22 | a | 603 | CLA | CMB-C2B-C3B | 3.81 | 131.82 | 124.88 |
| 22 | B | 606 | CLA | C4-C3-C5 | 3.82 | 121.87 | 115.29 |
| 22 | c | 503 | CLA | O2D-CGD-CBD | 3.82 | 118.05 | 111.28 |
| 22 | B | 606 | CLA | O2D-CGD-CBD | 3.82 | 118.06 | 111.28 |
| 22 | b | 606 | CLA | O2D-CGD-CBD | 3.83 | 118.08 | 111.28 |
| 22 | C | 513 | CLA | C4A-NA-C1A | 3.83 | 111.27 | 106.32 |
| 29 | c | 519 | LMG | O7-C10-C11 | 3.84 | 119.64 | 111.55 |
| 22 | A | 603 | CLA | CMB-C2B-C3B | 3.84 | 131.87 | 124.88 |
| 22 | B | 602 | CLA | C4A-NA-C1A | 3.84 | 111.28 | 106.32 |
| 22 | b | 602 | CLA | C4A-NA-C1A | 3.85 | 111.28 | 106.32 |
| 22 | c | 513 | CLA | C3C-C4C-NC | 3.85 | 115.19 | 110.43 |
| 25 | l | 102 | SQD | O7-S-C6 | 3.85 | 111.51 | 106.94 |
| 22 | b | 615 | CLA | C3C-C4C-NC | 3.85 | 115.20 | 110.43 |
| 22 | B | 615 | CLA | C3C-C4C-NC | 3.86 | 115.20 | 110.43 |
| 22 | a | 607 | CLA | C3C-C4C-NC | 3.86 | 115.20 | 110.43 |
| 24 | B | 618 | BCR | C23-C24-C25 | 3.87 | 138.07 | 127.25 |
| 24 | T | 101 | BCR | C23-C24-C25 | 3.87 | 138.08 | 127.25 |
| 29 | C | 519 | LMG | O7-C10-C11 | 3.87 | 119.71 | 111.55 |
| 22 | B | 602 | CLA | C3C-C4C-NC | 3.87 | 115.22 | 110.43 |
| 22 | A | 603 | CLA | C3B-C4B-NB | 3.88 | 114.22 | 109.21 |
| 25 | b | 621 | SQD | O7-S-C6 | 3.88 | 111.56 | 106.94 |
| 22 | A | 607 | CLA | C3C-C4C-NC | 3.88 | 115.24 | 110.43 |
| 22 | C | 510 | CLA | C3B-C4B-NB | 3.89 | 114.23 | 109.21 |
| 29 | c | 520 | LMG | O7-C10-C11 | 3.89 | 119.74 | 111.55 |
| 22 | C | 513 | CLA | C3C-C4C-NC | 3.90 | 115.25 | 110.43 |
| 22 | C | 512 | CLA | C3C-C4C-NC | 3.90 | 115.25 | 110.43 |
| 22 | c | 510 | CLA | C3B-C4B-NB | 3.90 | 114.25 | 109.21 |
| 22 | a | 603 | CLA | C3B-C4B-NB | 3.90 | 114.25 | 109.21 |
| 24 | B | 622 | BCR | C27-C26-C25 | 3.92 | 128.49 | 122.74 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 29 | C | 520 | LMG | O7-C10-C11 | 3.92 | 119.81 | 111.55 |
| 22 | b | 603 | CLA | C3C-C4C-NC | 3.92 | 115.28 | 110.43 |
| 23 | A | 605 | PHO | C3C-C4C-NC | 3.92 | 116.46 | 110.24 |
| 22 | b | 602 | CLA | C3C-C4C-NC | 3.92 | 115.28 | 110.43 |
| 22 | b | 616 | CLA | C4A-NA-C1A | 3.93 | 111.38 | 106.32 |
| 22 | B | 616 | CLA | C4A-NA-C1A | 3.93 | 111.39 | 106.32 |
| 24 | b | 622 | BCR | C27-C26-C25 | 3.93 | 128.51 | 122.74 |
| 22 | c | 512 | CLA | C3C-C4C-NC | 3.93 | 115.29 | 110.43 |
| 22 | c | 510 | CLA | C3C-C4C-NC | 3.93 | 115.30 | 110.43 |
| 22 | b | 617 | CLA | O2D-CGD-CBD | 3.94 | 118.27 | 111.28 |
| 22 | B | 603 | CLA | O2D-CGD-CBD | 3.95 | 118.28 | 111.28 |
| 22 | C | 510 | CLA | C3C-C4C-NC | 3.95 | 115.31 | 110.43 |
| 23 | a | 605 | PHO | C3C-C4C-NC | 3.96 | 116.52 | 110.24 |
| 24 | A | 608 | BCR | C23-C24-C25 | 3.96 | 138.34 | 127.25 |
| 22 | B | 603 | CLA | C3C-C4C-NC | 3.96 | 115.33 | 110.43 |
| 29 | b | 619 | LMG | O7-C10-C11 | 3.96 | 119.91 | 111.55 |
| 22 | b | 603 | CLA | O2D-CGD-CBD | 3.96 | 118.31 | 111.28 |
| 29 | B | 620 | LMG | O7-C10-C11 | 3.97 | 119.93 | 111.55 |
| 24 | a | 608 | BCR | C23-C24-C25 | 3.98 | 138.38 | 127.25 |
| 22 | B | 617 | CLA | O2D-CGD-CBD | 3.98 | 118.33 | 111.28 |
| 22 | B | 607 | CLA | C3C-C4C-NC | 3.99 | 115.36 | 110.43 |
| 22 | b | 607 | CLA | C3C-C4C-NC | 4.00 | 115.38 | 110.43 |
| 22 | C | 508 | CLA | C3C-C4C-NC | 4.01 | 115.39 | 110.43 |
| 25 | l | 102 | SQD | O47-C7-C8 | 4.01 | 120.01 | 111.55 |
| 25 | b | 621 | SQD | O47-C7-C8 | 4.03 | 120.03 | 111.55 |
| 24 | H | 101 | BCR | C8-C7-C6 | 4.03 | 138.54 | 127.25 |
| 24 | T | 102 | BCR | C33-C5-C6 | 4.03 | 129.02 | 124.51 |
| 23 | A | 605 | PHO | C2C-C1C-NC | 4.04 | 115.91 | 109.79 |
| 25 | D | 411 | SQD | O6-C1-C2 | 4.04 | 114.77 | 108.24 |
| 32 | e | 101 | LHG | O7-C7-C8 | 4.04 | 120.06 | 111.55 |
| 32 | E | 101 | LHG | O7-C7-C8 | 4.04 | 120.07 | 111.55 |
| 22 | c | 508 | CLA | C3C-C4C-NC | 4.04 | 115.43 | 110.43 |
| 25 | d | 411 | SQD | O6-C1-C2 | 4.04 | 114.78 | 108.24 |
| 24 | h | 101 | BCR | C8-C7-C6 | 4.05 | 138.58 | 127.25 |
| 23 | a | 606 | PHO | O2D-CGD-CBD | 4.05 | 118.47 | 111.28 |
| 24 | c | 515 | BCR | C8-C9-C10 | 4.06 | 125.17 | 118.94 |
| 23 | A | 606 | PHO | O2D-CGD-CBD | 4.06 | 118.48 | 111.28 |
| 22 | C | 502 | CLA | O2D-CGD-CBD | 4.06 | 118.48 | 111.28 |
| 23 | a | 605 | PHO | C2C-C1C-NC | 4.06 | 115.95 | 109.79 |
| 22 | c | 502 | CLA | O2D-CGD-CBD | 4.06 | 118.49 | 111.28 |
| 24 | b | 622 | BCR | C8-C9-C10 | 4.07 | 125.19 | 118.94 |
| 24 | B | 622 | BCR | C8-C9-C10 | 4.08 | 125.19 | 118.94 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 22 | b | 605 | CLA | C4A-NA-C1A | 4.08 | 111.58 | 106.32 |
| 24 | t | 101 | BCR | C33-C5-C6 | 4.08 | 129.08 | 124.51 |
| 24 | T | 101 | BCR | C29-C30-C25 | 4.09 | 116.87 | 110.48 |
| 22 | c | 503 | CLA | C3C-C4C-NC | 4.09 | 115.49 | 110.43 |
| 24 | C | 515 | BCR | C8-C9-C10 | 4.09 | 125.22 | 118.94 |
| 22 | B | 614 | CLA | C3C-C4C-NC | 4.09 | 115.49 | 110.43 |
| 22 | C | 509 | CLA | C3C-C4C-NC | 4.09 | 115.50 | 110.43 |
| 24 | B | 618 | BCR | C29-C30-C25 | 4.09 | 116.88 | 110.48 |
| 22 | C | 503 | CLA | C3C-C4C-NC | 4.10 | 115.50 | 110.43 |
| 24 | c | 514 | BCR | C23-C24-C25 | 4.10 | 138.73 | 127.25 |
| 22 | C | 505 | CLA | C3C-C4C-NC | 4.10 | 115.50 | 110.43 |
| 22 | c | 505 | CLA | C3C-C4C-NC | 4.11 | 115.51 | 110.43 |
| 24 | T | 101 | BCR | C38-C26-C25 | 4.11 | 129.11 | 124.51 |
| 22 | B | 605 | CLA | C4A-NA-C1A | 4.11 | 111.63 | 106.32 |
| 24 | C | 514 | BCR | C23-C24-C25 | 4.12 | 138.78 | 127.25 |
| 22 | c | 513 | CLA | C2C-C1C-NC | 4.12 | 114.36 | 110.09 |
| 24 | T | 102 | BCR | C2-C1-C6 | 4.12 | 116.93 | 110.48 |
| 24 | T | 102 | BCR | C23-C24-C25 | 4.13 | 138.80 | 127.25 |
| 22 | c | 509 | CLA | C3C-C4C-NC | 4.13 | 115.54 | 110.43 |
| 22 | a | 607 | CLA | O2D-CGD-CBD | 4.13 | 118.60 | 111.28 |
| 25 | l | 102 | SQD | O6-C1-C2 | 4.13 | 114.92 | 108.24 |
| 24 | t | 101 | BCR | C23-C24-C25 | 4.14 | 138.83 | 127.25 |
| 22 | C | 511 | CLA | O2D-CGD-CBD | 4.14 | 118.61 | 111.28 |
| 22 | b | 614 | CLA | C3C-C4C-NC | 4.14 | 115.55 | 110.43 |
| 22 | a | 604 | CLA | C3C-C4C-NC | 4.14 | 115.55 | 110.43 |
| 24 | t | 101 | BCR | C2-C1-C6 | 4.14 | 116.96 | 110.48 |
| 24 | B | 618 | BCR | C38-C26-C25 | 4.15 | 129.15 | 124.51 |
| 22 | C | 513 | CLA | C2C-C1C-NC | 4.15 | 114.39 | 110.09 |
| 22 | c | 511 | CLA | O2D-CGD-CBD | 4.15 | 118.65 | 111.28 |
| 22 | A | 604 | CLA | C3C-C4C-NC | 4.16 | 115.58 | 110.43 |
| 22 | A | 607 | CLA | O2D-CGD-CBD | 4.17 | 118.67 | 111.28 |
| 22 | b | 608 | CLA | C3B-C4B-NB | 4.17 | 114.60 | 109.21 |
| 25 | b | 621 | SQD | O6-C1-C2 | 4.17 | 114.98 | 108.24 |
| 23 | A | 606 | PHO | CAC-C3C-C4C | 4.17 | 129.68 | 125.19 |
| 23 | a | 606 | PHO | CAC-C3C-C4C | 4.17 | 129.68 | 125.19 |
| 22 | b | 610 | CLA | C3C-C4C-NC | 4.18 | 115.60 | 110.43 |
| 22 | C | 502 | CLA | C3C-C4C-NC | 4.19 | 115.62 | 110.43 |
| 22 | B | 604 | CLA | C3B-C4B-NB | 4.19 | 114.63 | 109.21 |
| 23 | A | 605 | PHO | C2D-C1D-ND | 4.20 | 116.16 | 109.79 |
| 24 | c | 514 | BCR | C23-C22-C21 | 4.20 | 125.39 | 118.94 |
| 22 | B | 608 | CLA | C3B-C4B-NB | 4.20 | 114.64 | 109.21 |
| 22 | b | 604 | CLA | C3B-C4B-NB | 4.20 | 114.64 | 109.21 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 24 | b | 618 | BCR | C33-C5-C6 | 4.21 | 129.22 | 124.51 |
| 22 | B | 603 | CLA | C2C-C1C-NC | 4.21 | 114.45 | 110.09 |
| 22 | c | 511 | CLA | C3C-C4C-NC | 4.21 | 115.64 | 110.43 |
| 22 | C | 511 | CLA | C3C-C4C-NC | 4.21 | 115.64 | 110.43 |
| 24 | C | 514 | BCR | C23-C22-C21 | 4.21 | 125.40 | 118.94 |
| 22 | b | 611 | CLA | C3C-C4C-NC | 4.22 | 115.65 | 110.43 |
| 23 | A | 605 | PHO | O2D-CGD-CBD | 4.22 | 118.77 | 111.28 |
| 24 | B | 619 | BCR | C33-C5-C6 | 4.23 | 129.24 | 124.51 |
| 22 | c | 502 | CLA | C3C-C4C-NC | 4.23 | 115.66 | 110.43 |
| 23 | a | 605 | PHO | C2D-C1D-ND | 4.23 | 116.21 | 109.79 |
| 23 | a | 605 | PHO | O2D-CGD-CBD | 4.23 | 118.79 | 111.28 |
| 22 | B | 611 | CLA | C3C-C4C-NC | 4.24 | 115.67 | 110.43 |
| 22 | C | 512 | CLA | C2C-C1C-NC | 4.24 | 114.48 | 110.09 |
| 24 | B | 619 | BCR | C8-C7-C6 | 4.24 | 139.13 | 127.25 |
| 22 | b | 612 | CLA | O2D-CGD-CBD | 4.24 | 118.81 | 111.28 |
| 24 | b | 618 | BCR | C8-C7-C6 | 4.24 | 139.13 | 127.25 |
| 22 | b | 603 | CLA | C2C-C1C-NC | 4.25 | 114.49 | 110.09 |
| 22 | a | 603 | CLA | C3C-C4C-NC | 4.25 | 115.69 | 110.43 |
| 22 | B | 612 | CLA | O2D-CGD-CBD | 4.26 | 118.83 | 111.28 |
| 22 | B | 610 | CLA | C3C-C4C-NC | 4.26 | 115.70 | 110.43 |
| 22 | b | 609 | CLA | C3C-C4C-NC | 4.27 | 115.71 | 110.43 |
| 22 | B | 609 | CLA | C3B-C4B-NB | 4.28 | 114.74 | 109.21 |
| 22 | c | 512 | CLA | C2C-C1C-NC | 4.28 | 114.52 | 110.09 |
| 22 | b | 613 | CLA | C3C-C4C-NC | 4.29 | 115.73 | 110.43 |
| 22 | A | 603 | CLA | C3C-C4C-NC | 4.29 | 115.73 | 110.43 |
| 25 | a | 609 | SQD | O9-S-C6 | 4.30 | 112.05 | 106.94 |
| 22 | b | 609 | CLA | C3B-C4B-NB | 4.30 | 114.77 | 109.21 |
| 25 | A | 609 | SQD | O9-S-C6 | 4.31 | 112.06 | 106.94 |
| 24 | T | 102 | BCR | C29-C30-C25 | 4.31 | 117.21 | 110.48 |
| 22 | B | 613 | CLA | C3C-C4C-NC | 4.31 | 115.76 | 110.43 |
| 22 | B | 609 | CLA | C3C-C4C-NC | 4.32 | 115.77 | 110.43 |
| 24 | t | 101 | BCR | C29-C30-C25 | 4.32 | 117.23 | 110.48 |
| 31 | c | 516 | DGD | O2G-C1B-C2B | 4.32 | 120.66 | 111.55 |
| 22 | c | 506 | CLA | C3C-C4C-NC | 4.32 | 115.78 | 110.43 |
| 22 | B | 604 | CLA | C3C-C4C-NC | 4.32 | 115.78 | 110.43 |
| 24 | d | 404 | BCR | C23-C24-C25 | 4.32 | 139.35 | 127.25 |
| 24 | D | 404 | BCR | C23-C24-C25 | 4.33 | 139.37 | 127.25 |
| 22 | b | 604 | CLA | C3C-C4C-NC | 4.34 | 115.80 | 110.43 |
| 31 | C | 516 | DGD | O2G-C1B-C2B | 4.35 | 120.71 | 111.55 |
| 22 | C | 513 | CLA | O2D-CGD-CBD | 4.35 | 118.99 | 111.28 |
| 24 | C | 514 | BCR | C32-C1-C6 | 4.35 | 117.36 | 110.31 |
| 22 | c | 513 | CLA | O2D-CGD-CBD | 4.36 | 119.00 | 111.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 22 | C | 506 | CLA | C3C-C4C-NC | 4.36 | 115.82 | 110.43 |
| 24 | c | 514 | BCR | C32-C1-C6 | 4.36 | 117.38 | 110.31 |
