



# Full wwPDB X-ray Structure Validation Report

Jul 18, 2014 – 01:58 AM EDT

PDB ID : 4TNK  
Title : RT XFEL structure of Photosystem II 250 microsec after the third illumination at 5.2 Å resolution  
Authors : Kern, J.; Tran, R.; Alonso-Mori, R.; Koroidov, S.; Echols, N.; Hattne, J.; Ibrahim, M.; Gul, S.; Laksmono, H.; Sierra, R.G.; Gildea, R.J.; Han, G.; Hellmich, J.; Lassalle-Kaiser, B.; Chatterjee, R.; Brewster, A.; Stan, C.A.; Gloeckner, C.; Lampe, A.; DiFiore, D.; Milathianaki, D.; Fry, A.R.; Seibert, M.M.; Koglin, J.E.; Gallo, E.; Uhlig, J.; Sokaras, D.; Weng, T.-C.; Zwart, P.H.; Skinner, D.E.; Bogan, M.J.; Messerschmidt, M.; Glatzel, P.; Williams, G.J.; Boutet, S.; Adams, P.D.; Zouni, A.; Messinger, J.; Sauter, N.K.; Bergmann, U.; Yano, J.; Yachandra, V.K.  
Deposited on : 2014-06-04  
Resolution : 5.20 Å (reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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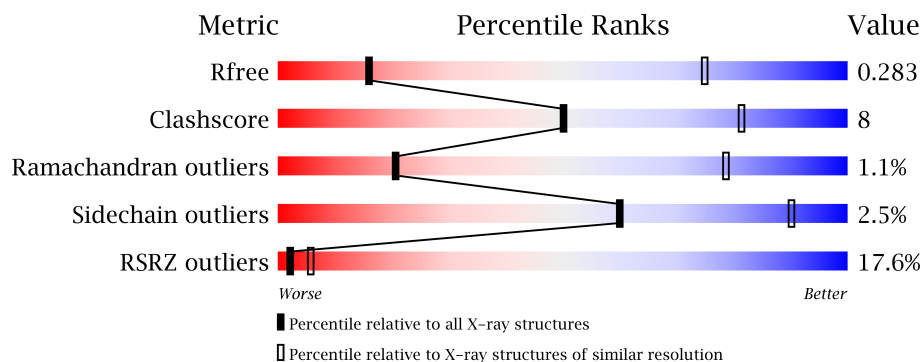
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable23161  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23161

# 1 Overall quality at a glance

The reported resolution of this entry is 5.20 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 66092                       | 1060 (6.80-3.50)                                      |
| Clashscore            | 79885                       | 1336 (6.80-3.50)                                      |
| Ramachandran outliers | 78287                       | 1250 (6.80-3.50)                                      |
| Sidechain outliers    | 78261                       | 1228 (6.80-3.50)                                      |
| RSRZ outliers         | 66119                       | 1059 (6.80-3.50)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 344    |                  |
| 1   | a     | 344    |                  |
| 2   | B     | 510    |                  |
| 2   | b     | 510    |                  |
| 3   | C     | 461    |                  |
| 3   | c     | 461    |                  |
| 4   | D     | 352    |                  |
| 4   | d     | 352    |                  |
| 5   | E     | 84     |                  |
| 5   | e     | 84     |                  |
| 6   | F     | 45     |                  |
| 6   | f     | 45     |                  |
| 7   | H     | 66     |                  |
| 7   | h     | 66     |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 8   | I     | 38     |                  |
| 8   | i     | 38     |                  |
| 9   | J     | 40     |                  |
| 9   | j     | 40     |                  |
| 10  | K     | 46     |                  |
| 10  | k     | 46     |                  |
| 11  | L     | 37     |                  |
| 11  | l     | 37     |                  |
| 12  | M     | 36     |                  |
| 12  | m     | 36     |                  |
| 13  | O     | 272    |                  |
| 13  | o     | 272    |                  |
| 14  | T     | 32     |                  |
| 14  | t     | 32     |                  |
| 15  | U     | 134    |                  |
| 15  | u     | 134    |                  |
| 16  | V     | 163    |                  |
| 16  | v     | 163    |                  |
| 17  | g     | 46     |                  |
| 17  | y     | 46     |                  |
| 18  | X     | 41     |                  |
| 18  | x     | 41     |                  |
| 19  | G     | 28     |                  |
| 19  | Y     | 28     |                  |
| 20  | Z     | 62     |                  |
| 20  | z     | 62     |                  |

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Geometry | Electron density |
|-----|------|-------|-----|----------|------------------|
| 22  | CLA  | A     | 406 | -        | X                |
| 22  | CLA  | B     | 601 | -        | X                |
| 22  | CLA  | B     | 603 | -        | X                |
| 22  | CLA  | B     | 604 | -        | X                |
| 22  | CLA  | B     | 605 | -        | X                |
| 22  | CLA  | B     | 608 | -        | X                |
| 22  | CLA  | B     | 609 | -        | X                |
| 22  | CLA  | B     | 614 | -        | X                |
| 22  | CLA  | B     | 615 | -        | X                |
| 22  | CLA  | C     | 502 | -        | X                |
| 22  | CLA  | C     | 506 | -        | X                |

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| Mol | Type | Chain | Res | Geometry | Electron density |
|-----|------|-------|-----|----------|------------------|
| 22  | CLA  | C     | 508 | -        | X                |
| 22  | CLA  | C     | 510 | -        | X                |
| 22  | CLA  | C     | 511 | -        | X                |
| 22  | CLA  | C     | 512 | -        | X                |
| 22  | CLA  | a     | 403 | -        | X                |
| 22  | CLA  | a     | 404 | -        | X                |
| 22  | CLA  | a     | 406 | -        | X                |
| 22  | CLA  | b     | 605 | -        | X                |
| 22  | CLA  | b     | 607 | -        | X                |
| 22  | CLA  | b     | 613 | -        | X                |
| 22  | CLA  | b     | 614 | -        | X                |
| 22  | CLA  | b     | 619 | -        | X                |
| 22  | CLA  | b     | 620 | -        | X                |
| 22  | CLA  | c     | 501 | -        | X                |
| 22  | CLA  | c     | 502 | -        | X                |
| 22  | CLA  | c     | 505 | -        | X                |
| 22  | CLA  | c     | 506 | -        | X                |
| 22  | CLA  | c     | 510 | -        | X                |
| 22  | CLA  | c     | 511 | -        | X                |
| 22  | CLA  | c     | 512 | -        | X                |
| 24  | PL9  | j     | 101 | -        | X                |
| 25  | BCR  | B     | 619 | -        | X                |
| 25  | BCR  | C     | 513 | -        | X                |
| 25  | BCR  | C     | 520 | -        | X                |
| 25  | BCR  | H     | 102 | -        | X                |
| 25  | BCR  | K     | 101 | -        | X                |
| 25  | BCR  | b     | 624 | -        | X                |
| 25  | BCR  | c     | 513 | -        | X                |
| 25  | BCR  | c     | 514 | -        | X                |
| 25  | BCR  | c     | 521 | -        | X                |
| 25  | BCR  | f     | 102 | -        | X                |
| 25  | BCR  | g     | 101 | -        | X                |
| 25  | BCR  | i     | 101 | -        | X                |
| 25  | BCR  | x     | 101 | -        | X                |
| 25  | BCR  | y     | 101 | -        | X                |
| 26  | DGD  | B     | 626 | -        | X                |
| 26  | DGD  | D     | 407 | -        | X                |
| 26  | DGD  | b     | 601 | -        | X                |
| 26  | DGD  | d     | 410 | -        | X                |
| 30  | SQD  | B     | 622 | -        | X                |
| 30  | SQD  | B     | 627 | -        | X                |
| 30  | SQD  | F     | 103 | -        | X                |

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| Mol | Type | Chain | Res | Geometry | Electron density |
|-----|------|-------|-----|----------|------------------|
| 30  | SQD  | a     | 401 | -        | X                |
| 30  | SQD  | d     | 403 | -        | X                |
| 30  | SQD  | f     | 103 | -        | X                |
| 31  | LMG  | C     | 517 | -        | X                |
| 31  | LMG  | I     | 101 | -        | X                |
| 31  | LMG  | b     | 627 | -        | X                |
| 31  | LMG  | c     | 518 | -        | X                |
| 31  | LMG  | i     | 102 | -        | X                |
| 31  | LMG  | m     | 101 | -        | X                |
| 32  | LMT  | B     | 623 | -        | X                |
| 32  | LMT  | B     | 628 | -        | X                |
| 32  | LMT  | D     | 408 | -        | X                |
| 32  | LMT  | I     | 102 | -        | X                |
| 32  | LMT  | b     | 628 | -        | X                |
| 32  | LMT  | b     | 629 | -        | X                |
| 32  | LMT  | d     | 411 | -        | X                |
| 32  | LMT  | i     | 103 | -        | X                |
| 34  | HEM  | v     | 201 | -        | X                |
| 35  | CA   | K     | 102 | -        | X                |
| 35  | CA   | o     | 301 | -        | X                |

## 2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 50244 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a protein called Photosystem Q(B) protein 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 335      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2628  | 1720 | 432 | 461 | 15 |         |         |       |
| 1   | a     | 335      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2628  | 1720 | 432 | 461 | 15 |         |         |       |

- Molecule 2 is a protein called Photosystem II core light harvesting protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | B     | 490      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3850  | 2528 | 641 | 668 | 13 |         |         |       |
| 2   | b     | 490      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3850  | 2528 | 641 | 668 | 13 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3   | C     | 447      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3444  | 2256 | 576 | 599 | 13 |         |         |       |
| 3   | c     | 447      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3444  | 2256 | 576 | 599 | 13 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 4   | D     | 340      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2706  | 1794 | 440 | 460 | 12 |         |         |       |
| 4   | d     | 340      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2706  | 1794 | 440 | 460 | 12 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 5   | E     | 82       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 666   | 434 | 108 | 124 |         |         |       |
| 5   | e     | 82       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 666   | 434 | 108 | 124 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 6   | F     | 35       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 282   | 192 | 46 | 43 | 1 |         |         |       |
| 6   | f     | 35       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 282   | 192 | 46 | 43 | 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     |
|     |       |          | 507   | 338 | 81 | 86 | 2 |         |         |       |
| 7   | h     | 65       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 507   | 338 | 81 | 86 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 8   | I     | 35       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 286   | 195 | 45 | 45 | 1 |         |         |       |
| 8   | i     | 35       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 286   | 195 | 45 | 45 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 9   | J     | 34       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 249   | 170 | 38 | 40 | 1 |         |         |       |
| 9   | j     | 34       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 249   | 170 | 38 | 40 | 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 |         |         |       |

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

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 11  | L     | 37       | Total | C   | N  | O  | S | 0       | 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     |
|     |       |          | 1845  | 1154 | 308 | 379 | 4 |         |         |       |
| 13  | o     | 243      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1845  | 1154 | 308 | 379 | 4 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 14  | T     | 32       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 275   | 192 | 40 | 41 | 2 |         |         |       |
| 14  | t     | 32       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 275   | 192 | 40 | 41 | 2 |         |         |       |

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

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



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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16  | V     | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1060  | 673 | 177 | 206 | 4 |         |         |       |
| 16  | v     | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1060  | 673 | 177 | 206 | 4 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 17  | y     | 28       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 201   | 134 | 33 | 31 | 3 |         |         |       |
| 17  | g     | 28       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 201   | 134 | 33 | 31 | 3 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|--|---------|---------|-------|
| 18  | X     | 37       | Total | C   | N  | O  |  | 0       | 0       | 0     |
|     |       |          | 270   | 182 | 41 | 47 |  |         |         |       |
| 18  | x     | 37       | Total | C   | N  | O  |  | 0       | 0       | 0     |
|     |       |          | 270   | 182 | 41 | 47 |  |         |         |       |

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

| Mol | Chain | Residues | Atoms |    |    |    |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|--|---------|---------|-------|
| 19  | Y     | 28       | Total | C  | N  | O  |  | 0       | 0       | 0     |
|     |       |          | 140   | 84 | 28 | 28 |  |         |         |       |
| 19  | G     | 28       | Total | C  | N  | O  |  | 0       | 0       | 0     |
|     |       |          | 140   | 84 | 28 | 28 |  |         |         |       |

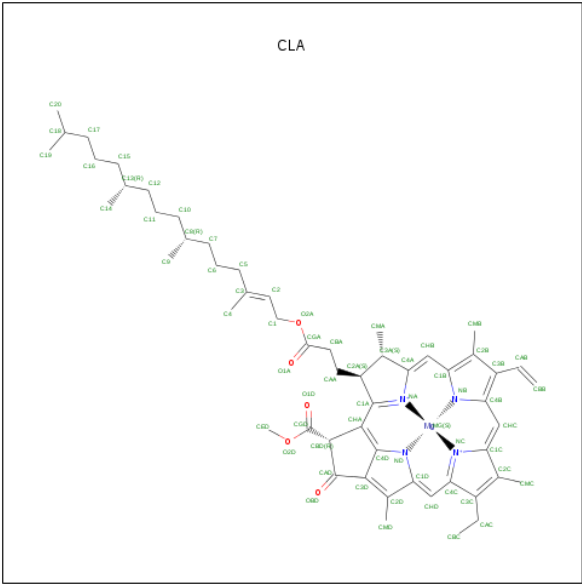
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 20  | Z     | 62       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 479   | 328 | 72 | 77 | 2 |         |         |       |
| 20  | z     | 62       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 479   | 328 | 72 | 77 | 2 |         |         |       |

- 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: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



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

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

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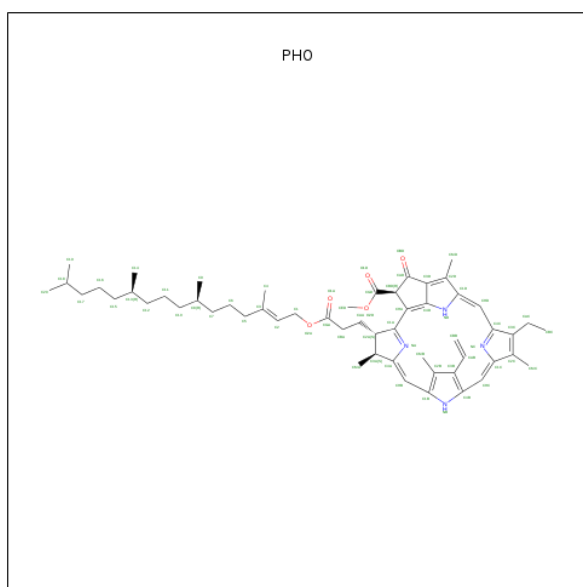
| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 22  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | D     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | D     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | H     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 22  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |

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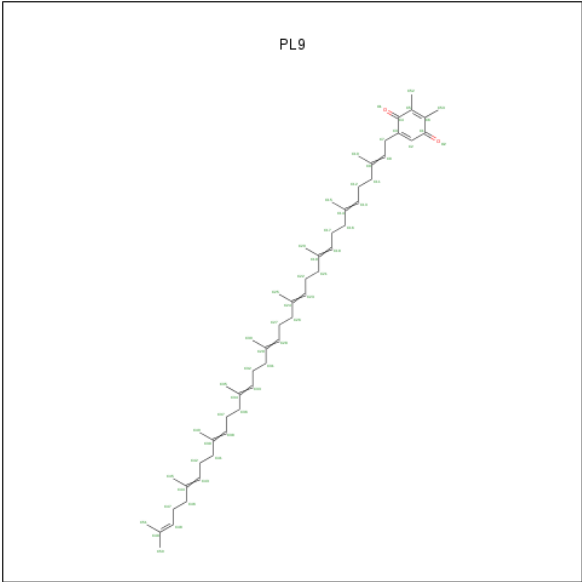
| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 22  | b     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 22  | b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

- Molecule 23 is PHEOPHYTIN A (three-letter code: PHO) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>5</sub>).



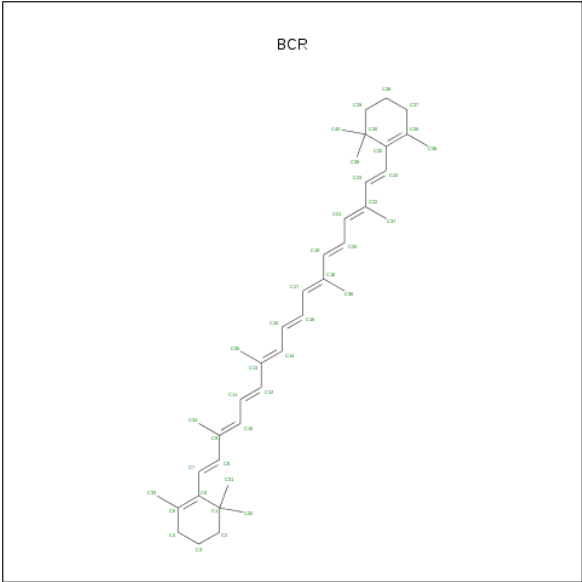
| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 23  | A     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |         |
| 23  | D     | 1        | Total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

- Molecule 24 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:  $C_{53}H_{80}O_2$ ).



| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 24  | A     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 45    | 43 | 2 |         |         |
| 24  | D     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 55    | 53 | 2 |         |         |
| 24  | J     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 35    | 33 | 2 |         |         |
| 24  | a     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 45    | 43 | 2 |         |         |
| 24  | d     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 55    | 53 | 2 |         |         |
| 24  | j     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 35    | 33 | 2 |         |         |

- Molecule 25 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 25  | A     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | B     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | B     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | B     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | B     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | C     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | C     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | F     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | H     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | J     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | K     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | y     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | b     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | b     | 1        | Total C<br>40 40 | 0       | 0       |

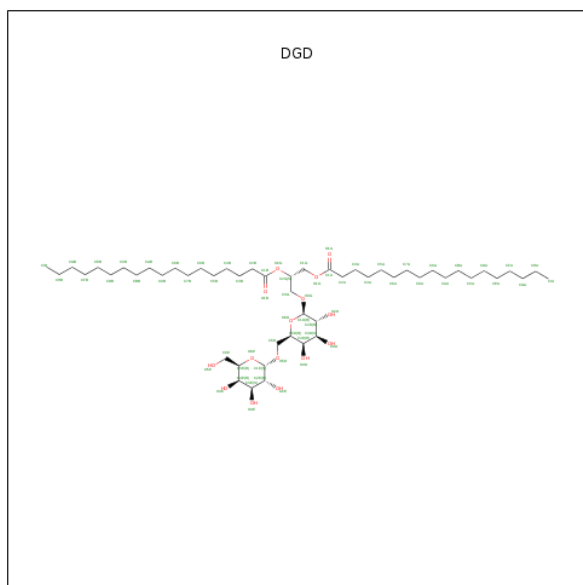
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| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 25  | b     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | b     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | c     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | c     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | c     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | f     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | i     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | j     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | g     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | x     | 1        | Total C<br>40 40 | 0       | 0       |

- Molecule 26 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



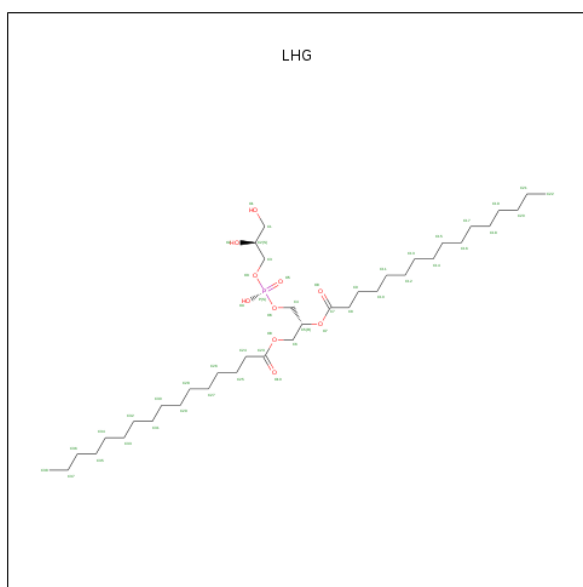
| Mol | Chain | Residues | Atoms                 | ZeroOcc | AltConf |
|-----|-------|----------|-----------------------|---------|---------|
| 26  | A     | 1        | Total C O<br>56 41 15 | 0       | 0       |

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| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 26  | B     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 58    | 43 | 15 |         |         |
| 26  | B     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 52    | 37 | 15 |         |         |
| 26  | C     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 53    | 38 | 15 |         |         |
| 26  | C     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 62    | 47 | 15 |         |         |
| 26  | C     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 66    | 51 | 15 |         |         |
| 26  | D     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 63    | 48 | 15 |         |         |
| 26  | a     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 56    | 41 | 15 |         |         |
| 26  | b     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 52    | 37 | 15 |         |         |
| 26  | b     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 58    | 43 | 15 |         |         |
| 26  | c     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 53    | 38 | 15 |         |         |
| 26  | c     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 62    | 47 | 15 |         |         |
| 26  | c     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 66    | 51 | 15 |         |         |
| 26  | d     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 63    | 48 | 15 |         |         |

- Molecule 27 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).

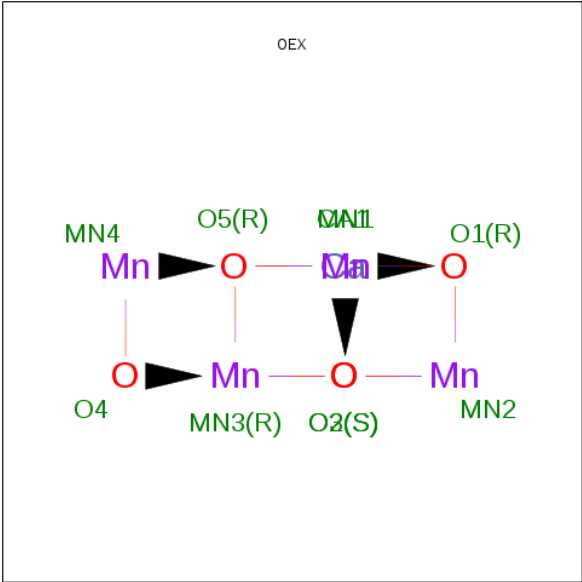


| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 27  | A     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 39    | 28 | 10 | 1 |         |         |
| 27  | C     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 37    | 26 | 10 | 1 |         |         |
| 27  | a     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 39    | 28 | 10 | 1 |         |         |
| 27  | c     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 37    | 26 | 10 | 1 |         |         |

- Molecule 28 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

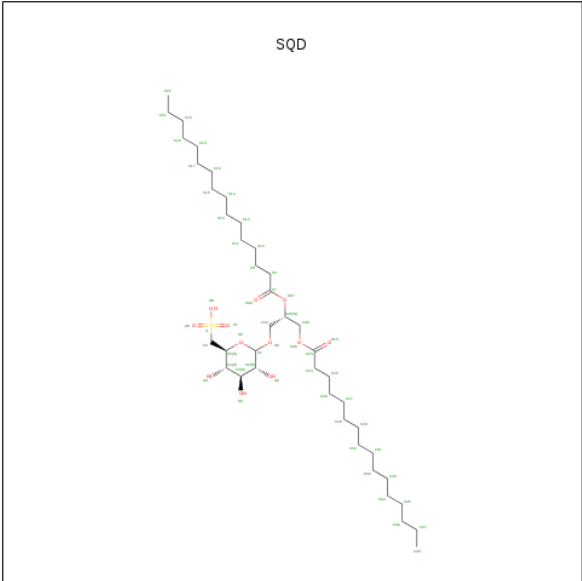
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 28  | A     | 1        | Total | Cl | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 28  | a     | 1        | Total | Cl | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 29 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 29  | A     | 1        | Total | Ca | Mn | O | 0       | 0       |
|     |       |          | 10    | 1  | 4  | 5 |         |         |
| 29  | a     | 1        | Total | Ca | Mn | O | 0       | 0       |
|     |       |          | 10    | 1  | 4  | 5 |         |         |

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



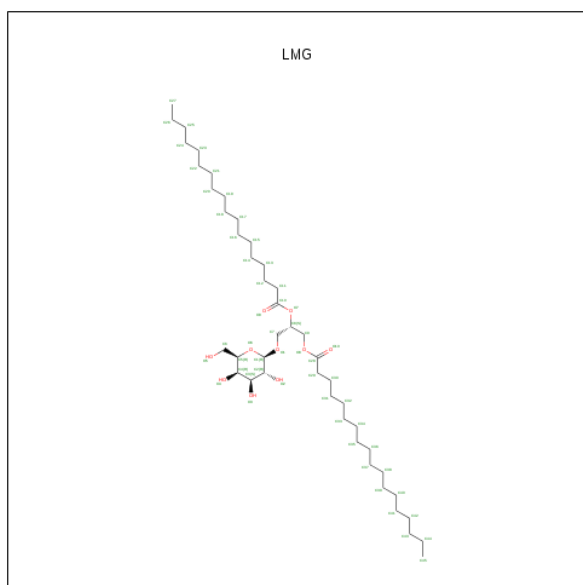
| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 30  | A     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 51    | 38 | 12 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 30  | A     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 54    | 41 | 12 | 1 |         |         |
| 30  | B     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 43    | 30 | 12 | 1 |         |         |
| 30  | B     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 47    | 34 | 12 | 1 |         |         |
| 30  | F     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 45    | 32 | 12 | 1 |         |         |
| 30  | a     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 54    | 41 | 12 | 1 |         |         |
| 30  | a     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 51    | 38 | 12 | 1 |         |         |
| 30  | b     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 47    | 34 | 12 | 1 |         |         |
| 30  | d     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 43    | 30 | 12 | 1 |         |         |
| 30  | f     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 45    | 32 | 12 | 1 |         |         |

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



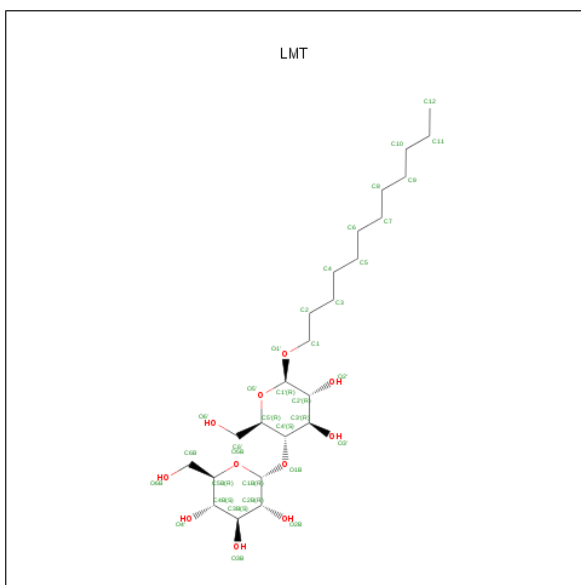
| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 31  | B     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 49    | 39 | 10 |         |         |
| 31  | B     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 49    | 39 | 10 |         |         |

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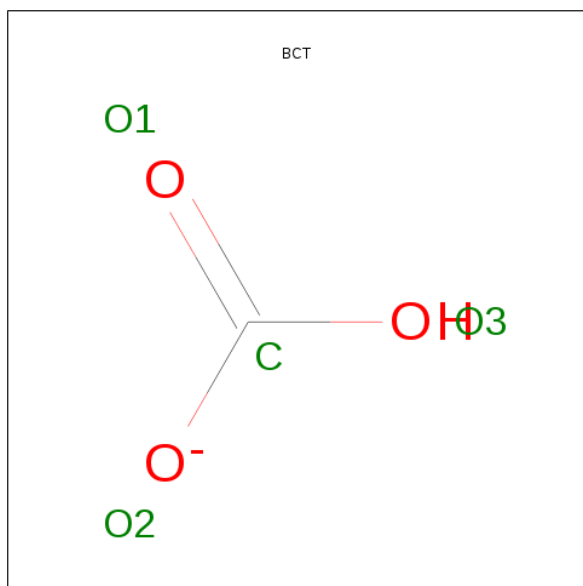
| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 31  | C     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 45    | 35 | 10 |         |         |
| 31  | C     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 48    | 38 | 10 |         |         |
| 31  | D     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 48    | 38 | 10 |         |         |
| 31  | D     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 46    | 36 | 10 |         |         |
| 31  | E     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 44    | 34 | 10 |         |         |
| 31  | I     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 43    | 33 | 10 |         |         |
| 31  | L     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 51    | 41 | 10 |         |         |
| 31  | M     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 42    | 32 | 10 |         |         |
| 31  | a     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 42    | 32 | 10 |         |         |
| 31  | b     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 49    | 39 | 10 |         |         |
| 31  | b     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 42    | 32 | 10 |         |         |
| 31  | c     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 45    | 35 | 10 |         |         |
| 31  | c     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 48    | 38 | 10 |         |         |
| 31  | d     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 49    | 39 | 10 |         |         |
| 31  | d     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 48    | 38 | 10 |         |         |
| 31  | d     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 46    | 36 | 10 |         |         |
| 31  | e     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 44    | 34 | 10 |         |         |
| 31  | i     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 43    | 33 | 10 |         |         |
| 31  | l     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 51    | 41 | 10 |         |         |
| 31  | m     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 42    | 32 | 10 |         |         |

- Molecule 32 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



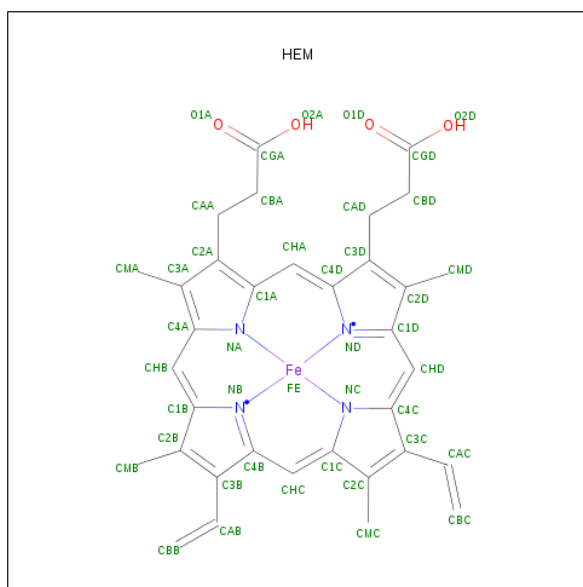
| Mol | Chain | Residues | Atoms       |         |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|---------|
| 32  | B     | 1        | Total<br>35 | C<br>24 | O<br>11 | 0       | 0       |
| 32  | B     | 1        | Total<br>35 | C<br>24 | O<br>11 | 0       | 0       |
| 32  | B     | 1        | Total<br>35 | C<br>24 | O<br>11 | 0       | 0       |
| 32  | B     | 1        | Total<br>35 | C<br>24 | O<br>11 | 0       | 0       |
| 32  | D     | 1        | Total<br>31 | C<br>20 | O<br>11 | 0       | 0       |
| 32  | I     | 1        | Total<br>35 | C<br>24 | O<br>11 | 0       | 0       |
| 32  | M     | 1        | Total<br>35 | C<br>24 | O<br>11 | 0       | 0       |
| 32  | M     | 1        | Total<br>35 | C<br>24 | O<br>11 | 0       | 0       |
| 32  | b     | 1        | Total<br>35 | C<br>24 | O<br>11 | 0       | 0       |
| 32  | b     | 1        | Total<br>35 | C<br>24 | O<br>11 | 0       | 0       |
| 32  | b     | 1        | Total<br>35 | C<br>24 | O<br>11 | 0       | 0       |
| 32  | b     | 1        | Total<br>35 | C<br>24 | O<br>11 | 0       | 0       |
| 32  | d     | 1        | Total<br>31 | C<br>20 | O<br>11 | 0       | 0       |
| 32  | i     | 1        | Total<br>35 | C<br>24 | O<br>11 | 0       | 0       |

- Molecule 33 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 33  | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 1 | 3 |         |         |
| 33  | d     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 1 | 3 |         |         |

- Molecule 34 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$ ).





| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 34  | F     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 34  | V     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 34  | f     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 34  | v     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |

- Molecule 35 is CALCIUM ION (three-letter code: CA) (formula: Ca).