| 22 | B | 602 | CLA | C2C-C1C-NC | 4.36 | 114.61 | 110.09 |
| 22 | c | 507 | CLA | O2D-CGD-CBD | 4.37 | 119.03 | 111.28 |
| 22 | c | 507 | CLA | C4A-NA-C1A | 4.37 | 111.96 | 106.32 |
| 24 | H | 101 | BCR | C28-C27-C26 | 4.38 | 121.68 | 113.99 |
| 22 | C | 507 | CLA | O2D-CGD-CBD | 4.39 | 119.06 | 111.28 |
| 22 | b | 602 | CLA | C2C-C1C-NC | 4.39 | 114.63 | 110.09 |
| 22 | C | 511 | CLA | C4A-NA-C1A | 4.39 | 111.98 | 106.32 |
| 24 | h | 101 | BCR | C28-C27-C26 | 4.39 | 121.70 | 113.99 |
| 24 | T | 102 | BCR | C8-C7-C6 | 4.39 | 139.55 | 127.25 |
| 24 | t | 101 | BCR | C8-C7-C6 | 4.40 | 139.56 | 127.25 |
| 22 | c | 511 | CLA | C4A-NA-C1A | 4.41 | 112.01 | 106.32 |
| 25 | a | 609 | SQD | O47-C7-C8 | 4.42 | 120.86 | 111.55 |
| 25 | A | 609 | SQD | O47-C7-C8 | 4.42 | 120.86 | 111.55 |
| 22 | d | 402 | CLA | O2D-CGD-CBD | 4.42 | 119.11 | 111.28 |
| 22 | C | 507 | CLA | C4A-NA-C1A | 4.42 | 112.02 | 106.32 |
| 22 | a | 604 | CLA | C3B-C4B-NB | 4.43 | 114.94 | 109.21 |
| 25 | l | 101 | SQD | O6-C1-C2 | 4.44 | 115.42 | 108.24 |
| 22 | D | 402 | CLA | O2D-CGD-CBD | 4.44 | 119.15 | 111.28 |
| 22 | d | 402 | CLA | C3C-C4C-NC | 4.47 | 115.95 | 110.43 |
| 22 | A | 604 | CLA | C3B-C4B-NB | 4.47 | 114.99 | 109.21 |
| 25 | L | 101 | SQD | O6-C1-C2 | 4.48 | 115.49 | 108.24 |
| 22 | D | 402 | CLA | C3C-C4C-NC | 4.49 | 115.98 | 110.43 |
| 24 | b | 618 | BCR | C2-C1-C6 | 4.49 | 117.50 | 110.48 |
| 22 | C | 505 | CLA | O2D-CGD-CBD | 4.49 | 119.24 | 111.28 |
| 22 | c | 505 | CLA | O2D-CGD-CBD | 4.50 | 119.25 | 111.28 |
| 22 | b | 616 | CLA | C3C-C4C-NC | 4.50 | 116.00 | 110.43 |
| 24 | B | 619 | BCR | C2-C1-C6 | 4.50 | 117.52 | 110.48 |
| 22 | c | 503 | CLA | C2C-C1C-NC | 4.51 | 114.76 | 110.09 |
| 22 | B | 616 | CLA | C3C-C4C-NC | 4.51 | 116.01 | 110.43 |
| 22 | C | 503 | CLA | C2C-C1C-NC | 4.52 | 114.77 | 110.09 |
| 22 | b | 610 | CLA | O2D-CGD-CBD | 4.53 | 119.31 | 111.28 |
| 22 | B | 610 | CLA | O2D-CGD-CBD | 4.53 | 119.31 | 111.28 |
| 25 | a | 609 | SQD | O6-C1-C2 | 4.55 | 115.59 | 108.24 |
| 22 | c | 507 | CLA | C2C-C1C-NC | 4.55 | 114.81 | 110.09 |
| 25 | A | 609 | SQD | O6-C1-C2 | 4.56 | 115.61 | 108.24 |
| 22 | c | 508 | CLA | O2D-CGD-CBD | 4.56 | 119.36 | 111.28 |
| 22 | C | 508 | CLA | O2D-CGD-CBD | 4.58 | 119.40 | 111.28 |
| 22 | B | 617 | CLA | C2C-C1C-NC | 4.58 | 114.83 | 110.09 |
| 31 | D | 410 | DGD | O2G-C1B-C2B | 4.60 | 121.25 | 111.55 |
| 31 | d | 410 | DGD | O2G-C1B-C2B | 4.61 | 121.27 | 111.55 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 24 | c | 514 | BCR | C27-C26-C25 | 4.62 | 129.53 | 122.74 |
| 22 | C | 507 | CLA | C2C-C1C-NC | 4.62 | 114.88 | 110.09 |
| 24 | C | 514 | BCR | C27-C26-C25 | 4.63 | 129.53 | 122.74 |
| 24 | B | 619 | BCR | C27-C26-C25 | 4.65 | 129.56 | 122.74 |
| 22 | D | 403 | CLA | C2C-C1C-NC | 4.65 | 114.90 | 110.09 |
| 22 | B | 615 | CLA | O2D-CGD-CBD | 4.65 | 119.52 | 111.28 |
| 24 | k | 101 | BCR | C23-C24-C25 | 4.65 | 140.28 | 127.25 |
| 22 | b | 615 | CLA | O2D-CGD-CBD | 4.65 | 119.53 | 111.28 |
| 24 | K | 101 | BCR | C23-C24-C25 | 4.66 | 140.29 | 127.25 |
| 24 | b | 618 | BCR | C27-C26-C25 | 4.66 | 129.58 | 122.74 |
| 22 | B | 617 | CLA | C3C-C4C-NC | 4.66 | 116.20 | 110.43 |
| 22 | b | 617 | CLA | C2C-C1C-NC | 4.67 | 114.92 | 110.09 |
| 22 | b | 617 | CLA | C3C-C4C-NC | 4.68 | 116.22 | 110.43 |
| 22 | d | 403 | CLA | C2C-C1C-NC | 4.68 | 114.94 | 110.09 |
| 22 | c | 509 | CLA | O2D-CGD-CBD | 4.70 | 119.62 | 111.28 |
| 22 | b | 616 | CLA | C2C-C1C-NC | 4.71 | 114.97 | 110.09 |
| 22 | b | 605 | CLA | C3C-C4C-NC | 4.72 | 116.27 | 110.43 |
| 22 | b | 611 | CLA | C2C-C1C-NC | 4.72 | 114.98 | 110.09 |
| 22 | B | 611 | CLA | C2C-C1C-NC | 4.72 | 114.98 | 110.09 |
| 22 | C | 509 | CLA | O2D-CGD-CBD | 4.72 | 119.66 | 111.28 |
| 24 | d | 404 | BCR | C4-C5-C6 | 4.73 | 129.69 | 122.74 |
| 22 | B | 613 | CLA | O2D-CGD-CBD | 4.74 | 119.68 | 111.28 |
| 22 | B | 613 | CLA | C2C-C1C-NC | 4.74 | 115.00 | 110.09 |
| 22 | b | 606 | CLA | C3C-C4C-NC | 4.74 | 116.30 | 110.43 |
| 22 | C | 508 | CLA | C2C-C1C-NC | 4.75 | 115.01 | 110.09 |
| 24 | D | 404 | BCR | C4-C5-C6 | 4.75 | 129.72 | 122.74 |
| 22 | b | 613 | CLA | O2D-CGD-CBD | 4.75 | 119.71 | 111.28 |
| 22 | B | 616 | CLA | C2C-C1C-NC | 4.76 | 115.02 | 110.09 |
| 29 | Z | 101 | LMG | O7-C10-C11 | 4.77 | 121.60 | 111.55 |
| 29 | z | 101 | LMG | O7-C10-C11 | 4.77 | 121.60 | 111.55 |
| 22 | b | 613 | CLA | C2C-C1C-NC | 4.77 | 115.03 | 110.09 |
| 22 | c | 511 | CLA | C2C-C1C-NC | 4.77 | 115.03 | 110.09 |
| 24 | b | 622 | BCR | C23-C22-C21 | 4.77 | 126.27 | 118.94 |
| 22 | C | 502 | CLA | C2C-C1C-NC | 4.77 | 115.03 | 110.09 |
| 22 | c | 502 | CLA | C2C-C1C-NC | 4.78 | 115.03 | 110.09 |
| 22 | B | 606 | CLA | C3C-C4C-NC | 4.78 | 116.34 | 110.43 |
| 24 | k | 101 | BCR | C4-C5-C6 | 4.78 | 129.76 | 122.74 |
| 22 | C | 511 | CLA | C2C-C1C-NC | 4.78 | 115.04 | 110.09 |
| 22 | D | 401 | CLA | C3C-C4C-NC | 4.79 | 116.35 | 110.43 |
| 22 | B | 605 | CLA | C3C-C4C-NC | 4.79 | 116.36 | 110.43 |
| 22 | c | 508 | CLA | C2C-C1C-NC | 4.79 | 115.05 | 110.09 |
| 24 | C | 514 | BCR | C2-C1-C6 | 4.79 | 117.97 | 110.48 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 24 | K | 101 | BCR | C4-C5-C6 | 4.80 | 129.78 | 122.74 |
| 22 | C | 505 | CLA | C2C-C1C-NC | 4.80 | 115.06 | 110.09 |
| 22 | B | 607 | CLA | C2C-C1C-NC | 4.81 | 115.07 | 110.09 |
| 24 | c | 515 | BCR | C38-C26-C25 | 4.81 | 129.89 | 124.51 |
| 24 | B | 622 | BCR | C23-C22-C21 | 4.81 | 126.32 | 118.94 |
| 22 | c | 505 | CLA | C2C-C1C-NC | 4.81 | 115.07 | 110.09 |
| 24 | C | 515 | BCR | C38-C26-C25 | 4.81 | 129.90 | 124.51 |
| 22 | B | 609 | CLA | O2D-CGD-CBD | 4.81 | 119.82 | 111.28 |
| 22 | b | 607 | CLA | C2C-C1C-NC | 4.82 | 115.08 | 110.09 |
| 24 | c | 514 | BCR | C2-C1-C6 | 4.82 | 118.02 | 110.48 |
| 22 | b | 609 | CLA | O2D-CGD-CBD | 4.83 | 119.84 | 111.28 |
| 22 | d | 401 | CLA | C3C-C4C-NC | 4.83 | 116.40 | 110.43 |
| 22 | a | 604 | CLA | O2D-CGD-CBD | 4.84 | 119.86 | 111.28 |
| 22 | A | 604 | CLA | O2D-CGD-CBD | 4.85 | 119.88 | 111.28 |
| 24 | d | 404 | BCR | C8-C7-C6 | 4.86 | 140.85 | 127.25 |
| 24 | D | 404 | BCR | C8-C7-C6 | 4.86 | 140.87 | 127.25 |
| 22 | b | 606 | CLA | C2C-C1C-NC | 4.87 | 115.13 | 110.09 |
| 22 | B | 606 | CLA | C2C-C1C-NC | 4.88 | 115.14 | 110.09 |
| 22 | c | 501 | CLA | C2C-C1C-NC | 4.88 | 115.14 | 110.09 |
| 22 | c | 504 | CLA | O2D-CGD-CBD | 4.88 | 119.94 | 111.28 |
| 22 | b | 604 | CLA | O2D-CGD-CBD | 4.89 | 119.94 | 111.28 |
| 22 | C | 504 | CLA | O2D-CGD-CBD | 4.89 | 119.95 | 111.28 |
| 24 | d | 404 | BCR | C7-C8-C9 | 4.89 | 133.56 | 126.21 |
| 24 | D | 404 | BCR | C7-C8-C9 | 4.89 | 133.57 | 126.21 |
| 22 | a | 603 | CLA | C2C-C1C-NC | 4.90 | 115.16 | 110.09 |
| 22 | A | 603 | CLA | C2C-C1C-NC | 4.90 | 115.17 | 110.09 |
| 22 | B | 604 | CLA | O2D-CGD-CBD | 4.90 | 119.98 | 111.28 |
| 22 | B | 612 | CLA | C3C-C4C-NC | 4.91 | 116.50 | 110.43 |
| 22 | C | 501 | CLA | C2C-C1C-NC | 4.91 | 115.17 | 110.09 |
| 24 | C | 515 | BCR | C29-C30-C25 | 4.91 | 118.15 | 110.48 |
| 22 | b | 612 | CLA | C3C-C4C-NC | 4.91 | 116.50 | 110.43 |
| 24 | B | 618 | BCR | C2-C1-C6 | 4.91 | 118.16 | 110.48 |
| 24 | c | 515 | BCR | C29-C30-C25 | 4.92 | 118.17 | 110.48 |
| 24 | T | 101 | BCR | C2-C1-C6 | 4.93 | 118.18 | 110.48 |
| 24 | T | 102 | BCR | C24-C23-C22 | 4.95 | 133.65 | 126.21 |
| 24 | h | 101 | BCR | C29-C30-C25 | 4.97 | 118.25 | 110.48 |
| 24 | t | 101 | BCR | C24-C23-C22 | 5.00 | 133.73 | 126.21 |
| 24 | H | 101 | BCR | C29-C30-C25 | 5.02 | 118.33 | 110.48 |
| 22 | c | 506 | CLA | C2C-C1C-NC | 5.05 | 115.32 | 110.09 |
| 24 | b | 618 | BCR | C40-C30-C25 | 5.07 | 118.53 | 110.31 |
| 22 | C | 506 | CLA | C2C-C1C-NC | 5.07 | 115.34 | 110.09 |
| 24 | B | 619 | BCR | C40-C30-C25 | 5.08 | 118.55 | 110.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 22 | C | 510 | CLA | C2C-C1C-NC | 5.09 | 115.36 | 110.09 |
| 22 | C | 506 | CLA | O2D-CGD-CBD | 5.11 | 120.35 | 111.28 |
| 22 | c | 506 | CLA | O2D-CGD-CBD | 5.11 | 120.35 | 111.28 |
| 22 | B | 614 | CLA | C2C-C1C-NC | 5.12 | 115.40 | 110.09 |
| 24 | d | 404 | BCR | C8-C9-C10 | 5.12 | 126.80 | 118.94 |
| 22 | c | 512 | CLA | O2D-CGD-CBD | 5.12 | 120.37 | 111.28 |
| 22 | c | 510 | CLA | C2C-C1C-NC | 5.13 | 115.40 | 110.09 |
| 22 | C | 512 | CLA | O2D-CGD-CBD | 5.14 | 120.39 | 111.28 |
| 24 | d | 404 | BCR | C24-C23-C22 | 5.14 | 133.93 | 126.21 |
| 22 | B | 615 | CLA | C2C-C1C-NC | 5.14 | 115.42 | 110.09 |
| 24 | k | 102 | BCR | C23-C24-C25 | 5.14 | 141.65 | 127.25 |
| 24 | K | 102 | BCR | C23-C24-C25 | 5.15 | 141.66 | 127.25 |
| 22 | b | 615 | CLA | C2C-C1C-NC | 5.15 | 115.42 | 110.09 |
| 22 | b | 614 | CLA | C2C-C1C-NC | 5.15 | 115.42 | 110.09 |
| 24 | D | 404 | BCR | C8-C9-C10 | 5.17 | 126.87 | 118.94 |
| 24 | C | 515 | BCR | C8-C7-C6 | 5.17 | 141.72 | 127.25 |
| 24 | c | 515 | BCR | C8-C7-C6 | 5.19 | 141.77 | 127.25 |
| 24 | D | 404 | BCR | C24-C23-C22 | 5.19 | 134.00 | 126.21 |
| 24 | k | 101 | BCR | C23-C22-C21 | 5.20 | 126.93 | 118.94 |
| 22 | b | 608 | CLA | C2C-C1C-NC | 5.21 | 115.48 | 110.09 |
| 24 | K | 101 | BCR | C8-C7-C6 | 5.22 | 141.87 | 127.25 |
| 24 | K | 101 | BCR | C23-C22-C21 | 5.23 | 126.96 | 118.94 |
| 24 | k | 101 | BCR | C8-C7-C6 | 5.24 | 141.91 | 127.25 |
| 24 | A | 608 | BCR | C24-C23-C22 | 5.26 | 134.11 | 126.21 |
| 22 | B | 608 | CLA | C2C-C1C-NC | 5.27 | 115.54 | 110.09 |
| 22 | D | 401 | CLA | C2C-C1C-NC | 5.27 | 115.55 | 110.09 |
| 22 | d | 401 | CLA | C2C-C1C-NC | 5.27 | 115.55 | 110.09 |
| 24 | a | 608 | BCR | C24-C23-C22 | 5.27 | 134.14 | 126.21 |
| 24 | C | 514 | BCR | C29-C30-C25 | 5.29 | 118.75 | 110.48 |
| 22 | c | 504 | CLA | C2C-C1C-NC | 5.29 | 115.57 | 110.09 |
| 22 | b | 612 | CLA | C2C-C1C-NC | 5.29 | 115.57 | 110.09 |
| 24 | c | 514 | BCR | C29-C30-C25 | 5.30 | 118.76 | 110.48 |
| 22 | C | 504 | CLA | C2C-C1C-NC | 5.31 | 115.59 | 110.09 |
| 22 | B | 612 | CLA | C2C-C1C-NC | 5.32 | 115.60 | 110.09 |
| 22 | b | 610 | CLA | C2C-C1C-NC | 5.33 | 115.61 | 110.09 |
| 22 | C | 509 | CLA | C2C-C1C-NC | 5.35 | 115.62 | 110.09 |
| 22 | B | 610 | CLA | C2C-C1C-NC | 5.35 | 115.63 | 110.09 |
| 22 | c | 509 | CLA | C2C-C1C-NC | 5.35 | 115.64 | 110.09 |
| 22 | A | 607 | CLA | C2C-C1C-NC | 5.36 | 115.64 | 110.09 |
| 24 | H | 101 | BCR | C33-C5-C6 | 5.37 | 130.52 | 124.51 |
| 22 | a | 607 | CLA | C2C-C1C-NC | 5.38 | 115.66 | 110.09 |
| 24 | K | 101 | BCR | C8-C9-C10 | 5.41 | 127.24 | 118.94 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 24 | B | 622 | BCR | C2-C1-C6 | 5.42 | 118.95 | 110.48 |
| 24 | b | 622 | BCR | C2-C1-C6 | 5.42 | 118.96 | 110.48 |
| 24 | k | 101 | BCR | C8-C9-C10 | 5.42 | 127.26 | 118.94 |
| 24 | h | 101 | BCR | C33-C5-C6 | 5.43 | 130.58 | 124.51 |
| 24 | k | 102 | BCR | C8-C9-C10 | 5.44 | 127.28 | 118.94 |
| 24 | K | 102 | BCR | C8-C9-C10 | 5.44 | 127.29 | 118.94 |
| 22 | B | 604 | CLA | C2C-C1C-NC | 5.47 | 115.75 | 110.09 |
| 22 | b | 604 | CLA | C2C-C1C-NC | 5.56 | 115.85 | 110.09 |
| 24 | k | 101 | BCR | C24-C23-C22 | 5.57 | 134.58 | 126.21 |
| 24 | K | 101 | BCR | C24-C23-C22 | 5.59 | 134.61 | 126.21 |
| 24 | b | 618 | BCR | C29-C30-C25 | 5.59 | 119.23 | 110.48 |
| 24 | B | 619 | BCR | C29-C30-C25 | 5.60 | 119.23 | 110.48 |
| 22 | b | 602 | CLA | O2D-CGD-CBD | 5.63 | 121.27 | 111.28 |
| 22 | B | 602 | CLA | O2D-CGD-CBD | 5.64 | 121.28 | 111.28 |
| 24 | c | 514 | BCR | C8-C7-C6 | 5.64 | 143.05 | 127.25 |
| 24 | C | 514 | BCR | C8-C7-C6 | 5.66 | 143.11 | 127.25 |
| 24 | d | 404 | BCR | C23-C22-C21 | 5.79 | 127.83 | 118.94 |
| 24 | D | 404 | BCR | C23-C22-C21 | 5.80 | 127.84 | 118.94 |
| 24 | c | 514 | BCR | C12-C13-C14 | 5.83 | 127.88 | 118.94 |
| 24 | C | 515 | BCR | C7-C8-C9 | 5.83 | 134.97 | 126.21 |
| 24 | c | 515 | BCR | C7-C8-C9 | 5.84 | 134.99 | 126.21 |
| 24 | C | 514 | BCR | C12-C13-C14 | 5.85 | 127.91 | 118.94 |
| 24 | c | 514 | BCR | C38-C26-C25 | 5.89 | 131.10 | 124.51 |
| 24 | C | 514 | BCR | C38-C26-C25 | 5.93 | 131.15 | 124.51 |
| 24 | c | 515 | BCR | C31-C1-C6 | 5.97 | 119.98 | 110.31 |
| 22 | B | 609 | CLA | C2C-C1C-NC | 5.97 | 116.28 | 110.09 |
| 22 | b | 609 | CLA | C2C-C1C-NC | 5.98 | 116.28 | 110.09 |
| 22 | C | 501 | CLA | O2D-CGD-CBD | 5.98 | 121.89 | 111.28 |
| 22 | c | 501 | CLA | O2D-CGD-CBD | 5.99 | 121.90 | 111.28 |
| 24 | C | 515 | BCR | C31-C1-C6 | 6.00 | 120.03 | 110.31 |
| 22 | b | 605 | CLA | C2C-C1C-NC | 6.01 | 116.31 | 110.09 |
| 22 | B | 605 | CLA | C2C-C1C-NC | 6.03 | 116.33 | 110.09 |
| 24 | T | 101 | BCR | C7-C8-C9 | 6.05 | 135.30 | 126.21 |
| 22 | A | 604 | CLA | C2C-C1C-NC | 6.06 | 116.37 | 110.09 |
| 22 | a | 604 | CLA | C2C-C1C-NC | 6.07 | 116.38 | 110.09 |
| 24 | B | 618 | BCR | C7-C8-C9 | 6.08 | 135.35 | 126.21 |
| 24 | b | 622 | BCR | C24-C23-C22 | 6.11 | 135.39 | 126.21 |
| 24 | k | 102 | BCR | C8-C7-C6 | 6.12 | 144.40 | 127.25 |
| 24 | K | 102 | BCR | C8-C7-C6 | 6.14 | 144.44 | 127.25 |
| 24 | B | 622 | BCR | C24-C23-C22 | 6.14 | 135.44 | 126.21 |
| 24 | c | 514 | BCR | C24-C23-C22 | 6.14 | 135.44 | 126.21 |
| 24 | C | 514 | BCR | C24-C23-C22 | 6.17 | 135.48 | 126.21 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 24 | b | 618 | BCR | C23-C24-C25 | 6.18 | 144.55 | 127.25 |
| 24 | B | 619 | BCR | C23-C24-C25 | 6.18 | 144.56 | 127.25 |
| 24 | t | 101 | BCR | C8-C9-C10 | 6.19 | 128.44 | 118.94 |
| 24 | b | 618 | BCR | C8-C9-C10 | 6.22 | 128.48 | 118.94 |
| 24 | a | 608 | BCR | C8-C9-C10 | 6.22 | 128.49 | 118.94 |
| 24 | T | 102 | BCR | C8-C9-C10 | 6.24 | 128.51 | 118.94 |
| 24 | B | 619 | BCR | C8-C9-C10 | 6.25 | 128.53 | 118.94 |
| 24 | b | 618 | BCR | C11-C12-C13 | 6.26 | 144.01 | 126.42 |
| 24 | B | 619 | BCR | C11-C12-C13 | 6.26 | 144.01 | 126.42 |
| 24 | A | 608 | BCR | C8-C9-C10 | 6.27 | 128.57 | 118.94 |
| 24 | H | 101 | BCR | C32-C1-C6 | 6.34 | 120.59 | 110.31 |
| 24 | h | 101 | BCR | C32-C1-C6 | 6.35 | 120.60 | 110.31 |
| 24 | K | 101 | BCR | C29-C30-C25 | 6.42 | 120.51 | 110.48 |
| 24 | k | 101 | BCR | C29-C30-C25 | 6.42 | 120.51 | 110.48 |
| 24 | C | 514 | BCR | C33-C5-C6 | 6.44 | 131.72 | 124.51 |
| 22 | D | 402 | CLA | C2C-C1C-NC | 6.45 | 116.77 | 110.09 |
| 22 | d | 402 | CLA | C2C-C1C-NC | 6.46 | 116.78 | 110.09 |
| 24 | c | 514 | BCR | C33-C5-C6 | 6.51 | 131.80 | 124.51 |
| 24 | c | 515 | BCR | C23-C22-C21 | 6.61 | 129.09 | 118.94 |
| 24 | c | 515 | BCR | C24-C23-C22 | 6.62 | 136.15 | 126.21 |
| 24 | B | 618 | BCR | C23-C22-C21 | 6.66 | 129.16 | 118.94 |
| 24 | C | 515 | BCR | C24-C23-C22 | 6.66 | 136.22 | 126.21 |
| 24 | C | 515 | BCR | C23-C22-C21 | 6.67 | 129.18 | 118.94 |
| 24 | h | 101 | BCR | C8-C9-C10 | 6.67 | 129.18 | 118.94 |
| 24 | H | 101 | BCR | C8-C9-C10 | 6.69 | 129.20 | 118.94 |
| 24 | T | 101 | BCR | C23-C22-C21 | 6.71 | 129.23 | 118.94 |
| 24 | b | 622 | BCR | C8-C7-C6 | 6.71 | 146.04 | 127.25 |
| 24 | B | 622 | BCR | C8-C7-C6 | 6.72 | 146.06 | 127.25 |
| 24 | B | 618 | BCR | C24-C23-C22 | 6.98 | 136.70 | 126.21 |
| 24 | T | 101 | BCR | C24-C23-C22 | 7.03 | 136.77 | 126.21 |
| 24 | B | 622 | BCR | C12-C13-C14 | 7.14 | 129.89 | 118.94 |
| 24 | b | 622 | BCR | C12-C13-C14 | 7.14 | 129.91 | 118.94 |
| 24 | t | 101 | BCR | C12-C13-C14 | 7.27 | 130.10 | 118.94 |
| 24 | T | 102 | BCR | C12-C13-C14 | 7.30 | 130.14 | 118.94 |
| 24 | D | 404 | BCR | C10-C11-C12 | 7.34 | 145.61 | 123.26 |
| 24 | d | 404 | BCR | C10-C11-C12 | 7.35 | 145.65 | 123.26 |
| 23 | A | 605 | PHO | CMD-C2D-C1D | 7.37 | 136.46 | 125.05 |
| 23 | a | 605 | PHO | CMD-C2D-C1D | 7.40 | 136.51 | 125.05 |
| 24 | K | 101 | BCR | C12-C13-C14 | 7.41 | 130.31 | 118.94 |
| 24 | B | 622 | BCR | C33-C5-C6 | 7.43 | 132.82 | 124.51 |
| 24 | k | 101 | BCR | C12-C13-C14 | 7.44 | 130.35 | 118.94 |
| 24 | b | 622 | BCR | C33-C5-C6 | 7.45 | 132.84 | 124.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 24 | K | 101 | BCR | C33-C5-C6 | 7.54 | 132.95 | 124.51 |
| 23 | a | 606 | PHO | CMD-C2D-C1D | 7.55 | 136.73 | 125.05 |
| 24 | A | 608 | BCR | C27-C26-C25 | 7.56 | 133.84 | 122.74 |
| 24 | k | 101 | BCR | C33-C5-C6 | 7.58 | 132.99 | 124.51 |
| 23 | A | 606 | PHO | CMD-C2D-C1D | 7.58 | 136.78 | 125.05 |
| 24 | a | 608 | BCR | C27-C26-C25 | 7.60 | 133.90 | 122.74 |
| 24 | K | 101 | BCR | C7-C8-C9 | 7.64 | 137.68 | 126.21 |
| 24 | k | 101 | BCR | C7-C8-C9 | 7.67 | 137.74 | 126.21 |
| 24 | T | 101 | BCR | C8-C9-C10 | 7.86 | 131.00 | 118.94 |
| 24 | H | 101 | BCR | C7-C8-C9 | 7.88 | 138.04 | 126.21 |
| 24 | h | 101 | BCR | C7-C8-C9 | 7.89 | 138.06 | 126.21 |
| 24 | B | 618 | BCR | C8-C9-C10 | 7.89 | 131.05 | 118.94 |
| 24 | b | 618 | BCR | C7-C8-C9 | 7.90 | 138.08 | 126.21 |
| 24 | B | 619 | BCR | C7-C8-C9 | 7.91 | 138.10 | 126.21 |
| 24 | a | 608 | BCR | C7-C8-C9 | 7.95 | 138.16 | 126.21 |
| 24 | b | 618 | BCR | C10-C11-C12 | 7.97 | 147.54 | 123.26 |
| 24 | B | 619 | BCR | C10-C11-C12 | 7.98 | 147.56 | 123.26 |
| 24 | D | 404 | BCR | C12-C13-C14 | 7.99 | 131.20 | 118.94 |
| 24 | d | 404 | BCR | C12-C13-C14 | 8.01 | 131.23 | 118.94 |
| 24 | K | 101 | BCR | C10-C11-C12 | 8.02 | 147.69 | 123.26 |
| 24 | k | 101 | BCR | C10-C11-C12 | 8.03 | 147.73 | 123.26 |
| 24 | A | 608 | BCR | C7-C8-C9 | 8.04 | 138.29 | 126.21 |
| 24 | d | 404 | BCR | C29-C30-C25 | 8.17 | 123.25 | 110.48 |
| 24 | D | 404 | BCR | C32-C1-C6 | 8.18 | 123.58 | 110.31 |
| 24 | d | 404 | BCR | C32-C1-C6 | 8.18 | 123.58 | 110.31 |
| 24 | D | 404 | BCR | C29-C30-C25 | 8.19 | 123.29 | 110.48 |
| 24 | c | 514 | BCR | C11-C10-C9 | 8.20 | 139.01 | 127.31 |
| 24 | C | 514 | BCR | C11-C10-C9 | 8.21 | 139.02 | 127.31 |
| 24 | B | 618 | BCR | C15-C14-C13 | 8.29 | 139.15 | 127.31 |
| 24 | T | 101 | BCR | C15-C14-C13 | 8.30 | 139.15 | 127.31 |
| 24 | K | 101 | BCR | C11-C12-C13 | 8.34 | 149.85 | 126.42 |
| 24 | k | 101 | BCR | C11-C12-C13 | 8.35 | 149.87 | 126.42 |
| 24 | k | 102 | BCR | C23-C22-C21 | 8.37 | 131.78 | 118.94 |
| 24 | K | 102 | BCR | C23-C22-C21 | 8.37 | 131.79 | 118.94 |
| 24 | c | 515 | BCR | C11-C12-C13 | 8.52 | 150.34 | 126.42 |
| 24 | a | 608 | BCR | C20-C19-C18 | 8.53 | 150.38 | 126.42 |
| 24 | C | 515 | BCR | C11-C12-C13 | 8.54 | 150.40 | 126.42 |
| 24 | A | 608 | BCR | C20-C19-C18 | 8.55 | 150.43 | 126.42 |
| 24 | B | 619 | BCR | C24-C23-C22 | 8.70 | 139.28 | 126.21 |
| 24 | b | 618 | BCR | C24-C23-C22 | 8.74 | 139.34 | 126.21 |
| 24 | h | 101 | BCR | C23-C22-C21 | 8.74 | 132.36 | 118.94 |
| 24 | H | 101 | BCR | C23-C22-C21 | 8.74 | 132.36 | 118.94 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 24 | T | 102 | BCR | C23-C22-C21 | 8.78 | 132.41 | 118.94 |
| 24 | t | 101 | BCR | C23-C22-C21 | 8.81 | 132.46 | 118.94 |
| 24 | B | 618 | BCR | C10-C11-C12 | 8.82 | 150.12 | 123.26 |
| 24 | T | 101 | BCR | C10-C11-C12 | 8.82 | 150.14 | 123.26 |
| 24 | k | 102 | BCR | C11-C10-C9 | 8.91 | 140.02 | 127.31 |
| 24 | K | 102 | BCR | C11-C10-C9 | 8.92 | 140.04 | 127.31 |
| 24 | b | 622 | BCR | C7-C8-C9 | 8.94 | 139.64 | 126.21 |
| 24 | B | 619 | BCR | C23-C22-C21 | 8.95 | 132.67 | 118.94 |
| 24 | B | 622 | BCR | C7-C8-C9 | 8.96 | 139.67 | 126.21 |
| 24 | b | 618 | BCR | C23-C22-C21 | 8.96 | 132.69 | 118.94 |
| 24 | H | 101 | BCR | C11-C12-C13 | 9.26 | 152.42 | 126.42 |
| 24 | h | 101 | BCR | C11-C12-C13 | 9.26 | 152.44 | 126.42 |
| 24 | t | 101 | BCR | C20-C19-C18 | 9.34 | 152.66 | 126.42 |
| 24 | t | 101 | BCR | C7-C8-C9 | 9.36 | 140.28 | 126.21 |
| 24 | T | 102 | BCR | C7-C8-C9 | 9.36 | 140.28 | 126.21 |
| 24 | T | 102 | BCR | C20-C19-C18 | 9.37 | 152.73 | 126.42 |
| 24 | k | 102 | BCR | C7-C8-C9 | 9.37 | 140.29 | 126.21 |
| 24 | K | 102 | BCR | C7-C8-C9 | 9.38 | 140.31 | 126.21 |
| 24 | B | 618 | BCR | C11-C12-C13 | 9.38 | 152.77 | 126.42 |
| 24 | T | 101 | BCR | C11-C12-C13 | 9.39 | 152.78 | 126.42 |
| 24 | D | 404 | BCR | C11-C12-C13 | 9.39 | 152.80 | 126.42 |
| 24 | d | 404 | BCR | C11-C12-C13 | 9.41 | 152.85 | 126.42 |