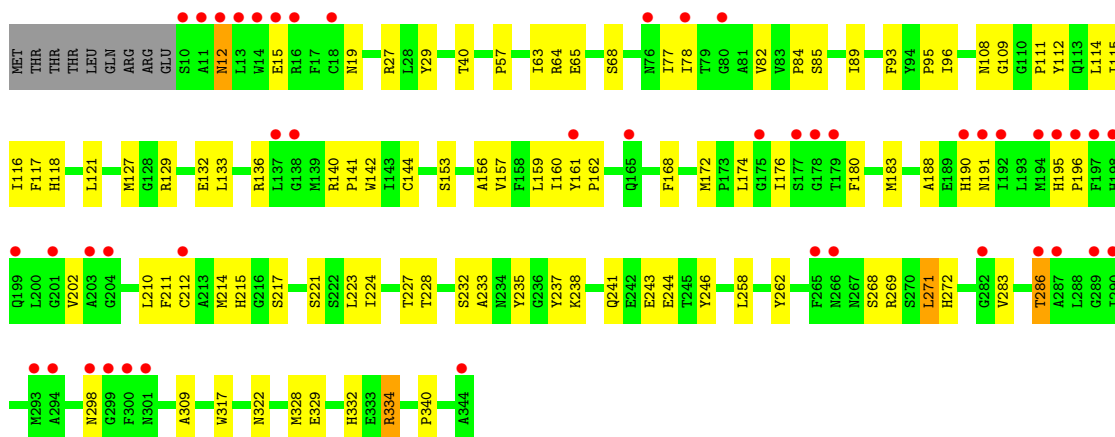
| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 35  | o     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 35  | O     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 35  | K     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 35  | k     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |

### 3 Residue-property plots

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

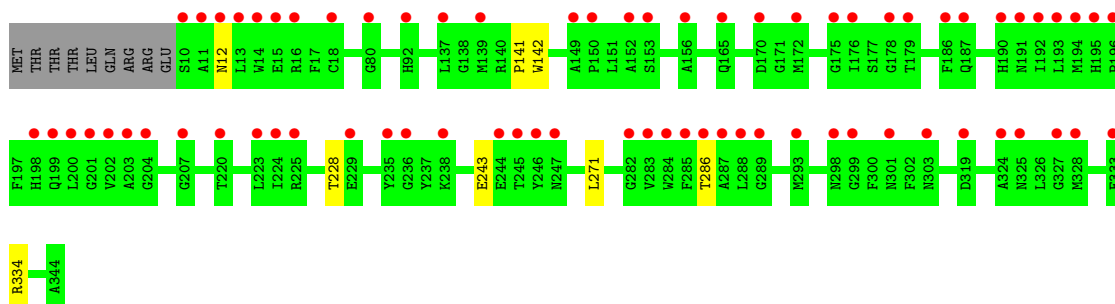
#### • Molecule 1: Photosystem Q(B) protein 1

Chain A: 



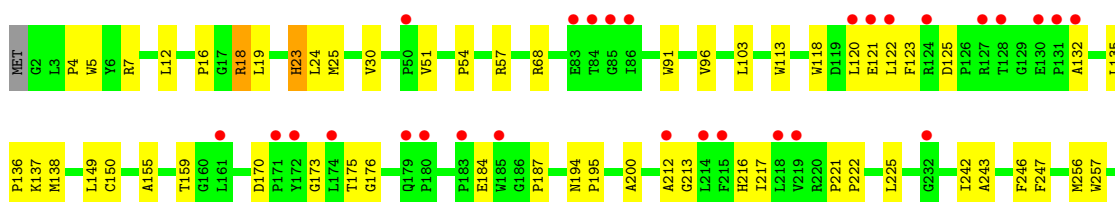
#### • Molecule 1: Photosystem Q(B) protein 1

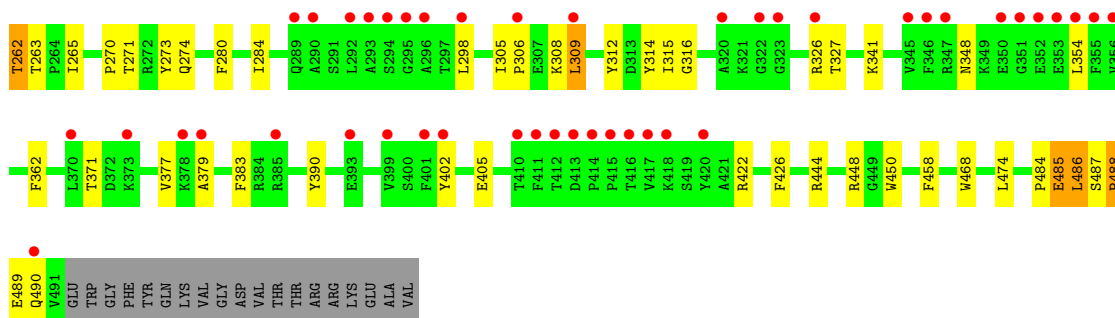
Chain a: 



#### • Molecule 2: Photosystem II core light harvesting protein

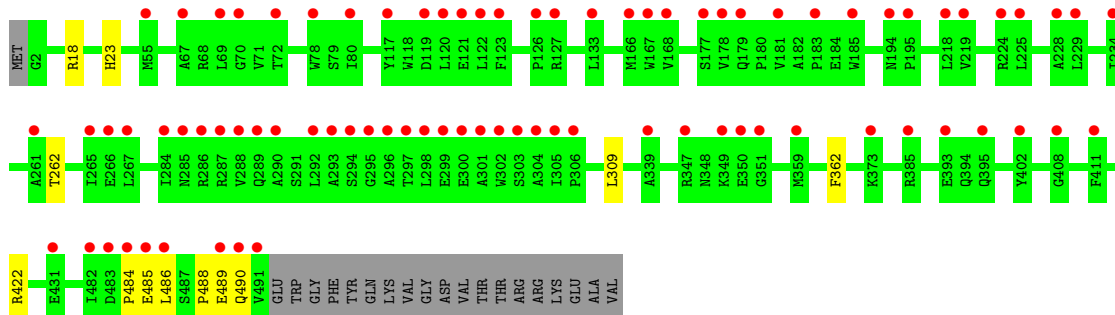
Chain B: 





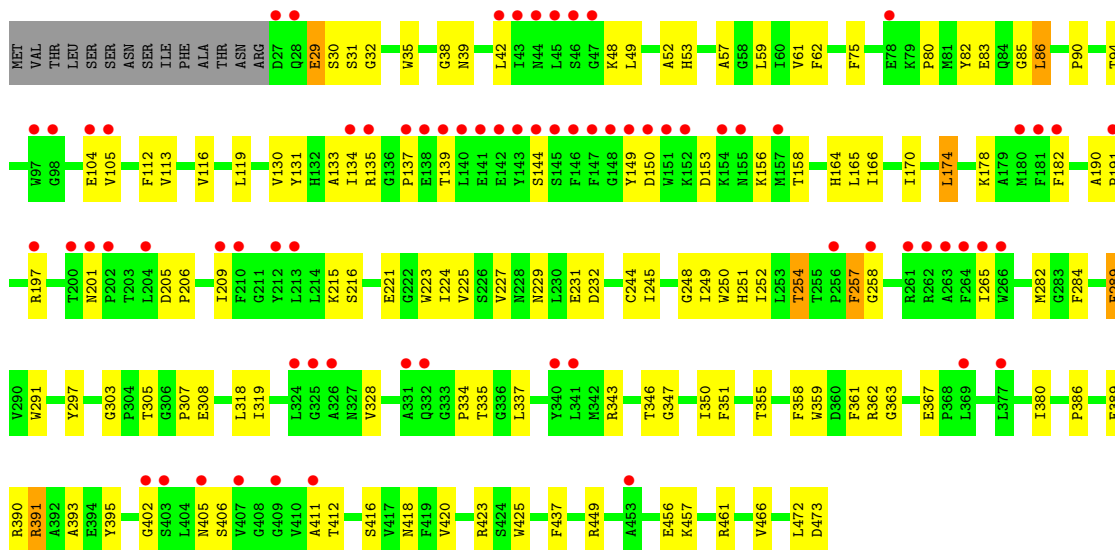
• Molecule 2: Photosystem II core light harvesting protein

Chain b:



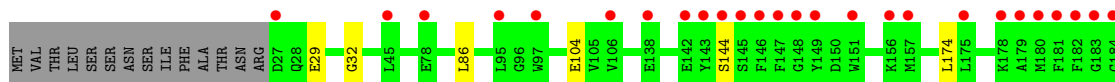
• Molecule 3: Photosystem II CP43 protein

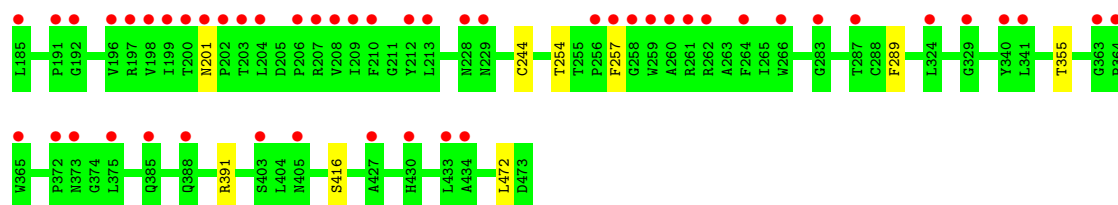
Chain C:



• Molecule 3: Photosystem II CP43 protein

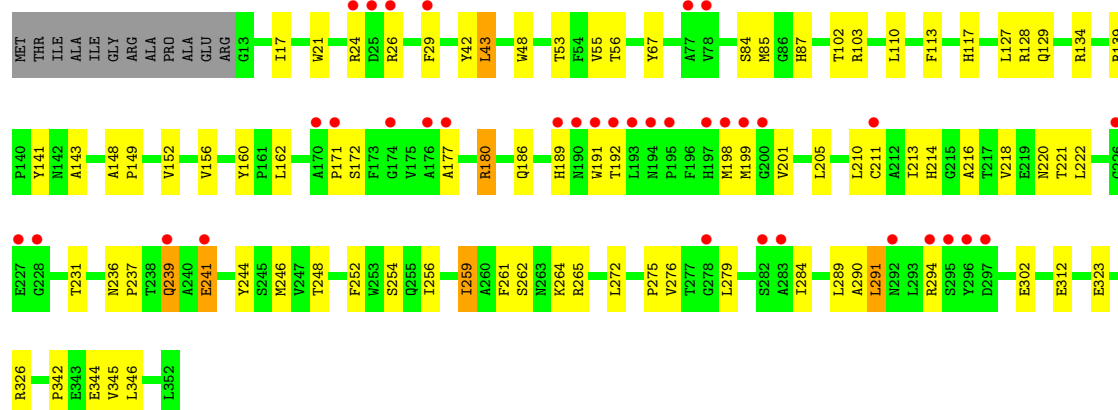
Chain c:





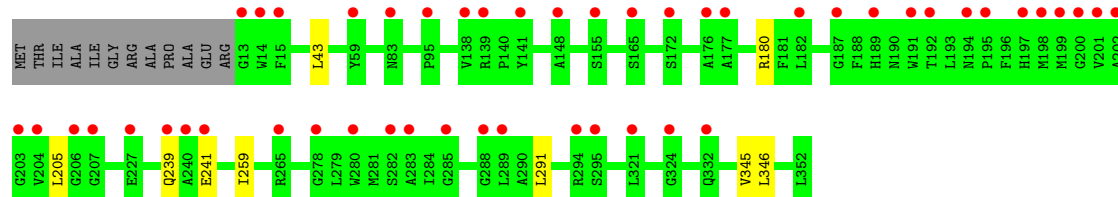
• Molecule 4: Photosystem II D2 protein

Chain D:



• Molecule 4: Photosystem II D2 protein

Chain d:



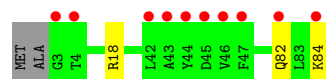
• Molecule 5: Cytochrome b559 subunit alpha

Chain E:



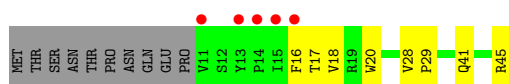
• Molecule 5: Cytochrome b559 subunit alpha

Chain e:



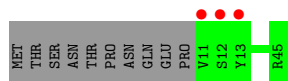
• Molecule 6: Cytochrome b559 subunit beta

Chain F:



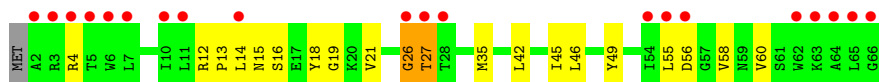
- Molecule 6: Cytochrome b559 subunit beta

Chain f:



- Molecule 7: Photosystem II reaction center protein H

Chain H:



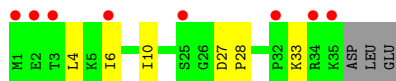
- Molecule 7: Photosystem II reaction center protein H

Chain h:



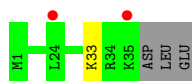
- Molecule 8: Photosystem II reaction center protein I

Chain I:



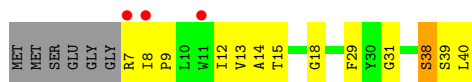
- Molecule 8: Photosystem II reaction center protein I

Chain i:



- Molecule 9: Photosystem II reaction center protein J

Chain J:



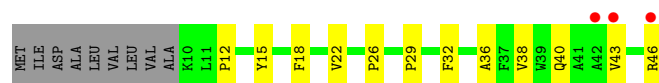
- Molecule 9: Photosystem II reaction center protein J

Chain j:



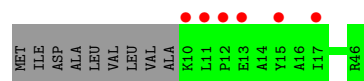
- Molecule 10: Photosystem II reaction center protein K

Chain K:



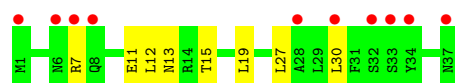
- Molecule 10: Photosystem II reaction center protein K

Chain k:



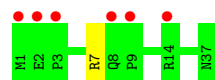
- Molecule 11: Photosystem II reaction center protein L

Chain L:



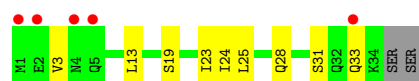
- Molecule 11: Photosystem II reaction center protein L

Chain l:



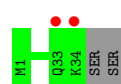
- Molecule 12: Photosystem II reaction center protein M

Chain M:



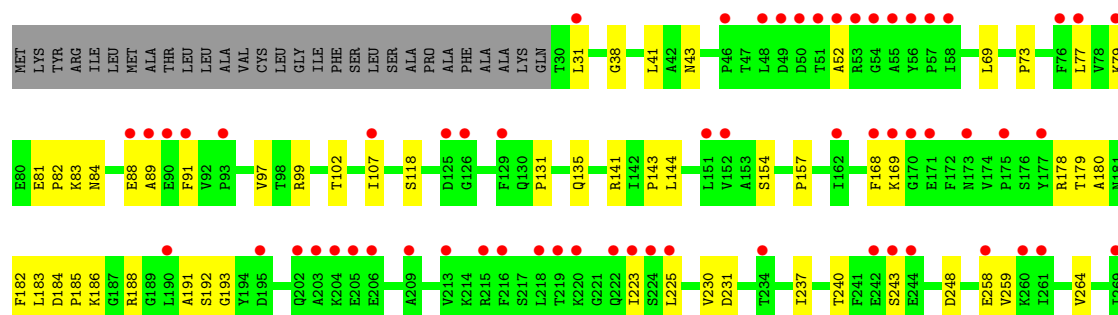
- Molecule 12: Photosystem II reaction center protein M

Chain m:



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

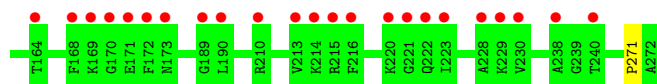
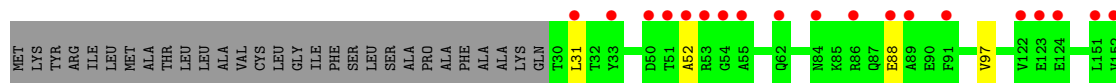
Chain O:





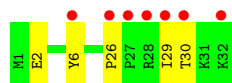
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:



- Molecule 14: Photosystem II reaction center protein T

Chain T:



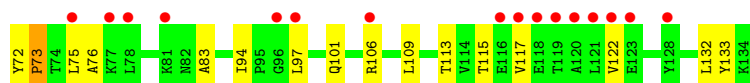
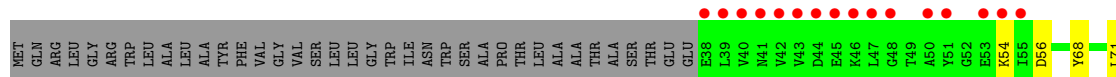
- Molecule 14: Photosystem II reaction center protein T

Chain t:



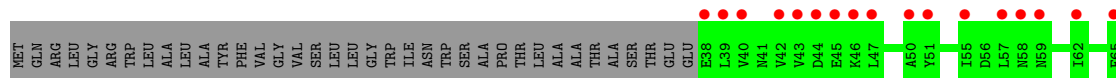
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:



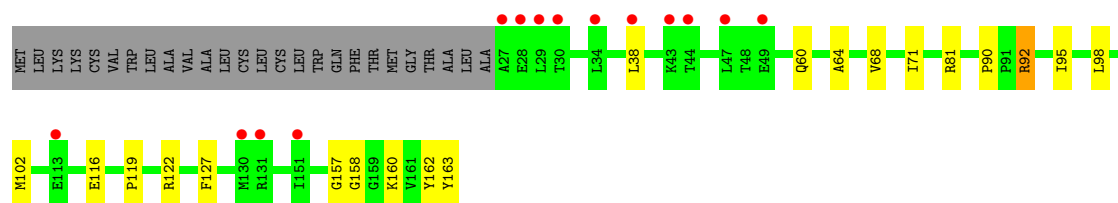
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:



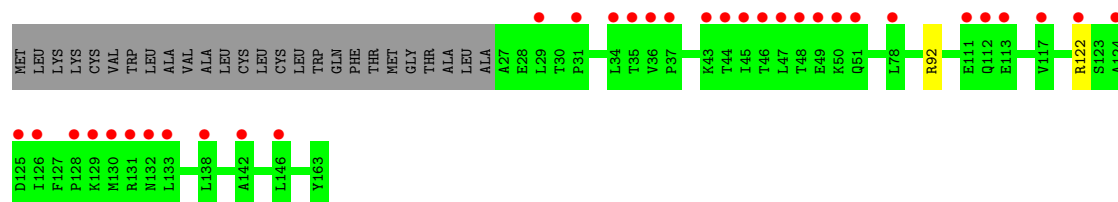
- Molecule 16: Cytochrome c-550

Chain V:



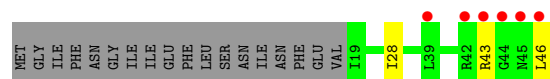
- Molecule 16: Cytochrome c-550

Chain v:



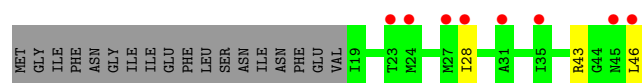
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:



- Molecule 17: Photosystem II reaction center protein Ycf12

Chain g:



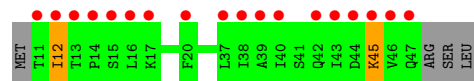
- Molecule 18: Photosystem II reaction center X protein

Chain X:



- Molecule 18: Photosystem II reaction center X protein

Chain x:



- Molecule 19: Photosystem II reaction center protein Y

Chain Y:

There are no outlier residues recorded for this chain.

- Molecule 19: Photosystem II reaction center protein Y

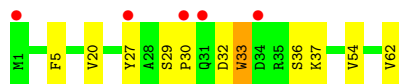
Chain G:



There are no outlier residues recorded for this chain.

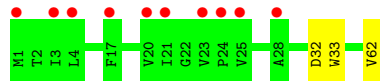
- Molecule 20: Photosystem II reaction center protein Z

Chain Z: 



- Molecule 20: Photosystem II reaction center protein Z

Chain z: 



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 132.62Å 229.30Å 306.82Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 68.41 – 5.20<br>68.41 – 5.20                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 98.0 (68.41-5.20)<br>97.9 (68.41-5.20)                      | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.59 (at 5.12Å)   | Xtriage          |
| Refinement program  | PHENIX (phenix.refine: dev_1635+SVN)                        | Depositor        |
| R, $R_{free}$   | 0.271 , 0.289<br>0.267 , 0.283                              | Depositor<br>DCC |
| $R_{free}$ test set   | 1751 reflections (4.87%)                                    | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 176.5   | Xtriage          |
| Anisotropy  | 0.214   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.32 , 152.8  | EDS              |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| L-test for twinning   | $\langle  L  \rangle = 0.33$ , $\langle L^2 \rangle = 0.15$ | Xtriage          |
| Outliers  | 0 of 35970 reflections                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.84  | EDS              |
| Total number of atoms   | 50244   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 207.0   | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.79% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, OEX, PHO, DGD, CL, CA, LMT, 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     | 0.25         | 0/2713      | 0.42        | 0/3700      |
| 1   | a     | 0.24         | 0/2713      | 0.42        | 0/3700      |
| 2   | B     | 0.24         | 0/3986      | 0.41        | 0/5433      |
| 2   | b     | 0.24         | 0/3986      | 0.41        | 0/5433      |
| 3   | C     | 0.23         | 0/3556      | 0.42        | 0/4842      |
| 3   | c     | 0.23         | 0/3556      | 0.42        | 0/4842      |
| 4   | D     | 0.24         | 0/2801      | 0.41        | 0/3818      |
| 4   | d     | 0.24         | 0/2801      | 0.41        | 0/3818      |
| 5   | E     | 0.23         | 0/685       | 0.44        | 0/933       |
| 5   | e     | 0.23         | 0/685       | 0.43        | 0/933       |
| 6   | F     | 0.23         | 0/291       | 0.40        | 0/397       |
| 6   | f     | 0.23         | 0/291       | 0.41        | 0/397       |
| 7   | H     | 0.24         | 0/520       | 0.46        | 0/709       |
| 7   | h     | 0.23         | 0/520       | 0.46        | 0/709       |
| 8   | I     | 0.25         | 0/293       | 0.44        | 0/395       |
| 8   | i     | 0.26         | 0/293       | 0.44        | 0/395       |
| 9   | J     | 0.21         | 0/255       | 0.41        | 0/346       |
| 9   | j     | 0.22         | 0/255       | 0.40        | 0/346       |
| 10  | K     | 0.27         | 0/303       | 0.49        | 0/416       |
| 10  | k     | 0.27         | 0/303       | 0.49        | 0/416       |
| 11  | L     | 0.23         | 0/311       | 0.40        | 0/422       |
| 11  | l     | 0.22         | 0/311       | 0.40        | 0/422       |
| 12  | M     | 0.24         | 0/270       | 0.44        | 0/367       |
| 12  | m     | 0.24         | 0/270       | 0.44        | 0/367       |
| 13  | O     | 0.23         | 0/1876      | 0.44        | 0/2548      |
| 13  | o     | 0.23         | 0/1876      | 0.44        | 0/2548      |
| 14  | T     | 0.25         | 0/284       | 0.41        | 0/381       |
| 14  | t     | 0.25         | 0/284       | 0.40        | 0/381       |
| 15  | U     | 0.23         | 0/785       | 0.43        | 0/1064      |
| 15  | u     | 0.23         | 0/785       | 0.44        | 0/1064      |
| 16  | V     | 0.22         | 0/1081      | 0.42        | 0/1468      |
| 16  | v     | 0.22         | 0/1081      | 0.41        | 0/1468      |

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 17  | g     | 0.22         | 0/202   | 0.46        | 0/272   |
| 17  | y     | 0.23         | 0/202   | 0.46        | 0/272   |
| 18  | X     | 0.27         | 0/273   | 0.44        | 0/370   |
| 18  | x     | 0.26         | 0/273   | 0.45        | 0/370   |
| 20  | Z     | 0.25         | 0/490   | 0.45        | 0/669   |
| 20  | z     | 0.24         | 0/490   | 0.45        | 0/669   |
| All | All   | 0.24         | 0/41950 | 0.42        | 0/57100 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2628  | 0        | 2524     | 82      | 0            |
| 1   | a     | 2628  | 0        | 2524     | 0       | 0            |
| 2   | B     | 3850  | 0        | 3718     | 90      | 0            |
| 2   | b     | 3850  | 0        | 3718     | 0       | 0            |
| 3   | C     | 3444  | 0        | 3365     | 100     | 0            |
| 3   | c     | 3444  | 0        | 3365     | 0       | 0            |
| 4   | D     | 2706  | 0        | 2608     | 83      | 0            |
| 4   | d     | 2706  | 0        | 2608     | 0       | 0            |
| 5   | E     | 666   | 0        | 651      | 16      | 0            |
| 5   | e     | 666   | 0        | 651      | 0       | 0            |
| 6   | F     | 282   | 0        | 291      | 8       | 0            |
| 6   | f     | 282   | 0        | 291      | 0       | 0            |
| 7   | H     | 507   | 0        | 521      | 22      | 0            |
| 7   | h     | 507   | 0        | 521      | 0       | 0            |
| 8   | I     | 286   | 0        | 308      | 4       | 0            |
| 8   | i     | 286   | 0        | 308      | 0       | 0            |
| 9   | J     | 249   | 0        | 262      | 10      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 9   | j     | 249   | 0        | 262      | 0       | 0            |
| 10  | K     | 293   | 0        | 305      | 10      | 0            |
| 10  | k     | 293   | 0        | 305      | 0       | 0            |
| 11  | L     | 304   | 0        | 316      | 9       | 0            |
| 11  | l     | 304   | 0        | 316      | 0       | 0            |
| 12  | M     | 267   | 0        | 289      | 8       | 0            |
| 12  | m     | 267   | 0        | 289      | 0       | 0            |
| 13  | O     | 1845  | 0        | 1801     | 34      | 0            |
| 13  | o     | 1845  | 0        | 1801     | 0       | 0            |
| 14  | T     | 275   | 0        | 288      | 3       | 0            |
| 14  | t     | 275   | 0        | 288      | 0       | 0            |
| 15  | U     | 774   | 0        | 773      | 10      | 0            |
| 15  | u     | 774   | 0        | 773      | 0       | 0            |
| 16  | V     | 1060  | 0        | 1068     | 12      | 0            |
| 16  | v     | 1060  | 0        | 1068     | 0       | 0            |
| 17  | g     | 201   | 0        | 226      | 0       | 0            |
| 17  | y     | 201   | 0        | 226      | 0       | 0            |
| 18  | X     | 270   | 0        | 299      | 10      | 0            |
| 18  | x     | 270   | 0        | 299      | 0       | 0            |
| 19  | G     | 140   | 0        | 31       | 0       | 0            |
| 19  | Y     | 140   | 0        | 31       | 0       | 0            |
| 20  | Z     | 479   | 0        | 516      | 9       | 0            |
| 20  | z     | 479   | 0        | 516      | 0       | 0            |
| 21  | A     | 1     | 0        | 0        | 0       | 0            |
| 21  | a     | 1     | 0        | 0        | 0       | 0            |
| 22  | A     | 260   | 0        | 288      | 42      | 0            |
| 22  | B     | 975   | 0        | 1080     | 103     | 0            |
| 22  | C     | 845   | 0        | 936      | 45      | 0            |
| 22  | D     | 130   | 0        | 144      | 13      | 0            |
| 22  | H     | 65    | 0        | 72       | 11      | 0            |
| 22  | a     | 260   | 0        | 288      | 0       | 0            |
| 22  | b     | 1040  | 0        | 1152     | 0       | 0            |
| 22  | c     | 845   | 0        | 936      | 0       | 0            |
| 22  | d     | 130   | 0        | 144      | 0       | 0            |
| 23  | A     | 64    | 0        | 74       | 6       | 0            |
| 23  | D     | 64    | 0        | 74       | 12      | 0            |
| 23  | d     | 128   | 0        | 148      | 0       | 0            |
| 24  | A     | 45    | 0        | 61       | 6       | 0            |
| 24  | D     | 55    | 0        | 80       | 10      | 0            |
| 24  | J     | 35    | 0        | 45       | 0       | 0            |
| 24  | a     | 45    | 0        | 61       | 0       | 0            |
| 24  | d     | 55    | 0        | 80       | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 24  | j     | 35    | 0        | 45       | 0       | 0            |
| 25  | A     | 40    | 0        | 56       | 3       | 0            |
| 25  | B     | 160   | 0        | 224      | 13      | 0            |
| 25  | C     | 80    | 0        | 112      | 15      | 0            |
| 25  | F     | 40    | 0        | 56       | 3       | 0            |
| 25  | H     | 40    | 0        | 56       | 2       | 0            |
| 25  | J     | 40    | 0        | 56       | 3       | 0            |
| 25  | K     | 40    | 0        | 56       | 3       | 0            |
| 25  | b     | 160   | 0        | 224      | 0       | 0            |
| 25  | c     | 120   | 0        | 168      | 0       | 0            |
| 25  | f     | 40    | 0        | 56       | 0       | 0            |
| 25  | g     | 40    | 0        | 56       | 0       | 0            |
| 25  | i     | 40    | 0        | 56       | 0       | 0            |
| 25  | j     | 40    | 0        | 56       | 0       | 0            |
| 25  | x     | 40    | 0        | 56       | 0       | 0            |
| 25  | y     | 40    | 0        | 56       | 0       | 0            |
| 26  | A     | 56    | 0        | 70       | 1       | 0            |
| 26  | B     | 110   | 0        | 136      | 4       | 0            |
| 26  | C     | 181   | 0        | 245      | 18      | 0            |
| 26  | D     | 63    | 0        | 87       | 2       | 0            |
| 26  | a     | 56    | 0        | 70       | 0       | 0            |
| 26  | b     | 110   | 0        | 136      | 0       | 0            |
| 26  | c     | 181   | 0        | 245      | 0       | 0            |
| 26  | d     | 63    | 0        | 87       | 0       | 0            |
| 27  | A     | 39    | 0        | 51       | 2       | 0            |
| 27  | C     | 37    | 0        | 44       | 3       | 0            |
| 27  | a     | 39    | 0        | 51       | 0       | 0            |
| 27  | c     | 37    | 0        | 44       | 0       | 0            |
| 28  | A     | 1     | 0        | 0        | 0       | 0            |
| 28  | a     | 1     | 0        | 0        | 0       | 0            |
| 29  | A     | 10    | 0        | 0        | 0       | 0            |
| 29  | a     | 10    | 0        | 0        | 0       | 0            |
| 30  | A     | 105   | 0        | 147      | 6       | 0            |
| 30  | B     | 90    | 0        | 111      | 3       | 0            |
| 30  | F     | 45    | 0        | 54       | 3       | 0            |
| 30  | a     | 105   | 0        | 147      | 0       | 0            |
| 30  | b     | 47    | 0        | 61       | 0       | 0            |
| 30  | d     | 43    | 0        | 50       | 0       | 0            |
| 30  | f     | 45    | 0        | 54       | 0       | 0            |
| 31  | B     | 98    | 0        | 136      | 6       | 0            |
| 31  | C     | 93    | 0        | 126      | 3       | 0            |
| 31  | D     | 94    | 0        | 128      | 15      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 31  | E     | 44    | 0        | 58       | 2       | 0            |
| 31  | I     | 43    | 0        | 56       | 1       | 0            |
| 31  | L     | 51    | 0        | 72       | 2       | 0            |
| 31  | M     | 42    | 0        | 54       | 3       | 0            |
| 31  | a     | 42    | 0        | 54       | 0       | 0            |
| 31  | b     | 91    | 0        | 122      | 0       | 0            |
| 31  | c     | 93    | 0        | 126      | 0       | 0            |
| 31  | d     | 143   | 0        | 196      | 0       | 0            |
| 31  | e     | 44    | 0        | 58       | 0       | 0            |
| 31  | i     | 43    | 0        | 56       | 0       | 0            |
| 31  | l     | 51    | 0        | 72       | 0       | 0            |
| 31  | m     | 42    | 0        | 54       | 0       | 0            |
| 32  | B     | 140   | 0        | 184      | 5       | 0            |
| 32  | D     | 31    | 0        | 35       | 0       | 0            |
| 32  | I     | 35    | 0        | 46       | 1       | 0            |
| 32  | M     | 70    | 0        | 92       | 0       | 0            |
| 32  | b     | 140   | 0        | 184      | 0       | 0            |
| 32  | d     | 31    | 0        | 35       | 0       | 0            |
| 32  | i     | 35    | 0        | 46       | 0       | 0            |
| 33  | D     | 4     | 0        | 1        | 0       | 0            |
| 33  | d     | 4     | 0        | 1        | 0       | 0            |
| 34  | F     | 43    | 0        | 30       | 5       | 0            |
| 34  | V     | 43    | 0        | 30       | 3       | 0            |
| 34  | f     | 43    | 0        | 30       | 0       | 0            |
| 34  | v     | 43    | 0        | 30       | 0       | 0            |
| 35  | K     | 1     | 0        | 0        | 0       | 0            |
| 35  | O     | 1     | 0        | 0        | 0       | 0            |
| 35  | k     | 1     | 0        | 0        | 0       | 0            |
| 35  | o     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 50244 | 0        | 51374    | 639     | 0            |

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (639) close contacts within the same asymmetric unit are listed below.

| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 3:C:39:ASN:HB2    | 22:C:507:CLA:HBA1 | 1.55        | 0.87     |
| 4:D:26:ARG:HD3    | 6:F:18:VAL:HG11   | 1.60        | 0.83     |
| 12:M:33:GLN:HB3   | 12:M:33:GLN:HB3   | 0.00        | 0.82     |
| 13:O:82:PRO:HG3   | 13:O:89:ALA:HB2   | 1.62        | 0.82     |
| 3:C:362:ARG:H     | 26:C:514:DGD:HE4  | 1.47        | 0.78     |
| 34:V:201:HEM:HBC2 | 34:V:201:HEM:HHD  | 1.67        | 0.77     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 3:C:362:ARG:H     | 26:C:515:DGD:HE4  | 24.14       | 0.77     |
| 4:D:199:MET:HG2   | 24:D:405:PL9:H322 | 1.69        | 0.74     |
| 1:A:129:ARG:HH21  | 4:D:256:ILE:HD12  | 1.53        | 0.73     |
| 2:B:121:GLU:HG2   | 7:H:4:ARG:HG2     | 1.69        | 0.73     |
| 4:D:29:PHE:O      | 4:D:128:ARG:NH2   | 2.22        | 0.73     |
| 34:F:101:HEM:HHC  | 34:F:101:HEM:HBB2 | 1.71        | 0.72     |
| 1:A:63:ILE:HB     | 3:C:335:THR:HG21  | 1.79        | 0.72     |
| 2:B:24:LEU:HD21   | 22:B:615:CLA:HAB  | 1.72        | 0.72     |
| 26:C:516:DGD:HAF2 | 22:C:519:CLA:H202 | 1.71        | 0.71     |
| 4:D:236:ASN:ND2   | 4:D:239:GLN:O     | 2.23        | 0.71     |
| 1:A:221:SER:HB3   | 4:D:141:TYR:HB2   | 1.72        | 0.71     |
| 13:O:69:LEU:HB3   | 13:O:107:ILE:HB   | 1.77        | 0.71     |
| 22:B:605:CLA:H72  | 25:B:619:BCR:H311 | 1.73        | 0.71     |
| 4:D:21:TRP:O      | 4:D:26:ARG:NH2    | 2.23        | 0.70     |
| 5:E:60:GLN:OE1    | 5:E:84:LYS:NZ     | 2.32        | 0.69     |
| 4:D:152:VAL:HG21  | 4:D:279:LEU:HD12  | 1.72        | 0.69     |
| 1:A:183:MET:HB3   | 22:A:402:CLA:HBC2 | 1.73        | 0.69     |
| 4:D:189:HIS:HA    | 4:D:294:ARG:HD2   | 1.84        | 0.69     |
| 4:D:259:ILE:HG12  | 31:D:409:LMG:H292 | 45.22       | 0.69     |
| 1:A:82:VAL:HB     | 1:A:174:LEU:HB2   | 1.74        | 0.68     |
| 22:C:503:CLA:H172 | 22:C:509:CLA:HBB2 | 1.74        | 0.68     |
| 12:M:31:SER:HA    | 31:M:101:LMG:HC1  | 1.79        | 0.67     |
| 3:C:178:LYS:HA    | 3:C:182:PHE:HB2   | 1.97        | 0.67     |
| 3:C:297:TYR:O     | 3:C:423:ARG:NH2   | 2.28        | 0.67     |
| 3:C:406:SER:O     | 3:C:418:ASN:ND2   | 2.28        | 0.67     |
| 2:B:187:PRO:HB3   | 22:B:601:CLA:HMB2 | 1.76        | 0.66     |
| 6:F:17:THR:HG23   | 6:F:20:TRP:H      | 1.60        | 0.66     |
| 2:B:474:LEU:O     | 4:D:134:ARG:NH1   | 2.54        | 0.66     |
| 4:D:186:GLN:HB2   | 22:D:403:CLA:HBC1 | 1.77        | 0.66     |
| 3:C:165:LEU:HD21  | 22:C:505:CLA:HAB  | 1.76        | 0.66     |
| 22:C:506:CLA:H112 | 25:C:513:BCR:H362 | 1.76        | 0.65     |
| 22:A:403:CLA:H122 | 23:D:401:PHO:H3A  | 31.92       | 0.65     |
| 3:C:250:TRP:O     | 3:C:254:THR:OG1   | 2.13        | 0.65     |
| 2:B:271:THR:HG22  | 2:B:273:TYR:H     | 1.63        | 0.65     |
| 3:C:291:TRP:O     | 3:C:305:THR:OG1   | 2.16        | 0.65     |
| 22:C:507:CLA:HBC3 | 22:C:509:CLA:H92  | 1.79        | 0.65     |
| 22:A:403:CLA:H71  | 22:A:404:CLA:HAB  | 27.47       | 0.65     |
| 20:Z:33:TRP:HA    | 20:Z:36:SER:HB3   | 1.80        | 0.64     |
| 22:B:612:CLA:H42  | 4:D:127:LEU:HD11  | 22.83       | 0.64     |
| 3:C:216:SER:HB3   | 3:C:221:GLU:HB2   | 1.84        | 0.64     |
| 1:A:174:LEU:HD22  | 23:D:401:PHO:H151 | 37.14       | 0.64     |
| 30:B:622:SQD:H171 | 30:B:622:SQD:H301 | 1.79        | 0.64     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 22:B:607:CLA:HBA2 | 30:B:622:SQD:H101 | 1.81        | 0.63     |
| 22:A:404:CLA:H142 | 22:D:403:CLA:H151 | 1.80        | 0.63     |
| 22:B:607:CLA:H42  | 4:D:127:LEU:HD11  | 1.80        | 0.63     |
| 22:A:403:CLA:HBB1 | 22:A:403:CLA:HHC  | 2.33        | 0.63     |
| 22:A:402:CLA:H71  | 22:A:403:CLA:HAB  | 1.80        | 0.63     |
| 4:D:24:ARG:NH2    | 18:X:44:ASP:O     | 2.35        | 0.63     |
| 3:C:49:LEU:O      | 3:C:53:HIS:ND1    | 2.30        | 0.62     |
| 2:B:341:LYS:HA    | 2:B:405:GLU:HB2   | 1.81        | 0.62     |
| 3:C:48:LYS:NZ     | 3:C:133:ALA:O     | 2.31        | 0.62     |
| 1:A:15:GLU:O      | 1:A:19:ASN:ND2    | 2.34        | 0.62     |
| 22:B:607:CLA:H193 | 7:H:42:LEU:HD12   | 10.41       | 0.62     |
| 13:O:77:LEU:HB3   | 13:O:91:PHE:HB3   | 1.84        | 0.62     |
| 22:B:602:CLA:H193 | 7:H:42:LEU:HD12   | 1.81        | 0.62     |
| 2:B:121:GLU:O     | 7:H:12:ARG:NH2    | 2.41        | 0.62     |
| 22:B:608:CLA:HMD1 | 7:H:27:THR:HB     | 1.82        | 0.61     |
| 1:A:140:ARG:NH2   | 27:A:410:LHG:O5   | 2.30        | 0.61     |
| 3:C:449:ARG:HE    | 22:C:504:CLA:HED1 | 1.65        | 0.61     |
| 22:A:404:CLA:H203 | 23:D:401:PHO:H71  | 15.37       | 0.61     |
| 4:D:214:HIS:ND1   | 24:D:405:PL9:O2   | 2.22        | 0.61     |
| 3:C:75:PHE:HZ     | 3:C:105:VAL:HG21  | 1.71        | 0.61     |
| 1:A:183:MET:HB3   | 22:A:403:CLA:HBC2 | 6.12        | 0.61     |
| 2:B:187:PRO:HB3   | 22:B:605:CLA:HMB2 | 29.63       | 0.61     |
| 2:B:149:LEU:HG    | 22:B:607:CLA:HBC1 | 22.33       | 0.61     |
| 30:A:413:SQD:H172 | 27:C:518:LHG:H172 | 1.83        | 0.61     |
| 4:D:216:ALA:O     | 4:D:220:ASN:ND2   | 2.35        | 0.61     |
| 9:J:15:THR:HG21   | 10:K:38:VAL:HG13  | 1.86        | 0.61     |
| 26:B:620:DGD:HAW2 | 22:H:101:CLA:H152 | 1.83        | 0.60     |
| 13:O:230:VAL:HG13 | 13:O:237:ILE:HG22 | 1.83        | 0.60     |
| 1:A:329:GLU:O     | 1:A:332:HIS:ND1   | 2.32        | 0.60     |
| 22:A:403:CLA:HED1 | 24:D:405:PL9:H372 | 1.83        | 0.60     |
| 11:L:13:ASN:ND2   | 31:L:101:LMG:O5   | 2.33        | 0.60     |
| 1:A:183:MET:HA    | 22:A:402:CLA:HMD2 | 1.83        | 0.60     |
| 3:C:42:LEU:HD21   | 22:C:510:CLA:H2A  | 1.83        | 0.60     |
| 4:D:259:ILE:HG12  | 31:D:406:LMG:H292 | 1.83        | 0.59     |
| 31:D:406:LMG:HO5  | 31:D:406:LMG:HO4  | 1.49        | 0.59     |
| 3:C:150:ASP:HB3   | 3:C:153:ASP:HB2   | 1.86        | 0.59     |
| 1:A:227:THR:HG21  | 1:A:233:ALA:HA    | 1.84        | 0.59     |
| 1:A:89:ILE:HD11   | 1:A:108:ASN:HB3   | 1.96        | 0.59     |
| 22:B:607:CLA:C2D  | 22:B:609:CLA:H2   | 16.50       | 0.59     |
| 4:D:192:THR:HG23  | 22:D:403:CLA:HBC2 | 1.84        | 0.59     |
| 1:A:174:LEU:HD22  | 23:A:405:PHO:H151 | 1.85        | 0.59     |
| 1:A:183:MET:HA    | 22:A:403:CLA:HMD2 | 8.57        | 0.58     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 22:B:606:CLA:HBB1 | 31:B:621:LMG:H341 | 1.84        | 0.58     |
| 22:B:606:CLA:HAA2 | 7:H:45:ILE:HD12   | 30.06       | 0.58     |
| 13:O:83:LYS:HG2   | 13:O:84:ASN:H     | 1.68        | 0.58     |
| 22:C:508:CLA:HBD  | 22:C:508:CLA:H121 | 1.84        | 0.58     |
| 5:E:18:ARG:NH1    | 34:F:101:HEM:O1A  | 2.37        | 0.58     |
| 34:V:201:HEM:HBB2 | 34:V:201:HEM:HMB1 | 1.85        | 0.58     |
| 22:B:613:CLA:HMD1 | 7:H:27:THR:HB     | 43.37       | 0.58     |
| 4:D:222:LEU:HD23  | 4:D:244:TYR:HB3   | 1.87        | 0.58     |
| 22:A:402:CLA:H122 | 23:A:405:PHO:H3A  | 1.84        | 0.58     |
| 2:B:327:THR:HG21  | 31:B:621:LMG:H111 | 1.85        | 0.58     |
| 2:B:379:ALA:HA    | 2:B:390:TYR:HB3   | 1.89        | 0.57     |
| 2:B:149:LEU:HG    | 22:B:602:CLA:HBC1 | 1.85        | 0.57     |
| 2:B:12:LEU:HB2    | 22:B:611:CLA:HMC2 | 1.85        | 0.57     |
| 22:C:505:CLA:HMC2 | 22:C:506:CLA:H102 | 1.87        | 0.57     |
| 1:A:29:TYR:O      | 1:A:129:ARG:NH1   | 2.53        | 0.57     |
| 31:D:406:LMG:O6   | 11:L:15:THR:HG21  | 2.05        | 0.57     |
| 2:B:487:SER:N     | 2:B:488:PRO:HD2   | 2.20        | 0.57     |
| 30:A:413:SQD:H223 | 26:C:516:DGD:HAE1 | 1.87        | 0.56     |
| 3:C:164:HIS:ND1   | 22:C:506:CLA:OBD  | 2.30        | 0.56     |
| 1:A:217:SER:HA    | 4:D:272:LEU:HD12  | 1.89        | 0.56     |
| 2:B:262:THR:HG22  | 2:B:263:THR:HG23  | 1.87        | 0.56     |
| 22:A:403:CLA:H203 | 23:A:405:PHO:H71  | 1.87        | 0.56     |
| 3:C:361:PHE:HD1   | 26:C:514:DGD:HE61 | 1.71        | 0.56     |
| 31:D:409:LMG:H171 | 25:F:102:BCR:H383 | 1.86        | 0.56     |
| 22:C:501:CLA:HMB3 | 25:C:513:BCR:H403 | 1.88        | 0.56     |
| 27:C:518:LHG:H271 | 27:C:518:LHG:H101 | 1.87        | 0.56     |
| 22:B:607:CLA:H151 | 22:B:608:CLA:H203 | 1.87        | 0.56     |
| 30:F:103:SQD:H162 | 18:X:33:THR:HA    | 1.88        | 0.56     |
| 13:O:240:THR:HG22 | 13:O:264:VAL:HG12 | 1.94        | 0.56     |
| 1:A:84:PRO:HA     | 1:A:112:TYR:CG    | 2.41        | 0.56     |
| 2:B:155:ALA:O     | 2:B:159:THR:OG1   | 2.18        | 0.56     |
| 3:C:215:LYS:HB3   | 3:C:223:TRP:HA    | 1.88        | 0.56     |
| 1:A:153:SER:HB3   | 22:A:402:CLA:HED1 | 1.88        | 0.55     |
| 22:B:606:CLA:H2   | 22:B:606:CLA:HBD  | 7.91        | 0.55     |
| 2:B:262:THR:OG1   | 22:B:607:CLA:O1D  | 28.18       | 0.55     |
| 13:O:73:PRO:HG2   | 13:O:102:THR:HB   | 1.89        | 0.55     |
| 20:Z:33:TRP:O     | 20:Z:37:LYS:HB2   | 2.06        | 0.55     |
| 10:K:12:PRO:HB2   | 10:K:15:TYR:HD2   | 1.72        | 0.55     |
| 15:U:68:TYR:HB2   | 15:U:71:LEU:HD12  | 1.88        | 0.55     |
| 1:A:212:CYS:HB2   | 4:D:211:CYS:HB2   | 1.89        | 0.55     |
| 1:A:65:GLU:OE2    | 1:A:334:ARG:NH2   | 2.57        | 0.55     |
| 22:C:501:CLA:C2D  | 22:C:503:CLA:H2   | 2.37        | 0.55     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 12:M:25:LEU:O     | 12:M:28:GLN:HG3   | 2.07        | 0.55     |
| 2:B:262:THR:OG1   | 22:B:602:CLA:O1D  | 2.24        | 0.55     |
| 22:H:101:CLA:H2   | 22:H:101:CLA:HBD  | 1.88        | 0.55     |
| 22:A:404:CLA:H93  | 22:D:403:CLA:H152 | 1.89        | 0.55     |
| 22:B:605:CLA:H18  | 22:B:615:CLA:H121 | 1.89        | 0.55     |
| 22:B:607:CLA:C3D  | 22:B:609:CLA:H2   | 17.27       | 0.55     |
| 22:B:613:CLA:H51  | 25:B:616:BCR:H372 | 1.87        | 0.54     |
| 26:B:626:DGD:O2D  | 26:B:626:DGD:O1B  | 2.25        | 0.54     |
| 31:D:409:LMG:O6   | 11:L:15:THR:HG21  | 54.03       | 0.54     |
| 7:H:55:LEU:HB2    | 7:H:58:VAL:HG12   | 1.90        | 0.54     |
| 22:D:404:CLA:H42  | 18:X:26:GLY:HA3   | 1.89        | 0.54     |
| 34:F:101:HEM:HMC2 | 34:F:101:HEM:HBC2 | 1.94        | 0.54     |
| 22:C:510:CLA:HMB2 | 25:K:101:BCR:H382 | 1.89        | 0.54     |
| 22:B:610:CLA:H41  | 22:B:613:CLA:HBC3 | 1.90        | 0.54     |
| 3:C:75:PHE:HD1    | 3:C:86:LEU:HD21   | 1.74        | 0.54     |
| 5:E:10:PHE:N      | 31:E:101:LMG:O3   | 2.40        | 0.54     |
| 3:C:229:ASN:HD22  | 3:C:231:GLU:HB2   | 1.74        | 0.54     |
| 2:B:103:LEU:HD21  | 22:B:609:CLA:HMC3 | 27.64       | 0.54     |
| 22:B:612:CLA:H51  | 22:B:613:CLA:H101 | 15.99       | 0.54     |
| 3:C:461:ARG:NH1   | 4:D:241:GLU:OE1   | 2.62        | 0.54     |
| 24:D:405:PL9:H352 | 31:L:101:LMG:H231 | 1.89        | 0.54     |
| 15:U:54:LYS:HD2   | 15:U:113:THR:HG23 | 2.00        | 0.54     |
| 2:B:256:MET:O     | 2:B:448:ARG:NH1   | 2.35        | 0.54     |
| 22:A:402:CLA:HBB1 | 22:A:402:CLA:HHC  | 1.89        | 0.54     |
| 4:D:43:LEU:HD23   | 4:D:117:HIS:CE1   | 2.44        | 0.54     |
| 2:B:150:CYS:HA    | 22:B:602:CLA:HBC2 | 1.90        | 0.53     |
| 3:C:305:THR:HG23  | 3:C:307:PRO:HD2   | 1.96        | 0.53     |
| 4:D:302:GLU:OE1   | 13:O:186:LYS:NZ   | 2.42        | 0.53     |
| 2:B:150:CYS:HA    | 22:B:607:CLA:HBC2 | 21.60       | 0.53     |
| 1:A:78:ILE:O      | 1:A:176:ILE:HB    | 2.08        | 0.53     |
| 2:B:184:GLU:H     | 2:B:200:ALA:HB2   | 1.74        | 0.53     |
| 22:B:610:CLA:OBD  | 32:B:628:LMT:O6'  | 53.46       | 0.53     |
| 2:B:122:LEU:O     | 7:H:15:ASN:ND2    | 2.42        | 0.53     |
| 2:B:247:PHE:HE1   | 22:H:101:CLA:H101 | 1.73        | 0.53     |
| 22:B:612:CLA:HMB1 | 22:B:612:CLA:HBB1 | 1.89        | 0.53     |
| 30:B:627:SQD:H1   | 30:B:627:SQD:H462 | 1.90        | 0.53     |
| 12:M:28:GLN:HA    | 12:M:28:GLN:HA    | 0.00        | 0.53     |
| 25:A:408:BCR:H321 | 30:A:414:SQD:H321 | 1.91        | 0.53     |
| 3:C:158:THR:O     | 3:C:251:HIS:HB3   | 2.09        | 0.53     |
| 4:D:172:SER:HB2   | 4:D:177:ALA:HB1   | 1.97        | 0.53     |
| 15:U:56:ASP:OD2   | 15:U:115:THR:OG1  | 2.19        | 0.53     |
| 5:E:57:ALA:HB3    | 5:E:60:GLN:HB3    | 1.91        | 0.53     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 4:D:103:ARG:HG3   | 5:E:73:LYS:HG3    | 1.93        | 0.53     |
| 2:B:458:PHE:HB3   | 22:B:608:CLA:HBC2 | 29.55       | 0.53     |
| 31:D:409:LMG:O5   | 31:D:409:LMG:O4   | 2.96        | 0.53     |
| 26:C:516:DGD:HA22 | 9:J:29:PHE:HE1    | 1.73        | 0.53     |
| 2:B:271:THR:HB    | 2:B:274:GLN:HG3   | 1.91        | 0.53     |
| 3:C:131:TYR:HE1   | 3:C:135:ARG:HD2   | 1.73        | 0.53     |
| 16:V:81:ARG:CZ    | 16:V:157:GLY:HA3  | 2.47        | 0.53     |
| 25:A:408:BCR:H342 | 30:A:414:SQD:H311 | 1.91        | 0.52     |
| 32:B:628:LMT:H62  | 8:I:4:LEU:HD22    | 82.15       | 0.52     |
| 4:D:262:SER:N     | 31:D:409:LMG:O3   | 52.73       | 0.52     |
| 2:B:4:PRO:HD2     | 2:B:7:ARG:HD2     | 1.92        | 0.52     |
| 2:B:458:PHE:HB3   | 22:B:603:CLA:HBC2 | 1.91        | 0.52     |
| 15:U:72:TYR:HB3   | 15:U:73:PRO:HD3   | 1.92        | 0.52     |
| 2:B:371:THR:HG22  | 2:B:377:VAL:HA    | 1.92        | 0.52     |
| 3:C:225:VAL:HG13  | 3:C:289:PHE:HA    | 2.01        | 0.52     |
| 4:D:191:TRP:CE3   | 4:D:289:LEU:HD11  | 2.48        | 0.52     |
| 3:C:85:GLY:N      | 26:C:515:DGD:HE4  | 2.24        | 0.52     |
| 13:O:180:ALA:HB1  | 13:O:191:ALA:HB2  | 1.92        | 0.52     |
| 1:A:188:ALA:HB2   | 1:A:328:MET:HB2   | 1.97        | 0.52     |
| 1:A:210:LEU:HG    | 23:D:401:PHO:NC   | 2.25        | 0.52     |
| 22:A:404:CLA:H161 | 24:A:407:PL9:H253 | 1.91        | 0.52     |
| 22:B:608:CLA:HBD  | 22:B:609:CLA:H43  | 22.44       | 0.52     |
| 4:D:275:PRO:O     | 4:D:279:LEU:HD23  | 2.15        | 0.52     |
| 1:A:12:ASN:HB3    | 1:A:15:GLU:HB3    | 1.91        | 0.52     |
| 1:A:64:ARG:O      | 13:O:178:ARG:NH2  | 2.43        | 0.52     |
| 2:B:103:LEU:HD21  | 22:B:604:CLA:HMC3 | 1.93        | 0.51     |
| 30:A:413:SQD:H311 | 22:C:507:CLA:H71  | 1.92        | 0.51     |
| 3:C:85:GLY:N      | 26:C:516:DGD:HE4  | 14.14       | 0.51     |
| 22:D:404:CLA:H43  | 18:X:23:LEU:HA    | 1.92        | 0.51     |
| 22:C:504:CLA:HBA1 | 22:C:504:CLA:HBD  | 1.94        | 0.51     |
| 22:B:602:CLA:C2D  | 22:B:604:CLA:H2   | 2.41        | 0.51     |
| 1:A:162:PRO:HB3   | 1:A:168:PHE:HA    | 1.93        | 0.51     |
| 1:A:317:TRP:CZ3   | 4:D:180:ARG:HD3   | 2.45        | 0.51     |
| 2:B:383:PHE:CZ    | 13:O:193:GLY:HA2  | 2.52        | 0.51     |
| 3:C:229:ASN:ND2   | 3:C:232:ASP:OD1   | 2.34        | 0.51     |
| 6:F:45:ARG:NH2    | 9:J:40:LEU:O      | 2.42        | 0.51     |
| 22:B:607:CLA:H2   | 22:B:609:CLA:H93  | 26.29       | 0.51     |
| 4:D:148:ALA:HB2   | 4:D:276:VAL:HG13  | 2.03        | 0.51     |
| 3:C:29:GLU:HB3    | 10:K:46:ARG:HH11  | 1.80        | 0.51     |
| 1:A:85:SER:HA     | 1:A:109:GLY:HA3   | 1.92        | 0.51     |
| 2:B:212:ALA:HB2   | 22:B:608:CLA:HMC3 | 1.92        | 0.51     |
| 1:A:224:ILE:O     | 4:D:265:ARG:NH2   | 2.46        | 0.51     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 22:A:403:CLA:HBA1 | 22:A:403:CLA:CHA  | 2.41        | 0.51     |
| 22:B:612:CLA:H151 | 22:B:613:CLA:H203 | 17.03       | 0.51     |
| 1:A:190:HIS:O     | 1:A:298:ASN:HB3   | 2.19        | 0.51     |
| 4:D:87:HIS:CD2    | 4:D:162:LEU:HA    | 2.49        | 0.51     |
| 4:D:85:MET:HA     | 5:E:69:ARG:HB3    | 2.00        | 0.51     |
| 1:A:57:PRO:HG3    | 1:A:68:SER:HB3    | 1.92        | 0.50     |
| 2:B:222:PRO:HG3   | 7:H:27:THR:H      | 1.79        | 0.50     |
| 4:D:261:PHE:HB2   | 24:D:405:PL9:H522 | 1.93        | 0.50     |
| 18:X:11:THR:HG23  | 18:X:12:ILE:HG22  | 1.93        | 0.50     |
| 2:B:51:VAL:HG13   | 2:B:308:LYS:HB2   | 1.93        | 0.50     |
| 2:B:327:THR:HG22  | 22:B:611:CLA:H12  | 31.54       | 0.50     |
| 25:B:617:BCR:H19C | 25:B:618:BCR:H363 | 1.92        | 0.50     |
| 23:D:401:PHO:H151 | 22:D:403:CLA:H172 | 1.92        | 0.50     |
| 25:C:513:BCR:H311 | 25:C:513:BCR:H343 | 3.34        | 0.50     |
| 10:K:40:GLN:HA    | 10:K:43:VAL:HG12  | 1.94        | 0.50     |
| 13:O:168:PHE:HB2  | 13:O:225:LEU:HB2  | 2.02        | 0.50     |
| 2:B:450:TRP:NE1   | 22:B:606:CLA:HBA1 | 2.27        | 0.50     |
| 1:A:271:LEU:HD11  | 24:A:407:PL9:C4   | 2.42        | 0.50     |
| 3:C:473:ASP:HB2   | 14:T:26:PRO:HB3   | 1.95        | 0.50     |
| 2:B:212:ALA:HB2   | 22:B:613:CLA:HMC3 | 34.89       | 0.50     |
| 2:B:256:MET:HA    | 2:B:263:THR:HG21  | 1.93        | 0.50     |
| 22:B:606:CLA:H193 | 11:L:27:LEU:HD11  | 1.92        | 0.50     |
| 22:B:606:CLA:HBC3 | 25:B:618:BCR:HC8  | 1.94        | 0.50     |
| 22:C:512:CLA:HAB  | 25:C:520:BCR:H371 | 1.94        | 0.50     |
| 2:B:150:CYS:HB2   | 22:B:607:CLA:HMC3 | 23.27       | 0.50     |
| 2:B:5:TRP:HZ3     | 22:B:610:CLA:H51  | 1.76        | 0.50     |
| 5:E:15:THR:HG23   | 9:J:8:ILE:O       | 2.18        | 0.49     |
| 22:B:606:CLA:H72  | 7:H:46:LEU:HD13   | 27.36       | 0.49     |
| 3:C:166:ILE:O     | 3:C:170:ILE:HG13  | 2.19        | 0.49     |
| 4:D:221:THR:HG23  | 4:D:244:TYR:HB2   | 2.00        | 0.49     |
| 22:B:609:CLA:H202 | 22:B:613:CLA:HBB2 | 16.74       | 0.49     |
| 3:C:305:THR:HG22  | 3:C:308:GLU:HB2   | 1.94        | 0.49     |
| 13:O:144:LEU:HD13 | 13:O:259:VAL:HG11 | 1.95        | 0.49     |
| 1:A:153:SER:HB3   | 22:A:403:CLA:HED1 | 17.31       | 0.49     |
| 3:C:361:PHE:HD1   | 26:C:515:DGD:HE61 | 20.65       | 0.49     |
| 10:K:26:PRO:O     | 10:K:29:PRO:HD2   | 2.12        | 0.49     |
| 1:A:77:ILE:HD11   | 14:T:6:TYR:HB3    | 1.94        | 0.49     |
| 22:A:404:CLA:CHA  | 22:A:404:CLA:HBA1 | 3.96        | 0.49     |
| 2:B:19:LEU:HG     | 2:B:23:HIS:CE1    | 2.48        | 0.49     |
| 13:O:118:SER:HB3  | 13:O:157:PRO:HA   | 1.95        | 0.49     |
| 27:A:410:LHG:H382 | 22:C:509:CLA:H93  | 1.95        | 0.49     |
| 22:B:612:CLA:H171 | 31:B:625:LMG:H401 | 1.95        | 0.49     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:132:GLU:O     | 1:A:136:ARG:HG2   | 2.13        | 0.49     |
| 3:C:86:LEU:HB3    | 3:C:90:PRO:HD3    | 1.94        | 0.49     |
| 1:A:211:PHE:HA    | 1:A:214:MET:HB2   | 1.96        | 0.49     |
| 1:A:244:GLU:HG3   | 1:A:246:TYR:H     | 1.79        | 0.49     |
| 2:B:19:LEU:O      | 2:B:23:HIS:ND1    | 2.45        | 0.49     |
| 3:C:284:PHE:HB3   | 26:C:515:DGD:HA51 | 19.67       | 0.49     |
| 31:D:406:LMG:H111 | 11:L:19:LEU:HD21  | 1.93        | 0.49     |
| 31:M:101:LMG:H142 | 31:M:101:LMG:H311 | 1.99        | 0.49     |
| 2:B:150:CYS:HB2   | 22:B:602:CLA:HMC3 | 1.95        | 0.49     |
| 3:C:80:PRO:HB3    | 3:C:82:TYR:CE1    | 2.50        | 0.49     |
| 22:C:501:CLA:H171 | 22:C:506:CLA:HMB3 | 1.96        | 0.49     |
| 4:D:48:TRP:CE2    | 23:D:401:PHO:H161 | 2.48        | 0.49     |
| 5:E:23:HIS:NE2    | 34:F:101:HEM:ND   | 2.63        | 0.49     |
| 4:D:17:ILE:HG21   | 18:X:42:GLN:HG3   | 1.94        | 0.49     |
| 1:A:114:LEU:O     | 1:A:118:HIS:ND1   | 2.42        | 0.48     |
| 1:A:136:ARG:NH2   | 8:I:27:ASP:OD1    | 2.43        | 0.48     |
| 2:B:170:ASP:OD1   | 2:B:175:THR:N     | 2.53        | 0.48     |
| 22:B:612:CLA:H18  | 22:B:613:CLA:H192 | 12.16       | 0.48     |
| 7:H:45:ILE:HD11   | 22:H:101:CLA:H42  | 1.94        | 0.48     |
| 22:B:603:CLA:HMD2 | 22:B:611:CLA:H193 | 1.95        | 0.48     |
| 3:C:425:TRP:CE2   | 22:C:519:CLA:HBA1 | 2.48        | 0.48     |
| 4:D:55:VAL:HG21   | 4:D:110:LEU:HD12  | 2.01        | 0.48     |
| 4:D:102:THR:OG1   | 26:D:407:DGD:HD62 | 2.13        | 0.48     |
| 22:A:404:CLA:HAB  | 22:D:403:CLA:H72  | 1.95        | 0.48     |
| 2:B:326:ARG:HB3   | 2:B:444:ARG:HG2   | 2.00        | 0.48     |
| 25:B:616:BCR:H333 | 12:M:13:LEU:HD12  | 1.96        | 0.48     |
| 22:B:605:CLA:OBD  | 32:B:623:LMT:O6'  | 2.24        | 0.48     |
| 2:B:120:LEU:HD13  | 22:B:615:CLA:HMD2 | 1.94        | 0.48     |
| 4:D:262:SER:N     | 31:D:406:LMG:O3   | 2.42        | 0.48     |
| 22:B:606:CLA:H41  | 22:B:606:CLA:H62  | 1.86        | 0.48     |
| 3:C:318:LEU:HG    | 3:C:328:VAL:HG11  | 1.96        | 0.48     |
| 4:D:43:LEU:HD23   | 4:D:117:HIS:HE1   | 1.78        | 0.48     |
| 26:D:407:DGD:O5E  | 26:D:407:DGD:O4E  | 2.24        | 0.48     |
| 13:O:240:THR:HA   | 13:O:264:VAL:HA   | 2.04        | 0.48     |
| 3:C:284:PHE:HB3   | 26:C:514:DGD:HA51 | 1.96        | 0.48     |
| 4:D:323:GLU:HG3   | 4:D:326:ARG:NH2   | 2.28        | 0.48     |
| 22:H:101:CLA:H41  | 22:H:101:CLA:H62  | 1.56        | 0.48     |
| 3:C:337:LEU:HA    | 13:O:131:PRO:HG3  | 2.07        | 0.48     |
| 13:O:230:VAL:HG12 | 13:O:231:ASP:H    | 1.77        | 0.48     |
| 23:A:405:PHO:H41  | 23:A:405:PHO:H62  | 1.46        | 0.47     |
| 1:A:89:ILE:HG12   | 13:O:99:ARG:NH2   | 2.36        | 0.47     |
| 2:B:96:VAL:HG22   | 22:B:610:CLA:HBA1 | 32.27       | 0.47     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 3:C:197:ARG:NH2   | 3:C:231:GLU:OE2   | 2.47        | 0.47     |
| 3:C:346:THR:HG21  | 13:O:38:GLY:HA2   | 2.00        | 0.47     |
| 22:B:602:CLA:C3D  | 22:B:604:CLA:H2   | 2.44        | 0.47     |
| 22:D:403:CLA:H61  | 22:D:403:CLA:H41  | 1.67        | 0.47     |
| 2:B:315:ILE:HG22  | 2:B:426:PHE:HB3   | 1.97        | 0.47     |
| 3:C:248:GLY:O     | 3:C:252:ILE:HG12  | 2.15        | 0.47     |
| 3:C:52:ALA:HA     | 22:C:510:CLA:HMB3 | 1.96        | 0.47     |
| 13:O:184:ASP:OD2  | 13:O:188:ARG:HB2  | 2.18        | 0.47     |
| 2:B:125:ASP:HB2   | 2:B:132:ALA:HB3   | 1.97        | 0.47     |
| 3:C:130:VAL:O     | 3:C:134:ILE:HG12  | 2.17        | 0.47     |
| 18:X:12:ILE:HG12  | 18:X:16:LEU:HD12  | 1.98        | 0.47     |
| 2:B:18:ARG:HD3    | 2:B:118:TRP:HB3   | 1.96        | 0.47     |
| 3:C:391:ARG:HD2   | 3:C:395:TYR:CZ    | 2.60        | 0.47     |
| 3:C:113:VAL:HG11  | 31:C:517:LMG:H132 | 1.97        | 0.47     |
| 13:O:135:GLN:HG2  | 13:O:141:ARG:HG3  | 2.11        | 0.47     |
| 22:A:403:CLA:HMA2 | 24:D:405:PL9:H411 | 1.95        | 0.47     |
| 2:B:54:PRO:HD2    | 2:B:57:ARG:HG3    | 1.96        | 0.47     |
| 2:B:68:ARG:HH22   | 22:B:603:CLA:HED1 | 1.80        | 0.47     |
| 15:U:75:LEU:HD21  | 15:U:101:GLN:HB3  | 1.96        | 0.47     |
| 22:B:603:CLA:H101 | 22:B:614:CLA:H2   | 1.97        | 0.47     |
| 25:B:619:BCR:H20C | 25:B:619:BCR:H361 | 1.76        | 0.47     |
| 2:B:30:VAL:HG12   | 22:B:609:CLA:HHD  | 22.16       | 0.47     |
| 22:B:611:CLA:H193 | 11:L:27:LEU:HD11  | 26.87       | 0.47     |
| 1:A:298:ASN:ND2   | 3:C:402:GLY:O     | 2.48        | 0.47     |
| 3:C:319:ILE:HG21  | 3:C:389:GLU:HG3   | 2.05        | 0.46     |
| 4:D:84:SER:HB2    | 4:D:85:MET:HE2    | 1.97        | 0.46     |
| 2:B:5:TRP:HZ3     | 22:B:615:CLA:H51  | 35.06       | 0.46     |
| 3:C:245:ILE:O     | 3:C:249:ILE:HG12  | 2.18        | 0.46     |
| 9:J:38:SER:OG     | 9:J:39:SER:N      | 2.47        | 0.46     |
| 22:A:402:CLA:H3A  | 22:A:402:CLA:HBA1 | 1.53        | 0.46     |
| 2:B:270:PRO:HG3   | 2:B:312:TYR:HD2   | 1.88        | 0.46     |
| 22:B:606:CLA:H162 | 22:B:606:CLA:H122 | 4.80        | 0.46     |
| 22:C:508:CLA:H62  | 22:C:508:CLA:H92  | 1.71        | 0.46     |
| 13:O:223:ILE:HG13 | 13:O:243:SER:HB3  | 2.01        | 0.46     |
| 3:C:347:GLY:HA3   | 13:O:43:ASN:HB2   | 2.00        | 0.46     |
| 2:B:121:GLU:HG2   | 7:H:4:ARG:HA      | 2.03        | 0.46     |
| 2:B:213:GLY:O     | 2:B:217:ILE:HG13  | 2.14        | 0.46     |
| 2:B:348:ASN:HB3   | 2:B:354:LEU:HD21  | 2.00        | 0.46     |
| 3:C:223:TRP:CD2   | 3:C:224:ILE:HG13  | 2.51        | 0.46     |
| 16:V:68:VAL:O     | 16:V:71:ILE:HG12  | 2.14        | 0.46     |
| 22:A:404:CLA:H161 | 22:A:404:CLA:H143 | 1.80        | 0.46     |
| 22:C:512:CLA:H3A  | 22:C:512:CLA:HBA2 | 1.70        | 0.46     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 22:A:404:CLA:H162 | 22:A:404:CLA:H202 | 4.12        | 0.46     |
| 1:A:317:TRP:HZ3   | 4:D:180:ARG:HD3   | 1.81        | 0.46     |