| 24 | h | 101 | BCR | C12-C13-C14 | 9.45 | 133.44 | 118.94 |
| 24 | H | 101 | BCR | C12-C13-C14 | 9.46 | 133.46 | 118.94 |
| 24 | B | 619 | BCR | C12-C13-C14 | 9.50 | 133.52 | 118.94 |
| 24 | d | 404 | BCR | C19-C18-C17 | 9.51 | 133.53 | 118.94 |
| 24 | D | 404 | BCR | C19-C18-C17 | 9.51 | 133.53 | 118.94 |
| 24 | b | 618 | BCR | C12-C13-C14 | 9.51 | 133.54 | 118.94 |
| 24 | d | 404 | BCR | C20-C19-C18 | 9.52 | 153.17 | 126.42 |
| 24 | D | 404 | BCR | C20-C19-C18 | 9.52 | 153.17 | 126.42 |
| 24 | c | 515 | BCR | C12-C13-C14 | 9.55 | 133.59 | 118.94 |
| 24 | C | 515 | BCR | C12-C13-C14 | 9.57 | 133.63 | 118.94 |
| 24 | C | 515 | BCR | C19-C18-C17 | 9.60 | 133.68 | 118.94 |
| 24 | c | 515 | BCR | C19-C18-C17 | 9.61 | 133.68 | 118.94 |
| 24 | k | 102 | BCR | C12-C13-C14 | 9.61 | 133.69 | 118.94 |
| 24 | K | 102 | BCR | C12-C13-C14 | 9.62 | 133.71 | 118.94 |
| 24 | H | 101 | BCR | C10-C11-C12 | 9.69 | 152.78 | 123.26 |
| 24 | c | 514 | BCR | C15-C14-C13 | 9.70 | 141.15 | 127.31 |
| 24 | C | 514 | BCR | C15-C14-C13 | 9.70 | 141.16 | 127.31 |
| 24 | h | 101 | BCR | C10-C11-C12 | 9.70 | 152.83 | 123.26 |
| 24 | A | 608 | BCR | C11-C12-C13 | 9.74 | 153.78 | 126.42 |
| 24 | a | 608 | BCR | C11-C12-C13 | 9.75 | 153.80 | 126.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24 | b | 622 | BCR | C19-C18-C17 | 9.77 | 133.93 | 118.94 |
| 24 | B | 622 | BCR | C19-C18-C17 | 9.77 | 133.93 | 118.94 |
| 24 | c | 514 | BCR | C7-C8-C9 | 9.77 | 140.90 | 126.21 |
| 24 | b | 622 | BCR | C15-C14-C13 | 9.83 | 141.34 | 127.31 |
| 24 | B | 622 | BCR | C15-C14-C13 | 9.83 | 141.34 | 127.31 |
| 24 | a | 608 | BCR | C10-C11-C12 | 9.83 | 153.22 | 123.26 |
| 24 | C | 514 | BCR | C7-C8-C9 | 9.83 | 140.99 | 126.21 |
| 24 | A | 608 | BCR | C10-C11-C12 | 9.84 | 153.24 | 123.26 |
| 24 | t | 101 | BCR | C11-C12-C13 | 10.11 | 154.81 | 126.42 |
| 24 | T | 102 | BCR | C11-C12-C13 | 10.11 | 154.83 | 126.42 |
| 24 | t | 101 | BCR | C15-C14-C13 | 10.28 | 141.99 | 127.31 |
| 24 | T | 102 | BCR | C15-C14-C13 | 10.34 | 142.07 | 127.31 |
| 24 | C | 515 | BCR | C10-C11-C12 | 10.35 | 154.81 | 123.26 |
| 24 | d | 404 | BCR | C11-C10-C9 | 10.36 | 142.10 | 127.31 |
| 24 | c | 515 | BCR | C10-C11-C12 | 10.37 | 154.85 | 123.26 |
| 24 | t | 101 | BCR | C10-C11-C12 | 10.37 | 154.86 | 123.26 |
| 24 | T | 102 | BCR | C10-C11-C12 | 10.39 | 154.93 | 123.26 |
| 24 | D | 404 | BCR | C11-C10-C9 | 10.39 | 142.15 | 127.31 |
| 24 | B | 622 | BCR | C21-C20-C19 | 10.40 | 154.94 | 123.26 |
| 24 | b | 622 | BCR | C21-C20-C19 | 10.42 | 155.00 | 123.26 |
| 24 | C | 514 | BCR | C19-C18-C17 | 10.54 | 135.11 | 118.94 |
| 24 | D | 404 | BCR | C15-C14-C13 | 10.55 | 142.36 | 127.31 |
| 24 | c | 514 | BCR | C19-C18-C17 | 10.56 | 135.15 | 118.94 |
| 24 | d | 404 | BCR | C15-C14-C13 | 10.58 | 142.41 | 127.31 |
| 24 | C | 514 | BCR | C11-C12-C13 | 10.59 | 156.18 | 126.42 |
| 24 | c | 514 | BCR | C11-C12-C13 | 10.60 | 156.18 | 126.42 |
| 24 | B | 619 | BCR | C20-C19-C18 | 10.69 | 156.44 | 126.42 |
| 24 | b | 618 | BCR | C20-C19-C18 | 10.71 | 156.50 | 126.42 |
| 24 | h | 101 | BCR | C19-C18-C17 | 10.72 | 135.40 | 118.94 |
| 24 | H | 101 | BCR | C19-C18-C17 | 10.72 | 135.40 | 118.94 |
| 24 | T | 101 | BCR | C20-C19-C18 | 10.73 | 156.55 | 126.42 |
| 24 | B | 618 | BCR | C20-C19-C18 | 10.74 | 156.58 | 126.42 |
| 24 | B | 622 | BCR | C20-C19-C18 | 10.75 | 156.61 | 126.42 |
| 24 | b | 622 | BCR | C20-C19-C18 | 10.76 | 156.64 | 126.42 |
| 24 | A | 608 | BCR | C15-C14-C13 | 10.77 | 142.68 | 127.31 |
| 24 | a | 608 | BCR | C15-C14-C13 | 10.79 | 142.71 | 127.31 |
| 24 | A | 608 | BCR | C12-C13-C14 | 10.85 | 135.59 | 118.94 |
| 24 | a | 608 | BCR | C12-C13-C14 | 10.86 | 135.60 | 118.94 |
| 24 | h | 101 | BCR | C20-C19-C18 | 10.89 | 157.02 | 126.42 |
| 24 | H | 101 | BCR | C20-C19-C18 | 10.90 | 157.04 | 126.42 |
| 24 | T | 101 | BCR | C11-C10-C9 | 11.01 | 143.03 | 127.31 |
| 24 | B | 618 | BCR | C11-C10-C9 | 11.03 | 143.05 | 127.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24 | K | 102 | BCR | C10-C11-C12 | 11.04 | 156.90 | 123.26 |
| 24 | k | 102 | BCR | C10-C11-C12 | 11.05 | 156.93 | 123.26 |
| 24 | A | 608 | BCR | C23-C22-C21 | 11.09 | 135.96 | 118.94 |
| 24 | a | 608 | BCR | C23-C22-C21 | 11.11 | 135.99 | 118.94 |
| 24 | k | 101 | BCR | C20-C19-C18 | 11.14 | 157.72 | 126.42 |
| 24 | K | 101 | BCR | C20-C19-C18 | 11.17 | 157.79 | 126.42 |
| 24 | K | 102 | BCR | C11-C12-C13 | 11.31 | 158.18 | 126.42 |
| 24 | k | 102 | BCR | C11-C12-C13 | 11.32 | 158.21 | 126.42 |
| 24 | K | 101 | BCR | C15-C14-C13 | 11.35 | 143.51 | 127.31 |
| 24 | a | 608 | BCR | C11-C10-C9 | 11.37 | 143.54 | 127.31 |
| 24 | k | 101 | BCR | C15-C14-C13 | 11.37 | 143.54 | 127.31 |
| 24 | A | 608 | BCR | C11-C10-C9 | 11.40 | 143.59 | 127.31 |
| 24 | T | 101 | BCR | C21-C20-C19 | 11.46 | 158.19 | 123.26 |
| 24 | B | 618 | BCR | C21-C20-C19 | 11.47 | 158.22 | 123.26 |
| 24 | c | 515 | BCR | C15-C14-C13 | 11.50 | 143.72 | 127.31 |
| 24 | C | 515 | BCR | C15-C14-C13 | 11.50 | 143.73 | 127.31 |
| 24 | h | 101 | BCR | C15-C14-C13 | 11.51 | 143.73 | 127.31 |
| 24 | H | 101 | BCR | C15-C14-C13 | 11.52 | 143.76 | 127.31 |
| 24 | B | 622 | BCR | C11-C12-C13 | 11.55 | 158.86 | 126.42 |
| 24 | b | 622 | BCR | C11-C12-C13 | 11.58 | 158.93 | 126.42 |
| 24 | B | 618 | BCR | C12-C13-C14 | 11.69 | 136.88 | 118.94 |
| 24 | T | 101 | BCR | C12-C13-C14 | 11.72 | 136.92 | 118.94 |
| 24 | B | 622 | BCR | C10-C11-C12 | 12.02 | 159.90 | 123.26 |
| 24 | b | 622 | BCR | C10-C11-C12 | 12.04 | 159.94 | 123.26 |
| 24 | C | 514 | BCR | C10-C11-C12 | 12.20 | 160.44 | 123.26 |
| 24 | c | 514 | BCR | C10-C11-C12 | 12.21 | 160.46 | 123.26 |
| 24 | K | 102 | BCR | C20-C19-C18 | 12.23 | 160.78 | 126.42 |
| 24 | K | 102 | BCR | C19-C18-C17 | 12.24 | 137.73 | 118.94 |
| 24 | k | 102 | BCR | C19-C18-C17 | 12.24 | 137.73 | 118.94 |
| 24 | k | 102 | BCR | C20-C19-C18 | 12.25 | 160.84 | 126.42 |
| 24 | B | 622 | BCR | C11-C10-C9 | 12.27 | 144.82 | 127.31 |
| 24 | b | 622 | BCR | C11-C10-C9 | 12.28 | 144.84 | 127.31 |
| 24 | c | 515 | BCR | C20-C19-C18 | 12.34 | 161.08 | 126.42 |
| 24 | C | 515 | BCR | C20-C19-C18 | 12.36 | 161.13 | 126.42 |
| 24 | a | 608 | BCR | C19-C18-C17 | 12.44 | 138.03 | 118.94 |
| 24 | A | 608 | BCR | C19-C18-C17 | 12.47 | 138.07 | 118.94 |
| 24 | t | 101 | BCR | C11-C10-C9 | 12.54 | 145.20 | 127.31 |
| 24 | T | 102 | BCR | C11-C10-C9 | 12.62 | 145.32 | 127.31 |
| 24 | k | 101 | BCR | C19-C18-C17 | 12.64 | 138.34 | 118.94 |
| 24 | c | 514 | BCR | C20-C19-C18 | 12.68 | 162.03 | 126.42 |
| 24 | C | 514 | BCR | C20-C19-C18 | 12.68 | 162.05 | 126.42 |
| 24 | K | 101 | BCR | C19-C18-C17 | 12.69 | 138.41 | 118.94 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24 | D | 404 | BCR | C21-C20-C19 | 12.96 | 162.75 | 123.26 |
| 24 | d | 404 | BCR | C21-C20-C19 | 12.96 | 162.76 | 123.26 |
| 24 | a | 608 | BCR | C21-C20-C19 | 12.99 | 162.84 | 123.26 |
| 24 | A | 608 | BCR | C21-C20-C19 | 13.01 | 162.90 | 123.26 |
| 24 | K | 101 | BCR | C11-C10-C9 | 13.01 | 145.88 | 127.31 |
| 24 | k | 101 | BCR | C11-C10-C9 | 13.02 | 145.89 | 127.31 |
| 24 | t | 101 | BCR | C19-C18-C17 | 13.20 | 139.20 | 118.94 |
| 24 | T | 102 | BCR | C19-C18-C17 | 13.25 | 139.28 | 118.94 |
| 24 | b | 618 | BCR | C11-C10-C9 | 13.30 | 146.29 | 127.31 |
| 24 | B | 619 | BCR | C11-C10-C9 | 13.32 | 146.32 | 127.31 |
| 24 | B | 618 | BCR | C16-C15-C14 | 13.54 | 152.35 | 123.46 |
| 24 | b | 618 | BCR | C15-C14-C13 | 13.55 | 146.65 | 127.31 |
| 24 | T | 101 | BCR | C16-C15-C14 | 13.56 | 152.40 | 123.46 |
| 24 | B | 619 | BCR | C15-C14-C13 | 13.56 | 146.66 | 127.31 |
| 24 | t | 101 | BCR | C21-C20-C19 | 13.62 | 164.76 | 123.26 |
| 24 | T | 102 | BCR | C21-C20-C19 | 13.64 | 164.81 | 123.26 |
| 24 | h | 101 | BCR | C11-C10-C9 | 13.82 | 147.04 | 127.31 |
| 24 | H | 101 | BCR | C11-C10-C9 | 13.83 | 147.04 | 127.31 |
| 24 | B | 622 | BCR | C20-C21-C22 | 13.98 | 147.26 | 127.31 |
| 24 | b | 622 | BCR | C20-C21-C22 | 13.99 | 147.27 | 127.31 |
| 24 | A | 608 | BCR | C16-C15-C14 | 14.03 | 153.41 | 123.46 |
| 24 | k | 102 | BCR | C21-C20-C19 | 14.04 | 166.03 | 123.26 |
| 24 | a | 608 | BCR | C16-C15-C14 | 14.04 | 153.43 | 123.46 |
| 24 | K | 102 | BCR | C21-C20-C19 | 14.04 | 166.04 | 123.26 |
| 24 | k | 102 | BCR | C15-C14-C13 | 14.15 | 147.51 | 127.31 |
| 24 | K | 102 | BCR | C15-C14-C13 | 14.16 | 147.51 | 127.31 |
| 24 | B | 619 | BCR | C19-C18-C17 | 14.37 | 140.99 | 118.94 |
| 24 | b | 618 | BCR | C19-C18-C17 | 14.37 | 141.00 | 118.94 |
| 24 | C | 515 | BCR | C11-C10-C9 | 14.47 | 147.96 | 127.31 |
| 24 | c | 515 | BCR | C11-C10-C9 | 14.47 | 147.97 | 127.31 |
| 24 | B | 619 | BCR | C21-C20-C19 | 14.93 | 168.76 | 123.26 |
| 24 | b | 618 | BCR | C21-C20-C19 | 14.95 | 168.82 | 123.26 |
| 24 | k | 101 | BCR | C21-C20-C19 | 14.96 | 168.83 | 123.26 |
| 24 | K | 101 | BCR | C21-C20-C19 | 14.96 | 168.84 | 123.26 |
| 24 | B | 619 | BCR | C16-C15-C14 | 15.22 | 155.96 | 123.46 |
| 24 | b | 618 | BCR | C16-C15-C14 | 15.23 | 155.97 | 123.46 |
| 24 | H | 101 | BCR | C21-C20-C19 | 15.31 | 169.92 | 123.26 |
| 24 | h | 101 | BCR | C21-C20-C19 | 15.31 | 169.92 | 123.26 |
| 24 | B | 619 | BCR | C15-C16-C17 | 15.39 | 156.31 | 123.46 |
| 24 | b | 618 | BCR | C15-C16-C17 | 15.40 | 156.33 | 123.46 |
| 24 | h | 101 | BCR | C16-C15-C14 | 15.44 | 156.42 | 123.46 |
| 24 | T | 101 | BCR | C19-C18-C17 | 15.46 | 142.66 | 118.94 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24 | H | 101 | BCR | C16-C15-C14 | 15.47 | 156.47 | 123.46 |
| 24 | B | 618 | BCR | C19-C18-C17 | 15.48 | 142.69 | 118.94 |
| 24 | K | 101 | BCR | C16-C15-C14 | 15.89 | 157.37 | 123.46 |
| 24 | k | 101 | BCR | C16-C15-C14 | 15.90 | 157.39 | 123.46 |
| 24 | c | 515 | BCR | C21-C20-C19 | 16.67 | 174.04 | 123.26 |
| 24 | C | 515 | BCR | C21-C20-C19 | 16.67 | 174.06 | 123.26 |
| 24 | b | 622 | BCR | C16-C17-C18 | 17.22 | 151.88 | 127.31 |