| 23:D:401:PHO:H62  | 23:D:401:PHO:H41  | 3.82        | 0.46     |
| 4:D:56:THR:HG21   | 5:E:50:PRO:HD3    | 2.02        | 0.46     |
| 3:C:149:TYR:HA    | 3:C:156:LYS:HD3   | 2.02        | 0.46     |
| 7:H:46:LEU:HD13   | 22:H:101:CLA:H72  | 1.98        | 0.46     |
| 1:A:334:ARG:NH2   | 4:D:312:GLU:OE2   | 2.49        | 0.46     |
| 10:K:12:PRO:HB2   | 10:K:15:TYR:CD2   | 2.49        | 0.46     |
| 22:C:510:CLA:H61  | 22:C:510:CLA:H93  | 1.80        | 0.46     |
| 1:A:93:PHE:CD2    | 1:A:95:PRO:HD3    | 2.55        | 0.46     |
| 3:C:343:ARG:NH1   | 3:C:347:GLY:O     | 2.49        | 0.46     |
| 3:C:456:GLU:N     | 3:C:456:GLU:OE1   | 2.48        | 0.46     |
| 16:V:98:LEU:O     | 16:V:102:MET:HG3  | 2.15        | 0.46     |
| 30:F:103:SQD:H131 | 18:X:36:VAL:HG11  | 2.00        | 0.46     |
| 22:B:609:CLA:H41  | 22:B:609:CLA:H62  | 1.95        | 0.45     |
| 2:B:306:PRO:HG2   | 2:B:309:LEU:HB2   | 2.03        | 0.45     |
| 26:C:516:DGD:HA22 | 9:J:29:PHE:CE1    | 2.50        | 0.45     |
| 22:B:607:CLA:H18  | 22:B:608:CLA:H192 | 1.98        | 0.45     |
| 3:C:166:ILE:HG23  | 3:C:245:ILE:HG23  | 2.05        | 0.45     |
| 3:C:386:PRO:HB3   | 16:V:116:GLU:HG2  | 1.99        | 0.45     |
| 3:C:59:LEU:HD13   | 22:C:509:CLA:HMD2 | 2.04        | 0.45     |
| 18:X:40:ILE:HA    | 18:X:43:ILE:HD12  | 1.99        | 0.45     |
| 25:C:513:BCR:H351 | 25:C:513:BCR:H15C | 1.83        | 0.45     |
| 4:D:244:TYR:OH    | 4:D:264:LYS:HE3   | 2.19        | 0.45     |
| 22:A:403:CLA:H62  | 22:A:403:CLA:H41  | 1.74        | 0.45     |
| 2:B:450:TRP:NE1   | 22:B:611:CLA:HBA1 | 27.87       | 0.45     |
| 25:B:618:BCR:H20C | 25:B:618:BCR:H361 | 1.81        | 0.45     |
| 22:A:403:CLA:HAA1 | 24:D:405:PL9:H362 | 1.99        | 0.45     |
| 1:A:271:LEU:HD21  | 24:A:407:PL9:HC71 | 1.97        | 0.45     |
| 13:O:178:ARG:HD2  | 13:O:182:PHE:CD1  | 2.52        | 0.45     |
| 1:A:29:TYR:CG     | 1:A:133:LEU:HD13  | 2.59        | 0.45     |
| 22:C:506:CLA:H92  | 22:C:506:CLA:H62  | 1.73        | 0.45     |
| 1:A:27:ARG:NH1    | 4:D:254:SER:O     | 2.48        | 0.45     |
| 25:K:101:BCR:H20C | 25:K:101:BCR:H361 | 1.77        | 0.45     |
| 22:B:614:CLA:H92  | 22:B:614:CLA:H62  | 1.78        | 0.45     |
| 22:H:101:CLA:H162 | 22:H:101:CLA:H122 | 1.55        | 0.45     |
| 31:D:409:LMG:H111 | 11:L:19:LEU:HD21  | 43.63       | 0.45     |
| 22:B:605:CLA:H161 | 22:B:605:CLA:HMD1 | 19.73       | 0.45     |
| 22:B:607:CLA:H92  | 22:B:607:CLA:HBB2 | 11.25       | 0.45     |
| 22:C:508:CLA:H11  | 22:C:508:CLA:H51  | 1.84        | 0.45     |
| 22:C:509:CLA:H61  | 22:C:509:CLA:H2   | 1.73        | 0.45     |
| 4:D:148:ALA:HB3   | 4:D:149:PRO:HD3   | 1.98        | 0.45     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 30:A:414:SQD:HO8  | 2:B:113:TRP:HE1   | 62.62       | 0.44     |
| 22:C:501:CLA:H193 | 22:C:506:CLA:H111 | 1.99        | 0.44     |
| 5:E:27:ILE:HB     | 5:E:28:PRO:HD3    | 2.02        | 0.44     |
| 22:A:403:CLA:H42  | 24:D:405:PL9:H162 | 1.98        | 0.44     |
| 3:C:137:PRO:HB2   | 3:C:139:THR:O     | 2.18        | 0.44     |
| 1:A:272:HIS:CD2   | 4:D:218:VAL:HG21  | 2.52        | 0.44     |
| 2:B:135:LEU:HA    | 2:B:138:MET:HE3   | 2.07        | 0.44     |
| 12:M:3:VAL:HG11   | 14:T:2:GLU:HG2    | 1.98        | 0.44     |
| 1:A:111:PRO:O     | 1:A:115:ILE:HG13  | 2.21        | 0.44     |
| 1:A:202:VAL:HB    | 22:A:402:CLA:HMB3 | 1.99        | 0.44     |
| 22:B:608:CLA:HMC2 | 25:H:102:BCR:H343 | 1.99        | 0.44     |
| 2:B:383:PHE:N     | 4:D:344:GLU:O     | 2.37        | 0.44     |
| 31:I:101:LMG:H181 | 32:I:102:LMT:H42  | 1.98        | 0.44     |
| 2:B:247:PHE:HB2   | 22:B:612:CLA:HBC1 | 22.36       | 0.44     |
| 25:B:616:BCR:H11C | 25:B:616:BCR:H341 | 1.88        | 0.44     |
| 3:C:350:ILE:HG21  | 3:C:359:TRP:HB2   | 2.00        | 0.44     |
| 3:C:318:LEU:HD21  | 3:C:380:ILE:HG23  | 2.00        | 0.44     |
| 26:C:516:DGD:HAW2 | 26:C:516:DGD:HA91 | 4.04        | 0.44     |
| 4:D:279:LEU:HG    | 23:D:401:PHO:HBC3 | 2.00        | 0.44     |
| 22:H:101:CLA:H93  | 22:H:101:CLA:H62  | 1.86        | 0.44     |
| 9:J:14:ALA:O      | 9:J:18:GLY:N      | 2.48        | 0.44     |
| 25:K:101:BCR:H343 | 25:K:101:BCR:H311 | 1.98        | 0.44     |
| 13:O:79:LYS:HB3   | 13:O:258:GLU:HB2  | 2.02        | 0.44     |
| 13:O:81:GLU:HA    | 13:O:82:PRO:HD3   | 1.81        | 0.44     |
| 16:V:38:LEU:HD12  | 16:V:95:ILE:HB    | 2.09        | 0.44     |
| 1:A:268:SER:O     | 1:A:272:HIS:ND1   | 2.42        | 0.44     |
| 2:B:135:LEU:HB2   | 2:B:136:PRO:HD3   | 2.01        | 0.44     |
| 3:C:90:PRO:O      | 3:C:94:THR:HG23   | 2.17        | 0.44     |
| 1:A:258:LEU:O     | 4:D:128:ARG:NH1   | 2.52        | 0.44     |
| 2:B:247:PHE:HB2   | 22:B:607:CLA:HBC1 | 2.00        | 0.44     |
| 22:B:614:CLA:H172 | 22:B:614:CLA:H111 | 2.00        | 0.44     |
| 26:B:620:DGD:HA71 | 22:H:101:CLA:H193 | 2.00        | 0.44     |
| 7:H:12:ARG:HD3    | 7:H:12:ARG:O      | 2.18        | 0.44     |
| 16:V:60:GLN:HA    | 16:V:64:ALA:HB2   | 1.99        | 0.44     |
| 3:C:131:TYR:CE1   | 3:C:135:ARG:HD2   | 2.52        | 0.44     |
| 3:C:190:ALA:HA    | 3:C:191:PRO:HD3   | 1.88        | 0.44     |
| 13:O:135:GLN:HB3  | 13:O:135:GLN:HE21 | 1.71        | 0.44     |
| 3:C:456:GLU:HG2   | 3:C:457:LYS:HG3   | 1.99        | 0.44     |
| 3:C:437:PHE:CZ    | 22:C:509:CLA:HMB3 | 2.52        | 0.44     |
| 3:C:112:PHE:HE2   | 25:C:520:BCR:HC31 | 1.82        | 0.44     |
| 8:I:6:ILE:O       | 8:I:10:ILE:HG12   | 2.25        | 0.43     |
| 2:B:16:PRO:HG2    | 2:B:123:PHE:HB3   | 2.01        | 0.43     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 22:B:612:CLA:H51  | 31:B:625:LMG:H231 | 1.99        | 0.43     |
| 3:C:209:ILE:HG23  | 25:C:513:BCR:H382 | 1.99        | 0.43     |
| 26:B:620:DGD:HAT2 | 22:H:101:CLA:H151 | 2.00        | 0.43     |
| 1:A:195:HIS:HA    | 1:A:196:PRO:HD3   | 1.92        | 0.43     |
| 3:C:42:LEU:HD13   | 22:C:510:CLA:HMA3 | 2.02        | 0.43     |
| 5:E:42:LEU:O      | 5:E:46:VAL:HG23   | 2.17        | 0.43     |
| 10:K:18:PHE:O     | 10:K:22:VAL:HG23  | 2.18        | 0.43     |
| 16:V:160:LYS:HA   | 16:V:163:TYR:CD2  | 2.54        | 0.43     |
| 20:Z:33:TRP:O     | 20:Z:33:TRP:CD1   | 2.72        | 0.43     |
| 25:B:616:BCR:H361 | 25:B:616:BCR:H20C | 1.78        | 0.43     |
| 3:C:307:PRO:HB3   | 3:C:358:PHE:HB3   | 2.01        | 0.43     |
| 26:C:515:DGD:HA91 | 26:C:515:DGD:HAW2 | 1.75        | 0.43     |
| 3:C:420:VAL:H     | 26:C:516:DGD:HE62 | 11.29       | 0.43     |
| 22:D:403:CLA:H92  | 22:D:403:CLA:H62  | 1.83        | 0.43     |
| 1:A:156:ALA:HA    | 1:A:160:ILE:HB    | 1.99        | 0.43     |
| 1:A:238:LYS:O     | 1:A:241:GLN:HG3   | 2.18        | 0.43     |
| 1:A:93:PHE:HZ     | 22:A:406:CLA:HAA1 | 1.93        | 0.43     |
| 3:C:393:ALA:HB1   | 34:V:201:HEM:HBC1 | 2.06        | 0.43     |
| 22:C:510:CLA:H141 | 20:Z:20:VAL:HG13  | 2.00        | 0.43     |
| 4:D:160:TYR:HA    | 4:D:290:ALA:HB2   | 2.02        | 0.43     |
| 7:H:45:ILE:HD12   | 22:H:101:CLA:HAA2 | 1.99        | 0.43     |
| 1:A:269:ARG:NH1   | 4:D:231:THR:HB    | 2.33        | 0.43     |
| 22:A:402:CLA:H51  | 23:A:405:PHO:C3B  | 2.49        | 0.43     |
| 22:B:602:CLA:H92  | 22:B:602:CLA:HBB2 | 2.01        | 0.43     |
| 3:C:29:GLU:HB2    | 3:C:30:SER:H      | 1.64        | 0.43     |
| 4:D:129:GLN:OE1   | 4:D:143:ALA:HA    | 2.18        | 0.43     |
| 4:D:53:THR:HG22   | 4:D:67:TYR:CD2    | 2.54        | 0.43     |
| 22:B:610:CLA:H3A  | 22:B:610:CLA:HBA2 | 3.06        | 0.43     |
| 32:B:629:LMT:H3O2 | 32:B:629:LMT:H2O1 | 5.77        | 0.43     |
| 23:D:401:PHO:CHB  | 22:D:403:CLA:H101 | 2.49        | 0.43     |
| 13:O:192:SER:OG   | 13:O:193:GLY:N    | 2.51        | 0.43     |
| 22:C:507:CLA:H172 | 26:C:515:DGD:HBW2 | 2.00        | 0.43     |
| 6:F:16:PHE:HB3    | 30:F:103:SQD:H241 | 2.01        | 0.43     |
| 1:A:237:TYR:OH    | 4:D:246:MET:HG2   | 2.27        | 0.43     |
| 1:A:317:TRP:CD1   | 4:D:177:ALA:HB2   | 2.54        | 0.43     |
| 2:B:280:PHE:O     | 2:B:284:ILE:HG13  | 2.18        | 0.43     |
| 2:B:298:LEU:HD23  | 2:B:402:TYR:CZ    | 2.53        | 0.43     |
| 3:C:466:VAL:HG21  | 4:D:248:THR:HG23  | 2.00        | 0.43     |
| 2:B:16:PRO:HB2    | 2:B:123:PHE:CG    | 2.54        | 0.43     |
| 20:Z:29:SER:HA    | 20:Z:30:PRO:HD3   | 1.83        | 0.43     |
| 1:A:40:THR:HG21   | 1:A:121:LEU:HD23  | 2.01        | 0.42     |
| 2:B:194:ASN:HA    | 2:B:195:PRO:HD3   | 1.90        | 0.42     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 22:B:611:CLA:H162 | 22:B:611:CLA:H122 | 1.74        | 0.42     |
| 25:C:513:BCR:H24C | 25:C:513:BCR:H371 | 1.89        | 0.42     |
| 6:F:17:THR:OG1    | 6:F:18:VAL:N      | 2.52        | 0.42     |
| 3:C:62:PHE:CE2    | 10:K:29:PRO:HD3   | 2.57        | 0.42     |
| 22:A:404:CLA:H11  | 22:A:404:CLA:H51  | 4.37        | 0.42     |
| 3:C:363:GLY:O     | 3:C:367:GLU:HG2   | 2.23        | 0.42     |
| 1:A:322:ASN:OD1   | 3:C:412:THR:HA    | 2.22        | 0.42     |
| 25:C:513:BCR:H11C | 25:C:513:BCR:H341 | 1.90        | 0.42     |
| 3:C:405:ASN:HB2   | 26:C:516:DGD:HG31 | 2.01        | 0.42     |
| 3:C:35:TRP:CZ2    | 27:C:518:LHG:H261 | 2.54        | 0.42     |
| 1:A:127:MET:HG3   | 1:A:144:CYS:HB2   | 2.02        | 0.42     |
| 22:A:403:CLA:H162 | 22:A:403:CLA:H202 | 1.76        | 0.42     |
| 2:B:485:GLU:HG3   | 2:B:486:LEU:N     | 2.34        | 0.42     |
| 22:B:603:CLA:HBD  | 22:B:604:CLA:H43  | 2.02        | 0.42     |
| 22:B:605:CLA:H3A  | 22:B:605:CLA:HBA2 | 1.23        | 0.42     |
| 3:C:224:ILE:O     | 3:C:227:VAL:HG23  | 2.20        | 0.42     |
| 3:C:303:GLY:O     | 3:C:423:ARG:NE    | 2.39        | 0.42     |
| 1:A:157:VAL:HG13  | 1:A:172:MET:HB3   | 2.07        | 0.42     |
| 1:A:283:VAL:O     | 1:A:286:THR:HG22  | 2.19        | 0.42     |
| 22:A:406:CLA:H141 | 22:A:406:CLA:H162 | 1.68        | 0.42     |
| 24:A:407:PL9:H351 | 24:A:407:PL9:H371 | 1.84        | 0.42     |
| 22:B:602:CLA:H162 | 22:B:602:CLA:H192 | 1.76        | 0.42     |
| 22:C:512:CLA:HAB  | 25:C:520:BCR:H24C | 2.00        | 0.42     |
| 25:C:513:BCR:H391 | 10:K:36:ALA:HB2   | 35.91       | 0.42     |
| 1:A:161:TYR:HB3   | 1:A:162:PRO:HD3   | 2.03        | 0.42     |
| 2:B:25:MET:HG2    | 25:B:616:BCR:H23C | 2.00        | 0.42     |
| 22:B:604:CLA:H202 | 22:B:608:CLA:HBB2 | 2.01        | 0.42     |
| 3:C:38:GLY:HA3    | 22:C:510:CLA:HMD3 | 2.03        | 0.42     |
| 25:C:513:BCR:H20C | 25:C:513:BCR:H361 | 1.85        | 0.42     |
| 31:D:409:LMG:HC1  | 31:D:409:LMG:O9   | 4.10        | 0.42     |
| 2:B:137:LYS:HD2   | 7:H:14:LEU:O      | 2.20        | 0.42     |
| 13:O:143:PRO:HG2  | 13:O:248:ASP:HB3  | 2.00        | 0.42     |
| 16:V:90:PRO:O     | 16:V:92:ARG:HD3   | 2.18        | 0.42     |
| 1:A:340:PRO:HG3   | 15:U:133:TYR:CG   | 2.58        | 0.42     |
| 31:B:621:LMG:H421 | 4:D:284:ILE:HD13  | 2.01        | 0.42     |
| 3:C:318:LEU:HD13  | 3:C:351:PHE:HE1   | 1.90        | 0.42     |
| 25:H:102:BCR:H20C | 25:H:102:BCR:H361 | 1.79        | 0.42     |
| 7:H:12:ARG:N      | 7:H:13:PRO:HD2    | 2.35        | 0.42     |
| 31:C:517:LMG:H292 | 31:C:517:LMG:H111 | 2.00        | 0.42     |
| 1:A:221:SER:HB2   | 4:D:139:ARG:O     | 2.19        | 0.42     |
| 1:A:129:ARG:NH2   | 4:D:256:ILE:HD12  | 2.28        | 0.42     |
| 13:O:154:SER:N    | 13:O:169:LYS:O    | 2.51        | 0.42     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 15:U:72:TYR:O     | 15:U:76:ALA:HB3   | 2.21        | 0.42     |
| 20:Z:5:PHE:CE1    | 20:Z:54:VAL:HG13  | 2.55        | 0.42     |
| 1:A:153:SER:HB2   | 22:A:402:CLA:H43  | 2.00        | 0.42     |
| 1:A:176:ILE:HD12  | 22:A:404:CLA:HED3 | 27.29       | 0.42     |
| 2:B:327:THR:HG22  | 22:B:606:CLA:H12  | 2.01        | 0.42     |
| 22:B:604:CLA:H62  | 22:B:604:CLA:H41  | 1.81        | 0.42     |
| 22:B:615:CLA:H143 | 22:B:615:CLA:H111 | 1.78        | 0.42     |
| 25:B:617:BCR:H15C | 25:B:617:BCR:H351 | 1.87        | 0.42     |
| 25:B:618:BCR:H24C | 25:B:618:BCR:H371 | 1.82        | 0.42     |
| 4:D:87:HIS:CD2    | 4:D:162:LEU:HD23  | 2.54        | 0.42     |
| 1:A:159:LEU:C     | 1:A:162:PRO:HD2   | 2.40        | 0.42     |
| 2:B:91:TRP:CH2    | 22:B:605:CLA:H12  | 2.55        | 0.42     |
| 22:C:501:CLA:H162 | 22:C:501:CLA:H141 | 1.77        | 0.42     |
| 25:C:520:BCR:H371 | 25:C:520:BCR:H24C | 1.84        | 0.42     |
| 4:D:201:VAL:O     | 4:D:205:LEU:HB2   | 2.20        | 0.42     |
| 22:B:603:CLA:H11  | 22:B:604:CLA:H42  | 2.02        | 0.42     |
| 1:A:191:ASN:HB2   | 3:C:411:ALA:HB1   | 2.11        | 0.42     |
| 22:C:507:CLA:H172 | 26:C:516:DGD:HBW2 | 12.23       | 0.42     |
| 16:V:158:GLY:HA3  | 16:V:162:TYR:CD2  | 2.75        | 0.42     |
| 22:C:510:CLA:H171 | 20:Z:20:VAL:HA    | 2.10        | 0.42     |
| 23:A:405:PHO:H13  | 23:A:405:PHO:H102 | 1.86        | 0.41     |
| 22:B:607:CLA:HBA1 | 22:B:607:CLA:CHA  | 2.49        | 0.41     |
| 4:D:205:LEU:HA    | 4:D:205:LEU:HD12  | 1.84        | 0.41     |
| 4:D:252:PHE:O     | 4:D:256:ILE:HG22  | 2.23        | 0.41     |
| 23:D:401:PHO:H102 | 23:D:401:PHO:H13  | 4.39        | 0.41     |
| 7:H:19:GLY:O      | 7:H:21:VAL:HG13   | 2.20        | 0.41     |
| 15:U:94:ILE:HB    | 15:U:97:LEU:HD11  | 2.06        | 0.41     |
| 22:A:403:CLA:HED2 | 4:D:198:MET:SD    | 2.60        | 0.41     |
| 22:B:607:CLA:H41  | 22:B:607:CLA:H61  | 3.46        | 0.41     |
| 22:B:612:CLA:H161 | 22:B:612:CLA:H143 | 4.29        | 0.41     |
| 3:C:80:PRO:HB2    | 3:C:83:GLU:HG3    | 2.18        | 0.41     |
| 4:D:236:ASN:HA    | 4:D:237:PRO:HD2   | 1.96        | 0.41     |
| 22:D:403:CLA:H3A  | 22:D:403:CLA:HBA1 | 1.86        | 0.41     |
| 5:E:60:GLN:HG2    | 5:E:62:SER:H      | 1.85        | 0.41     |
| 6:F:28:VAL:HB     | 6:F:29:PRO:HD3    | 2.06        | 0.41     |
| 1:A:215:HIS:HA    | 24:A:407:PL9:O1   | 2.21        | 0.41     |
| 2:B:242:ILE:HG12  | 22:B:610:CLA:HBB1 | 2.02        | 0.41     |
| 2:B:468:TRP:HH2   | 31:B:625:LMG:HO2  | 1.65        | 0.41     |
| 31:C:521:LMG:H112 | 25:J:102:BCR:H373 | 2.02        | 0.41     |
| 24:D:405:PL9:H13  | 31:D:406:LMG:H132 | 2.02        | 0.41     |
| 25:F:102:BCR:H341 | 25:F:102:BCR:H11C | 1.94        | 0.41     |
| 3:C:135:ARG:HB2   | 20:Z:27:TYR:HB3   | 2.02        | 0.41     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 25:A:408:BCR:H11C | 25:A:408:BCR:H341 | 1.95        | 0.41     |
| 26:A:409:DGD:HG32 | 26:A:409:DGD:HD2  | 1.73        | 0.41     |
| 2:B:221:PRO:HA    | 2:B:222:PRO:HD3   | 1.93        | 0.41     |
| 3:C:205:ASP:HA    | 3:C:206:PRO:HD2   | 1.93        | 0.41     |
| 4:D:148:ALA:HB1   | 4:D:279:LEU:HB2   | 2.02        | 0.41     |
| 31:D:406:LMG:O9   | 31:D:406:LMG:HC1  | 2.20        | 0.41     |
| 22:C:510:CLA:H122 | 10:K:32:PHE:HE1   | 1.86        | 0.41     |
| 1:A:232:SER:HB3   | 1:A:235:TYR:HD1   | 1.98        | 0.41     |
| 22:A:403:CLA:HBA1 | 22:A:403:CLA:H3A  | 3.98        | 0.41     |
| 3:C:282:MET:HG2   | 22:C:501:CLA:H61  | 2.12        | 0.41     |
| 4:D:113:PHE:O     | 4:D:117:HIS:HB2   | 2.24        | 0.41     |
| 4:D:156:VAL:HG12  | 4:D:171:PRO:HG3   | 2.02        | 0.41     |
| 4:D:210:LEU:HA    | 4:D:213:ILE:HG22  | 2.07        | 0.41     |
| 5:E:14:ILE:HG22   | 9:J:13:VAL:HG11   | 2.08        | 0.41     |
| 25:J:102:BCR:H351 | 25:J:102:BCR:H15C | 1.75        | 0.41     |
| 18:X:17:LYS:O     | 18:X:21:ILE:HG13  | 2.22        | 0.41     |
| 22:A:403:CLA:H151 | 23:D:401:PHO:H72  | 39.38       | 0.41     |
| 2:B:222:PRO:HD2   | 2:B:225:LEU:HD12  | 2.15        | 0.41     |
| 22:B:607:CLA:H51  | 22:B:608:CLA:H101 | 2.02        | 0.41     |
| 22:B:612:CLA:CHA  | 22:B:612:CLA:HBA1 | 5.05        | 0.41     |
| 3:C:265:ILE:HD11  | 8:I:28:PRO:HB3    | 2.02        | 0.41     |
| 4:D:110:LEU:HA    | 4:D:110:LEU:HD23  | 1.93        | 0.41     |
| 22:B:613:CLA:H91  | 22:B:613:CLA:H112 | 1.85        | 0.41     |
| 3:C:116:VAL:HG21  | 25:C:520:BCR:HC21 | 2.02        | 0.41     |
| 22:C:505:CLA:H161 | 22:C:505:CLA:H202 | 1.90        | 0.41     |
| 4:D:312:GLU:HB2   | 13:O:185:PRO:CG   | 2.50        | 0.41     |
| 5:E:10:PHE:HE1    | 34:F:101:HEM:HBD2 | 1.98        | 0.41     |
| 25:F:102:BCR:H15C | 25:F:102:BCR:H351 | 1.92        | 0.41     |
| 16:V:158:GLY:HA3  | 16:V:162:TYR:HD2  | 2.03        | 0.41     |
| 1:A:309:ALA:HA    | 6:F:45:ARG:HB2    | 2.07        | 0.41     |
| 2:B:305:ILE:HA    | 2:B:306:PRO:HD2   | 1.95        | 0.41     |
| 2:B:30:VAL:HG12   | 22:B:604:CLA:HHD  | 2.02        | 0.41     |
| 2:B:314:TYR:CE2   | 2:B:316:GLY:HA3   | 2.55        | 0.41     |
| 22:B:609:CLA:H12  | 22:B:609:CLA:H51  | 1.88        | 0.41     |
| 4:D:342:PRO:O     | 4:D:345:VAL:HG12  | 2.23        | 0.41     |
| 5:E:50:PRO:HB3    | 5:E:54:SER:O      | 2.30        | 0.41     |
| 6:F:41:GLN:OE1    | 9:J:31:GLY:HA3    | 2.31        | 0.41     |
| 2:B:243:ALA:HA    | 2:B:246:PHE:CE2   | 2.56        | 0.41     |
| 22:B:604:CLA:H141 | 22:B:604:CLA:H161 | 1.88        | 0.41     |
| 22:B:614:CLA:H51  | 22:B:614:CLA:H12  | 3.14        | 0.41     |
| 3:C:334:PRO:HA    | 13:O:179:THR:OG1  | 2.21        | 0.41     |
| 3:C:386:PRO:O     | 3:C:390:ARG:HG2   | 2.27        | 0.41     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 3:C:57:ALA:O      | 3:C:61:VAL:HG23   | 2.22        | 0.41     |
| 4:D:48:TRP:CD2    | 23:D:401:PHO:H161 | 2.56        | 0.41     |
| 22:B:606:CLA:H61  | 7:H:46:LEU:HB2    | 31.05       | 0.41     |
| 25:J:102:BCR:H11C | 25:J:102:BCR:H341 | 1.82        | 0.41     |
| 1:A:262:TYR:CZ    | 31:E:101:LMG:HC5  | 2.71        | 0.41     |
| 32:B:624:LMT:H102 | 7:H:35:MET:SD     | 2.61        | 0.41     |
| 3:C:437:PHE:HZ    | 22:C:509:CLA:HMB3 | 1.86        | 0.41     |
| 1:A:334:ARG:NH1   | 13:O:183:LEU:O    | 2.66        | 0.41     |
| 2:B:173:GLY:HA3   | 2:B:265:ILE:HD11  | 2.03        | 0.41     |
| 22:B:602:CLA:H61  | 22:B:602:CLA:H41  | 1.64        | 0.41     |
| 3:C:119:LEU:HG    | 25:C:513:BCR:H10C | 39.47       | 0.41     |
| 11:L:11:GLU:HG2   | 11:L:12:LEU:N     | 2.35        | 0.41     |
| 12:M:19:SER:O     | 12:M:23:ILE:HG13  | 2.25        | 0.41     |
| 1:A:116:ILE:HG13  | 1:A:117:PHE:N     | 2.35        | 0.40     |
| 1:A:223:LEU:HD13  | 4:D:265:ARG:HD3   | 2.16        | 0.40     |
| 1:A:96:ILE:HD12   | 22:A:406:CLA:HMD1 | 2.06        | 0.40     |
| 22:B:602:CLA:CBB  | 22:B:604:CLA:H152 | 2.51        | 0.40     |
| 22:B:606:CLA:H41  | 22:B:606:CLA:H93  | 4.04        | 0.40     |
| 3:C:29:GLU:OE1    | 3:C:31:SER:HB2    | 2.34        | 0.40     |
| 5:E:84:LYS:HZ2    | 5:E:84:LYS:HB2    | 1.85        | 0.40     |
| 13:O:41:LEU:HD12  | 13:O:41:LEU:HA    | 1.95        | 0.40     |
| 2:B:222:PRO:HG3   | 7:H:26:GLY:HA3    | 2.12        | 0.40     |
| 2:B:257:TRP:CE2   | 4:D:291:LEU:HD12  | 2.57        | 0.40     |
| 3:C:257:PHE:HB3   | 3:C:258:GLY:H     | 1.61        | 0.40     |
| 4:D:261:PHE:HA    | 31:D:409:LMG:O2   | 48.82       | 0.40     |
| 20:Z:33:TRP:O     | 20:Z:33:TRP:HD1   | 2.05        | 0.40     |
| 2:B:137:LYS:HE3   | 2:B:137:LYS:HB2   | 1.97        | 0.40     |
| 2:B:212:ALA:O     | 2:B:216:HIS:ND1   | 2.52        | 0.40     |
| 9:J:9:PRO:HB2     | 9:J:12:ILE:HG13   | 2.03        | 0.40     |
| 12:M:24:ILE:HG21  | 31:M:101:LMG:H322 | 9.50        | 0.40     |
| 1:A:180:PHE:HA    | 1:A:183:MET:HE3   | 2.04        | 0.40     |
| 3:C:174:LEU:HD13  | 22:C:502:CLA:H111 | 2.07        | 0.40     |
| 22:C:519:CLA:H161 | 22:C:519:CLA:H141 | 1.90        | 0.40     |
| 24:D:405:PL9:H372 | 11:L:30:LEU:HD13  | 2.03        | 0.40     |
| 15:U:117:VAL:HG13 | 15:U:122:VAL:HG21 | 2.04        | 0.40     |
| 16:V:119:PRO:HA   | 16:V:127:PHE:CD2  | 2.63        | 0.40     |
| 16:V:81:ARG:NE    | 16:V:157:GLY:HA3  | 2.53        | 0.40     |
| 22:A:403:CLA:H11  | 22:A:403:CLA:H51  | 1.85        | 0.40     |
| 22:A:404:CLA:HAB  | 22:D:403:CLA:H42  | 2.03        | 0.40     |
| 24:A:407:PL9:H301 | 4:D:42:TYR:HA     | 2.03        | 0.40     |
| 22:B:607:CLA:H141 | 22:B:607:CLA:H161 | 2.86        | 0.40     |
| 22:B:613:CLA:H152 | 22:B:613:CLA:H112 | 1.81        | 0.40     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 25:B:616:BCR:H351 | 25:B:616:BCR:H15C | 1.88        | 0.40     |
| 22:C:511:CLA:H61  | 22:C:511:CLA:H13  | 2.04        | 0.40     |
| 15:U:106:ARG:HA   | 15:U:109:LEU:HG   | 2.03        | 0.40     |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 333/344 (97%) | 311 (93%) | 18 (5%) | 4 (1%)   | 19          | 77  |
| 1   | a     | 333/344 (97%) | 311 (93%) | 18 (5%) | 4 (1%)   | 19          | 77  |
| 2   | B     | 488/510 (96%) | 451 (92%) | 33 (7%) | 4 (1%)   | 27          | 83  |
| 2   | b     | 488/510 (96%) | 449 (92%) | 36 (7%) | 3 (1%)   | 33          | 86  |
| 3   | C     | 445/461 (96%) | 405 (91%) | 36 (8%) | 4 (1%)   | 25          | 81  |
| 3   | c     | 445/461 (96%) | 405 (91%) | 36 (8%) | 4 (1%)   | 25          | 81  |
| 4   | D     | 338/352 (96%) | 316 (94%) | 21 (6%) | 1 (0%)   | 50          | 91  |
| 4   | d     | 338/352 (96%) | 316 (94%) | 21 (6%) | 1 (0%)   | 50          | 91  |
| 5   | E     | 80/84 (95%)   | 76 (95%)  | 3 (4%)  | 1 (1%)   | 18          | 75  |
| 5   | e     | 80/84 (95%)   | 76 (95%)  | 3 (4%)  | 1 (1%)   | 18          | 75  |
| 6   | F     | 33/45 (73%)   | 29 (88%)  | 4 (12%) | 0        | 100         | 100 |
| 6   | f     | 33/45 (73%)   | 29 (88%)  | 4 (12%) | 0        | 100         | 100 |
| 7   | H     | 63/66 (96%)   | 54 (86%)  | 6 (10%) | 3 (5%)   | 4           | 44  |
| 7   | h     | 63/66 (96%)   | 54 (86%)  | 6 (10%) | 3 (5%)   | 4           | 44  |
| 8   | I     | 33/38 (87%)   | 27 (82%)  | 6 (18%) | 0        | 100         | 100 |
| 8   | i     | 33/38 (87%)   | 27 (82%)  | 6 (18%) | 0        | 100         | 100 |
| 9   | J     | 32/40 (80%)   | 28 (88%)  | 3 (9%)  | 1 (3%)   | 7           | 57  |
| 9   | j     | 32/40 (80%)   | 28 (88%)  | 3 (9%)  | 1 (3%)   | 7           | 57  |
| 10  | K     | 35/46 (76%)   | 32 (91%)  | 3 (9%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 10  | k     | 35/46 (76%)     | 32 (91%)   | 3 (9%)   | 0        | 100         | 100 |
| 11  | L     | 35/37 (95%)     | 33 (94%)   | 2 (6%)   | 0        | 100         | 100 |
| 11  | l     | 35/37 (95%)     | 33 (94%)   | 2 (6%)   | 0        | 100         | 100 |
| 12  | M     | 32/36 (89%)     | 29 (91%)   | 3 (9%)   | 0        | 100         | 100 |
| 12  | m     | 32/36 (89%)     | 29 (91%)   | 3 (9%)   | 0        | 100         | 100 |
| 13  | O     | 241/272 (89%)   | 207 (86%)  | 31 (13%) | 3 (1%)   | 19          | 77  |
| 13  | o     | 241/272 (89%)   | 208 (86%)  | 30 (12%) | 3 (1%)   | 19          | 77  |
| 14  | T     | 30/32 (94%)     | 27 (90%)   | 2 (7%)   | 1 (3%)   | 6           | 55  |
| 14  | t     | 30/32 (94%)     | 26 (87%)   | 3 (10%)  | 1 (3%)   | 6           | 55  |
| 15  | U     | 95/134 (71%)    | 87 (92%)   | 6 (6%)   | 2 (2%)   | 11          | 66  |
| 15  | u     | 95/134 (71%)    | 87 (92%)   | 6 (6%)   | 2 (2%)   | 11          | 66  |
| 16  | V     | 135/163 (83%)   | 123 (91%)  | 12 (9%)  | 0        | 100         | 100 |
| 16  | v     | 135/163 (83%)   | 124 (92%)  | 11 (8%)  | 0        | 100         | 100 |
| 17  | g     | 26/46 (56%)     | 19 (73%)   | 6 (23%)  | 1 (4%)   | 5           | 51  |
| 17  | y     | 26/46 (56%)     | 19 (73%)   | 6 (23%)  | 1 (4%)   | 5           | 51  |
| 18  | X     | 35/41 (85%)     | 31 (89%)   | 2 (6%)   | 2 (6%)   | 3           | 39  |
| 18  | x     | 35/41 (85%)     | 31 (89%)   | 2 (6%)   | 2 (6%)   | 3           | 39  |
| 20  | Z     | 60/62 (97%)     | 54 (90%)   | 5 (8%)   | 1 (2%)   | 14          | 70  |
| 20  | z     | 60/62 (97%)     | 54 (90%)   | 5 (8%)   | 1 (2%)   | 14          | 70  |
| All | All   | 5138/5618 (92%) | 4677 (91%) | 406 (8%) | 55 (1%)  | 21          | 78  |