| 24 | B | 622 | BCR | C16-C17-C18 | 17.24 | 151.91 | 127.31 |
| 24 | c | 514 | BCR | C21-C20-C19 | 17.31 | 176.01 | 123.26 |
| 24 | C | 514 | BCR | C21-C20-C19 | 17.33 | 176.07 | 123.26 |
| 24 | a | 608 | BCR | C15-C16-C17 | 17.40 | 160.60 | 123.46 |
| 24 | A | 608 | BCR | C15-C16-C17 | 17.41 | 160.63 | 123.46 |
| 24 | t | 101 | BCR | C16-C15-C14 | 17.66 | 161.15 | 123.46 |
| 24 | T | 102 | BCR | C16-C15-C14 | 17.67 | 161.18 | 123.46 |
| 24 | T | 101 | BCR | C20-C21-C22 | 18.05 | 153.07 | 127.31 |
| 24 | B | 618 | BCR | C20-C21-C22 | 18.05 | 153.07 | 127.31 |
| 24 | K | 102 | BCR | C16-C15-C14 | 18.43 | 162.80 | 123.46 |
| 24 | k | 102 | BCR | C16-C15-C14 | 18.46 | 162.86 | 123.46 |
| 24 | k | 102 | BCR | C16-C17-C18 | 18.72 | 154.02 | 127.31 |
| 24 | K | 102 | BCR | C16-C17-C18 | 18.73 | 154.04 | 127.31 |
| 24 | B | 618 | BCR | C15-C16-C17 | 18.88 | 163.77 | 123.46 |
| 24 | T | 101 | BCR | C15-C16-C17 | 18.93 | 163.86 | 123.46 |
| 24 | d | 404 | BCR | C16-C15-C14 | 19.37 | 164.81 | 123.46 |
| 24 | D | 404 | BCR | C16-C15-C14 | 19.38 | 164.82 | 123.46 |
| 24 | b | 622 | BCR | C16-C15-C14 | 19.53 | 165.14 | 123.46 |
| 24 | B | 622 | BCR | C16-C15-C14 | 19.54 | 165.18 | 123.46 |
| 24 | k | 101 | BCR | C15-C16-C17 | 19.88 | 165.89 | 123.46 |
| 24 | K | 101 | BCR | C15-C16-C17 | 19.88 | 165.89 | 123.46 |
| 24 | C | 514 | BCR | C16-C15-C14 | 19.88 | 165.91 | 123.46 |
| 24 | c | 514 | BCR | C16-C15-C14 | 19.90 | 165.94 | 123.46 |
| 24 | b | 622 | BCR | C15-C16-C17 | 20.30 | 166.79 | 123.46 |
| 24 | B | 622 | BCR | C15-C16-C17 | 20.33 | 166.85 | 123.46 |
| 24 | H | 101 | BCR | C16-C17-C18 | 20.52 | 156.59 | 127.31 |
| 24 | h | 101 | BCR | C16-C17-C18 | 20.53 | 156.61 | 127.31 |
| 24 | c | 515 | BCR | C16-C17-C18 | 20.61 | 156.72 | 127.31 |
| 24 | C | 515 | BCR | C16-C17-C18 | 20.61 | 156.73 | 127.31 |
| 24 | b | 618 | BCR | C16-C17-C18 | 20.62 | 156.74 | 127.31 |
| 24 | B | 619 | BCR | C16-C17-C18 | 20.63 | 156.75 | 127.31 |
| 24 | c | 515 | BCR | C16-C15-C14 | 20.92 | 168.10 | 123.46 |
| 24 | k | 102 | BCR | C20-C21-C22 | 20.93 | 157.18 | 127.31 |
| 24 | C | 515 | BCR | C16-C15-C14 | 20.94 | 168.15 | 123.46 |
| 24 | K | 102 | BCR | C20-C21-C22 | 20.98 | 157.25 | 127.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24 | K | 102 | BCR | C15-C16-C17 | 21.47 | 169.28 | 123.46 |
| 24 | k | 102 | BCR | C15-C16-C17 | 21.49 | 169.34 | 123.46 |
| 24 | a | 608 | BCR | C16-C17-C18 | 21.52 | 158.03 | 127.31 |
| 24 | A | 608 | BCR | C16-C17-C18 | 21.54 | 158.06 | 127.31 |
| 24 | B | 619 | BCR | C20-C21-C22 | 21.92 | 158.59 | 127.31 |
| 24 | b | 618 | BCR | C20-C21-C22 | 21.92 | 158.60 | 127.31 |
| 24 | d | 404 | BCR | C15-C16-C17 | 22.28 | 171.02 | 123.46 |
| 24 | D | 404 | BCR | C15-C16-C17 | 22.30 | 171.05 | 123.46 |
| 24 | D | 404 | BCR | C16-C17-C18 | 22.31 | 159.15 | 127.31 |
| 24 | d | 404 | BCR | C16-C17-C18 | 22.32 | 159.16 | 127.31 |
| 24 | D | 404 | BCR | C20-C21-C22 | 22.47 | 159.38 | 127.31 |
| 24 | d | 404 | BCR | C20-C21-C22 | 22.49 | 159.41 | 127.31 |
| 24 | c | 515 | BCR | C15-C16-C17 | 22.73 | 171.97 | 123.46 |
| 24 | C | 515 | BCR | C15-C16-C17 | 22.76 | 172.04 | 123.46 |
| 24 | c | 514 | BCR | C20-C21-C22 | 23.05 | 160.21 | 127.31 |
| 24 | C | 514 | BCR | C20-C21-C22 | 23.07 | 160.23 | 127.31 |
| 24 | K | 101 | BCR | C16-C17-C18 | 23.32 | 160.59 | 127.31 |
| 24 | k | 101 | BCR | C16-C17-C18 | 23.33 | 160.61 | 127.31 |
| 24 | B | 618 | BCR | C16-C17-C18 | 24.19 | 161.83 | 127.31 |
| 24 | T | 101 | BCR | C16-C17-C18 | 24.20 | 161.85 | 127.31 |
| 24 | H | 101 | BCR | C15-C16-C17 | 24.29 | 175.32 | 123.46 |
| 24 | h | 101 | BCR | C15-C16-C17 | 24.30 | 175.33 | 123.46 |
| 24 | T | 102 | BCR | C15-C16-C17 | 24.33 | 175.40 | 123.46 |
| 24 | t | 101 | BCR | C15-C16-C17 | 24.35 | 175.44 | 123.46 |
| 24 | C | 514 | BCR | C16-C17-C18 | 25.06 | 163.08 | 127.31 |
| 24 | c | 514 | BCR | C16-C17-C18 | 25.08 | 163.11 | 127.31 |
| 24 | A | 608 | BCR | C20-C21-C22 | 25.15 | 163.21 | 127.31 |
| 24 | a | 608 | BCR | C20-C21-C22 | 25.16 | 163.21 | 127.31 |
| 24 | T | 102 | BCR | C16-C17-C18 | 25.43 | 163.60 | 127.31 |
| 24 | t | 101 | BCR | C16-C17-C18 | 25.44 | 163.61 | 127.31 |
| 24 | k | 101 | BCR | C20-C21-C22 | 25.55 | 163.77 | 127.31 |
| 24 | K | 101 | BCR | C20-C21-C22 | 25.57 | 163.81 | 127.31 |
| 24 | c | 515 | BCR | C20-C21-C22 | 25.67 | 163.95 | 127.31 |
| 24 | C | 514 | BCR | C15-C16-C17 | 25.71 | 178.33 | 123.46 |
| 24 | C | 515 | BCR | C20-C21-C22 | 25.73 | 164.04 | 127.31 |
| 24 | c | 514 | BCR | C15-C16-C17 | 25.75 | 178.43 | 123.46 |
| 24 | t | 101 | BCR | C20-C21-C22 | 26.58 | 165.24 | 127.31 |
| 24 | T | 102 | BCR | C20-C21-C22 | 26.60 | 165.27 | 127.31 |
| 24 | h | 101 | BCR | C20-C21-C22 | 26.91 | 165.71 | 127.31 |
| 24 | H | 101 | BCR | C20-C21-C22 | 26.91 | 165.72 | 127.31 |

All (166) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 22 | B | 617 | CLA | NC |
| 22 | B | 617 | CLA | ND |
| 22 | B | 617 | CLA | NA |
| 22 | c | 513 | CLA | NC |
| 22 | c | 513 | CLA | NA |
| 22 | A | 607 | CLA | NC |
| 22 | d | 402 | CLA | NA |
| 22 | c | 511 | CLA | NC |
| 22 | c | 511 | CLA | NA |
| 22 | B | 610 | CLA | NC |
| 22 | B | 610 | CLA | ND |
| 22 | c | 502 | CLA | NA |
| 22 | B | 614 | CLA | NC |
| 22 | B | 614 | CLA | ND |
| 22 | B | 614 | CLA | NA |
| 22 | b | 602 | CLA | ND |
| 22 | b | 602 | CLA | NA |
| 22 | D | 403 | CLA | NC |
| 22 | D | 403 | CLA | NA |
| 22 | c | 508 | CLA | NC |
| 22 | c | 508 | CLA | NA |
| 22 | b | 612 | CLA | NC |
| 22 | b | 612 | CLA | NA |
| 22 | B | 609 | CLA | NC |
| 22 | b | 605 | CLA | NC |
| 22 | b | 605 | CLA | ND |
| 22 | b | 605 | CLA | NA |
| 22 | B | 606 | CLA | NC |
| 22 | B | 606 | CLA | ND |
| 22 | B | 606 | CLA | NA |
| 22 | B | 612 | CLA | NC |
| 22 | B | 612 | CLA | NA |
| 22 | b | 617 | CLA | NC |
| 22 | b | 617 | CLA | ND |
| 22 | b | 617 | CLA | NA |
| 22 | B | 605 | CLA | NC |
| 22 | B | 605 | CLA | ND |
| 22 | B | 605 | CLA | NA |
| 22 | C | 505 | CLA | ND |
| 22 | A | 603 | CLA | NC |
| 22 | A | 603 | CLA | ND |
| 22 | A | 603 | CLA | NA |
| 22 | C | 501 | CLA | NC |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 22 | C | 501 | CLA | NA |
| 22 | c | 503 | CLA | NC |
| 22 | c | 503 | CLA | ND |
| 22 | c | 503 | CLA | NA |
| 22 | b | 613 | CLA | NA |
| 22 | b | 613 | CLA | NC |
| 22 | b | 613 | CLA | ND |
| 22 | b | 608 | CLA | NC |
| 22 | b | 608 | CLA | ND |
| 22 | b | 608 | CLA | NA |
| 22 | b | 606 | CLA | NC |
| 22 | b | 606 | CLA | ND |
| 22 | b | 606 | CLA | NA |
| 22 | B | 603 | CLA | NC |
| 22 | B | 603 | CLA | ND |
| 22 | B | 603 | CLA | NA |
| 22 | c | 504 | CLA | NC |
| 22 | c | 504 | CLA | ND |
| 22 | c | 504 | CLA | NA |
| 22 | B | 602 | CLA | ND |
| 22 | B | 602 | CLA | NA |
| 22 | c | 507 | CLA | NC |
| 22 | c | 507 | CLA | ND |
| 22 | c | 507 | CLA | NA |
| 22 | b | 610 | CLA | NC |
| 22 | b | 610 | CLA | ND |
| 22 | B | 616 | CLA | NC |
| 22 | B | 616 | CLA | ND |
| 22 | B | 616 | CLA | NA |
| 22 | D | 401 | CLA | ND |
| 22 | c | 509 | CLA | NC |
| 22 | c | 509 | CLA | ND |
| 22 | c | 509 | CLA | NA |
| 22 | b | 611 | CLA | NC |
| 22 | b | 611 | CLA | ND |
| 22 | b | 611 | CLA | NA |
| 22 | c | 510 | CLA | NC |
| 22 | c | 510 | CLA | ND |
| 22 | c | 510 | CLA | NA |
| 22 | B | 607 | CLA | NC |
| 22 | B | 607 | CLA | NA |
| 22 | C | 508 | CLA | NC |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 22 | C | 508 | CLA | NA |
| 22 | C | 504 | CLA | NC |
| 22 | C | 504 | CLA | ND |
| 22 | C | 504 | CLA | NA |
| 22 | d | 401 | CLA | ND |
| 22 | c | 501 | CLA | NC |
| 22 | c | 501 | CLA | NA |
| 22 | B | 608 | CLA | NC |
| 22 | B | 608 | CLA | ND |
| 22 | B | 608 | CLA | NA |
| 22 | b | 604 | CLA | NC |
| 22 | b | 604 | CLA | ND |
| 22 | b | 604 | CLA | NA |
| 22 | C | 513 | CLA | NC |
| 22 | C | 513 | CLA | NA |
| 22 | b | 616 | CLA | NC |
| 22 | b | 616 | CLA | ND |
| 22 | b | 616 | CLA | NA |
| 22 | a | 603 | CLA | NC |
| 22 | a | 603 | CLA | ND |
| 22 | a | 603 | CLA | NA |
| 22 | D | 402 | CLA | NA |
| 22 | C | 502 | CLA | NA |
| 22 | b | 607 | CLA | NC |
| 22 | b | 607 | CLA | NA |
| 22 | a | 604 | CLA | NC |
| 22 | a | 604 | CLA | NA |
| 22 | c | 505 | CLA | ND |
| 22 | b | 603 | CLA | NC |
| 22 | b | 603 | CLA | ND |
| 22 | b | 603 | CLA | NA |
| 22 | b | 609 | CLA | NC |
| 22 | A | 604 | CLA | NC |
| 22 | A | 604 | CLA | NA |
| 22 | B | 611 | CLA | NC |
| 22 | B | 611 | CLA | ND |
| 22 | B | 611 | CLA | NA |
| 22 | C | 512 | CLA | NC |
| 22 | C | 512 | CLA | NA |
| 22 | C | 512 | CLA | ND |
| 22 | b | 615 | CLA | NC |
| 22 | b | 615 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 22 | b | 615 | CLA | NA |
| 22 | C | 506 | CLA | NC |
| 22 | C | 506 | CLA | ND |
| 22 | C | 506 | CLA | NA |
| 22 | C | 507 | CLA | NC |
| 22 | C | 507 | CLA | ND |
| 22 | C | 507 | CLA | NA |
| 22 | B | 613 | CLA | NA |
| 22 | B | 613 | CLA | NC |
| 22 | B | 613 | CLA | ND |
| 22 | c | 512 | CLA | NC |
| 22 | c | 512 | CLA | NA |
| 22 | c | 512 | CLA | ND |
| 22 | B | 615 | CLA | NC |
| 22 | B | 615 | CLA | ND |
| 22 | B | 615 | CLA | NA |
| 22 | c | 506 | CLA | NC |
| 22 | c | 506 | CLA | ND |
| 22 | c | 506 | CLA | NA |
| 22 | d | 403 | CLA | NC |
| 22 | d | 403 | CLA | NA |
| 22 | B | 604 | CLA | NC |
| 22 | B | 604 | CLA | ND |
| 22 | B | 604 | CLA | NA |
| 22 | C | 509 | CLA | NC |
| 22 | C | 509 | CLA | ND |
| 22 | C | 509 | CLA | NA |
| 22 | a | 607 | CLA | NC |
| 22 | C | 511 | CLA | NC |
| 22 | C | 511 | CLA | NA |
| 22 | C | 510 | CLA | NC |
| 22 | C | 510 | CLA | ND |
| 22 | C | 510 | CLA | NA |
| 22 | b | 614 | CLA | NC |
| 22 | b | 614 | CLA | ND |
| 22 | b | 614 | CLA | NA |
| 22 | C | 503 | CLA | NC |
| 22 | C | 503 | CLA | ND |
| 22 | C | 503 | CLA | NA |

All (2) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 29 | z | 101 | LMG | C7-O1-C1-O6 |
| 29 | Z | 101 | LMG | C7-O1-C1-O6 |

There are no ring outliers.

62 monomers are involved in 148 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 22 | A | 603 | CLA | 5 | 0 |
| 22 | A | 604 | CLA | 3 | 0 |
| 23 | A | 605 | PHO | 2 | 0 |
| 23 | A | 606 | PHO | 4 | 0 |
| 22 | A | 607 | CLA | 2 | 0 |
| 24 | A | 608 | BCR | 1 | 0 |
| 25 | A | 609 | SQD | 2 | 0 |
| 28 | A | 613 | PL9 | 8 | 0 |
| 29 | A | 614 | LMG | 3 | 0 |
| 25 | B | 601 | SQD | 4 | 0 |
| 22 | B | 603 | CLA | 1 | 0 |
| 22 | B | 604 | CLA | 2 | 0 |
| 22 | B | 605 | CLA | 2 | 0 |
| 22 | B | 606 | CLA | 5 | 0 |
| 22 | B | 607 | CLA | 2 | 0 |
| 22 | B | 609 | CLA | 2 | 0 |
| 22 | B | 611 | CLA | 4 | 0 |
| 22 | B | 612 | CLA | 2 | 0 |
| 22 | B | 613 | CLA | 3 | 0 |
| 22 | B | 614 | CLA | 5 | 0 |
| 22 | B | 615 | CLA | 3 | 0 |
| 22 | B | 616 | CLA | 2 | 0 |
| 22 | B | 617 | CLA | 4 | 0 |
| 24 | B | 618 | BCR | 3 | 0 |
| 24 | B | 619 | BCR | 1 | 0 |
| 29 | B | 620 | LMG | 3 | 0 |
| 24 | B | 622 | BCR | 4 | 0 |
| 22 | C | 501 | CLA | 2 | 0 |
| 22 | C | 502 | CLA | 3 | 0 |
| 22 | C | 503 | CLA | 3 | 0 |
| 22 | C | 504 | CLA | 1 | 0 |
| 22 | C | 505 | CLA | 2 | 0 |
| 22 | C | 506 | CLA | 4 | 0 |
| 22 | C | 507 | CLA | 1 | 0 |
| 22 | C | 508 | CLA | 3 | 0 |
| 22 | C | 509 | CLA | 2 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 22 | C | 510 | CLA | 6 | 0 |
| 22 | C | 511 | CLA | 2 | 0 |
| 22 | C | 512 | CLA | 3 | 0 |
| 22 | C | 513 | CLA | 1 | 0 |
| 31 | C | 516 | DGD | 2 | 0 |
| 31 | C | 517 | DGD | 2 | 0 |
| 31 | C | 518 | DGD | 1 | 0 |
| 29 | C | 519 | LMG | 1 | 0 |
| 22 | D | 401 | CLA | 1 | 0 |
| 22 | D | 402 | CLA | 4 | 0 |
| 22 | D | 403 | CLA | 3 | 0 |
| 24 | D | 404 | BCR | 3 | 0 |
| 29 | D | 406 | LMG | 2 | 0 |
| 32 | D | 409 | LHG | 13 | 0 |
| 31 | D | 410 | DGD | 3 | 0 |
| 32 | E | 101 | LHG | 2 | 0 |
| 33 | F | 101 | HEM | 1 | 0 |
| 24 | H | 101 | BCR | 1 | 0 |
| 31 | H | 102 | DGD | 1 | 0 |
| 24 | K | 102 | BCR | 1 | 0 |
| 25 | L | 101 | SQD | 5 | 0 |
| 32 | L | 102 | LHG | 1 | 0 |
| 24 | T | 101 | BCR | 7 | 0 |
| 24 | T | 102 | BCR | 2 | 0 |
| 33 | V | 201 | HEM | 9 | 0 |
| 29 | Z | 101 | LMG | 1 | 0 |

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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 | 334/334 (100%) | 0.59 | 19 (5%) 24 22 | 16, 22, 43, 53 | 0 |
| 1 | a | 334/334 (100%) | 0.60 | 26 (7%) 13 13 | 16, 22, 43, 53 | 0 |
| 2 | B | 504/504 (100%) | 0.48 | 33 (6%) 19 17 | 18, 27, 49, 70 | 0 |
| 2 | b | 504/504 (100%) | 0.76 | 72 (14%) 2 4 | 18, 27, 49, 70 | 0 |
| 3 | C | 451/461 (97%) | 0.64 | 44 (9%) 7 8 | 21, 31, 44, 56 | 0 |
| 3 | c | 451/461 (97%) | 0.52 | 37 (8%) 11 12 | 21, 31, 44, 56 | 0 |
| 4 | D | 342/342 (100%) | 0.78 | 32 (9%) 8 9 | 17, 23, 39, 61 | 0 |
| 4 | d | 342/342 (100%) | 0.70 | 24 (7%) 16 15 | 17, 23, 39, 61 | 0 |
| 5 | E | 81/81 (100%) | 0.83 | 10 (12%) 4 6 | 27, 40, 57, 63 | 0 |
| 5 | e | 81/81 (100%) | 0.42 | 9 (11%) 5 6 | 27, 40, 57, 63 | 0 |
| 6 | F | 34/34 (100%) | 0.36 | 1 (2%) 51 42 | 28, 33, 58, 61 | 0 |
| 6 | f | 34/34 (100%) | -0.00 | 0 100 100 | 28, 33, 58, 61 | 0 |
| 7 | H | 65/65 (100%) | 0.66 | 10 (15%) 2 3 | 23, 34, 40, 58 | 0 |
| 7 | h | 65/65 (100%) | 1.42 | 19 (29%) 0 1 | 23, 34, 40, 58 | 0 |
| 8 | I | 38/38 (100%) | 0.54 | 4 (10%) 6 7 | 30, 34, 65, 68 | 0 |
| 8 | i | 38/38 (100%) | 0.08 | 4 (10%) 6 7 | 30, 34, 65, 68 | 0 |
| 9 | J | 38/40 (95%) | 0.56 | 3 (7%) 12 12 | 26, 37, 68, 72 | 0 |
| 9 | j | 38/40 (95%) | -0.14 | 0 100 100 | 26, 37, 68, 72 | 0 |
| 10 | K | 37/37 (100%) | 0.51 | 2 (5%) 26 24 | 33, 38, 45, 47 | 0 |
| 10 | k | 37/37 (100%) | 0.60 | 4 (10%) 6 6 | 33, 38, 45, 47 | 0 |
| 11 | L | 37/37 (100%) | 0.59 | 1 (2%) 54 46 | 17, 22, 50, 59 | 0 |
| 11 | l | 37/37 (100%) | 0.59 | 3 (8%) 12 12 | 17, 22, 50, 59 | 0 |
| 12 | M | 34/34 (100%) | 1.02 | 6 (17%) 1 3 | 21, 23, 36, 52 | 0 |
| 12 | m | 34/34 (100%) | 0.74 | 3 (8%) 10 10 | 21, 23, 36, 52 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 13 | O | 243/243 (100%) | 0.38 | 8 (3%) 46 38 | 18, 32, 55, 71 | 0 |
| 13 | o | 243/243 (100%) | 0.56 | 15 (6%) 20 19 | 18, 32, 55, 71 | 0 |
| 14 | T | 30/30 (100%) | 0.86 | 3 (10%) 7 8 | 19, 23, 44, 52 | 0 |
| 14 | t | 30/30 (100%) | 0.84 | 1 (3%) 46 38 | 19, 23, 44, 52 | 0 |
| 15 | U | 97/97 (100%) | 0.30 | 2 (2%) 63 55 | 23, 30, 48, 50 | 0 |
| 15 | u | 97/97 (100%) | 0.55 | 6 (6%) 20 19 | 23, 30, 48, 50 | 0 |
| 16 | V | 137/137 (100%) | 0.22 | 2 (1%) 73 65 | 23, 28, 39, 48 | 0 |
| 16 | v | 137/137 (100%) | 0.38 | 6 (4%) 34 30 | 23, 28, 39, 48 | 0 |
| 17 | X | 39/39 (100%) | 0.99 | 7 (17%) 1 3 | 33, 40, 66, 68 | 0 |
| 17 | x | 39/39 (100%) | 1.00 | 7 (17%) 1 3 | 33, 40, 66, 68 | 0 |
| 18 | Y | 29/29 (100%) | 0.68 | 3 (10%) 6 7 | 42, 48, 75, 77 | 0 |
| 18 | y | 29/29 (100%) | 0.29 | 0 100 100 | 42, 48, 75, 77 | 0 |
| 19 | Z | 62/62 (100%) | 0.48 | 2 (3%) 47 39 | 39, 48, 68, 72 | 0 |
| 19 | z | 62/62 (100%) | 0.69 | 7 (11%) 5 6 | 39, 48, 68, 72 | 0 |
| All | All | 5264/5288 (99%) | 0.59 | 435 (8%) 11 11 | 16, 29, 51, 77 | 0 |

All (435) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 17 | X | 2 | THR | 7.3 |
| 4 | D | 59 | TYR | 6.8 |
| 9 | J | 3 | SER | 6.6 |
| 4 | D | 56 | THR | 5.7 |
| 4 | d | 136 | VAL | 5.5 |
| 1 | a | 140 | ARG | 5.4 |
| 4 | D | 136 | VAL | 5.4 |
| 2 | b | 270 | PRO | 5.3 |
| 1 | a | 138 | GLY | 5.2 |
| 3 | C | 24 | THR | 5.2 |
| 4 | d | 59 | TYR | 5.1 |
| 2 | b | 499 | VAL | 5.0 |
| 17 | x | 2 | THR | 5.0 |
| 2 | b | 262 | THR | 5.0 |
| 3 | C | 256 | PRO | 5.0 |
| 4 | d | 135 | LEU | 4.9 |
| 1 | a | 139 | MET | 4.8 |
| 7 | H | 56 | ASP | 4.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3 | C | 265 | ILE | 4.8 |
| 3 | c | 146 | PHE | 4.7 |
| 4 | d | 107 | LEU | 4.7 |
| 3 | c | 198 | VAL | 4.7 |
| 2 | b | 187 | PRO | 4.6 |
| 4 | d | 106 | GLN | 4.6 |
| 2 | b | 435 | GLU | 4.5 |
| 3 | C | 137 | PRO | 4.5 |
| 1 | a | 245 | THR | 4.5 |
| 2 | b | 131 | PRO | 4.4 |
| 4 | D | 106 | GLN | 4.4 |
| 3 | C | 264 | PHE | 4.4 |
| 2 | b | 500 | GLY | 4.4 |
| 12 | M | 2 | GLU | 4.3 |
| 7 | h | 23 | PRO | 4.3 |
| 3 | C | 138 | GLU | 4.3 |
| 3 | c | 228 | ASN | 4.2 |
| 3 | C | 97 | TRP | 4.2 |
| 3 | c | 86 | LEU | 4.1 |
| 2 | B | 136 | PRO | 4.1 |
| 4 | D | 135 | LEU | 4.1 |
| 5 | E | 49 | THR | 4.1 |
| 6 | F | 12 | SER | 4.1 |
| 4 | D | 55 | VAL | 4.1 |
| 7 | H | 55 | LEU | 4.1 |
| 17 | X | 40 | SER | 4.1 |
| 2 | b | 71 | VAL | 4.1 |
| 1 | A | 245 | THR | 4.1 |
| 2 | b | 261 | ALA | 4.0 |
| 3 | c | 197 | ARG | 4.0 |
| 7 | h | 55 | LEU | 4.0 |
| 3 | C | 266 | TRP | 3.9 |
| 4 | d | 137 | GLY | 3.9 |
| 19 | z | 62 | VAL | 3.9 |
| 2 | b | 361 | ALA | 3.9 |
| 19 | Z | 1 | MET | 3.9 |
| 4 | D | 137 | GLY | 3.9 |
| 17 | x | 40 | SER | 3.9 |
| 2 | b | 188 | ASP | 3.8 |
| 3 | C | 25 | ASN | 3.8 |
| 4 | d | 264 | LYS | 3.8 |
| 2 | b | 267 | LEU | 3.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 16 | v | 21 | LEU | 3.7 |
| 1 | a | 246 | TYR | 3.7 |
| 3 | c | 127 | PHE | 3.7 |
| 3 | C | 400 | PRO | 3.7 |
| 1 | A | 11 | ALA | 3.7 |
| 3 | C | 146 | PHE | 3.6 |
| 1 | A | 262 | TYR | 3.6 |
| 1 | A | 317 | TRP | 3.6 |
| 17 | x | 3 | ILE | 3.6 |
| 2 | b | 70 | GLY | 3.6 |
| 2 | b | 190 | PHE | 3.5 |
| 15 | U | 8 | GLU | 3.5 |
| 4 | d | 29 | PHE | 3.5 |
| 4 | D | 107 | LEU | 3.5 |
| 3 | C | 263 | ALA | 3.5 |
| 4 | d | 221 | THR | 3.5 |
| 2 | b | 218 | LEU | 3.5 |
| 7 | h | 54 | ILE | 3.5 |
| 19 | z | 23 | VAL | 3.5 |
| 19 | z | 61 | VAL | 3.5 |
| 2 | b | 229 | LEU | 3.5 |
| 4 | D | 27 | PHE | 3.5 |
| 2 | B | 43 | ALA | 3.5 |
| 19 | z | 1 | MET | 3.5 |
| 3 | c | 373 | ASN | 3.4 |
| 3 | C | 457 | LYS | 3.4 |
| 13 | o | 243 | ILE | 3.4 |
| 5 | e | 84 | LYS | 3.4 |
| 2 | B | 499 | VAL | 3.4 |
| 1 | A | 137 | LEU | 3.4 |
| 1 | A | 139 | MET | 3.4 |
| 4 | d | 54 | PHE | 3.3 |
| 18 | Y | 46 | LEU | 3.3 |
| 7 | h | 56 | ASP | 3.3 |
| 2 | B | 367 | PRO | 3.3 |
| 2 | B | 362 | PHE | 3.3 |
| 4 | D | 93 | TRP | 3.3 |
| 7 | h | 27 | THR | 3.3 |
| 7 | h | 53 | LEU | 3.3 |
| 2 | B | 183 | PRO | 3.3 |
| 13 | O | 243 | ILE | 3.2 |
| 7 | H | 65 | LEU | 3.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | a | 137 | LEU | 3.2 |
| 2 | b | 133 | LEU | 3.2 |
| 4 | D | 32 | TRP | 3.2 |
| 18 | Y | 43 | ARG | 3.2 |
| 3 | c | 264 | PHE | 3.2 |
| 17 | x | 38 | GLN | 3.2 |
| 4 | D | 54 | PHE | 3.2 |
| 17 | X | 3 | ILE | 3.1 |
| 3 | c | 457 | LYS | 3.1 |
| 10 | k | 18 | PHE | 3.1 |
| 2 | b | 123 | PHE | 3.1 |
| 2 | b | 219 | VAL | 3.1 |
| 5 | e | 55 | TYR | 3.1 |
| 8 | i | 38 | GLU | 3.1 |
| 13 | O | 169 | ASP | 3.1 |
| 2 | b | 305 | ILE | 3.1 |
| 3 | C | 127 | PHE | 3.1 |
| 2 | b | 87 | ASP | 3.1 |
| 2 | b | 119 | ASP | 3.1 |
| 2 | b | 72 | THR | 3.1 |
| 8 | I | 25 | SER | 3.1 |
| 4 | D | 264 | LYS | 3.1 |
| 1 | A | 306 | VAL | 3.1 |
| 4 | d | 11 | GLU | 3.0 |
| 2 | B | 44 | THR | 3.0 |
| 7 | h | 2 | ALA | 3.0 |
| 3 | C | 452 | ALA | 3.0 |
| 3 | c | 422 | PRO | 3.0 |
| 2 | b | 217 | ILE | 3.0 |
| 2 | B | 187 | PRO | 3.0 |
| 4 | d | 28 | VAL | 3.0 |
| 2 | B | 378 | LYS | 3.0 |
| 2 | B | 368 | VAL | 3.0 |
| 1 | A | 246 | TYR | 3.0 |
| 1 | A | 12 | ASN | 3.0 |
| 2 | B | 262 | THR | 3.0 |
| 15 | u | 66 | GLY | 3.0 |
| 2 | b | 356 | VAL | 3.0 |
| 2 | B | 69 | LEU | 3.0 |
| 4 | D | 12 | ARG | 3.0 |
| 8 | i | 37 | LEU | 3.0 |
| 4 | d | 98 | GLN | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 4 | d | 138 | VAL | 3.0 |
| 2 | b | 497 | GLN | 3.0 |
| 2 | B | 309 | LEU | 3.0 |
| 2 | B | 500 | GLY | 3.0 |
| 3 | C | 147 | PHE | 3.0 |
| 1 | a | 257 | ARG | 2.9 |
| 13 | o | 129 | THR | 2.9 |
| 3 | c | 400 | PRO | 2.9 |
| 1 | a | 268 | SER | 2.9 |
| 2 | b | 302 | TRP | 2.9 |
| 16 | v | 3 | LEU | 2.9 |
| 17 | X | 38 | GLN | 2.9 |