All (55) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 12  | ASN  |
| 2   | B     | 484 | PRO  |
| 2   | B     | 488 | PRO  |
| 7   | H     | 18  | TYR  |
| 13  | O     | 52  | ALA  |
| 1   | a     | 12  | ASN  |
| 2   | b     | 484 | PRO  |
| 2   | b     | 488 | PRO  |
| 7   | h     | 18  | TYR  |
| 1   | A     | 141 | PRO  |
| 3   | C     | 257 | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 416 | SER  |
| 14  | T     | 30  | THR  |
| 17  | y     | 43  | ARG  |
| 18  | X     | 12  | ILE  |
| 18  | X     | 45  | LYS  |
| 20  | Z     | 32  | ASP  |
| 1   | a     | 141 | PRO  |
| 3   | c     | 257 | PHE  |
| 3   | c     | 416 | SER  |
| 13  | o     | 52  | ALA  |
| 14  | t     | 30  | THR  |
| 17  | g     | 43  | ARG  |
| 18  | x     | 12  | ILE  |
| 18  | x     | 45  | LYS  |
| 20  | z     | 32  | ASP  |
| 2   | B     | 489 | GLU  |
| 3   | C     | 32  | GLY  |
| 4   | D     | 239 | GLN  |
| 7   | H     | 26  | GLY  |
| 9   | J     | 38  | SER  |
| 13  | O     | 88  | GLU  |
| 13  | O     | 271 | PRO  |
| 2   | b     | 489 | GLU  |
| 3   | c     | 32  | GLY  |
| 4   | d     | 239 | GLN  |
| 5   | e     | 82  | GLN  |
| 9   | j     | 38  | SER  |
| 13  | o     | 88  | GLU  |
| 1   | A     | 142 | TRP  |
| 1   | A     | 334 | ARG  |
| 5   | E     | 82  | GLN  |
| 1   | a     | 334 | ARG  |
| 13  | o     | 271 | PRO  |
| 15  | u     | 73  | PRO  |
| 7   | H     | 16  | SER  |
| 15  | U     | 73  | PRO  |
| 3   | c     | 144 | SER  |
| 7   | h     | 16  | SER  |
| 7   | h     | 26  | GLY  |
| 3   | C     | 144 | SER  |
| 15  | U     | 83  | ALA  |
| 1   | a     | 142 | TRP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | u     | 83  | ALA  |
| 2   | B     | 176 | GLY  |