| 7 | h | 26 | GLY | 2.9 |
| 16 | v | 120 | LEU | 2.9 |
| 1 | A | 265 | PHE | 2.9 |
| 3 | C | 399 | ALA | 2.9 |
| 3 | c | 291 | TRP | 2.9 |
| 1 | A | 257 | ARG | 2.9 |
| 3 | c | 336 | GLY | 2.9 |
| 2 | b | 343 | HIS | 2.9 |
| 15 | u | 56 | GLU | 2.9 |
| 12 | M | 1 | MET | 2.9 |
| 5 | E | 70 | PHE | 2.9 |
| 3 | C | 255 | THR | 2.9 |
| 3 | c | 69 | LEU | 2.9 |
| 1 | a | 240 | GLY | 2.9 |
| 4 | D | 96 | GLU | 2.8 |
| 2 | b | 264 | PRO | 2.8 |
| 19 | z | 24 | PRO | 2.8 |
| 2 | B | 347 | ARG | 2.8 |
| 3 | c | 112 | PHE | 2.8 |
| 4 | D | 333 | ASP | 2.8 |
| 5 | E | 47 | PHE | 2.8 |
| 7 | h | 47 | GLU | 2.8 |
| 8 | I | 30 | ARG | 2.8 |
| 3 | c | 200 | THR | 2.8 |
| 3 | C | 199 | ILE | 2.8 |
| 15 | u | 103 | TYR | 2.8 |
| 13 | o | 181 | GLU | 2.8 |
| 10 | K | 32 | PHE | 2.8 |
| 1 | a | 244 | GLU | 2.8 |
| 2 | B | 306 | PRO | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 5 | e | 56 | TYR | 2.8 |
| 4 | d | 56 | THR | 2.7 |
| 2 | B | 70 | GLY | 2.7 |
| 19 | z | 27 | TYR | 2.7 |
| 2 | B | 366 | PHE | 2.7 |
| 3 | C | 268 | GLY | 2.7 |
| 7 | H | 66 | GLY | 2.7 |
| 9 | J | 5 | GLY | 2.7 |
| 3 | c | 134 | ILE | 2.7 |
| 4 | D | 95 | PRO | 2.7 |
| 7 | h | 14 | LEU | 2.7 |
| 1 | A | 261 | GLN | 2.7 |
| 12 | M | 3 | VAL | 2.7 |
| 4 | d | 108 | GLY | 2.7 |
| 8 | I | 32 | PRO | 2.7 |
| 3 | C | 139 | THR | 2.7 |
| 2 | b | 16 | PRO | 2.7 |
| 4 | D | 103 | ARG | 2.7 |
| 19 | Z | 35 | ARG | 2.7 |
| 2 | B | 305 | ILE | 2.7 |
| 2 | b | 490 | GLN | 2.7 |
| 3 | c | 181 | PHE | 2.7 |
| 15 | U | 32 | ILE | 2.7 |
| 19 | z | 40 | ILE | 2.7 |
| 4 | d | 262 | SER | 2.7 |
| 13 | o | 190 | PHE | 2.6 |
| 5 | e | 66 | VAL | 2.6 |
| 2 | B | 229 | LEU | 2.6 |
| 2 | B | 166 | MET | 2.6 |
| 2 | B | 498 | LYS | 2.6 |
| 3 | C | 99 | VAL | 2.6 |
| 3 | C | 202 | PRO | 2.6 |
| 3 | c | 296 | VAL | 2.6 |
| 3 | C | 204 | LEU | 2.6 |
| 3 | c | 147 | PHE | 2.6 |
| 2 | B | 87 | ASP | 2.6 |
| 2 | b | 491 | VAL | 2.6 |
| 15 | u | 8 | GLU | 2.6 |
| 2 | b | 268 | PHE | 2.6 |
| 2 | b | 494 | GLY | 2.6 |
| 13 | o | 87 | VAL | 2.6 |
| 17 | x | 39 | ARG | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | a | 74 | GLY | 2.6 |
| 3 | C | 81 | MET | 2.6 |
| 3 | c | 199 | ILE | 2.6 |
| 4 | d | 23 | LYS | 2.6 |
| 2 | b | 234 | ILE | 2.6 |
| 3 | c | 458 | GLY | 2.6 |
| 3 | c | 81 | MET | 2.6 |
| 2 | b | 318 | ASN | 2.6 |
| 8 | i | 36 | ASP | 2.6 |
| 3 | C | 365 | TRP | 2.5 |
| 14 | T | 30 | THR | 2.5 |
| 1 | a | 223 | LEU | 2.5 |
| 2 | B | 185 | TRP | 2.5 |
| 3 | c | 143 | TYR | 2.5 |
| 4 | D | 110 | LEU | 2.5 |
| 2 | b | 220 | ARG | 2.5 |
| 17 | X | 34 | ILE | 2.5 |
| 3 | c | 227 | VAL | 2.5 |
| 2 | b | 317 | ASN | 2.5 |
| 3 | C | 267 | SER | 2.5 |
| 13 | O | 164 | LEU | 2.5 |
| 1 | A | 268 | SER | 2.5 |
| 13 | o | 184 | ARG | 2.5 |
| 2 | b | 438 | ASN | 2.5 |
| 1 | a | 250 | ALA | 2.5 |
| 11 | l | 33 | SER | 2.5 |
| 4 | D | 180 | ARG | 2.5 |
| 2 | b | 392 | PHE | 2.5 |
| 3 | c | 238 | ILE | 2.5 |
| 2 | b | 443 | PHE | 2.5 |
| 2 | b | 120 | LEU | 2.4 |
| 1 | a | 222 | SER | 2.4 |
| 5 | e | 54 | SER | 2.4 |
| 1 | a | 239 | PHE | 2.4 |
| 1 | a | 317 | TRP | 2.4 |
| 4 | d | 32 | TRP | 2.4 |
| 2 | B | 195 | PRO | 2.4 |
| 12 | m | 7 | GLY | 2.4 |
| 5 | e | 64 | PRO | 2.4 |
| 1 | A | 244 | GLU | 2.4 |
| 4 | D | 60 | THR | 2.4 |
| 1 | A | 219 | VAL | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2 | B | 497 | GLN | 2.4 |
| 2 | b | 362 | PHE | 2.4 |
| 2 | b | 447 | PRO | 2.4 |
| 2 | b | 353 | GLU | 2.4 |
| 2 | B | 71 | VAL | 2.4 |
| 7 | h | 22 | ALA | 2.4 |
| 5 | E | 84 | LYS | 2.4 |
| 5 | E | 64 | PRO | 2.4 |
| 2 | b | 195 | PRO | 2.4 |
| 8 | I | 24 | LEU | 2.4 |
| 2 | B | 77 | GLY | 2.4 |
| 1 | a | 224 | ILE | 2.4 |
| 2 | b | 183 | PRO | 2.4 |
| 15 | u | 101 | GLY | 2.4 |
| 13 | O | 120 | PHE | 2.3 |
| 13 | o | 211 | ILE | 2.3 |
| 16 | v | 116 | ALA | 2.3 |
| 2 | b | 189 | GLY | 2.3 |
| 7 | H | 57 | GLY | 2.3 |
| 4 | D | 138 | VAL | 2.3 |
| 2 | B | 490 | GLN | 2.3 |
| 7 | h | 3 | ARG | 2.3 |
| 4 | D | 25 | ASP | 2.3 |
| 5 | e | 57 | ALA | 2.3 |
| 17 | X | 39 | ARG | 2.3 |
| 7 | h | 65 | LEU | 2.3 |
| 3 | c | 456 | GLU | 2.3 |
| 2 | b | 274 | GLN | 2.3 |
| 4 | d | 60 | THR | 2.3 |
| 4 | D | 28 | VAL | 2.3 |
| 17 | x | 37 | VAL | 2.3 |
| 2 | b | 122 | LEU | 2.3 |
| 1 | a | 76 | ASN | 2.3 |
| 3 | C | 296 | VAL | 2.3 |
| 3 | C | 203 | THR | 2.3 |
| 1 | A | 85 | SER | 2.3 |
| 3 | C | 23 | ALA | 2.3 |
| 13 | O | 20 | PRO | 2.3 |
| 5 | e | 60 | GLN | 2.3 |
| 12 | m | 33 | GLN | 2.3 |
| 7 | H | 53 | LEU | 2.3 |
| 10 | K | 11 | LEU | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 7 | H | 64 | ALA | 2.3 |
| 1 | a | 306 | VAL | 2.3 |
| 1 | a | 141 | PRO | 2.3 |
| 2 | b | 306 | PRO | 2.3 |
| 3 | c | 82 | TYR | 2.3 |
| 4 | D | 300 | SER | 2.3 |
| 5 | E | 17 | VAL | 2.3 |
| 5 | E | 18 | ARG | 2.3 |
| 1 | A | 143 | ILE | 2.2 |
| 7 | h | 24 | GLY | 2.2 |
| 13 | o | 42 | ARG | 2.2 |
| 3 | C | 234 | VAL | 2.2 |
| 2 | B | 505 | ARG | 2.2 |
| 3 | C | 238 | ILE | 2.2 |
| 3 | C | 336 | GLY | 2.2 |
| 7 | H | 47 | GLU | 2.2 |
| 2 | b | 309 | LEU | 2.2 |
| 3 | c | 149 | TYR | 2.2 |
| 5 | E | 5 | THR | 2.2 |
| 7 | h | 20 | LYS | 2.2 |
| 3 | C | 200 | THR | 2.2 |
| 3 | c | 203 | THR | 2.2 |
| 2 | b | 182 | ALA | 2.2 |
| 2 | b | 369 | ILE | 2.2 |
| 3 | c | 263 | ALA | 2.2 |
| 5 | E | 22 | ILE | 2.2 |
| 12 | M | 4 | ASN | 2.2 |
| 11 | l | 8 | GLN | 2.2 |
| 2 | b | 185 | TRP | 2.2 |
| 4 | d | 292 | ASN | 2.2 |
| 5 | E | 12 | ASP | 2.2 |
| 11 | L | 33 | SER | 2.2 |
| 13 | O | 87 | VAL | 2.2 |
| 1 | a | 80 | GLY | 2.2 |
| 2 | b | 84 | THR | 2.2 |
| 12 | M | 5 | GLN | 2.2 |
| 14 | T | 2 | GLU | 2.2 |
| 4 | d | 308 | ASP | 2.2 |
| 13 | O | 154 | ALA | 2.2 |
| 2 | b | 436 | THR | 2.2 |
| 1 | A | 304 | HIS | 2.2 |
| 3 | C | 72 | LEU | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2 | b | 132 | ALA | 2.2 |
| 3 | c | 249 | ILE | 2.2 |
| 7 | H | 54 | ILE | 2.2 |
| 7 | h | 48 | ILE | 2.2 |
| 13 | o | 40 | ILE | 2.2 |
| 3 | C | 213 | LEU | 2.2 |
| 10 | k | 21 | LEU | 2.2 |
| 14 | t | 3 | THR | 2.2 |
| 1 | a | 247 | ASN | 2.2 |
| 3 | C | 291 | TRP | 2.2 |
| 2 | b | 367 | PRO | 2.1 |
| 4 | d | 341 | PHE | 2.1 |
| 7 | h | 28 | THR | 2.1 |
| 3 | C | 124 | VAL | 2.1 |
| 4 | D | 350 | ASN | 2.1 |
| 17 | x | 36 | LYS | 2.1 |
| 18 | Y | 45 | ASN | 2.1 |
| 3 | C | 466 | VAL | 2.1 |
| 4 | D | 79 | SER | 2.1 |
| 13 | o | 150 | SER | 2.1 |
| 1 | a | 75 | ASN | 2.1 |
| 9 | J | 4 | GLU | 2.1 |
| 1 | a | 340 | PRO | 2.1 |
| 16 | v | 90 | GLU | 2.1 |
| 12 | M | 7 | GLY | 2.1 |
| 3 | C | 86 | LEU | 2.1 |
| 15 | u | 77 | GLU | 2.1 |
| 13 | O | 76 | THR | 2.1 |
| 11 | l | 1 | MET | 2.1 |
| 2 | b | 445 | THR | 2.1 |
| 3 | C | 95 | LEU | 2.1 |
| 4 | D | 89 | LEU | 2.1 |
| 14 | T | 3 | THR | 2.1 |
| 4 | D | 307 | GLU | 2.1 |
| 4 | d | 35 | ILE | 2.1 |
| 2 | b | 420 | TYR | 2.1 |
| 4 | D | 308 | ASP | 2.1 |
| 7 | h | 66 | GLY | 2.1 |
| 2 | b | 344 | ALA | 2.1 |
| 13 | o | 140 | THR | 2.1 |
| 2 | b | 192 | PRO | 2.1 |
| 10 | k | 15 | TYR | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 12 | m | 4 | ASN | 2.1 |
| 2 | b | 284 | ILE | 2.1 |
| 3 | C | 111 | PHE | 2.1 |
| 3 | c | 292 | PHE | 2.1 |
| 17 | X | 36 | LYS | 2.1 |
| 3 | c | 230 | LEU | 2.1 |
| 16 | V | 125 | ILE | 2.1 |
| 4 | D | 23 | LYS | 2.1 |
| 3 | C | 269 | GLU | 2.1 |
| 1 | a | 79 | THR | 2.1 |
| 13 | o | 176 | GLN | 2.1 |
| 2 | b | 428 | GLU | 2.1 |
| 13 | o | 101 | ILE | 2.1 |
| 3 | c | 256 | PRO | 2.0 |
| 3 | c | 447 | ARG | 2.0 |
| 1 | a | 236 | GLY | 2.0 |
| 3 | c | 243 | ILE | 2.0 |
| 13 | o | 112 | GLY | 2.0 |
| 7 | H | 63 | LYS | 2.0 |
| 4 | D | 85 | MET | 2.0 |
| 2 | B | 379 | ALA | 2.0 |
| 2 | b | 304 | ALA | 2.0 |
| 2 | b | 311 | PHE | 2.0 |
| 5 | e | 37 | PHE | 2.0 |
| 1 | A | 194 | MET | 2.0 |
| 13 | o | 20 | PRO | 2.0 |
| 2 | B | 503 | THR | 2.0 |
| 2 | b | 136 | PRO | 2.0 |
| 2 | b | 194 | ASN | 2.0 |
| 8 | i | 32 | PRO | 2.0 |
| 2 | b | 85 | GLY | 2.0 |
| 10 | k | 14 | ALA | 2.0 |
| 2 | b | 231 | MET | 2.0 |
| 2 | B | 421 | ALA | 2.0 |
| 2 | b | 421 | ALA | 2.0 |
| 16 | V | 120 | LEU | 2.0 |
| 3 | C | 364 | PRO | 2.0 |
| 16 | v | 10 | VAL | 2.0 |
| 7 | h | 46 | LEU | 2.0 |

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 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. 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 | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 26 | CL | U | 201 | 1/1 | 0.01 | 0.17 | 50,50,50,50 | 0 |
| 26 | CL | u | 201 | 1/1 | 0.03 | 0.36 | 50,50,50,50 | 0 |
| 29 | LMG | c | 520 | 51/55 | 0.21 | 1.84 | 43,76,81,82 | 0 |
| 30 | CA | B | 621 | 1/1 | 0.26 | 0.72 | 76,76,76,76 | 0 |
| 28 | PL9 | a | 613 | 55/55 | 0.26 | 1.48 | 52,69,78,78 | 0 |
| 29 | LMG | z | 101 | 37/55 | 0.27 | 1.47 | 55,84,88,88 | 0 |
| 30 | CA | f | 102 | 1/1 | 0.28 | 0.74 | 56,56,56,56 | 0 |
| 24 | BCR | k | 101 | 40/40 | 0.29 | 1.14 | 34,38,39,39 | 0 |
| 29 | LMG | C | 520 | 51/55 | 0.31 | 1.34 | 43,76,81,82 | 0 |
| 29 | LMG | Z | 101 | 37/55 | 0.33 | 1.65 | 55,84,88,88 | 0 |
| 24 | BCR | d | 404 | 40/40 | 0.34 | 1.17 | 25,30,48,49 | 0 |
| 28 | PL9 | A | 613 | 55/55 | 0.34 | 1.95 | 52,69,78,78 | 0 |
| 24 | BCR | a | 608 | 40/40 | 0.39 | 0.47 | 22,27,32,32 | 0 |
| 24 | BCR | D | 404 | 40/40 | 0.40 | 1.52 | 25,30,48,49 | 0 |
| 24 | BCR | T | 102 | 40/40 | 0.41 | 1.10 | 27,33,39,39 | 0 |
| 29 | LMG | C | 519 | 51/55 | 0.42 | 0.86 | 31,57,72,73 | 0 |
| 24 | BCR | A | 608 | 40/40 | 0.45 | 0.70 | 22,27,32,32 | 0 |
| 24 | BCR | t | 101 | 40/40 | 0.47 | 0.63 | 27,33,39,39 | 0 |
| 31 | DGD | D | 410 | 62/66 | 0.48 | 1.24 | 77,89,103,103 | 0 |