### 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     | 271/280 (97%) | 267 (98%) | 4 (2%)   | 76          | 94  |
| 1   | a     | 271/280 (97%) | 267 (98%) | 4 (2%)   | 76          | 94  |
| 2   | B     | 390/407 (96%) | 381 (98%) | 9 (2%)   | 63          | 91  |
| 2   | b     | 390/407 (96%) | 381 (98%) | 9 (2%)   | 63          | 91  |
| 3   | C     | 347/362 (96%) | 336 (97%) | 11 (3%)  | 51          | 87  |
| 3   | c     | 347/362 (96%) | 336 (97%) | 11 (3%)  | 51          | 87  |
| 4   | D     | 275/283 (97%) | 269 (98%) | 6 (2%)   | 64          | 91  |
| 4   | d     | 275/283 (97%) | 267 (97%) | 8 (3%)   | 55          | 88  |
| 5   | E     | 72/73 (99%)   | 70 (97%)  | 2 (3%)   | 56          | 88  |
| 5   | e     | 72/73 (99%)   | 70 (97%)  | 2 (3%)   | 56          | 88  |
| 6   | F     | 29/39 (74%)   | 29 (100%) | 0        | 100         | 100 |
| 6   | f     | 29/39 (74%)   | 29 (100%) | 0        | 100         | 100 |
| 7   | H     | 53/55 (96%)   | 49 (92%)  | 4 (8%)   | 19          | 65  |
| 7   | h     | 53/55 (96%)   | 49 (92%)  | 4 (8%)   | 19          | 65  |
| 8   | I     | 32/35 (91%)   | 31 (97%)  | 1 (3%)   | 52          | 88  |
| 8   | i     | 32/35 (91%)   | 31 (97%)  | 1 (3%)   | 52          | 88  |
| 9   | J     | 24/28 (86%)   | 23 (96%)  | 1 (4%)   | 40          | 82  |
| 9   | j     | 24/28 (86%)   | 23 (96%)  | 1 (4%)   | 40          | 82  |
| 10  | K     | 30/37 (81%)   | 30 (100%) | 0        | 100         | 100 |
| 10  | k     | 30/37 (81%)   | 30 (100%) | 0        | 100         | 100 |
| 11  | L     | 35/35 (100%)  | 34 (97%)  | 1 (3%)   | 55          | 88  |
| 11  | l     | 35/35 (100%)  | 34 (97%)  | 1 (3%)   | 55          | 88  |
| 12  | M     | 31/33 (94%)   | 31 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 12  | m     | 31/33 (94%)     | 31 (100%)  | 0        | 100         | 100 |
| 13  | O     | 202/228 (89%)   | 200 (99%)  | 2 (1%)   | 85          | 96  |
| 13  | o     | 202/228 (89%)   | 200 (99%)  | 2 (1%)   | 85          | 96  |
| 14  | T     | 29/29 (100%)    | 28 (97%)   | 1 (3%)   | 49          | 87  |
| 14  | t     | 29/29 (100%)    | 28 (97%)   | 1 (3%)   | 49          | 87  |
| 15  | U     | 84/112 (75%)    | 83 (99%)   | 1 (1%)   | 82          | 95  |
| 15  | u     | 84/112 (75%)    | 83 (99%)   | 1 (1%)   | 82          | 95  |
| 16  | V     | 116/138 (84%)   | 114 (98%)  | 2 (2%)   | 73          | 93  |
| 16  | v     | 116/138 (84%)   | 114 (98%)  | 2 (2%)   | 73          | 93  |
| 17  | g     | 20/37 (54%)     | 18 (90%)   | 2 (10%)  | 11          | 50  |
| 17  | y     | 20/37 (54%)     | 18 (90%)   | 2 (10%)  | 11          | 50  |
| 18  | X     | 30/34 (88%)     | 28 (93%)   | 2 (7%)   | 23          | 70  |
| 18  | x     | 30/34 (88%)     | 28 (93%)   | 2 (7%)   | 23          | 70  |
| 20  | Z     | 52/52 (100%)    | 50 (96%)   | 2 (4%)   | 44          | 85  |
| 20  | z     | 52/52 (100%)    | 50 (96%)   | 2 (4%)   | 44          | 85  |
| All | All   | 4244/4594 (92%) | 4140 (98%) | 104 (2%) | 60          | 90  |

All (104) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 228 | THR  |
| 1   | A     | 243 | GLU  |
| 1   | A     | 271 | LEU  |
| 1   | A     | 286 | THR  |
| 2   | B     | 18  | ARG  |
| 2   | B     | 23  | HIS  |
| 2   | B     | 262 | THR  |
| 2   | B     | 309 | LEU  |
| 2   | B     | 362 | PHE  |
| 2   | B     | 422 | ARG  |
| 2   | B     | 485 | GLU  |
| 2   | B     | 486 | LEU  |
| 2   | B     | 490 | GLN  |
| 3   | C     | 29  | GLU  |
| 3   | C     | 86  | LEU  |
| 3   | C     | 104 | GLU  |
| 3   | C     | 174 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 201 | ASN  |
| 3   | C     | 244 | CYS  |
| 3   | C     | 254 | THR  |
| 3   | C     | 289 | PHE  |
| 3   | C     | 355 | THR  |
| 3   | C     | 391 | ARG  |
| 3   | C     | 472 | LEU  |
| 4   | D     | 43  | LEU  |
| 4   | D     | 180 | ARG  |
| 4   | D     | 241 | GLU  |
| 4   | D     | 259 | ILE  |
| 4   | D     | 291 | LEU  |
| 4   | D     | 346 | LEU  |
| 5   | E     | 18  | ARG  |
| 5   | E     | 84  | LYS  |
| 7   | H     | 27  | THR  |
| 7   | H     | 49  | TYR  |
| 7   | H     | 56  | ASP  |
| 7   | H     | 60  | VAL  |
| 8   | I     | 33  | LYS  |
| 9   | J     | 7   | ARG  |
| 11  | L     | 7   | ARG  |
| 13  | O     | 31  | LEU  |
| 13  | O     | 97  | VAL  |
| 14  | T     | 29  | ILE  |
| 15  | U     | 132 | LEU  |
| 16  | V     | 92  | ARG  |
| 16  | V     | 122 | ARG  |
| 17  | y     | 28  | ILE  |
| 17  | y     | 46  | LEU  |
| 18  | X     | 12  | ILE  |
| 18  | X     | 45  | LYS  |
| 20  | Z     | 33  | TRP  |
| 20  | Z     | 62  | VAL  |
| 1   | a     | 228 | THR  |
| 1   | a     | 243 | GLU  |
| 1   | a     | 271 | LEU  |
| 1   | a     | 286 | THR  |
| 2   | b     | 18  | ARG  |
| 2   | b     | 23  | HIS  |
| 2   | b     | 262 | THR  |
| 2   | b     | 309 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | b     | 362 | PHE  |
| 2   | b     | 422 | ARG  |
| 2   | b     | 485 | GLU  |
| 2   | b     | 486 | LEU  |
| 2   | b     | 490 | GLN  |
| 3   | c     | 29  | GLU  |
| 3   | c     | 86  | LEU  |
| 3   | c     | 104 | GLU  |
| 3   | c     | 174 | LEU  |
| 3   | c     | 201 | ASN  |
| 3   | c     | 244 | CYS  |
| 3   | c     | 254 | THR  |
| 3   | c     | 289 | PHE  |
| 3   | c     | 355 | THR  |
| 3   | c     | 391 | ARG  |
| 3   | c     | 472 | LEU  |
| 4   | d     | 43  | LEU  |
| 4   | d     | 180 | ARG  |
| 4   | d     | 205 | LEU  |
| 4   | d     | 241 | GLU  |
| 4   | d     | 259 | ILE  |
| 4   | d     | 291 | LEU  |
| 4   | d     | 345 | VAL  |
| 4   | d     | 346 | LEU  |
| 5   | e     | 18  | ARG  |
| 5   | e     | 84  | LYS  |
| 7   | h     | 27  | THR  |
| 7   | h     | 49  | TYR  |
| 7   | h     | 56  | ASP  |
| 7   | h     | 60  | VAL  |
| 8   | i     | 33  | LYS  |
| 9   | j     | 7   | ARG  |
| 11  | l     | 7   | ARG  |
| 13  | o     | 31  | LEU  |
| 13  | o     | 97  | VAL  |
| 14  | t     | 29  | ILE  |
| 15  | u     | 132 | LEU  |
| 16  | v     | 92  | ARG  |
| 16  | v     | 122 | ARG  |
| 17  | g     | 28  | ILE  |
| 17  | g     | 46  | LEU  |
| 18  | x     | 12  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18  | x     | 45  | LYS  |
| 20  | z     | 33  | TRP  |
| 20  | z     | 62  | VAL  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 241 | GLN  |
| 1   | A     | 266 | ASN  |
| 4   | D     | 117 | HIS  |
| 4   | D     | 332 | GLN  |
| 1   | a     | 241 | GLN  |
| 4   | d     | 117 | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA chains 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 184 ligands modelled in this entry, 8 are monoatomic - leaving 176 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 |
| 22  | CLA  | A     | 402 | -    | 73,73,73     | 1.64  | 10 (13%) | 96,113,113  | 1.19 | 11 (11%) |
| 22  | CLA  | A     | 403 | -    | 73,73,73     | 1.61  | 11 (15%) | 96,113,113  | 1.22 | 11 (11%) |
| 22  | CLA  | A     | 404 | -    | 73,73,73     | 1.59  | 10 (13%) | 96,113,113  | 1.24 | 13 (13%) |
| 23  | PHO  | A     | 405 | -    | 69,69,69     | 1.24  | 11 (15%) | 92,99,99    | 1.16 | 8 (8%)   |
| 22  | CLA  | A     | 406 | -    | 73,73,73     | 1.59  | 10 (13%) | 96,113,113  | 1.23 | 12 (12%) |
| 24  | PL9  | A     | 407 | -    | 45,45,55     | 1.09  | 3 (6%)   | 55,57,69    | 1.71 | 12 (21%) |
| 25  | BCR  | A     | 408 | -    | 41,41,41     | 1.06  | 2 (4%)   | 56,56,56    | 1.22 | 7 (12%)  |
| 26  | DGD  | A     | 409 | -    | 57,57,67     | 2.23  | 2 (3%)   | 71,71,81    | 1.58 | 9 (12%)  |
| 27  | LHG  | A     | 410 | -    | 38,38,48     | 2.38  | 2 (5%)   | 44,44,54    | 1.43 | 6 (13%)  |
| 29  | OEX  | A     | 412 | 1,3  | 8,15,15      | 10.59 | 8 (100%) | 0,32,32     | 0.00 | -        |
| 30  | SQD  | A     | 413 | -    | 51,51,54     | 1.53  | 4 (7%)   | 62,62,65    | 2.01 | 11 (17%) |
| 30  | SQD  | A     | 414 | -    | 54,54,54     | 0.92  | 3 (5%)   | 65,65,65    | 1.74 | 12 (18%) |
| 22  | CLA  | B     | 601 | -    | 73,73,73     | 1.62  | 10 (13%) | 96,113,113  | 1.24 | 11 (11%) |
| 22  | CLA  | B     | 602 | -    | 73,73,73     | 1.58  | 10 (13%) | 96,113,113  | 1.26 | 14 (14%) |
| 22  | CLA  | B     | 603 | -    | 73,73,73     | 1.61  | 10 (13%) | 96,113,113  | 1.30 | 14 (14%) |
| 22  | CLA  | B     | 604 | -    | 73,73,73     | 1.60  | 10 (13%) | 96,113,113  | 1.27 | 13 (13%) |
| 22  | CLA  | B     | 605 | -    | 73,73,73     | 1.57  | 10 (13%) | 96,113,113  | 1.27 | 13 (13%) |
| 22  | CLA  | B     | 606 | -    | 73,73,73     | 1.58  | 10 (13%) | 96,113,113  | 1.23 | 13 (13%) |
| 22  | CLA  | B     | 607 | -    | 73,73,73     | 1.59  | 10 (13%) | 96,113,113  | 1.25 | 14 (14%) |
| 22  | CLA  | B     | 608 | -    | 73,73,73     | 1.63  | 10 (13%) | 96,113,113  | 1.23 | 13 (13%) |
| 22  | CLA  | B     | 609 | -    | 73,73,73     | 1.57  | 10 (13%) | 96,113,113  | 1.26 | 12 (12%) |
| 22  | CLA  | B     | 610 | -    | 73,73,73     | 1.57  | 11 (15%) | 96,113,113  | 1.45 | 14 (14%) |
| 22  | CLA  | B     | 611 | -    | 73,73,73     | 1.59  | 10 (13%) | 96,113,113  | 1.26 | 14 (14%) |
| 22  | CLA  | B     | 612 | -    | 73,73,73     | 1.58  | 10 (13%) | 96,113,113  | 1.30 | 14 (14%) |
| 22  | CLA  | B     | 613 | -    | 73,73,73     | 1.60  | 10 (13%) | 96,113,113  | 1.27 | 13 (13%) |
| 22  | CLA  | B     | 614 | -    | 73,73,73     | 1.62  | 10 (13%) | 96,113,113  | 1.24 | 13 (13%) |
| 22  | CLA  | B     | 615 | -    | 73,73,73     | 1.61  | 11 (15%) | 96,113,113  | 1.23 | 12 (12%) |
| 25  | BCR  | B     | 616 | -    | 41,41,41     | 1.09  | 2 (4%)   | 56,56,56    | 1.22 | 7 (12%)  |
| 25  | BCR  | B     | 617 | -    | 41,41,41     | 1.02  | 2 (4%)   | 56,56,56    | 1.33 | 7 (12%)  |
| 25  | BCR  | B     | 618 | -    | 41,41,41     | 1.08  | 2 (4%)   | 56,56,56    | 1.36 | 9 (16%)  |
| 25  | BCR  | B     | 619 | -    | 41,41,41     | 1.06  | 2 (4%)   | 56,56,56    | 1.25 | 8 (14%)  |
| 26  | DGD  | B     | 620 | -    | 59,59,67     | 2.24  | 2 (3%)   | 73,73,81    | 1.45 | 7 (9%)   |
| 31  | LMG  | B     | 621 | -    | 49,49,55     | 2.34  | 4 (8%)   | 57,57,63    | 1.40 | 9 (15%)  |
| 30  | SQD  | B     | 622 | -    | 43,43,54     | 1.25  | 4 (9%)   | 54,54,65    | 2.03 | 11 (20%) |
| 32  | LMT  | B     | 623 | -    | 36,36,36     | 1.09  | 4 (11%)  | 47,47,47    | 1.03 | 2 (4%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 32  | LMT  | B     | 624 | -    | 36,36,36     | 1.06 | 3 (8%)   | 47,47,47    | 1.03 | 2 (4%)   |
| 31  | LMG  | B     | 625 | -    | 49,49,55     | 2.52 | 2 (4%)   | 57,57,63    | 1.43 | 8 (14%)  |
| 26  | DGD  | B     | 626 | -    | 53,53,67     | 2.29 | 6 (11%)  | 67,67,81    | 1.46 | 10 (14%) |
| 30  | SQD  | B     | 627 | -    | 47,47,54     | 1.08 | 4 (8%)   | 58,58,65    | 2.03 | 11 (18%) |
| 32  | LMT  | B     | 628 | -    | 36,36,36     | 1.08 | 5 (13%)  | 47,47,47    | 1.03 | 2 (4%)   |
| 32  | LMT  | B     | 629 | -    | 36,36,36     | 1.10 | 4 (11%)  | 47,47,47    | 1.05 | 1 (2%)   |
| 22  | CLA  | C     | 501 | -    | 73,73,73     | 1.61 | 11 (15%) | 96,113,113  | 1.20 | 12 (12%) |
| 22  | CLA  | C     | 502 | -    | 73,73,73     | 1.60 | 11 (15%) | 96,113,113  | 1.25 | 11 (11%) |
| 22  | CLA  | C     | 503 | -    | 73,73,73     | 1.60 | 10 (13%) | 96,113,113  | 1.26 | 13 (13%) |
| 22  | CLA  | C     | 504 | -    | 73,73,73     | 1.58 | 11 (15%) | 96,113,113  | 1.27 | 15 (15%) |
| 22  | CLA  | C     | 505 | -    | 73,73,73     | 1.59 | 10 (13%) | 96,113,113  | 1.28 | 15 (15%) |
| 22  | CLA  | C     | 506 | -    | 73,73,73     | 1.59 | 10 (13%) | 96,113,113  | 1.27 | 13 (13%) |
| 22  | CLA  | C     | 507 | -    | 73,73,73     | 1.61 | 10 (13%) | 96,113,113  | 1.30 | 13 (13%) |
| 22  | CLA  | C     | 508 | -    | 73,73,73     | 1.60 | 10 (13%) | 96,113,113  | 1.24 | 11 (11%) |
| 22  | CLA  | C     | 509 | -    | 73,73,73     | 1.60 | 10 (13%) | 96,113,113  | 1.22 | 11 (11%) |
| 22  | CLA  | C     | 510 | 3    | 73,73,73     | 1.60 | 10 (13%) | 96,113,113  | 1.29 | 13 (13%) |
| 22  | CLA  | C     | 511 | -    | 73,73,73     | 1.62 | 10 (13%) | 96,113,113  | 1.27 | 14 (14%) |
| 22  | CLA  | C     | 512 | -    | 73,73,73     | 1.60 | 10 (13%) | 96,113,113  | 1.26 | 13 (13%) |
| 25  | BCR  | C     | 513 | -    | 41,41,41     | 1.07 | 2 (4%)   | 56,56,56    | 1.27 | 8 (14%)  |
| 26  | DGD  | C     | 514 | -    | 54,54,67     | 2.40 | 4 (7%)   | 68,68,81    | 1.34 | 10 (14%) |
| 26  | DGD  | C     | 515 | -    | 63,63,67     | 1.49 | 2 (3%)   | 77,77,81    | 1.44 | 12 (15%) |
| 26  | DGD  | C     | 516 | -    | 67,67,67     | 0.86 | 2 (2%)   | 81,81,81    | 1.44 | 12 (14%) |
| 31  | LMG  | C     | 517 | -    | 45,45,55     | 2.64 | 2 (4%)   | 53,53,63    | 1.45 | 8 (15%)  |
| 27  | LHG  | C     | 518 | -    | 36,36,48     | 2.39 | 2 (5%)   | 42,42,54    | 1.53 | 7 (16%)  |
| 22  | CLA  | C     | 519 | -    | 73,73,73     | 1.59 | 10 (13%) | 96,113,113  | 1.22 | 12 (12%) |
| 25  | BCR  | C     | 520 | -    | 41,41,41     | 1.04 | 2 (4%)   | 56,56,56    | 1.18 | 9 (16%)  |
| 31  | LMG  | C     | 521 | -    | 48,48,55     | 2.37 | 2 (4%)   | 56,56,63    | 1.42 | 9 (16%)  |
| 23  | PHO  | D     | 401 | -    | 69,69,69     | 1.23 | 10 (14%) | 92,99,99    | 1.15 | 10 (10%) |
| 33  | BCT  | D     | 402 | 21   | 0,3,3        | 0.00 | -        | 0,3,3       | 0.00 | -        |
| 22  | CLA  | D     | 403 | -    | 73,73,73     | 1.60 | 10 (13%) | 96,113,113  | 1.22 | 12 (12%) |
| 22  | CLA  | D     | 404 | -    | 73,73,73     | 1.59 | 10 (13%) | 96,113,113  | 1.28 | 15 (15%) |
| 24  | PL9  | D     | 405 | -    | 55,55,55     | 1.22 | 3 (5%)   | 69,69,69    | 1.68 | 16 (23%) |
| 31  | LMG  | D     | 406 | -    | 48,48,55     | 2.41 | 3 (6%)   | 56,56,63    | 1.51 | 7 (12%)  |
| 26  | DGD  | D     | 407 | -    | 64,64,67     | 1.41 | 3 (4%)   | 78,78,81    | 1.34 | 7 (8%)   |
| 32  | LMT  | D     | 408 | -    | 32,32,36     | 2.79 | 6 (18%)  | 43,43,47    | 1.07 | 2 (4%)   |



| Mol | Type | Chain | Res | Link | Bond lengths |       |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|-------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ  | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 31  | LMG  | D     | 409 | -    | 46,46,55     | 2.57  | 4 (8%)   | 54,54,63    | 1.43 | 6 (11%)  |
| 31  | LMG  | E     | 101 | -    | 44,44,55     | 2.64  | 3 (6%)   | 52,52,63    | 1.41 | 6 (11%)  |
| 34  | HEM  | F     | 101 | 5,6  | 42,50,50     | 3.65  | 13 (30%) | 27,82,82    | 1.14 | 1 (3%)   |
| 25  | BCR  | F     | 102 | -    | 41,41,41     | 1.09  | 2 (4%)   | 56,56,56    | 1.20 | 6 (10%)  |
| 30  | SQD  | F     | 103 | -    | 45,45,54     | 1.39  | 5 (11%)  | 56,56,65    | 1.92 | 12 (21%) |
| 22  | CLA  | H     | 101 | -    | 73,73,73     | 1.62  | 10 (13%) | 96,113,113  | 1.21 | 13 (13%) |
| 25  | BCR  | H     | 102 | -    | 41,41,41     | 1.07  | 2 (4%)   | 56,56,56    | 1.20 | 4 (7%)   |
| 31  | LMG  | I     | 101 | -    | 43,43,55     | 2.37  | 3 (6%)   | 51,51,63    | 1.35 | 7 (13%)  |
| 32  | LMT  | I     | 102 | -    | 36,36,36     | 1.07  | 5 (13%)  | 47,47,47    | 1.10 | 2 (4%)   |
| 24  | PL9  | J     | 101 | -    | 35,35,55     | 1.16  | 1 (2%)   | 43,45,69    | 1.85 | 8 (18%)  |
| 25  | BCR  | J     | 102 | -    | 41,41,41     | 1.03  | 2 (4%)   | 56,56,56    | 1.59 | 13 (23%) |
| 25  | BCR  | K     | 101 | -    | 41,41,41     | 1.08  | 2 (4%)   | 56,56,56    | 1.31 | 8 (14%)  |
| 31  | LMG  | L     | 101 | -    | 51,51,55     | 2.34  | 3 (5%)   | 59,59,63    | 1.43 | 8 (13%)  |
| 31  | LMG  | M     | 101 | -    | 42,42,55     | 2.38  | 3 (7%)   | 50,50,63    | 1.33 | 5 (10%)  |
| 32  | LMT  | M     | 102 | -    | 36,36,36     | 1.10  | 4 (11%)  | 47,47,47    | 1.04 | 2 (4%)   |
| 32  | LMT  | M     | 103 | -    | 36,36,36     | 1.09  | 5 (13%)  | 47,47,47    | 1.03 | 3 (6%)   |
| 34  | HEM  | V     | 201 | 16   | 42,50,50     | 3.69  | 12 (28%) | 27,82,82    | 1.14 | 2 (7%)   |
| 30  | SQD  | a     | 401 | -    | 54,54,54     | 0.92  | 3 (5%)   | 65,65,65    | 1.74 | 10 (15%) |
| 31  | LMG  | a     | 402 | -    | 42,42,55     | 2.53  | 4 (9%)   | 50,50,63    | 1.33 | 5 (10%)  |
| 22  | CLA  | a     | 403 | -    | 73,73,73     | 1.64  | 10 (13%) | 96,113,113  | 1.21 | 11 (11%) |
| 22  | CLA  | a     | 404 | -    | 73,73,73     | 1.58  | 10 (13%) | 96,113,113  | 1.22 | 11 (11%) |
| 22  | CLA  | a     | 405 | -    | 73,73,73     | 1.61  | 10 (13%) | 96,113,113  | 1.22 | 11 (11%) |
| 22  | CLA  | a     | 406 | -    | 73,73,73     | 1.59  | 10 (13%) | 96,113,113  | 1.25 | 13 (13%) |
| 24  | PL9  | a     | 407 | -    | 45,45,55     | 1.13  | 3 (6%)   | 55,57,69    | 1.74 | 13 (23%) |
| 26  | DGD  | a     | 408 | -    | 57,57,67     | 2.29  | 2 (3%)   | 71,71,81    | 1.54 | 9 (12%)  |
| 27  | LHG  | a     | 409 | -    | 38,38,48     | 2.34  | 2 (5%)   | 44,44,54    | 1.43 | 6 (13%)  |
| 29  | OEX  | a     | 411 | 1,3  | 8,15,15      | 10.48 | 8 (100%) | 0,32,32     | 0.00 | -        |
| 30  | SQD  | a     | 412 | -    | 51,51,54     | 1.55  | 4 (7%)   | 62,62,65    | 2.00 | 12 (19%) |
| 26  | DGD  | b     | 601 | -    | 53,53,67     | 2.29  | 6 (11%)  | 67,67,81    | 1.47 | 10 (14%) |
| 30  | SQD  | b     | 602 | -    | 47,47,54     | 1.10  | 4 (8%)   | 58,58,65    | 2.05 | 10 (17%) |
| 32  | LMT  | b     | 603 | -    | 36,36,36     | 1.09  | 5 (13%)  | 47,47,47    | 0.99 | 1 (2%)   |
| 32  | LMT  | b     | 604 | -    | 36,36,36     | 1.09  | 5 (13%)  | 47,47,47    | 1.06 | 1 (2%)   |
| 22  | CLA  | b     | 605 | -    | 73,73,73     | 1.63  | 11 (15%) | 96,113,113  | 1.24 | 11 (11%) |
| 22  | CLA  | b     | 606 | -    | 73,73,73     | 1.59  | 11 (15%) | 96,113,113  | 1.24 | 12 (12%) |
| 22  | CLA  | b     | 607 | -    | 73,73,73     | 1.59  | 10 (13%) | 96,113,113  | 1.23 | 12 (12%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 22  | CLA  | b     | 608 | -    | 73,73,73     | 1.60 | 10 (13%) | 96,113,113  | 1.29 | 15 (15%) |
| 22  | CLA  | b     | 609 | -    | 73,73,73     | 1.59 | 10 (13%) | 96,113,113  | 1.26 | 12 (12%) |
| 22  | CLA  | b     | 610 | -    | 73,73,73     | 1.60 | 10 (13%) | 96,113,113  | 1.24 | 13 (13%) |
| 22  | CLA  | b     | 611 | -    | 73,73,73     | 1.59 | 10 (13%) | 96,113,113  | 1.20 | 11 (11%) |
| 22  | CLA  | b     | 612 | -    | 73,73,73     | 1.60 | 10 (13%) | 96,113,113  | 1.23 | 12 (12%) |
| 22  | CLA  | b     | 613 | -    | 73,73,73     | 1.61 | 10 (13%) | 96,113,113  | 1.23 | 13 (13%) |
| 22  | CLA  | b     | 614 | -    | 73,73,73     | 1.58 | 10 (13%) | 96,113,113  | 1.26 | 12 (12%) |
| 22  | CLA  | b     | 615 | -    | 73,73,73     | 1.57 | 11 (15%) | 96,113,113  | 1.43 | 16 (16%) |
| 22  | CLA  | b     | 616 | -    | 73,73,73     | 1.61 | 10 (13%) | 96,113,113  | 1.23 | 13 (13%) |
| 22  | CLA  | b     | 617 | -    | 73,73,73     | 1.59 | 10 (13%) | 96,113,113  | 1.28 | 14 (14%) |
| 22  | CLA  | b     | 618 | -    | 73,73,73     | 1.60 | 10 (13%) | 96,113,113  | 1.25 | 12 (12%) |
| 22  | CLA  | b     | 619 | -    | 73,73,73     | 1.61 | 10 (13%) | 96,113,113  | 1.24 | 14 (14%) |
| 22  | CLA  | b     | 620 | -    | 73,73,73     | 1.62 | 11 (15%) | 96,113,113  | 1.21 | 11 (11%) |
| 25  | BCR  | b     | 621 | -    | 41,41,41     | 1.07 | 2 (4%)   | 56,56,56    | 1.20 | 6 (10%)  |
| 25  | BCR  | b     | 622 | -    | 41,41,41     | 1.04 | 2 (4%)   | 56,56,56    | 1.32 | 8 (14%)  |
| 25  | BCR  | b     | 623 | -    | 41,41,41     | 1.08 | 2 (4%)   | 56,56,56    | 1.36 | 10 (17%) |
| 25  | BCR  | b     | 624 | -    | 41,41,41     | 1.08 | 2 (4%)   | 56,56,56    | 1.29 | 9 (16%)  |
| 26  | DGD  | b     | 625 | -    | 59,59,67     | 2.24 | 2 (3%)   | 73,73,81    | 1.48 | 7 (9%)   |
| 31  | LMG  | b     | 626 | -    | 49,49,55     | 2.36 | 3 (6%)   | 57,57,63    | 1.42 | 10 (17%) |
| 31  | LMG  | b     | 627 | -    | 42,42,55     | 2.45 | 3 (7%)   | 50,50,63    | 1.34 | 5 (10%)  |
| 32  | LMT  | b     | 628 | -    | 36,36,36     | 1.09 | 4 (11%)  | 47,47,47    | 1.03 | 2 (4%)   |
| 32  | LMT  | b     | 629 | -    | 36,36,36     | 1.07 | 5 (13%)  | 47,47,47    | 1.06 | 3 (6%)   |
| 22  | CLA  | c     | 501 | -    | 73,73,73     | 1.62 | 11 (15%) | 96,113,113  | 1.19 | 13 (13%) |
| 22  | CLA  | c     | 502 | -    | 73,73,73     | 1.61 | 10 (13%) | 96,113,113  | 1.26 | 12 (12%) |
| 22  | CLA  | c     | 503 | -    | 73,73,73     | 1.62 | 10 (13%) | 96,113,113  | 1.25 | 13 (13%) |
| 22  | CLA  | c     | 504 | -    | 73,73,73     | 1.60 | 10 (13%) | 96,113,113  | 1.25 | 13 (13%) |
| 22  | CLA  | c     | 505 | -    | 73,73,73     | 1.60 | 10 (13%) | 96,113,113  | 1.30 | 13 (13%) |
| 22  | CLA  | c     | 506 | -    | 73,73,73     | 1.59 | 10 (13%) | 96,113,113  | 1.28 | 13 (13%) |
| 22  | CLA  | c     | 507 | -    | 73,73,73     | 1.59 | 10 (13%) | 96,113,113  | 1.32 | 14 (14%) |
| 22  | CLA  | c     | 508 | -    | 73,73,73     | 1.61 | 10 (13%) | 96,113,113  | 1.25 | 13 (13%) |
| 22  | CLA  | c     | 509 | -    | 73,73,73     | 1.62 | 10 (13%) | 96,113,113  | 1.24 | 12 (12%) |
| 22  | CLA  | c     | 510 | 3    | 73,73,73     | 1.63 | 11 (15%) | 96,113,113  | 1.25 | 13 (13%) |
| 22  | CLA  | c     | 511 | -    | 73,73,73     | 1.63 | 10 (13%) | 96,113,113  | 1.24 | 14 (14%) |
| 22  | CLA  | c     | 512 | -    | 73,73,73     | 1.63 | 10 (13%) | 96,113,113  | 1.23 | 13 (13%) |
| 25  | BCR  | c     | 513 | -    | 41,41,41     | 1.07 | 2 (4%)   | 56,56,56    | 1.31 | 9 (16%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 25  | BCR  | c     | 514 | -    | 41,41,41     | 1.06 | 2 (4%)   | 56,56,56    | 1.28 | 8 (14%)  |
| 26  | DGD  | c     | 515 | -    | 54,54,67     | 2.45 | 3 (5%)   | 68,68,81    | 1.38 | 10 (14%) |
| 26  | DGD  | c     | 516 | -    | 63,63,67     | 1.46 | 2 (3%)   | 77,77,81    | 1.46 | 12 (15%) |
| 26  | DGD  | c     | 517 | -    | 67,67,67     | 0.88 | 2 (2%)   | 81,81,81    | 1.40 | 9 (11%)  |
| 31  | LMG  | c     | 518 | -    | 45,45,55     | 2.53 | 2 (4%)   | 53,53,63    | 1.43 | 8 (15%)  |
| 27  | LHG  | c     | 519 | -    | 36,36,48     | 2.33 | 3 (8%)   | 42,42,54    | 1.53 | 8 (19%)  |
| 22  | CLA  | c     | 520 | -    | 73,73,73     | 1.60 | 10 (13%) | 96,113,113  | 1.22 | 12 (12%) |
| 25  | BCR  | c     | 521 | -    | 41,41,41     | 1.04 | 2 (4%)   | 56,56,56    | 1.21 | 7 (12%)  |
| 31  | LMG  | c     | 522 | -    | 48,48,55     | 2.36 | 3 (6%)   | 56,56,63    | 1.41 | 9 (16%)  |
| 23  | PHO  | d     | 401 | -    | 69,69,69     | 1.22 | 10 (14%) | 92,99,99    | 1.19 | 9 (9%)   |
| 23  | PHO  | d     | 402 | -    | 69,69,69     | 1.26 | 11 (15%) | 92,99,99    | 1.17 | 10 (10%) |
| 30  | SQD  | d     | 403 | -    | 43,43,54     | 1.23 | 4 (9%)   | 54,54,65    | 1.97 | 11 (20%) |
| 33  | BCT  | d     | 404 | 21   | 0,3,3        | 0.00 | -        | 0,3,3       | 0.00 | -        |
| 22  | CLA  | d     | 405 | -    | 73,73,73     | 1.62 | 10 (13%) | 96,113,113  | 1.19 | 13 (13%) |
| 22  | CLA  | d     | 406 | -    | 73,73,73     | 1.61 | 10 (13%) | 96,113,113  | 1.25 | 13 (13%) |
| 24  | PL9  | d     | 407 | -    | 55,55,55     | 1.15 | 3 (5%)   | 69,69,69    | 1.68 | 15 (21%) |
| 31  | LMG  | d     | 408 | -    | 49,49,55     | 2.51 | 2 (4%)   | 57,57,63    | 1.44 | 8 (14%)  |
| 31  | LMG  | d     | 409 | -    | 48,48,55     | 2.39 | 3 (6%)   | 56,56,63    | 1.52 | 6 (10%)  |
| 26  | DGD  | d     | 410 | -    | 64,64,67     | 1.48 | 2 (3%)   | 78,78,81    | 1.37 | 9 (11%)  |
| 32  | LMT  | d     | 411 | -    | 32,32,36     | 2.81 | 6 (18%)  | 43,43,47    | 1.07 | 2 (4%)   |
| 31  | LMG  | d     | 412 | -    | 46,46,55     | 2.61 | 4 (8%)   | 54,54,63    | 1.41 | 7 (12%)  |
| 31  | LMG  | e     | 101 | -    | 44,44,55     | 2.69 | 3 (6%)   | 52,52,63    | 1.41 | 7 (13%)  |
| 34  | HEM  | f     | 101 | 5,6  | 42,50,50     | 3.62 | 13 (30%) | 27,82,82    | 1.27 | 3 (11%)  |
| 25  | BCR  | f     | 102 | -    | 41,41,41     | 1.07 | 2 (4%)   | 56,56,56    | 1.19 | 6 (10%)  |
| 30  | SQD  | f     | 103 | -    | 45,45,54     | 1.40 | 4 (8%)   | 56,56,65    | 1.92 | 12 (21%) |
| 25  | BCR  | g     | 101 | -    | 41,41,41     | 1.10 | 3 (7%)   | 56,56,56    | 1.28 | 8 (14%)  |
| 25  | BCR  | i     | 101 | -    | 41,41,41     | 1.06 | 2 (4%)   | 56,56,56    | 1.19 | 6 (10%)  |
| 31  | LMG  | i     | 102 | -    | 43,43,55     | 2.33 | 2 (4%)   | 51,51,63    | 1.34 | 6 (11%)  |
| 32  | LMT  | i     | 103 | -    | 36,36,36     | 1.06 | 4 (11%)  | 47,47,47    | 1.08 | 2 (4%)   |
| 24  | PL9  | j     | 101 | -    | 35,35,55     | 1.24 | 2 (5%)   | 43,45,69    | 1.81 | 8 (18%)  |
| 25  | BCR  | j     | 102 | -    | 41,41,41     | 1.02 | 2 (4%)   | 56,56,56    | 1.52 | 12 (21%) |
| 31  | LMG  | l     | 101 | -    | 51,51,55     | 2.34 | 3 (5%)   | 59,59,63    | 1.41 | 8 (13%)  |
| 31  | LMG  | m     | 101 | -    | 42,42,55     | 2.47 | 4 (9%)   | 50,50,63    | 1.35 | 5 (10%)  |
| 34  | HEM  | v     | 201 | 16   | 42,50,50     | 3.70 | 14 (33%) | 27,82,82    | 1.12 | 1 (3%)   |
| 25  | BCR  | x     | 101 | -    | 41,41,41     | 1.06 | 2 (4%)   | 56,56,56    | 1.16 | 4 (7%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 25  | BCR  | y     | 101 | -    | 41,41,41     | 1.09 | 3 (7%)   | 56,56,56    | 1.23 | 5 (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   |
|-----|------|-------|-----|------|---------|--------------|---------|
| 22  | CLA  | A     | 402 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | A     | 403 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | A     | 404 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 23  | PHO  | A     | 405 | -    | -       | 0/49/103/103 | 0/1/6/6 |
| 22  | CLA  | A     | 406 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 24  | PL9  | A     | 407 | -    | -       | 0/41/61/73   | 0/1/1/1 |
| 25  | BCR  | A     | 408 | -    | -       | 0/29/63/63   | 0/2/2/2 |
| 26  | DGD  | A     | 409 | -    | -       | 0/45/85/95   | 0/2/2/2 |
| 27  | LHG  | A     | 410 | -    | -       | 0/43/43/53   | 0/0/0/0 |
| 29  | OEX  | A     | 412 | 1,3  | -       | 0/0/68/68    | 0/0/6/6 |
| 30  | SQD  | A     | 413 | -    | -       | 0/46/66/69   | 0/1/1/1 |
| 30  | SQD  | A     | 414 | -    | -       | 0/49/69/69   | 0/1/1/1 |
| 22  | CLA  | B     | 601 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | B     | 602 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | B     | 603 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | B     | 604 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | B     | 605 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | B     | 606 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | B     | 607 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | B     | 608 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | B     | 609 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | B     | 610 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | B     | 611 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | B     | 612 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | B     | 613 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | B     | 614 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | B     | 615 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 25  | BCR  | B     | 616 | -    | -       | 0/29/63/63   | 0/2/2/2 |
| 25  | BCR  | B     | 617 | -    | -       | 0/29/63/63   | 0/2/2/2 |
| 25  | BCR  | B     | 618 | -    | -       | 0/29/63/63   | 0/2/2/2 |
| 25  | BCR  | B     | 619 | -    | -       | 0/29/63/63   | 0/2/2/2 |
| 26  | DGD  | B     | 620 | -    | -       | 0/47/87/95   | 0/2/2/2 |
| 31  | LMG  | B     | 621 | -    | -       | 0/44/64/70   | 0/1/1/1 |
| 30  | SQD  | B     | 622 | -    | -       | 1/38/58/69   | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions     | Rings   |
|-----|------|-------|-----|------|---------|--------------|---------|
| 32  | LMT  | B     | 623 | -    | -       | 0/21/61/61   | 0/2/2/2 |
| 32  | LMT  | B     | 624 | -    | -       | 0/21/61/61   | 0/2/2/2 |
| 31  | LMG  | B     | 625 | -    | -       | 0/44/64/70   | 0/1/1/1 |
| 26  | DGD  | B     | 626 | -    | -       | 0/41/81/95   | 0/2/2/2 |
| 30  | SQD  | B     | 627 | -    | -       | 0/42/62/69   | 0/1/1/1 |
| 32  | LMT  | B     | 628 | -    | -       | 0/21/61/61   | 0/2/2/2 |
| 32  | LMT  | B     | 629 | -    | -       | 0/21/61/61   | 0/2/2/2 |
| 22  | CLA  | C     | 501 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | C     | 502 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | C     | 503 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | C     | 504 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | C     | 505 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | C     | 506 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | C     | 507 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | C     | 508 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | C     | 509 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | C     | 510 | 3    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | C     | 511 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | C     | 512 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 25  | BCR  | C     | 513 | -    | -       | 0/29/63/63   | 0/2/2/2 |
| 26  | DGD  | C     | 514 | -    | -       | 0/42/82/95   | 0/2/2/2 |
| 26  | DGD  | C     | 515 | -    | -       | 1/51/91/95   | 0/2/2/2 |
| 26  | DGD  | C     | 516 | -    | -       | 0/55/95/95   | 0/2/2/2 |
| 31  | LMG  | C     | 517 | -    | -       | 0/40/60/70   | 0/1/1/1 |
| 27  | LHG  | C     | 518 | -    | -       | 0/41/41/53   | 0/0/0/0 |
| 22  | CLA  | C     | 519 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 25  | BCR  | C     | 520 | -    | -       | 0/29/63/63   | 0/2/2/2 |
| 31  | LMG  | C     | 521 | -    | -       | 0/43/63/70   | 0/1/1/1 |
| 23  | PHO  | D     | 401 | -    | -       | 0/49/103/103 | 0/1/6/6 |
| 33  | BCT  | D     | 402 | 21   | -       | 0/0/0/0      | 0/0/0/0 |
| 22  | CLA  | D     | 403 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | D     | 404 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 24  | PL9  | D     | 405 | -    | -       | 0/53/73/73   | 0/1/1/1 |
| 31  | LMG  | D     | 406 | -    | -       | 0/43/63/70   | 0/1/1/1 |
| 26  | DGD  | D     | 407 | -    | -       | 0/52/92/95   | 0/2/2/2 |
| 32  | LMT  | D     | 408 | -    | -       | 0/17/57/61   | 0/2/2/2 |
| 31  | LMG  | D     | 409 | -    | -       | 0/41/61/70   | 0/1/1/1 |
| 31  | LMG  | E     | 101 | -    | -       | 0/39/59/70   | 0/1/1/1 |
| 34  | HEM  | F     | 101 | 5,6  | -       | 0/14/114/114 | 0/0/8/8 |
| 25  | BCR  | F     | 102 | -    | -       | 0/29/63/63   | 0/2/2/2 |
| 30  | SQD  | F     | 103 | -    | -       | 0/40/60/69   | 0/1/1/1 |
| 22  | CLA  | H     | 101 | -    | -       | 0/37/135/135 | 0/0/9/9 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions     | Rings   |
|-----|------|-------|-----|------|---------|--------------|---------|
| 25  | BCR  | H     | 102 | -    | -       | 0/29/63/63   | 0/2/2/2 |
| 31  | LMG  | I     | 101 | -    | -       | 0/38/58/70   | 0/1/1/1 |
| 32  | LMT  | I     | 102 | -    | -       | 0/21/61/61   | 0/2/2/2 |
| 24  | PL9  | J     | 101 | -    | -       | 0/29/49/73   | 0/1/1/1 |
| 25  | BCR  | J     | 102 | -    | -       | 0/29/63/63   | 0/2/2/2 |
| 25  | BCR  | K     | 101 | -    | -       | 0/29/63/63   | 0/2/2/2 |
| 31  | LMG  | L     | 101 | -    | -       | 0/46/66/70   | 0/1/1/1 |
| 31  | LMG  | M     | 101 | -    | -       | 0/37/57/70   | 0/1/1/1 |
| 32  | LMT  | M     | 102 | -    | -       | 0/21/61/61   | 0/2/2/2 |
| 32  | LMT  | M     | 103 | -    | -       | 0/21/61/61   | 0/2/2/2 |
| 34  | HEM  | V     | 201 | 16   | -       | 0/14/114/114 | 0/0/8/8 |
| 30  | SQD  | a     | 401 | -    | -       | 0/49/69/69   | 0/1/1/1 |
| 31  | LMG  | a     | 402 | -    | -       | 0/37/57/70   | 0/1/1/1 |
| 22  | CLA  | a     | 403 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | a     | 404 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | a     | 405 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | a     | 406 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 24  | PL9  | a     | 407 | -    | -       | 0/41/61/73   | 0/1/1/1 |
| 26  | DGD  | a     | 408 | -    | -       | 0/45/85/95   | 0/2/2/2 |
| 27  | LHG  | a     | 409 | -    | -       | 0/43/43/53   | 0/0/0/0 |
| 29  | OEX  | a     | 411 | 1,3  | -       | 0/0/68/68    | 0/0/6/6 |
| 30  | SQD  | a     | 412 | -    | -       | 0/46/66/69   | 0/1/1/1 |
| 26  | DGD  | b     | 601 | -    | -       | 0/41/81/95   | 0/2/2/2 |
| 30  | SQD  | b     | 602 | -    | -       | 0/42/62/69   | 0/1/1/1 |
| 32  | LMT  | b     | 603 | -    | -       | 0/21/61/61   | 0/2/2/2 |
| 32  | LMT  | b     | 604 | -    | -       | 0/21/61/61   | 0/2/2/2 |
| 22  | CLA  | b     | 605 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | b     | 606 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | b     | 607 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | b     | 608 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | b     | 609 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | b     | 610 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | b     | 611 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | b     | 612 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | b     | 613 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | b     | 614 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | b     | 615 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | b     | 616 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | b     | 617 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | b     | 618 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | b     | 619 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | b     | 620 | -    | -       | 0/37/135/135 | 0/0/9/9 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions     | Rings   |
|-----|------|-------|-----|------|---------|--------------|---------|
| 25  | BCR  | b     | 621 | -    | -       | 0/29/63/63   | 0/2/2/2 |
| 25  | BCR  | b     | 622 | -    | -       | 0/29/63/63   | 0/2/2/2 |
| 25  | BCR  | b     | 623 | -    | -       | 0/29/63/63   | 0/2/2/2 |
| 25  | BCR  | b     | 624 | -    | -       | 0/29/63/63   | 0/2/2/2 |
| 26  | DGD  | b     | 625 | -    | -       | 0/47/87/95   | 0/2/2/2 |
| 31  | LMG  | b     | 626 | -    | -       | 0/44/64/70   | 0/1/1/1 |
| 31  | LMG  | b     | 627 | -    | -       | 0/37/57/70   | 0/1/1/1 |
| 32  | LMT  | b     | 628 | -    | -       | 0/21/61/61   | 0/2/2/2 |
| 32  | LMT  | b     | 629 | -    | -       | 0/21/61/61   | 0/2/2/2 |
| 22  | CLA  | c     | 501 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | c     | 502 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | c     | 503 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | c     | 504 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | c     | 505 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | c     | 506 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | c     | 507 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | c     | 508 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | c     | 509 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | c     | 510 | 3    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | c     | 511 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | c     | 512 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 25  | BCR  | c     | 513 | -    | -       | 0/29/63/63   | 0/2/2/2 |
| 25  | BCR  | c     | 514 | -    | -       | 0/29/63/63   | 0/2/2/2 |
| 26  | DGD  | c     | 515 | -    | -       | 0/42/82/95   | 0/2/2/2 |
| 26  | DGD  | c     | 516 | -    | -       | 1/51/91/95   | 0/2/2/2 |
| 26  | DGD  | c     | 517 | -    | -       | 0/55/95/95   | 0/2/2/2 |
| 31  | LMG  | c     | 518 | -    | -       | 0/40/60/70   | 0/1/1/1 |
| 27  | LHG  | c     | 519 | -    | -       | 0/41/41/53   | 0/0/0/0 |
| 22  | CLA  | c     | 520 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 25  | BCR  | c     | 521 | -    | -       | 0/29/63/63   | 0/2/2/2 |
| 31  | LMG  | c     | 522 | -    | -       | 0/43/63/70   | 0/1/1/1 |
| 23  | PHO  | d     | 401 | -    | -       | 0/49/103/103 | 0/1/6/6 |
| 23  | PHO  | d     | 402 | -    | -       | 0/49/103/103 | 0/1/6/6 |
| 30  | SQD  | d     | 403 | -    | -       | 1/38/58/69   | 0/1/1/1 |
| 33  | BCT  | d     | 404 | 21   | -       | 0/0/0/0      | 0/0/0/0 |
| 22  | CLA  | d     | 405 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 22  | CLA  | d     | 406 | -    | -       | 0/37/135/135 | 0/0/9/9 |
| 24  | PL9  | d     | 407 | -    | -       | 0/53/73/73   | 0/1/1/1 |
| 31  | LMG  | d     | 408 | -    | -       | 0/44/64/70   | 0/1/1/1 |
| 31  | LMG  | d     | 409 | -    | -       | 0/43/63/70   | 0/1/1/1 |
| 26  | DGD  | d     | 410 | -    | -       | 0/52/92/95   | 0/2/2/2 |
| 32  | LMT  | d     | 411 | -    | -       | 0/17/57/61   | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions     | Rings   |
|-----|------|-------|-----|------|---------|--------------|---------|
| 31  | LMG  | d     | 412 | -    | -       | 0/41/61/70   | 0/1/1/1 |
| 31  | LMG  | e     | 101 | -    | -       | 0/39/59/70   | 0/1/1/1 |
| 34  | HEM  | f     | 101 | 5,6  | -       | 0/14/114/114 | 0/0/8/8 |
| 25  | BCR  | f     | 102 | -    | -       | 0/29/63/63   | 0/2/2/2 |
| 30  | SQD  | f     | 103 | -    | -       | 0/40/60/69   | 0/1/1/1 |
| 25  | BCR  | g     | 101 | -    | -       | 0/29/63/63   | 0/2/2/2 |
| 25  | BCR  | i     | 101 | -    | -       | 0/29/63/63   | 0/2/2/2 |
| 31  | LMG  | i     | 102 | -    | -       | 0/38/58/70   | 0/1/1/1 |
| 32  | LMT  | i     | 103 | -    | -       | 0/21/61/61   | 0/2/2/2 |
| 24  | PL9  | j     | 101 | -    | -       | 0/29/49/73   | 0/1/1/1 |
| 25  | BCR  | j     | 102 | -    | -       | 0/29/63/63   | 0/2/2/2 |
| 31  | LMG  | l     | 101 | -    | -       | 0/46/66/70   | 0/1/1/1 |
| 31  | LMG  | m     | 101 | -    | -       | 0/37/57/70   | 0/1/1/1 |
| 34  | HEM  | v     | 201 | 16   | -       | 0/14/114/114 | 0/0/8/8 |
| 25  | BCR  | x     | 101 | -    | -       | 0/29/63/63   | 0/2/2/2 |
| 25  | BCR  | y     | 101 | -    | -       | 0/29/63/63   | 0/2/2/2 |

All (1105) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 34  | V     | 201 | HEM  | C3C-C2C | -14.70 | 1.33        | 1.45     |
| 32  | d     | 411 | LMT  | C8-C7   | -14.56 | 1.49        | 1.55     |
| 29  | A     | 412 | OEX  | O1-MN1  | -14.52 | 1.88        | 2.02     |
| 34  | v     | 201 | HEM  | C3C-C2C | -14.52 | 1.34        | 1.45     |
| 29  | A     | 412 | OEX  | O3-MN1  | -14.45 | 1.88        | 2.02     |
| 32  | D     | 408 | LMT  | C8-C7   | -14.38 | 1.49        | 1.55     |
| 29  | a     | 411 | OEX  | O1-MN1  | -14.31 | 1.88        | 2.02     |
| 29  | a     | 411 | OEX  | O3-MN1  | -14.10 | 1.88        | 2.02     |
| 27  | A     | 410 | LHG  | C12-C11 | -14.03 | 1.49        | 1.55     |
| 26  | c     | 515 | DGD  | C9B-C8B | -13.92 | 1.49        | 1.55     |
| 27  | a     | 409 | LHG  | C12-C11 | -13.84 | 1.49        | 1.55     |
| 26  | a     | 408 | DGD  | CDB-CCB | -13.70 | 1.49        | 1.55     |
| 26  | A     | 409 | DGD  | CDB-CCB | -13.49 | 1.49        | 1.55     |
| 26  | C     | 514 | DGD  | C9B-C8B | -13.32 | 1.49        | 1.55     |
| 34  | F     | 101 | HEM  | C3C-C2C | -13.24 | 1.35        | 1.45     |
| 26  | b     | 601 | DGD  | CDB-CCB | -13.09 | 1.49        | 1.55     |
| 26  | B     | 626 | DGD  | CDB-CCB | -13.01 | 1.50        | 1.55     |
| 34  | f     | 101 | HEM  | C3C-C2C | -12.98 | 1.35        | 1.45     |
| 26  | b     | 625 | DGD  | CDB-CCB | -12.81 | 1.50        | 1.55     |
| 26  | B     | 620 | DGD  | CDB-CCB | -12.69 | 1.50        | 1.55     |
| 34  | F     | 101 | HEM  | C3B-C2B | -12.45 | 1.33        | 1.45     |
| 34  | f     | 101 | HEM  | C3B-C2B | -12.32 | 1.33        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 31  | a     | 402 | LMG  | C22-C21 | -12.27 | 1.50        | 1.55     |
| 31  | B     | 625 | LMG  | C41-C40 | -12.17 | 1.50        | 1.55     |
| 31  | e     | 101 | LMG  | C39-C38 | -12.17 | 1.50        | 1.55     |
| 31  | d     | 408 | LMG  | C41-C40 | -12.16 | 1.50        | 1.55     |
| 31  | d     | 412 | LMG  | C22-C21 | -12.09 | 1.50        | 1.55     |
| 31  | e     | 101 | LMG  | C22-C21 | -12.04 | 1.50        | 1.55     |
| 31  | C     | 517 | LMG  | C40-C39 | -12.01 | 1.50        | 1.55     |
| 31  | C     | 517 | LMG  | C22-C21 | -12.00 | 1.50        | 1.55     |
| 31  | E     | 101 | LMG  | C39-C38 | -11.92 | 1.50        | 1.55     |
| 31  | D     | 409 | LMG  | C41-C40 | -11.81 | 1.50        | 1.55     |
| 31  | E     | 101 | LMG  | C22-C21 | -11.78 | 1.50        | 1.55     |
| 31  | d     | 412 | LMG  | C41-C40 | -11.73 | 1.50        | 1.55     |
| 31  | C     | 521 | LMG  | C23-C22 | -11.69 | 1.50        | 1.55     |
| 31  | D     | 409 | LMG  | C22-C21 | -11.69 | 1.50        | 1.55     |
| 31  | m     | 101 | LMG  | C22-C21 | -11.68 | 1.50        | 1.55     |
| 31  | D     | 406 | LMG  | C40-C39 | -11.61 | 1.50        | 1.55     |
| 31  | b     | 627 | LMG  | C22-C21 | -11.59 | 1.50        | 1.55     |
| 31  | B     | 625 | LMG  | C25-C24 | -11.55 | 1.50        | 1.55     |
| 31  | I     | 101 | LMG  | C23-C22 | -11.53 | 1.50        | 1.55     |
| 31  | d     | 408 | LMG  | C25-C24 | -11.50 | 1.50        | 1.55     |
| 31  | i     | 102 | LMG  | C23-C22 | -11.48 | 1.50        | 1.55     |
| 31  | c     | 518 | LMG  | C40-C39 | -11.47 | 1.50        | 1.55     |
| 31  | c     | 518 | LMG  | C22-C21 | -11.38 | 1.50        | 1.55     |
| 31  | l     | 101 | LMG  | C43-C42 | -11.29 | 1.50        | 1.55     |
| 31  | c     | 522 | LMG  | C23-C22 | -11.29 | 1.50        | 1.55     |
| 31  | d     | 409 | LMG  | C25-C24 | -11.29 | 1.50        | 1.55     |
| 31  | M     | 101 | LMG  | C22-C21 | -11.24 | 1.50        | 1.55     |
| 31  | L     | 101 | LMG  | C43-C42 | -11.23 | 1.50        | 1.55     |
| 29  | A     | 412 | OEX  | O1-MN2  | -11.21 | 1.91        | 2.02     |
| 29  | a     | 411 | OEX  | O1-MN2  | -11.18 | 1.91        | 2.02     |
| 31  | B     | 621 | LMG  | C23-C22 | -11.16 | 1.50        | 1.55     |
| 31  | L     | 101 | LMG  | C25-C24 | -11.13 | 1.50        | 1.55     |
| 31  | l     | 101 | LMG  | C25-C24 | -11.12 | 1.50        | 1.55     |
| 31  | b     | 626 | LMG  | C23-C22 | -11.12 | 1.50        | 1.55     |
| 31  | d     | 409 | LMG  | C40-C39 | -10.87 | 1.50        | 1.55     |
| 34  | V     | 201 | HEM  | C3B-C2B | -10.86 | 1.35        | 1.45     |
| 31  | b     | 626 | LMG  | C43-C42 | -10.86 | 1.50        | 1.55     |
| 31  | D     | 406 | LMG  | C25-C24 | -10.77 | 1.50        | 1.55     |
| 34  | v     | 201 | HEM  | C3B-C2B | -10.73 | 1.35        | 1.45     |
| 29  | a     | 411 | OEX  | O3-MN3  | -10.72 | 1.88        | 2.06     |
| 31  | B     | 621 | LMG  | C43-C42 | -10.65 | 1.50        | 1.55     |
| 29  | A     | 412 | OEX  | O3-MN3  | -10.59 | 1.88        | 2.06     |