| 22 | CLA | b | 607 | 65/65 | 0.51 | 0.88 | 24,28,40,41 | 0 |
| 32 | LHG | e | 101 | 42/49 | 0.52 | 0.61 | 69,83,86,86 | 0 |
| 31 | DGD | d | 410 | 62/66 | 0.53 | 0.76 | 77,89,103,103 | 0 |
| 30 | CA | b | 620 | 1/1 | 0.53 | 1.25 | 76,76,76,76 | 0 |
| 32 | LHG | E | 101 | 42/49 | 0.55 | 1.29 | 69,83,86,86 | 0 |
| 26 | CL | a | 610 | 1/1 | 0.57 | 0.55 | 24,24,24,24 | 0 |
| 22 | CLA | a | 604 | 65/65 | 0.57 | 0.86 | 19,21,63,65 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 29 | LMG | B | 620 | 51/55 | 0.58 | 0.38 | 29,39,51,54 | 0 |
| 24 | BCR | K | 101 | 40/40 | 0.61 | 1.40 | 34,38,39,39 | 0 |
| 25 | SQD | d | 411 | 43/54 | 0.61 | 0.91 | 67,74,78,79 | 0 |
| 22 | CLA | B | 607 | 65/65 | 0.61 | 0.62 | 24,28,40,41 | 0 |
| 22 | CLA | b | 602 | 65/65 | 0.61 | 1.48 | 32,41,66,66 | 0 |
| 22 | CLA | B | 602 | 65/65 | 0.62 | 1.02 | 32,41,66,66 | 0 |
| 29 | LMG | A | 614 | 51/55 | 0.63 | 0.85 | 53,59,64,65 | 0 |
| 25 | SQD | a | 609 | 54/54 | 0.64 | 0.53 | 49,57,66,67 | 0 |
| 25 | SQD | A | 609 | 54/54 | 0.65 | 0.63 | 49,57,66,67 | 0 |
| 25 | SQD | D | 411 | 43/54 | 0.66 | 1.27 | 67,74,78,79 | 0 |
| 22 | CLA | C | 513 | 65/65 | 0.66 | 1.10 | 39,45,64,64 | 0 |
| 22 | CLA | c | 512 | 65/65 | 0.66 | 1.57 | 37,41,62,63 | 0 |
| 22 | CLA | b | 615 | 65/65 | 0.67 | 0.44 | 20,24,60,61 | 0 |
| 24 | BCR | B | 622 | 40/40 | 0.67 | 0.43 | 25,37,44,45 | 0 |
| 24 | BCR | H | 101 | 40/40 | 0.67 | 1.33 | 26,33,42,42 | 0 |
| 22 | CLA | b | 617 | 65/65 | 0.67 | 0.91 | 22,29,77,78 | 0 |
| 29 | LMG | b | 619 | 51/55 | 0.67 | 0.38 | 29,39,51,54 | 0 |
| 22 | CLA | c | 502 | 65/65 | 0.68 | 0.96 | 24,26,39,42 | 0 |
| 29 | LMG | a | 614 | 51/55 | 0.68 | 0.80 | 53,59,64,65 | 0 |
| 22 | CLA | c | 513 | 65/65 | 0.68 | 1.01 | 39,45,64,64 | 0 |
| 24 | BCR | b | 622 | 40/40 | 0.69 | 0.48 | 25,37,44,45 | 0 |
| 22 | CLA | B | 617 | 65/65 | 0.69 | 0.51 | 22,29,77,78 | 0 |
| 22 | CLA | C | 507 | 65/65 | 0.70 | 1.34 | 29,33,52,53 | 0 |
| 24 | BCR | k | 102 | 40/40 | 0.70 | 2.16 | 29,33,37,37 | 0 |
| 30 | CA | F | 102 | 1/1 | 0.70 | 0.49 | 56,56,56,56 | 0 |
| 34 | MG | j | 101 | 1/1 | 0.70 | 0.29 | 27,27,27,27 | 0 |
| 22 | CLA | C | 512 | 65/65 | 0.70 | 1.32 | 37,41,62,63 | 0 |
| 22 | CLA | D | 403 | 65/65 | 0.70 | 1.20 | 24,27,65,67 | 0 |
| 28 | PL9 | D | 408 | 55/55 | 0.70 | 0.51 | 19,23,29,32 | 0 |
| 24 | BCR | c | 514 | 40/40 | 0.72 | 1.69 | 37,43,47,47 | 0 |
| 22 | CLA | c | 501 | 65/65 | 0.72 | 1.66 | 29,32,44,46 | 0 |
| 22 | CLA | C | 508 | 65/65 | 0.73 | 0.74 | 25,29,54,58 | 0 |
| 24 | BCR | C | 515 | 40/40 | 0.73 | 1.99 | 30,37,40,41 | 0 |
| 25 | SQD | B | 601 | 54/54 | 0.73 | 0.35 | 50,63,68,68 | 0 |
| 25 | SQD | b | 601 | 54/54 | 0.73 | 0.49 | 50,63,68,68 | 0 |
| 24 | BCR | B | 619 | 40/40 | 0.73 | 0.31 | 21,28,40,40 | 0 |
| 22 | CLA | a | 603 | 65/65 | 0.73 | 0.60 | 15,19,25,34 | 0 |
| 22 | CLA | b | 614 | 65/65 | 0.73 | 0.45 | 19,22,45,47 | 0 |
| 22 | CLA | B | 615 | 65/65 | 0.74 | 0.38 | 20,24,60,61 | 0 |
| 22 | CLA | d | 403 | 65/65 | 0.74 | 1.19 | 24,27,65,67 | 0 |
| 31 | DGD | C | 518 | 62/66 | 0.75 | 0.64 | 22,31,52,56 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 24 | BCR | b | 618 | 40/40 | 0.75 | 0.42 | 21,28,40,40 | 0 |
| 22 | CLA | A | 604 | 65/65 | 0.75 | 1.02 | 19,21,63,65 | 0 |
| 32 | LHG | D | 409 | 49/49 | 0.75 | 0.75 | 26,33,62,64 | 0 |
| 22 | CLA | c | 507 | 65/65 | 0.76 | 1.38 | 29,33,52,53 | 0 |
| 22 | CLA | a | 607 | 65/65 | 0.76 | 0.81 | 21,24,71,72 | 0 |
| 32 | LHG | D | 405 | 49/49 | 0.76 | 0.38 | 29,34,41,41 | 0 |
| 22 | CLA | C | 506 | 65/65 | 0.76 | 0.96 | 31,38,74,75 | 0 |
| 29 | LMG | d | 406 | 51/55 | 0.76 | 0.50 | 26,35,65,67 | 0 |
| 24 | BCR | C | 514 | 40/40 | 0.76 | 1.48 | 37,43,47,47 | 0 |
| 25 | SQD | b | 621 | 54/54 | 0.77 | 0.40 | 58,66,80,80 | 0 |
| 28 | PL9 | d | 408 | 55/55 | 0.77 | 0.40 | 19,23,29,32 | 0 |
| 25 | SQD | L | 101 | 54/54 | 0.77 | 0.41 | 57,69,84,85 | 0 |
| 23 | PHO | A | 605 | 64/64 | 0.77 | 0.59 | 16,21,25,26 | 0 |
| 22 | CLA | A | 603 | 65/65 | 0.77 | 0.67 | 15,19,25,34 | 0 |
| 22 | CLA | b | 612 | 65/65 | 0.77 | 0.43 | 19,21,32,34 | 0 |
| 32 | LHG | d | 409 | 49/49 | 0.77 | 0.71 | 26,33,62,64 | 0 |
| 22 | CLA | D | 402 | 65/65 | 0.77 | 0.53 | 14,18,29,35 | 0 |
| 29 | LMG | D | 406 | 51/55 | 0.78 | 0.80 | 26,35,65,67 | 0 |
| 22 | CLA | d | 402 | 65/65 | 0.78 | 0.47 | 14,18,29,35 | 0 |
| 24 | BCR | c | 515 | 40/40 | 0.78 | 1.59 | 30,37,40,41 | 0 |
| 22 | CLA | B | 616 | 65/65 | 0.78 | 0.74 | 25,27,45,46 | 0 |
| 22 | CLA | b | 606 | 65/65 | 0.78 | 0.84 | 19,23,34,35 | 0 |
| 24 | BCR | T | 101 | 40/40 | 0.79 | 0.40 | 23,27,28,29 | 0 |
| 22 | CLA | C | 501 | 65/65 | 0.79 | 1.23 | 29,32,44,46 | 0 |
| 32 | LHG | d | 407 | 49/49 | 0.80 | 0.37 | 24,28,37,40 | 0 |
| 26 | CL | A | 610 | 1/1 | 0.80 | 0.45 | 24,24,24,24 | 0 |
| 23 | PHO | a | 605 | 64/64 | 0.81 | 0.52 | 16,21,25,26 | 0 |
| 22 | CLA | C | 504 | 65/65 | 0.81 | 0.70 | 25,28,54,54 | 0 |
| 31 | DGD | c | 518 | 62/66 | 0.81 | 0.53 | 22,31,52,56 | 0 |
| 24 | BCR | K | 102 | 40/40 | 0.81 | 2.31 | 29,33,37,37 | 0 |
| 22 | CLA | B | 609 | 65/65 | 0.81 | 0.88 | 20,24,31,31 | 0 |
| 32 | LHG | d | 405 | 49/49 | 0.81 | 0.44 | 29,34,41,41 | 0 |
| 24 | BCR | h | 101 | 40/40 | 0.81 | 1.31 | 26,33,42,42 | 0 |
| 22 | CLA | c | 509 | 65/65 | 0.81 | 1.18 | 29,32,46,47 | 0 |
| 22 | CLA | b | 616 | 65/65 | 0.81 | 1.25 | 25,27,45,46 | 0 |
| 24 | BCR | B | 618 | 40/40 | 0.81 | 0.31 | 23,27,28,29 | 0 |
| 25 | SQD | l | 102 | 54/54 | 0.82 | 0.32 | 58,66,80,80 | 0 |
| 22 | CLA | A | 607 | 65/65 | 0.82 | 0.78 | 21,24,71,72 | 0 |
| 23 | PHO | A | 606 | 64/64 | 0.82 | 1.13 | 19,22,28,32 | 0 |
| 22 | CLA | b | 605 | 65/65 | 0.82 | 0.78 | 19,22,50,51 | 0 |
| 31 | DGD | h | 102 | 62/66 | 0.82 | 0.90 | 26,32,38,40 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 22 | CLA | c | 503 | 65/65 | 0.82 | 1.11 | 27,31,35,36 | 0 |
| 23 | PHO | a | 606 | 64/64 | 0.82 | 0.79 | 19,22,28,32 | 0 |
| 32 | LHG | D | 407 | 49/49 | 0.82 | 0.49 | 24,28,37,40 | 0 |
| 25 | SQD | l | 101 | 54/54 | 0.82 | 0.32 | 57,69,84,85 | 0 |
| 29 | LMG | c | 519 | 51/55 | 0.83 | 0.67 | 31,57,72,73 | 0 |
| 21 | FE2 | a | 602 | 1/1 | 0.83 | 0.35 | 26,26,26,26 | 0 |
| 22 | CLA | c | 511 | 65/65 | 0.83 | 0.89 | 29,34,37,38 | 0 |
| 22 | CLA | B | 606 | 65/65 | 0.83 | 0.84 | 19,23,34,35 | 0 |
| 22 | CLA | b | 603 | 65/65 | 0.83 | 1.17 | 23,26,32,32 | 0 |
| 22 | CLA | b | 609 | 65/65 | 0.83 | 1.02 | 20,24,31,31 | 0 |
| 31 | DGD | C | 517 | 62/66 | 0.83 | 0.53 | 23,35,62,63 | 0 |
| 22 | CLA | D | 401 | 65/65 | 0.83 | 0.95 | 13,18,34,35 | 0 |
| 22 | CLA | B | 603 | 65/65 | 0.83 | 1.15 | 23,26,32,32 | 0 |
| 32 | LHG | L | 102 | 49/49 | 0.84 | 0.35 | 23,31,43,44 | 0 |
| 22 | CLA | C | 510 | 65/65 | 0.84 | 0.81 | 24,28,35,37 | 0 |
| 22 | CLA | B | 612 | 65/65 | 0.84 | 0.44 | 19,21,32,34 | 0 |
| 22 | CLA | b | 611 | 65/65 | 0.84 | 0.94 | 21,25,32,37 | 0 |
| 26 | CL | A | 611 | 1/1 | 0.85 | 0.35 | 21,21,21,21 | 0 |
| 31 | DGD | H | 102 | 62/66 | 0.85 | 1.00 | 26,32,38,40 | 0 |
| 31 | DGD | C | 516 | 62/66 | 0.85 | 0.58 | 23,33,61,62 | 0 |
| 22 | CLA | c | 506 | 65/65 | 0.85 | 0.93 | 31,38,74,75 | 0 |
| 32 | LHG | l | 103 | 49/49 | 0.85 | 0.33 | 23,31,43,44 | 0 |
| 22 | CLA | b | 610 | 65/65 | 0.86 | 1.10 | 23,28,31,32 | 0 |
| 22 | CLA | c | 510 | 65/65 | 0.86 | 0.85 | 24,28,35,37 | 0 |
| 34 | MG | J | 101 | 1/1 | 0.86 | 0.11 | 27,27,27,27 | 0 |
| 22 | CLA | b | 613 | 65/65 | 0.86 | 0.75 | 20,24,30,31 | 0 |
| 22 | CLA | C | 502 | 65/65 | 0.86 | 0.79 | 24,26,39,42 | 0 |
| 22 | CLA | B | 613 | 65/65 | 0.87 | 0.73 | 20,24,30,31 | 0 |
| 22 | CLA | c | 508 | 65/65 | 0.87 | 0.60 | 25,29,54,58 | 0 |
| 22 | CLA | b | 608 | 65/65 | 0.87 | 0.43 | 17,20,32,34 | 0 |
| 31 | DGD | c | 516 | 62/66 | 0.87 | 0.55 | 23,33,61,62 | 0 |
| 22 | CLA | c | 505 | 65/65 | 0.87 | 0.82 | 28,30,44,45 | 0 |
| 22 | CLA | b | 604 | 65/65 | 0.88 | 1.31 | 18,22,31,35 | 0 |
| 22 | CLA | B | 604 | 65/65 | 0.88 | 1.04 | 18,22,31,35 | 0 |
| 22 | CLA | B | 605 | 65/65 | 0.89 | 0.57 | 19,22,50,51 | 0 |
| 33 | HEM | F | 101 | 43/43 | 0.89 | 0.80 | 39,42,45,47 | 0 |
| 27 | BCT | A | 612 | 4/4 | 0.89 | 1.01 | 39,39,40,42 | 0 |
| 31 | DGD | c | 517 | 62/66 | 0.89 | 0.40 | 23,35,62,63 | 0 |
| 22 | CLA | d | 401 | 65/65 | 0.90 | 0.84 | 13,18,34,35 | 0 |
| 22 | CLA | B | 611 | 65/65 | 0.90 | 1.00 | 21,25,32,37 | 0 |
| 22 | CLA | B | 610 | 65/65 | 0.90 | 0.83 | 23,28,31,32 | 0 |
| 22 | CLA | C | 505 | 65/65 | 0.90 | 0.90 | 28,30,44,45 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 22 | CLA | C | 503 | 65/65 | 0.90 | 0.81 | 27,31,35,36 | 0 |
| 26 | CL | a | 611 | 1/1 | 0.91 | 0.37 | 21,21,21,21 | 0 |
| 33 | HEM | f | 101 | 43/43 | 0.91 | 0.69 | 39,42,45,47 | 0 |
| 22 | CLA | C | 511 | 65/65 | 0.91 | 1.24 | 29,34,37,38 | 0 |
| 22 | CLA | B | 608 | 65/65 | 0.91 | 0.41 | 17,20,32,34 | 0 |
| 22 | CLA | c | 504 | 65/65 | 0.91 | 0.51 | 25,28,54,54 | 0 |
| 22 | CLA | B | 614 | 65/65 | 0.91 | 0.38 | 19,22,45,47 | 0 |
| 33 | HEM | V | 201 | 43/43 | 0.91 | 0.69 | 23,24,27,29 | 0 |
| 33 | HEM | v | 201 | 43/43 | 0.92 | 0.72 | 23,24,27,29 | 0 |
| 20 | OEX | A | 601 | 10/10 | 0.92 | 0.40 | 22,23,26,26 | 0 |
| 30 | CA | O | 301 | 1/1 | 0.93 | 0.14 | 49,49,49,49 | 0 |
| 27 | BCT | a | 612 | 4/4 | 0.93 | 1.21 | 39,39,40,42 | 0 |
| 22 | CLA | C | 509 | 65/65 | 0.93 | 1.30 | 29,32,46,47 | 0 |
| 20 | OEX | a | 601 | 10/10 | 0.94 | 0.41 | 22,23,26,26 | 0 |
| 30 | CA | o | 301 | 1/1 | 0.95 | 0.28 | 49,49,49,49 | 0 |
| 21 | FE2 | A | 602 | 1/1 | 0.96 | 0.16 | 26,26,26,26 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.