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| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 31  | c     | 522 | LMG  | C42-C41 | -10.59 | 1.50        | 1.55     |
| 29  | A     | 412 | OEX  | O2-MN3  | -10.48 | 1.88        | 2.06     |
| 29  | a     | 411 | OEX  | O2-MN3  | -10.28 | 1.88        | 2.06     |
| 31  | C     | 521 | LMG  | C42-C41 | -10.26 | 1.51        | 1.55     |
| 27  | C     | 518 | LHG  | C30-C29 | -9.89  | 1.51        | 1.55     |
| 27  | c     | 519 | LHG  | C30-C29 | -9.71  | 1.51        | 1.55     |
| 27  | C     | 518 | LHG  | C18-C17 | -9.52  | 1.51        | 1.55     |
| 26  | C     | 515 | DGD  | CEA-CDA | -9.44  | 1.51        | 1.55     |
| 31  | m     | 101 | LMG  | C37-C36 | -9.39  | 1.51        | 1.55     |
| 31  | b     | 627 | LMG  | C37-C36 | -9.38  | 1.51        | 1.55     |
| 31  | a     | 402 | LMG  | C37-C36 | -9.31  | 1.51        | 1.55     |
| 26  | B     | 620 | DGD  | CFA-CEA | -9.26  | 1.51        | 1.55     |
| 26  | d     | 410 | DGD  | CFA-CEA | -9.20  | 1.51        | 1.55     |
| 26  | b     | 625 | DGD  | CFA-CEA | -9.15  | 1.51        | 1.55     |
| 26  | C     | 514 | DGD  | CEA-CDA | -9.12  | 1.51        | 1.55     |
| 26  | c     | 516 | DGD  | CEA-CDA | -9.10  | 1.51        | 1.55     |
| 27  | c     | 519 | LHG  | C18-C17 | -9.04  | 1.51        | 1.55     |
| 31  | M     | 101 | LMG  | C37-C36 | -9.00  | 1.51        | 1.55     |
| 26  | c     | 515 | DGD  | CEA-CDA | -8.97  | 1.51        | 1.55     |
| 31  | I     | 101 | LMG  | C37-C36 | -8.84  | 1.51        | 1.55     |
| 30  | a     | 412 | SQD  | C35-C34 | -8.80  | 1.51        | 1.55     |
| 30  | A     | 413 | SQD  | C35-C34 | -8.67  | 1.51        | 1.55     |
| 31  | i     | 102 | LMG  | C37-C36 | -8.50  | 1.51        | 1.55     |
| 26  | D     | 407 | DGD  | CFA-CEA | -8.30  | 1.51        | 1.55     |
| 29  | A     | 412 | OEX  | O3-MN2  | -7.68  | 1.94        | 2.02     |
| 26  | a     | 408 | DGD  | CDA-CCA | -7.64  | 1.52        | 1.55     |
| 22  | A     | 402 | CLA  | C3B-C4B | 7.55   | 1.50        | 1.41     |
| 29  | a     | 411 | OEX  | O3-MN2  | -7.49  | 1.95        | 2.02     |
| 22  | a     | 403 | CLA  | C3B-C4B | 7.49   | 1.50        | 1.41     |
| 22  | c     | 508 | CLA  | C3B-C4B | 7.27   | 1.50        | 1.41     |
| 26  | B     | 626 | DGD  | C9A-C8A | -7.21  | 1.52        | 1.55     |
| 22  | A     | 403 | CLA  | C3B-C4B | 7.17   | 1.49        | 1.41     |
| 22  | B     | 613 | CLA  | C3B-C4B | 7.12   | 1.49        | 1.41     |
| 22  | c     | 509 | CLA  | C3B-C4B | 7.11   | 1.49        | 1.41     |
| 22  | c     | 512 | CLA  | C3B-C4B | 7.11   | 1.49        | 1.41     |
| 22  | b     | 612 | CLA  | C3B-C4B | 7.10   | 1.49        | 1.41     |
| 22  | c     | 511 | CLA  | C3B-C4B | 7.10   | 1.49        | 1.41     |
| 22  | c     | 505 | CLA  | C3B-C4B | 7.06   | 1.49        | 1.41     |
| 26  | A     | 409 | DGD  | CDA-CCA | -7.05  | 1.52        | 1.55     |
| 22  | b     | 605 | CLA  | C3B-C4B | 7.05   | 1.49        | 1.41     |
| 22  | b     | 616 | CLA  | C3B-C4B | 7.05   | 1.49        | 1.41     |
| 22  | a     | 405 | CLA  | C3B-C4B | 7.03   | 1.49        | 1.41     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | C     | 508 | CLA  | C3B-C4B | 7.02  | 1.49        | 1.41     |
| 22  | b     | 613 | CLA  | C3B-C4B | 7.00  | 1.49        | 1.41     |
| 22  | c     | 510 | CLA  | C3B-C4B | 7.00  | 1.49        | 1.41     |
| 22  | B     | 608 | CLA  | C3B-C4B | 7.00  | 1.49        | 1.41     |
| 22  | H     | 101 | CLA  | C3B-C4B | 6.99  | 1.49        | 1.41     |
| 22  | b     | 620 | CLA  | C3B-C4B | 6.99  | 1.49        | 1.41     |
| 22  | C     | 519 | CLA  | C3B-C4B | 6.99  | 1.49        | 1.41     |
| 22  | C     | 511 | CLA  | C3B-C4B | 6.98  | 1.49        | 1.41     |
| 22  | B     | 612 | CLA  | C3B-C4B | 6.97  | 1.49        | 1.41     |
| 26  | b     | 601 | DGD  | C9A-C8A | -6.96 | 1.52        | 1.55     |
| 22  | D     | 404 | CLA  | C3B-C4B | 6.96  | 1.49        | 1.41     |
| 22  | B     | 601 | CLA  | C3B-C4B | 6.96  | 1.49        | 1.41     |
| 22  | d     | 406 | CLA  | C3B-C4B | 6.94  | 1.49        | 1.41     |
| 22  | b     | 606 | CLA  | C3B-C4B | 6.94  | 1.49        | 1.41     |
| 22  | B     | 607 | CLA  | C3B-C4B | 6.94  | 1.49        | 1.41     |
| 22  | b     | 607 | CLA  | C3B-C4B | 6.92  | 1.49        | 1.41     |
| 22  | c     | 520 | CLA  | C3B-C4B | 6.92  | 1.49        | 1.41     |
| 22  | a     | 404 | CLA  | C3B-C4B | 6.91  | 1.49        | 1.41     |
| 22  | B     | 615 | CLA  | C3B-C4B | 6.91  | 1.49        | 1.41     |
| 22  | B     | 614 | CLA  | C3B-C4B | 6.90  | 1.49        | 1.41     |
| 22  | c     | 507 | CLA  | C3B-C4B | 6.90  | 1.49        | 1.41     |
| 22  | C     | 505 | CLA  | C3B-C4B | 6.90  | 1.49        | 1.41     |
| 22  | b     | 619 | CLA  | C3B-C4B | 6.90  | 1.49        | 1.41     |
| 22  | A     | 404 | CLA  | C3B-C4B | 6.87  | 1.49        | 1.41     |
| 22  | C     | 509 | CLA  | C3B-C4B | 6.87  | 1.49        | 1.41     |
| 22  | C     | 507 | CLA  | C3B-C4B | 6.86  | 1.49        | 1.41     |
| 22  | C     | 510 | CLA  | C3B-C4B | 6.85  | 1.49        | 1.41     |
| 22  | B     | 611 | CLA  | C3B-C4B | 6.84  | 1.49        | 1.41     |
| 22  | b     | 610 | CLA  | C3B-C4B | 6.84  | 1.49        | 1.41     |
| 22  | b     | 617 | CLA  | C3B-C4B | 6.81  | 1.49        | 1.41     |
| 22  | b     | 618 | CLA  | C3B-C4B | 6.81  | 1.49        | 1.41     |
| 22  | B     | 604 | CLA  | C3B-C4B | 6.80  | 1.49        | 1.41     |
| 22  | c     | 506 | CLA  | C3B-C4B | 6.79  | 1.49        | 1.41     |
| 22  | D     | 403 | CLA  | C3B-C4B | 6.79  | 1.49        | 1.41     |
| 22  | c     | 501 | CLA  | C3B-C4B | 6.77  | 1.49        | 1.41     |
| 22  | d     | 405 | CLA  | C3B-C4B | 6.75  | 1.49        | 1.41     |
| 22  | b     | 614 | CLA  | C3B-C4B | 6.74  | 1.49        | 1.41     |
| 22  | c     | 502 | CLA  | C3B-C4B | 6.74  | 1.49        | 1.41     |
| 22  | a     | 406 | CLA  | C3B-C4B | 6.73  | 1.49        | 1.41     |
| 22  | B     | 606 | CLA  | C3B-C4B | 6.72  | 1.49        | 1.41     |
| 22  | c     | 503 | CLA  | C3B-C4B | 6.72  | 1.49        | 1.41     |
| 22  | A     | 406 | CLA  | C3B-C4B | 6.72  | 1.49        | 1.41     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | B     | 602 | CLA  | C3B-C4B | 6.71  | 1.49        | 1.41     |
| 22  | b     | 608 | CLA  | C3B-C4B | 6.71  | 1.49        | 1.41     |
| 22  | C     | 502 | CLA  | C3B-C4B | 6.70  | 1.49        | 1.41     |
| 22  | b     | 609 | CLA  | C3B-C4B | 6.68  | 1.49        | 1.41     |
| 22  | C     | 512 | CLA  | C3B-C4B | 6.68  | 1.49        | 1.41     |
| 22  | b     | 611 | CLA  | C3B-C4B | 6.66  | 1.49        | 1.41     |
| 22  | C     | 506 | CLA  | C3B-C4B | 6.66  | 1.49        | 1.41     |
| 22  | B     | 609 | CLA  | C3B-C4B | 6.66  | 1.49        | 1.41     |
| 22  | C     | 503 | CLA  | C3B-C4B | 6.64  | 1.49        | 1.41     |
| 22  | B     | 603 | CLA  | C3B-C4B | 6.61  | 1.49        | 1.41     |
| 22  | C     | 501 | CLA  | C3B-C4B | 6.59  | 1.49        | 1.41     |
| 22  | B     | 605 | CLA  | C3B-C4B | 6.59  | 1.49        | 1.41     |
| 22  | C     | 504 | CLA  | C3B-C4B | 6.40  | 1.48        | 1.41     |
| 22  | c     | 504 | CLA  | C3B-C4B | 6.38  | 1.48        | 1.41     |
| 29  | A     | 412 | OEX  | O5-MN3  | -6.32 | 1.85        | 2.11     |
| 29  | a     | 411 | OEX  | O5-MN3  | -6.27 | 1.85        | 2.11     |
| 22  | b     | 615 | CLA  | C3B-C4B | 5.98  | 1.48        | 1.41     |
| 22  | B     | 610 | CLA  | C3B-C4B | 5.95  | 1.48        | 1.41     |
| 34  | V     | 201 | HEM  | CMB-C2B | 5.88  | 1.55        | 1.45     |
| 34  | f     | 101 | HEM  | CMC-C2C | 5.88  | 1.55        | 1.45     |
| 34  | v     | 201 | HEM  | CMB-C2B | 5.86  | 1.55        | 1.45     |
| 34  | v     | 201 | HEM  | CMD-C2D | 5.85  | 1.55        | 1.45     |
| 34  | V     | 201 | HEM  | CMD-C2D | 5.85  | 1.55        | 1.45     |
| 29  | a     | 411 | OEX  | O2-MN2  | -5.83 | 1.96        | 2.02     |
| 34  | F     | 101 | HEM  | CMC-C2C | 5.83  | 1.55        | 1.45     |
| 34  | v     | 201 | HEM  | CMC-C2C | 5.77  | 1.54        | 1.45     |
| 34  | F     | 101 | HEM  | CMD-C2D | 5.71  | 1.54        | 1.45     |
| 34  | V     | 201 | HEM  | CMC-C2C | 5.69  | 1.54        | 1.45     |
| 34  | f     | 101 | HEM  | CMD-C2D | 5.65  | 1.54        | 1.45     |
| 29  | A     | 412 | OEX  | O2-MN2  | -5.64 | 1.96        | 2.02     |
| 34  | f     | 101 | HEM  | CMB-C2B | 5.64  | 1.54        | 1.45     |
| 34  | F     | 101 | HEM  | CMB-C2B | 5.63  | 1.54        | 1.45     |
| 30  | f     | 103 | SQD  | C19-C18 | -5.56 | 1.52        | 1.55     |
| 30  | F     | 103 | SQD  | C19-C18 | -5.30 | 1.53        | 1.55     |
| 24  | D     | 405 | PL9  | C7-C3   | -5.27 | 1.47        | 1.51     |
| 22  | c     | 509 | CLA  | C4B-NB  | 4.85  | 1.42        | 1.34     |
| 24  | d     | 407 | PL9  | C7-C3   | -4.78 | 1.47        | 1.51     |
| 22  | A     | 402 | CLA  | C4B-NB  | 4.78  | 1.42        | 1.34     |
| 22  | a     | 403 | CLA  | C4B-NB  | 4.77  | 1.42        | 1.34     |
| 22  | B     | 601 | CLA  | C4B-NB  | 4.77  | 1.42        | 1.34     |
| 22  | b     | 605 | CLA  | C4B-NB  | 4.76  | 1.42        | 1.34     |
| 22  | C     | 508 | CLA  | C4B-NB  | 4.75  | 1.42        | 1.34     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | c     | 508 | CLA  | C4B-NB  | 4.75  | 1.42        | 1.34     |
| 24  | j     | 101 | PL9  | C7-C3   | -4.75 | 1.47        | 1.51     |
| 22  | c     | 512 | CLA  | C4B-NB  | 4.74  | 1.42        | 1.34     |
| 22  | B     | 614 | CLA  | C4B-NB  | 4.74  | 1.42        | 1.34     |
| 22  | b     | 620 | CLA  | C4B-NB  | 4.72  | 1.42        | 1.34     |
| 22  | C     | 509 | CLA  | C4B-NB  | 4.72  | 1.42        | 1.34     |
| 22  | B     | 615 | CLA  | C4B-NB  | 4.71  | 1.42        | 1.34     |
| 22  | c     | 511 | CLA  | C4B-NB  | 4.69  | 1.42        | 1.34     |
| 22  | c     | 505 | CLA  | C4B-NB  | 4.69  | 1.42        | 1.34     |
| 22  | c     | 503 | CLA  | C4B-NB  | 4.69  | 1.42        | 1.34     |
| 22  | d     | 406 | CLA  | C4B-NB  | 4.69  | 1.42        | 1.34     |
| 22  | C     | 507 | CLA  | C4B-NB  | 4.69  | 1.42        | 1.34     |
| 34  | f     | 101 | HEM  | C3C-CAC | 4.68  | 1.55        | 1.40     |
| 22  | B     | 610 | CLA  | C4B-NB  | 4.68  | 1.42        | 1.34     |
| 22  | c     | 510 | CLA  | C4B-NB  | 4.68  | 1.42        | 1.34     |
| 34  | V     | 201 | HEM  | C3B-CAB | 4.67  | 1.55        | 1.40     |
| 22  | b     | 615 | CLA  | C4B-NB  | 4.67  | 1.42        | 1.34     |
| 22  | c     | 507 | CLA  | C4B-NB  | 4.67  | 1.42        | 1.34     |
| 22  | B     | 608 | CLA  | C4B-NB  | 4.67  | 1.42        | 1.34     |
| 22  | c     | 520 | CLA  | C4B-NB  | 4.66  | 1.42        | 1.34     |
| 34  | v     | 201 | HEM  | C3B-CAB | 4.65  | 1.55        | 1.40     |
| 22  | b     | 616 | CLA  | C4B-NB  | 4.65  | 1.42        | 1.34     |
| 22  | C     | 511 | CLA  | C4B-NB  | 4.64  | 1.42        | 1.34     |
| 22  | H     | 101 | CLA  | C4B-NB  | 4.64  | 1.42        | 1.34     |
| 22  | A     | 403 | CLA  | C4B-NB  | 4.63  | 1.42        | 1.34     |
| 22  | c     | 501 | CLA  | C4B-NB  | 4.63  | 1.42        | 1.34     |
| 34  | F     | 101 | HEM  | C3C-CAC | 4.63  | 1.55        | 1.40     |
| 22  | B     | 604 | CLA  | C4B-NB  | 4.63  | 1.42        | 1.34     |
| 22  | a     | 405 | CLA  | C4B-NB  | 4.63  | 1.42        | 1.34     |
| 22  | A     | 406 | CLA  | C4B-NB  | 4.63  | 1.42        | 1.34     |
| 22  | b     | 611 | CLA  | C4B-NB  | 4.62  | 1.42        | 1.34     |
| 22  | b     | 619 | CLA  | C4B-NB  | 4.62  | 1.42        | 1.34     |
| 34  | V     | 201 | HEM  | C3C-CAC | 4.61  | 1.55        | 1.40     |
| 34  | v     | 201 | HEM  | C3C-CAC | 4.61  | 1.55        | 1.40     |
| 22  | C     | 505 | CLA  | C4B-NB  | 4.61  | 1.41        | 1.34     |
| 22  | b     | 613 | CLA  | C4B-NB  | 4.61  | 1.41        | 1.34     |
| 22  | D     | 404 | CLA  | C4B-NB  | 4.60  | 1.41        | 1.34     |
| 22  | d     | 405 | CLA  | C4B-NB  | 4.59  | 1.41        | 1.34     |
| 22  | B     | 611 | CLA  | C4B-NB  | 4.59  | 1.41        | 1.34     |
| 22  | C     | 512 | CLA  | C4B-NB  | 4.58  | 1.41        | 1.34     |
| 22  | b     | 610 | CLA  | C4B-NB  | 4.58  | 1.41        | 1.34     |
| 22  | b     | 612 | CLA  | C4B-NB  | 4.57  | 1.41        | 1.34     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22  | C     | 503 | CLA  | C4B-NB  | 4.57 | 1.41        | 1.34     |
| 22  | C     | 510 | CLA  | C4B-NB  | 4.57 | 1.41        | 1.34     |
| 22  | C     | 501 | CLA  | C4B-NB  | 4.56 | 1.41        | 1.34     |
| 22  | b     | 617 | CLA  | C4B-NB  | 4.56 | 1.41        | 1.34     |
| 22  | B     | 603 | CLA  | C4B-NB  | 4.55 | 1.41        | 1.34     |
| 22  | c     | 504 | CLA  | C4B-NB  | 4.55 | 1.41        | 1.34     |
| 22  | b     | 614 | CLA  | C4B-NB  | 4.54 | 1.41        | 1.34     |
| 22  | b     | 609 | CLA  | C4B-NB  | 4.54 | 1.41        | 1.34     |
| 22  | D     | 403 | CLA  | C4B-NB  | 4.53 | 1.41        | 1.34     |
| 22  | c     | 502 | CLA  | C4B-NB  | 4.52 | 1.41        | 1.34     |
| 34  | f     | 101 | HEM  | C3B-CAB | 4.52 | 1.55        | 1.40     |
| 22  | C     | 502 | CLA  | C4B-NB  | 4.51 | 1.41        | 1.34     |
| 22  | a     | 406 | CLA  | C4B-NB  | 4.51 | 1.41        | 1.34     |
| 22  | a     | 404 | CLA  | C4B-NB  | 4.51 | 1.41        | 1.34     |
| 22  | b     | 608 | CLA  | C4B-NB  | 4.50 | 1.41        | 1.34     |
| 22  | B     | 606 | CLA  | C4B-NB  | 4.50 | 1.41        | 1.34     |
| 22  | c     | 506 | CLA  | C4B-NB  | 4.50 | 1.41        | 1.34     |
| 22  | A     | 404 | CLA  | C4B-NB  | 4.48 | 1.41        | 1.34     |
| 22  | B     | 609 | CLA  | C4B-NB  | 4.48 | 1.41        | 1.34     |
| 22  | C     | 506 | CLA  | C4B-NB  | 4.48 | 1.41        | 1.34     |
| 22  | B     | 605 | CLA  | C4B-NB  | 4.48 | 1.41        | 1.34     |
| 22  | b     | 618 | CLA  | C4B-NB  | 4.48 | 1.41        | 1.34     |
| 22  | C     | 519 | CLA  | C4B-NB  | 4.47 | 1.41        | 1.34     |
| 34  | F     | 101 | HEM  | C3B-CAB | 4.47 | 1.55        | 1.40     |
| 22  | B     | 607 | CLA  | C4B-NB  | 4.47 | 1.41        | 1.34     |
| 22  | B     | 612 | CLA  | C4B-NB  | 4.44 | 1.41        | 1.34     |
| 22  | C     | 504 | CLA  | C4B-NB  | 4.44 | 1.41        | 1.34     |
| 22  | c     | 503 | CLA  | CHB-C4A | 4.43 | 1.39        | 1.33     |
| 22  | d     | 405 | CLA  | CHB-C4A | 4.42 | 1.39        | 1.33     |
| 22  | b     | 606 | CLA  | C4B-NB  | 4.42 | 1.41        | 1.34     |
| 22  | B     | 602 | CLA  | C4B-NB  | 4.41 | 1.41        | 1.34     |
| 22  | B     | 613 | CLA  | C4B-NB  | 4.40 | 1.41        | 1.34     |
| 22  | b     | 607 | CLA  | C4B-NB  | 4.40 | 1.41        | 1.34     |
| 22  | c     | 504 | CLA  | CHB-C4A | 4.34 | 1.39        | 1.33     |
| 22  | B     | 603 | CLA  | CHB-C4A | 4.33 | 1.39        | 1.33     |
| 22  | b     | 608 | CLA  | CHB-C4A | 4.23 | 1.39        | 1.33     |
| 22  | C     | 512 | CLA  | CHB-C4A | 4.22 | 1.39        | 1.33     |
| 22  | C     | 501 | CLA  | CHB-C4A | 4.21 | 1.39        | 1.33     |
| 22  | b     | 610 | CLA  | CHB-C4A | 4.21 | 1.39        | 1.33     |
| 22  | c     | 510 | CLA  | CHB-C4A | 4.19 | 1.39        | 1.33     |
| 22  | B     | 614 | CLA  | CHB-C4A | 4.19 | 1.39        | 1.33     |
| 22  | C     | 503 | CLA  | CHB-C4A | 4.19 | 1.39        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | b     | 616 | CLA  | CHB-C4A | 4.18  | 1.39        | 1.33     |
| 22  | C     | 504 | CLA  | CHB-C4A | 4.18  | 1.39        | 1.33     |
| 22  | c     | 501 | CLA  | CHB-C4A | 4.18  | 1.39        | 1.33     |
| 22  | C     | 507 | CLA  | CHB-C4A | 4.17  | 1.39        | 1.33     |
| 22  | C     | 502 | CLA  | CHB-C4A | 4.16  | 1.39        | 1.33     |
| 22  | b     | 620 | CLA  | CHB-C4A | 4.16  | 1.39        | 1.33     |
| 22  | c     | 502 | CLA  | CHB-C4A | 4.15  | 1.39        | 1.33     |
| 34  | v     | 201 | HEM  | C3D-C2D | 4.15  | 1.54        | 1.43     |
| 22  | B     | 611 | CLA  | CHB-C4A | 4.14  | 1.39        | 1.33     |
| 24  | a     | 407 | PL9  | C7-C3   | -4.14 | 1.48        | 1.51     |
| 22  | c     | 512 | CLA  | CHB-C4A | 4.13  | 1.39        | 1.33     |
| 34  | V     | 201 | HEM  | C3D-C2D | 4.13  | 1.54        | 1.43     |
| 22  | b     | 619 | CLA  | CHB-C4A | 4.13  | 1.39        | 1.33     |
| 22  | c     | 503 | CLA  | C1A-NA  | 4.13  | 1.41        | 1.32     |
| 22  | B     | 603 | CLA  | C1A-NA  | 4.11  | 1.41        | 1.32     |
| 22  | B     | 610 | CLA  | C1A-NA  | 4.11  | 1.41        | 1.32     |
| 22  | c     | 510 | CLA  | C1A-NA  | 4.10  | 1.41        | 1.32     |
| 22  | b     | 605 | CLA  | CHB-C4A | 4.10  | 1.38        | 1.33     |
| 22  | H     | 101 | CLA  | CHB-C4A | 4.10  | 1.38        | 1.33     |
| 22  | b     | 618 | CLA  | CHB-C4A | 4.10  | 1.38        | 1.33     |
| 22  | c     | 511 | CLA  | CHB-C4A | 4.09  | 1.38        | 1.33     |
| 22  | b     | 617 | CLA  | CHB-C4A | 4.09  | 1.38        | 1.33     |
| 24  | J     | 101 | PL9  | C7-C3   | -4.09 | 1.48        | 1.51     |
| 22  | B     | 608 | CLA  | CHB-C4A | 4.08  | 1.38        | 1.33     |
| 22  | C     | 511 | CLA  | CHB-C4A | 4.08  | 1.38        | 1.33     |
| 22  | b     | 615 | CLA  | C1A-NA  | 4.08  | 1.41        | 1.32     |
| 22  | b     | 620 | CLA  | C1B-C2B | 4.08  | 1.50        | 1.43     |
| 22  | D     | 403 | CLA  | CHB-C4A | 4.07  | 1.38        | 1.33     |
| 22  | A     | 402 | CLA  | CHB-C4A | 4.07  | 1.38        | 1.33     |
| 22  | d     | 405 | CLA  | C1B-C2B | 4.05  | 1.50        | 1.43     |
| 22  | C     | 510 | CLA  | C1A-NA  | 4.04  | 1.41        | 1.32     |
| 22  | c     | 501 | CLA  | C1B-C2B | 4.04  | 1.50        | 1.43     |
| 22  | B     | 615 | CLA  | CHB-C4A | 4.04  | 1.38        | 1.33     |
| 22  | B     | 608 | CLA  | C1A-NA  | 4.03  | 1.41        | 1.32     |
| 22  | c     | 504 | CLA  | C1A-NA  | 4.03  | 1.41        | 1.32     |
| 22  | c     | 520 | CLA  | CHB-C4A | 4.03  | 1.38        | 1.33     |
| 22  | a     | 403 | CLA  | CHB-C4A | 4.02  | 1.38        | 1.33     |
| 22  | b     | 608 | CLA  | C1A-NA  | 4.02  | 1.41        | 1.32     |
| 22  | B     | 613 | CLA  | CHB-C4A | 4.02  | 1.38        | 1.33     |
| 22  | B     | 604 | CLA  | CHB-C4A | 4.02  | 1.38        | 1.33     |
| 22  | c     | 511 | CLA  | C1A-NA  | 4.01  | 1.41        | 1.32     |
| 22  | c     | 502 | CLA  | C1A-NA  | 4.01  | 1.41        | 1.32     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22  | C     | 511 | CLA  | C1A-NA  | 4.01 | 1.41        | 1.32     |
| 22  | b     | 619 | CLA  | C1A-NA  | 4.01 | 1.41        | 1.32     |
| 22  | B     | 601 | CLA  | CHB-C4A | 4.00 | 1.38        | 1.33     |
| 22  | C     | 502 | CLA  | C1A-NA  | 4.00 | 1.41        | 1.32     |
| 22  | C     | 506 | CLA  | C1A-NA  | 4.00 | 1.41        | 1.32     |
| 22  | d     | 405 | CLA  | C1A-NA  | 4.00 | 1.41        | 1.32     |
| 22  | C     | 501 | CLA  | C1B-C2B | 4.00 | 1.50        | 1.43     |
| 22  | C     | 512 | CLA  | C1A-NA  | 3.99 | 1.41        | 1.32     |
| 22  | b     | 605 | CLA  | C1A-NA  | 3.98 | 1.41        | 1.32     |
| 22  | C     | 510 | CLA  | CHB-C4A | 3.98 | 1.38        | 1.33     |
| 22  | C     | 503 | CLA  | C1A-NA  | 3.98 | 1.41        | 1.32     |
| 22  | H     | 101 | CLA  | C1A-NA  | 3.98 | 1.41        | 1.32     |
| 22  | C     | 501 | CLA  | C1A-NA  | 3.98 | 1.41        | 1.32     |
| 22  | C     | 509 | CLA  | CHB-C4A | 3.98 | 1.38        | 1.33     |
| 22  | a     | 405 | CLA  | CHB-C4A | 3.98 | 1.38        | 1.33     |
| 22  | B     | 605 | CLA  | CHB-C4A | 3.98 | 1.38        | 1.33     |
| 22  | b     | 618 | CLA  | C1A-NA  | 3.97 | 1.41        | 1.32     |
| 22  | b     | 609 | CLA  | C1A-NA  | 3.97 | 1.41        | 1.32     |
| 22  | C     | 507 | CLA  | C1A-NA  | 3.96 | 1.41        | 1.32     |
| 22  | d     | 406 | CLA  | CHB-C4A | 3.96 | 1.38        | 1.33     |
| 22  | b     | 611 | CLA  | CHB-C4A | 3.96 | 1.38        | 1.33     |
| 22  | C     | 506 | CLA  | CHB-C4A | 3.96 | 1.38        | 1.33     |
| 22  | B     | 615 | CLA  | C1B-C2B | 3.96 | 1.49        | 1.43     |
| 22  | c     | 512 | CLA  | C1A-NA  | 3.96 | 1.41        | 1.32     |
| 22  | b     | 613 | CLA  | C1A-NA  | 3.96 | 1.41        | 1.32     |
| 22  | c     | 507 | CLA  | CHB-C4A | 3.96 | 1.38        | 1.33     |
| 22  | A     | 406 | CLA  | CHB-C4A | 3.95 | 1.38        | 1.33     |
| 22  | c     | 506 | CLA  | C1A-NA  | 3.95 | 1.41        | 1.32     |
| 22  | B     | 614 | CLA  | C1B-C2B | 3.95 | 1.49        | 1.43     |
| 22  | c     | 504 | CLA  | C1B-C2B | 3.95 | 1.49        | 1.43     |
| 22  | b     | 610 | CLA  | C1B-C2B | 3.95 | 1.49        | 1.43     |
| 34  | F     | 101 | HEM  | C3D-C2D | 3.95 | 1.53        | 1.43     |
| 22  | b     | 616 | CLA  | C1B-C2B | 3.95 | 1.49        | 1.43     |
| 22  | b     | 610 | CLA  | C1A-NA  | 3.94 | 1.40        | 1.32     |
| 22  | c     | 511 | CLA  | C1B-C2B | 3.94 | 1.49        | 1.43     |
| 22  | B     | 601 | CLA  | C1A-NA  | 3.94 | 1.40        | 1.32     |
| 22  | b     | 609 | CLA  | CHB-C4A | 3.93 | 1.38        | 1.33     |
| 22  | c     | 508 | CLA  | C1A-NA  | 3.93 | 1.40        | 1.32     |
| 22  | c     | 501 | CLA  | C1A-NA  | 3.93 | 1.40        | 1.32     |
| 22  | c     | 520 | CLA  | C1A-NA  | 3.93 | 1.40        | 1.32     |
| 22  | a     | 406 | CLA  | CHB-C4A | 3.93 | 1.38        | 1.33     |
| 22  | a     | 406 | CLA  | C1A-NA  | 3.93 | 1.40        | 1.32     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22  | D     | 403 | CLA  | C1A-NA  | 3.93 | 1.40        | 1.32     |
| 22  | c     | 503 | CLA  | C1B-C2B | 3.92 | 1.49        | 1.43     |
| 22  | A     | 403 | CLA  | C1A-NA  | 3.92 | 1.40        | 1.32     |
| 22  | B     | 603 | CLA  | C1B-C2B | 3.92 | 1.49        | 1.43     |
| 22  | A     | 403 | CLA  | CHB-C4A | 3.91 | 1.38        | 1.33     |
| 22  | C     | 504 | CLA  | C1A-NA  | 3.91 | 1.40        | 1.32     |
| 22  | B     | 602 | CLA  | C1A-NA  | 3.91 | 1.40        | 1.32     |
| 22  | c     | 510 | CLA  | C1B-C2B | 3.91 | 1.49        | 1.43     |
| 22  | B     | 614 | CLA  | C1A-NA  | 3.91 | 1.40        | 1.32     |
| 34  | F     | 101 | HEM  | FE-ND   | 3.91 | 2.11        | 1.95     |
| 22  | C     | 504 | CLA  | C1B-C2B | 3.90 | 1.49        | 1.43     |
| 22  | c     | 505 | CLA  | C1A-NA  | 3.90 | 1.40        | 1.32     |
| 22  | c     | 509 | CLA  | CHB-C4A | 3.90 | 1.38        | 1.33     |
| 22  | b     | 608 | CLA  | C1B-C2B | 3.90 | 1.49        | 1.43     |
| 22  | b     | 613 | CLA  | CHB-C4A | 3.90 | 1.38        | 1.33     |
| 22  | b     | 614 | CLA  | C1A-NA  | 3.90 | 1.40        | 1.32     |
| 22  | A     | 404 | CLA  | CHB-C4A | 3.89 | 1.38        | 1.33     |
| 22  | b     | 617 | CLA  | C1A-NA  | 3.89 | 1.40        | 1.32     |
| 22  | b     | 612 | CLA  | CHB-C4A | 3.89 | 1.38        | 1.33     |
| 22  | H     | 101 | CLA  | C1B-C2B | 3.89 | 1.49        | 1.43     |
| 22  | c     | 507 | CLA  | C1A-NA  | 3.89 | 1.40        | 1.32     |
| 22  | D     | 403 | CLA  | C1B-C2B | 3.88 | 1.49        | 1.43     |
| 22  | B     | 602 | CLA  | CHB-C4A | 3.88 | 1.38        | 1.33     |
| 22  | b     | 620 | CLA  | C1A-NA  | 3.88 | 1.40        | 1.32     |
| 22  | C     | 511 | CLA  | C1B-C2B | 3.87 | 1.49        | 1.43     |
| 22  | B     | 611 | CLA  | C1B-C2B | 3.87 | 1.49        | 1.43     |
| 22  | B     | 606 | CLA  | CHB-C4A | 3.86 | 1.38        | 1.33     |
| 22  | A     | 404 | CLA  | C1A-NA  | 3.86 | 1.40        | 1.32     |
| 22  | d     | 406 | CLA  | C1A-NA  | 3.86 | 1.40        | 1.32     |
| 22  | b     | 615 | CLA  | CHB-C4A | 3.86 | 1.38        | 1.33     |
| 22  | b     | 607 | CLA  | CHB-C4A | 3.85 | 1.38        | 1.33     |
| 22  | B     | 609 | CLA  | C1A-NA  | 3.85 | 1.40        | 1.32     |
| 22  | a     | 405 | CLA  | C1A-NA  | 3.85 | 1.40        | 1.32     |
| 22  | b     | 616 | CLA  | C1A-NA  | 3.85 | 1.40        | 1.32     |
| 22  | B     | 612 | CLA  | CHB-C4A | 3.85 | 1.38        | 1.33     |
| 22  | b     | 617 | CLA  | C1B-C2B | 3.84 | 1.49        | 1.43     |
| 34  | v     | 201 | HEM  | FE-NB   | 3.84 | 2.09        | 1.95     |
| 34  | f     | 101 | HEM  | C3D-C2D | 3.84 | 1.53        | 1.43     |
| 22  | b     | 619 | CLA  | C1B-C2B | 3.84 | 1.49        | 1.43     |
| 34  | v     | 201 | HEM  | FE-ND   | 3.84 | 2.11        | 1.95     |
| 22  | B     | 612 | CLA  | C1A-NA  | 3.84 | 1.40        | 1.32     |
| 22  | c     | 509 | CLA  | C1A-NA  | 3.84 | 1.40        | 1.32     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22  | B     | 604 | CLA  | C1A-NA  | 3.84 | 1.40        | 1.32     |
| 22  | b     | 607 | CLA  | C1A-NA  | 3.83 | 1.40        | 1.32     |
| 22  | B     | 611 | CLA  | C1A-NA  | 3.83 | 1.40        | 1.32     |
| 22  | B     | 610 | CLA  | CHB-C4A | 3.83 | 1.38        | 1.33     |
| 22  | B     | 613 | CLA  | C1A-NA  | 3.83 | 1.40        | 1.32     |
| 22  | a     | 405 | CLA  | C1B-C2B | 3.83 | 1.49        | 1.43     |
| 22  | C     | 509 | CLA  | C1A-NA  | 3.83 | 1.40        | 1.32     |
| 22  | A     | 406 | CLA  | C1A-NA  | 3.82 | 1.40        | 1.32     |
| 22  | b     | 614 | CLA  | CHB-C4A | 3.82 | 1.38        | 1.33     |
| 22  | C     | 519 | CLA  | C1A-NA  | 3.82 | 1.40        | 1.32     |
| 22  | B     | 615 | CLA  | C1A-NA  | 3.82 | 1.40        | 1.32     |
| 22  | B     | 605 | CLA  | C1A-NA  | 3.82 | 1.40        | 1.32     |
| 22  | C     | 510 | CLA  | C1B-C2B | 3.81 | 1.49        | 1.43     |
| 22  | c     | 512 | CLA  | C1B-C2B | 3.81 | 1.49        | 1.43     |
| 22  | c     | 506 | CLA  | CHB-C4A | 3.80 | 1.38        | 1.33     |
| 22  | B     | 607 | CLA  | CHB-C4A | 3.80 | 1.38        | 1.33     |
| 22  | C     | 503 | CLA  | C1B-C2B | 3.80 | 1.49        | 1.43     |
| 22  | a     | 403 | CLA  | C1A-NA  | 3.80 | 1.40        | 1.32     |
| 22  | C     | 508 | CLA  | C1A-NA  | 3.80 | 1.40        | 1.32     |
| 22  | B     | 604 | CLA  | C1B-C2B | 3.80 | 1.49        | 1.43     |
| 22  | C     | 505 | CLA  | C1A-NA  | 3.80 | 1.40        | 1.32     |
| 22  | D     | 404 | CLA  | CHB-C4A | 3.79 | 1.38        | 1.33     |
| 22  | C     | 508 | CLA  | CHB-C4A | 3.79 | 1.38        | 1.33     |
| 22  | B     | 606 | CLA  | C1A-NA  | 3.79 | 1.40        | 1.32     |
| 22  | a     | 404 | CLA  | CHB-C4A | 3.79 | 1.38        | 1.33     |
| 22  | A     | 402 | CLA  | C1A-NA  | 3.79 | 1.40        | 1.32     |
| 22  | B     | 607 | CLA  | C1A-NA  | 3.79 | 1.40        | 1.32     |
| 22  | D     | 404 | CLA  | C1A-NA  | 3.79 | 1.40        | 1.32     |
| 22  | b     | 612 | CLA  | C1A-NA  | 3.78 | 1.40        | 1.32     |
| 22  | d     | 406 | CLA  | C1B-C2B | 3.78 | 1.49        | 1.43     |
| 22  | c     | 502 | CLA  | C1B-C2B | 3.78 | 1.49        | 1.43     |
| 22  | c     | 505 | CLA  | CHB-C4A | 3.77 | 1.38        | 1.33     |
| 22  | B     | 609 | CLA  | CHB-C4A | 3.77 | 1.38        | 1.33     |
| 22  | b     | 605 | CLA  | C1B-C2B | 3.76 | 1.49        | 1.43     |
| 22  | C     | 519 | CLA  | CHB-C4A | 3.76 | 1.38        | 1.33     |
| 34  | V     | 201 | HEM  | FE-ND   | 3.76 | 2.10        | 1.95     |
| 22  | C     | 512 | CLA  | C1B-C2B | 3.76 | 1.49        | 1.43     |
| 22  | c     | 520 | CLA  | C1B-C2B | 3.76 | 1.49        | 1.43     |
| 22  | b     | 611 | CLA  | C1A-NA  | 3.76 | 1.40        | 1.32     |
| 22  | c     | 508 | CLA  | CHB-C4A | 3.76 | 1.38        | 1.33     |
| 22  | a     | 404 | CLA  | C1A-NA  | 3.76 | 1.40        | 1.32     |
| 22  | b     | 606 | CLA  | C1A-NA  | 3.75 | 1.40        | 1.32     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | B     | 613 | CLA  | C1B-C2B | 3.74  | 1.49        | 1.43     |
| 22  | C     | 502 | CLA  | C1B-C2B | 3.74  | 1.49        | 1.43     |
| 22  | B     | 601 | CLA  | C1B-C2B | 3.74  | 1.49        | 1.43     |
| 24  | A     | 407 | PL9  | C7-C3   | -3.74 | 1.48        | 1.51     |
| 22  | C     | 505 | CLA  | CHB-C4A | 3.74  | 1.38        | 1.33     |
| 22  | A     | 404 | CLA  | C1B-C2B | 3.74  | 1.49        | 1.43     |
| 22  | B     | 608 | CLA  | C1B-C2B | 3.73  | 1.49        | 1.43     |
| 22  | C     | 506 | CLA  | C1B-C2B | 3.73  | 1.49        | 1.43     |
| 22  | b     | 606 | CLA  | CHB-C4A | 3.72  | 1.38        | 1.33     |
| 22  | b     | 618 | CLA  | C1B-C2B | 3.72  | 1.49        | 1.43     |
| 22  | b     | 607 | CLA  | C1B-C2B | 3.72  | 1.49        | 1.43     |
| 22  | c     | 509 | CLA  | C1B-C2B | 3.72  | 1.49        | 1.43     |
| 22  | C     | 507 | CLA  | C1B-C2B | 3.71  | 1.49        | 1.43     |
| 34  | f     | 101 | HEM  | FE-ND   | 3.71  | 2.10        | 1.95     |
| 22  | A     | 406 | CLA  | C1B-C2B | 3.71  | 1.49        | 1.43     |
| 22  | b     | 611 | CLA  | C1B-C2B | 3.70  | 1.49        | 1.43     |
| 22  | B     | 605 | CLA  | C1B-C2B | 3.70  | 1.49        | 1.43     |
| 22  | C     | 509 | CLA  | C1B-C2B | 3.70  | 1.49        | 1.43     |
| 22  | B     | 612 | CLA  | C1B-C2B | 3.69  | 1.49        | 1.43     |
| 22  | D     | 404 | CLA  | C1B-C2B | 3.69  | 1.49        | 1.43     |
| 30  | F     | 103 | SQD  | C32-C31 | -3.68 | 1.53        | 1.55     |
| 22  | C     | 505 | CLA  | C1B-C2B | 3.68  | 1.49        | 1.43     |
| 22  | b     | 609 | CLA  | C1B-C2B | 3.67  | 1.49        | 1.43     |
| 22  | c     | 505 | CLA  | C1B-C2B | 3.67  | 1.49        | 1.43     |
| 22  | B     | 602 | CLA  | C1B-C2B | 3.66  | 1.49        | 1.43     |
| 22  | b     | 613 | CLA  | C1B-C2B | 3.66  | 1.49        | 1.43     |
| 22  | A     | 402 | CLA  | C1B-C2B | 3.65  | 1.49        | 1.43     |
| 22  | B     | 606 | CLA  | C1B-C2B | 3.64  | 1.49        | 1.43     |
| 22  | b     | 615 | CLA  | CMB-C2B | -3.63 | 1.44        | 1.51     |
| 22  | B     | 610 | CLA  | CMB-C2B | -3.63 | 1.44        | 1.51     |
| 22  | a     | 406 | CLA  | C1B-C2B | 3.62  | 1.49        | 1.43     |
| 22  | C     | 508 | CLA  | C1B-C2B | 3.62  | 1.49        | 1.43     |
| 22  | A     | 403 | CLA  | C1B-C2B | 3.62  | 1.49        | 1.43     |
| 22  | c     | 506 | CLA  | C1B-C2B | 3.62  | 1.49        | 1.43     |
| 22  | b     | 606 | CLA  | C1B-C2B | 3.61  | 1.49        | 1.43     |
| 30  | f     | 103 | SQD  | C32-C31 | -3.59 | 1.53        | 1.55     |
| 22  | a     | 404 | CLA  | C1B-C2B | 3.59  | 1.49        | 1.43     |
| 22  | b     | 612 | CLA  | C1B-C2B | 3.58  | 1.49        | 1.43     |
| 22  | b     | 614 | CLA  | C1B-C2B | 3.58  | 1.49        | 1.43     |
| 22  | C     | 519 | CLA  | C1B-C2B | 3.57  | 1.49        | 1.43     |
| 22  | a     | 403 | CLA  | C1B-C2B | 3.55  | 1.49        | 1.43     |
| 22  | c     | 508 | CLA  | C1B-C2B | 3.54  | 1.49        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | c     | 507 | CLA  | C1B-C2B | 3.52  | 1.49        | 1.43     |
| 30  | B     | 622 | SQD  | C18-C17 | -3.52 | 1.53        | 1.55     |
| 25  | F     | 102 | BCR  | C1-C6   | -3.47 | 1.48        | 1.53     |
| 25  | H     | 102 | BCR  | C1-C6   | -3.46 | 1.48        | 1.53     |
| 34  | f     | 101 | HEM  | FE-NB   | 3.46  | 2.07        | 1.95     |
| 22  | B     | 609 | CLA  | C1B-C2B | 3.45  | 1.49        | 1.43     |
| 34  | V     | 201 | HEM  | FE-NB   | 3.45  | 2.07        | 1.95     |
| 22  | B     | 607 | CLA  | C1B-C2B | 3.45  | 1.49        | 1.43     |
| 25  | x     | 101 | BCR  | C1-C6   | -3.42 | 1.48        | 1.53     |
| 25  | f     | 102 | BCR  | C1-C6   | -3.40 | 1.48        | 1.53     |
| 23  | d     | 402 | PHO  | C1D-ND  | 3.40  | 1.41        | 1.36     |
| 30  | d     | 403 | SQD  | C18-C17 | -3.39 | 1.53        | 1.55     |
| 23  | A     | 405 | PHO  | C1D-ND  | 3.32  | 1.41        | 1.36     |
| 23  | D     | 401 | PHO  | C4B-C3B | 3.32  | 1.50        | 1.42     |
| 23  | d     | 402 | PHO  | C4B-C3B | 3.30  | 1.50        | 1.42     |
| 25  | g     | 101 | BCR  | C30-C25 | -3.30 | 1.49        | 1.53     |
| 25  | B     | 616 | BCR  | C1-C6   | -3.30 | 1.49        | 1.53     |
| 23  | D     | 401 | PHO  | C1D-ND  | 3.29  | 1.41        | 1.36     |
| 30  | b     | 602 | SQD  | C31-C30 | -3.26 | 1.53        | 1.55     |
| 30  | B     | 622 | SQD  | C31-C30 | -3.26 | 1.53        | 1.55     |
| 25  | y     | 101 | BCR  | C1-C6   | -3.25 | 1.49        | 1.53     |
| 25  | b     | 621 | BCR  | C1-C6   | -3.25 | 1.49        | 1.53     |
| 23  | d     | 401 | PHO  | C1D-ND  | 3.23  | 1.41        | 1.36     |
| 25  | C     | 513 | BCR  | C1-C6   | -3.20 | 1.49        | 1.53     |
| 25  | c     | 514 | BCR  | C1-C6   | -3.19 | 1.49        | 1.53     |
| 25  | b     | 623 | BCR  | C30-C25 | -3.18 | 1.49        | 1.53     |
| 25  | y     | 101 | BCR  | C30-C25 | -3.17 | 1.49        | 1.53     |
| 25  | J     | 102 | BCR  | C30-C25 | -3.17 | 1.49        | 1.53     |
| 25  | g     | 101 | BCR  | C1-C6   | -3.17 | 1.49        | 1.53     |
| 30  | b     | 602 | SQD  | O48-C23 | 3.16  | 1.43        | 1.33     |
| 25  | b     | 622 | BCR  | C1-C6   | -3.15 | 1.49        | 1.53     |
| 25  | B     | 618 | BCR  | C30-C25 | -3.13 | 1.49        | 1.53     |
| 25  | j     | 102 | BCR  | C30-C25 | -3.12 | 1.49        | 1.53     |
| 23  | A     | 405 | PHO  | C4B-C3B | 3.12  | 1.49        | 1.42     |
| 25  | c     | 513 | BCR  | C1-C6   | -3.11 | 1.49        | 1.53     |
| 25  | b     | 624 | BCR  | C30-C25 | -3.11 | 1.49        | 1.53     |
| 23  | d     | 401 | PHO  | C4B-C3B | 3.11  | 1.49        | 1.42     |
| 25  | K     | 101 | BCR  | C1-C6   | -3.10 | 1.49        | 1.53     |
| 25  | C     | 520 | BCR  | C30-C25 | -3.10 | 1.49        | 1.53     |
| 30  | B     | 622 | SQD  | O48-C23 | 3.08  | 1.42        | 1.33     |
| 30  | B     | 627 | SQD  | O48-C23 | 3.07  | 1.42        | 1.33     |
| 30  | d     | 403 | SQD  | C31-C30 | -3.07 | 1.53        | 1.55     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25  | F     | 102 | BCR  | C30-C25 | -3.06 | 1.49        | 1.53     |
| 25  | B     | 619 | BCR  | C30-C25 | -3.06 | 1.49        | 1.53     |
| 30  | B     | 627 | SQD  | C31-C30 | -3.06 | 1.53        | 1.55     |
| 30  | a     | 401 | SQD  | O48-C23 | 3.04  | 1.42        | 1.33     |
| 25  | B     | 616 | BCR  | C30-C25 | -3.03 | 1.49        | 1.53     |
| 34  | F     | 101 | HEM  | FE-NB   | 3.02  | 2.06        | 1.95     |
| 30  | F     | 103 | SQD  | O48-C23 | 3.02  | 1.42        | 1.33     |
| 25  | i     | 101 | BCR  | C1-C6   | -3.01 | 1.49        | 1.53     |
| 30  | A     | 414 | SQD  | O48-C23 | 3.01  | 1.42        | 1.33     |
| 25  | b     | 624 | BCR  | C1-C6   | -3.00 | 1.49        | 1.53     |
| 25  | A     | 408 | BCR  | C30-C25 | -3.00 | 1.49        | 1.53     |
| 30  | a     | 412 | SQD  | O48-C23 | 3.00  | 1.42        | 1.33     |
| 30  | f     | 103 | SQD  | O48-C23 | 3.00  | 1.42        | 1.33     |
| 25  | c     | 521 | BCR  | C30-C25 | -2.99 | 1.49        | 1.53     |
| 25  | B     | 617 | BCR  | C1-C6   | -2.97 | 1.49        | 1.53     |
| 25  | i     | 101 | BCR  | C30-C25 | -2.97 | 1.49        | 1.53     |
| 25  | f     | 102 | BCR  | C30-C25 | -2.97 | 1.49        | 1.53     |
| 30  | d     | 403 | SQD  | O48-C23 | 2.96  | 1.42        | 1.33     |
| 25  | B     | 619 | BCR  | C1-C6   | -2.96 | 1.49        | 1.53     |
| 25  | B     | 618 | BCR  | C1-C6   | -2.95 | 1.49        | 1.53     |
| 25  | b     | 621 | BCR  | C30-C25 | -2.94 | 1.49        | 1.53     |
| 25  | A     | 408 | BCR  | C1-C6   | -2.94 | 1.49        | 1.53     |
| 25  | b     | 623 | BCR  | C1-C6   | -2.94 | 1.49        | 1.53     |
| 23  | D     | 401 | PHO  | C1B-C2B | 2.93  | 1.50        | 1.42     |
| 30  | A     | 413 | SQD  | O48-C23 | 2.93  | 1.42        | 1.33     |
| 23  | d     | 402 | PHO  | C3D-C4D | 2.93  | 1.44        | 1.40     |
| 23  | A     | 405 | PHO  | C1B-C2B | 2.93  | 1.50        | 1.42     |
| 23  | d     | 402 | PHO  | C1B-C2B | 2.92  | 1.49        | 1.42     |
| 23  | d     | 401 | PHO  | C3D-C4D | 2.92  | 1.44        | 1.40     |
| 23  | D     | 401 | PHO  | C3D-C4D | 2.92  | 1.44        | 1.40     |
| 25  | C     | 513 | BCR  | C30-C25 | -2.91 | 1.49        | 1.53     |
| 23  | A     | 405 | PHO  | C3D-C4D | 2.89  | 1.44        | 1.40     |
| 25  | K     | 101 | BCR  | C30-C25 | -2.88 | 1.49        | 1.53     |
| 25  | C     | 520 | BCR  | C1-C6   | -2.85 | 1.49        | 1.53     |
| 23  | d     | 401 | PHO  | C1B-C2B | 2.84  | 1.49        | 1.42     |
| 22  | b     | 615 | CLA  | C1B-C2B | 2.80  | 1.48        | 1.43     |
| 25  | c     | 521 | BCR  | C1-C6   | -2.78 | 1.49        | 1.53     |
| 25  | c     | 514 | BCR  | C30-C25 | -2.77 | 1.49        | 1.53     |
| 25  | H     | 102 | BCR  | C30-C25 | -2.77 | 1.49        | 1.53     |
| 26  | b     | 601 | DGD  | C1E-C2E | 2.77  | 1.60        | 1.52     |
| 25  | x     | 101 | BCR  | C30-C25 | -2.75 | 1.49        | 1.53     |
| 30  | B     | 622 | SQD  | O47-C7  | 2.75  | 1.42        | 1.34     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25  | c     | 513 | BCR  | C30-C25 | -2.74 | 1.49        | 1.53     |
| 26  | B     | 626 | DGD  | C1E-C2E | 2.74  | 1.60        | 1.52     |
| 26  | C     | 514 | DGD  | O2G-C2G | -2.72 | 1.39        | 1.46     |
| 30  | d     | 403 | SQD  | O47-C7  | 2.72  | 1.42        | 1.34     |
| 24  | D     | 405 | PL9  | C3-C4   | -2.72 | 1.44        | 1.49     |
| 30  | a     | 412 | SQD  | O47-C7  | 2.71  | 1.42        | 1.34     |
| 30  | A     | 414 | SQD  | O47-C7  | 2.70  | 1.42        | 1.34     |
| 30  | a     | 401 | SQD  | O47-C7  | 2.70  | 1.42        | 1.34     |
| 22  | B     | 610 | CLA  | C1B-C2B | 2.70  | 1.48        | 1.43     |
| 30  | A     | 413 | SQD  | O47-C7  | 2.69  | 1.42        | 1.34     |
| 30  | F     | 103 | SQD  | O47-C7  | 2.68  | 1.42        | 1.34     |
| 30  | B     | 627 | SQD  | O47-C7  | 2.68  | 1.42        | 1.34     |
| 30  | b     | 602 | SQD  | O47-C7  | 2.66  | 1.42        | 1.34     |
| 22  | C     | 507 | CLA  | CMB-C2B | -2.66 | 1.46        | 1.51     |
| 22  | B     | 611 | CLA  | CMD-C2D | -2.64 | 1.45        | 1.51     |
| 22  | c     | 507 | CLA  | CMB-C2B | -2.63 | 1.46        | 1.51     |
| 25  | B     | 617 | BCR  | C30-C25 | -2.63 | 1.50        | 1.53     |
| 25  | b     | 622 | BCR  | C30-C25 | -2.61 | 1.50        | 1.53     |
| 25  | j     | 102 | BCR  | C1-C6   | -2.59 | 1.50        | 1.53     |
| 30  | f     | 103 | SQD  | O47-C7  | 2.59  | 1.42        | 1.34     |
| 23  | d     | 402 | PHO  | CHD-C4C | 2.59  | 1.36        | 1.35     |
| 25  | J     | 102 | BCR  | C1-C6   | -2.58 | 1.50        | 1.53     |
| 22  | B     | 607 | CLA  | CMB-C2B | -2.57 | 1.46        | 1.51     |
| 22  | B     | 603 | CLA  | CMB-C2B | -2.55 | 1.46        | 1.51     |
| 22  | a     | 403 | CLA  | CMB-C2B | -2.54 | 1.46        | 1.51     |
| 22  | b     | 609 | CLA  | C1D-C2D | 2.54  | 1.49        | 1.42     |
| 32  | b     | 629 | LMT  | O3'-C3' | -2.53 | 1.36        | 1.43     |
| 22  | b     | 616 | CLA  | CMD-C2D | -2.53 | 1.46        | 1.51     |
| 22  | b     | 612 | CLA  | CMB-C2B | -2.53 | 1.46        | 1.51     |
| 22  | C     | 510 | CLA  | C4D-C3D | 2.53  | 1.48        | 1.42     |
| 34  | f     | 101 | HEM  | FE-NC   | 2.53  | 2.05        | 1.95     |
| 22  | A     | 403 | CLA  | CMB-C2B | -2.52 | 1.46        | 1.51     |
| 22  | A     | 406 | CLA  | CMB-C2B | -2.51 | 1.46        | 1.51     |
| 22  | C     | 501 | CLA  | CMB-C2B | -2.51 | 1.46        | 1.51     |
| 22  | B     | 608 | CLA  | CHC-C1C | 2.51  | 1.43        | 1.35     |
| 22  | a     | 403 | CLA  | C1D-C2D | 2.51  | 1.48        | 1.42     |
| 22  | B     | 609 | CLA  | C1D-C2D | 2.51  | 1.48        | 1.42     |
| 22  | b     | 609 | CLA  | CMB-C2B | -2.50 | 1.46        | 1.51     |
| 22  | C     | 504 | CLA  | CMB-C2B | -2.50 | 1.46        | 1.51     |
| 22  | B     | 609 | CLA  | CMB-C2B | -2.50 | 1.46        | 1.51     |
| 22  | C     | 509 | CLA  | CMB-C2B | -2.50 | 1.46        | 1.51     |
| 22  | a     | 406 | CLA  | CMB-C2B | -2.50 | 1.46        | 1.51     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | c     | 510 | CLA  | C4D-C3D | 2.49  | 1.48        | 1.42     |
| 32  | b     | 603 | LMT  | O3'-C3' | -2.49 | 1.36        | 1.43     |
| 32  | d     | 411 | LMT  | O3'-C3' | -2.49 | 1.36        | 1.43     |
| 22  | C     | 511 | CLA  | C4D-C3D | 2.49  | 1.48        | 1.42     |
| 22  | b     | 611 | CLA  | C1D-C2D | 2.49  | 1.48        | 1.42     |
| 22  | H     | 101 | CLA  | CMB-C2B | -2.49 | 1.46        | 1.51     |
| 22  | B     | 605 | CLA  | CMB-C2B | -2.49 | 1.46        | 1.51     |
| 32  | M     | 103 | LMT  | O3'-C3' | -2.49 | 1.36        | 1.43     |
| 22  | C     | 512 | CLA  | CMB-C2B | -2.49 | 1.46        | 1.51     |
| 22  | A     | 402 | CLA  | CMB-C2B | -2.49 | 1.46        | 1.51     |
| 22  | C     | 503 | CLA  | CMB-C2B | -2.49 | 1.46        | 1.51     |
| 22  | C     | 501 | CLA  | C1D-C2D | 2.48  | 1.48        | 1.42     |
| 22  | C     | 502 | CLA  | CMB-C2B | -2.48 | 1.46        | 1.51     |
| 22  | B     | 601 | CLA  | CMB-C2B | -2.48 | 1.46        | 1.51     |
| 32  | b     | 628 | LMT  | O3'-C3' | -2.48 | 1.37        | 1.43     |
| 22  | c     | 504 | CLA  | CMB-C2B | -2.48 | 1.46        | 1.51     |
| 32  | B     | 624 | LMT  | O3'-C3' | -2.48 | 1.37        | 1.43     |
| 22  | c     | 511 | CLA  | C4D-C3D | 2.48  | 1.48        | 1.42     |
| 22  | a     | 404 | CLA  | CMB-C2B | -2.48 | 1.46        | 1.51     |
| 22  | c     | 504 | CLA  | CMD-C2D | -2.48 | 1.46        | 1.51     |
| 22  | b     | 614 | CLA  | CMB-C2B | -2.47 | 1.46        | 1.51     |
| 22  | C     | 512 | CLA  | C4D-C3D | 2.47  | 1.48        | 1.42     |
| 22  | c     | 501 | CLA  | CMB-C2B | -2.47 | 1.46        | 1.51     |
| 24  | d     | 407 | PL9  | C3-C4   | -2.47 | 1.45        | 1.49     |
| 22  | c     | 502 | CLA  | CMB-C2B | -2.47 | 1.46        | 1.51     |
| 22  | b     | 605 | CLA  | CMB-C2B | -2.47 | 1.46        | 1.51     |
| 22  | b     | 618 | CLA  | CMB-C2B | -2.47 | 1.46        | 1.51     |
| 22  | c     | 501 | CLA  | C1D-C2D | 2.47  | 1.48        | 1.42     |
| 22  | c     | 520 | CLA  | CMB-C2B | -2.47 | 1.46        | 1.51     |
| 22  | C     | 510 | CLA  | C1D-C2D | 2.47  | 1.48        | 1.42     |
| 22  | C     | 508 | CLA  | CMB-C2B | -2.47 | 1.46        | 1.51     |
| 22  | b     | 613 | CLA  | CHC-C1C | 2.47  | 1.43        | 1.35     |
| 22  | b     | 611 | CLA  | CMB-C2B | -2.47 | 1.46        | 1.51     |
| 22  | c     | 509 | CLA  | CMD-C2D | -2.47 | 1.46        | 1.51     |
| 22  | C     | 519 | CLA  | CMB-C2B | -2.46 | 1.46        | 1.51     |
| 32  | B     | 623 | LMT  | O3'-C3' | -2.46 | 1.37        | 1.43     |
| 22  | b     | 608 | CLA  | CMB-C2B | -2.46 | 1.46        | 1.51     |
| 22  | c     | 510 | CLA  | C1D-C2D | 2.46  | 1.48        | 1.42     |
| 22  | b     | 614 | CLA  | C1D-C2D | 2.46  | 1.48        | 1.42     |
| 22  | C     | 512 | CLA  | C1D-C2D | 2.46  | 1.48        | 1.42     |
| 22  | B     | 606 | CLA  | CMB-C2B | -2.46 | 1.46        | 1.51     |
| 22  | a     | 406 | CLA  | C4D-C3D | 2.45  | 1.48        | 1.42     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | B     | 608 | CLA  | CMB-C2B | -2.46 | 1.46        | 1.51     |
| 32  | M     | 102 | LMT  | O3'-C3' | -2.45 | 1.37        | 1.43     |
| 32  | D     | 408 | LMT  | O3'-C3' | -2.45 | 1.37        | 1.43     |
| 22  | c     | 505 | CLA  | CMB-C2B | -2.45 | 1.46        | 1.51     |
| 22  | C     | 501 | CLA  | C4D-C3D | 2.45  | 1.48        | 1.42     |
| 22  | B     | 604 | CLA  | CMB-C2B | -2.45 | 1.46        | 1.51     |
| 22  | c     | 520 | CLA  | C1D-C2D | 2.45  | 1.48        | 1.42     |
| 22  | b     | 606 | CLA  | CHC-C1C | 2.45  | 1.43        | 1.35     |
| 22  | b     | 613 | CLA  | CMB-C2B | -2.45 | 1.46        | 1.51     |
| 22  | b     | 606 | CLA  | CMB-C2B | -2.45 | 1.46        | 1.51     |
| 22  | C     | 503 | CLA  | C4D-C3D | 2.45  | 1.48        | 1.42     |
| 22  | c     | 509 | CLA  | CMB-C2B | -2.45 | 1.46        | 1.51     |
| 34  | v     | 201 | HEM  | C4D-ND  | 2.45  | 1.39        | 1.33     |
| 22  | A     | 403 | CLA  | C1D-C2D | 2.44  | 1.48        | 1.42     |
| 22  | b     | 612 | CLA  | CHC-C1C | 2.44  | 1.43        | 1.35     |
| 32  | I     | 102 | LMT  | O3'-C3' | -2.44 | 1.37        | 1.43     |
| 22  | c     | 508 | CLA  | CMB-C2B | -2.44 | 1.46        | 1.51     |
| 22  | c     | 503 | CLA  | CMB-C2B | -2.44 | 1.46        | 1.51     |
| 22  | d     | 406 | CLA  | CMB-C2B | -2.44 | 1.46        | 1.51     |
| 22  | C     | 505 | CLA  | CMB-C2B | -2.44 | 1.46        | 1.51     |
| 22  | b     | 609 | CLA  | C4D-C3D | 2.44  | 1.48        | 1.42     |
| 22  | B     | 613 | CLA  | CHC-C1C | 2.44  | 1.43        | 1.35     |
| 22  | c     | 508 | CLA  | C4D-C3D | 2.44  | 1.48        | 1.42     |
| 22  | c     | 512 | CLA  | C1D-C2D | 2.43  | 1.48        | 1.42     |
| 22  | D     | 404 | CLA  | CMB-C2B | -2.43 | 1.46        | 1.51     |
| 22  | B     | 604 | CLA  | C1D-C2D | 2.43  | 1.48        | 1.42     |
| 22  | C     | 504 | CLA  | CMD-C2D | -2.43 | 1.46        | 1.51     |
| 22  | c     | 512 | CLA  | CMB-C2B | -2.43 | 1.46        | 1.51     |
| 34  | v     | 201 | HEM  | FE-NC   | 2.43  | 2.05        | 1.95     |
| 22  | B     | 610 | CLA  | C1D-C2D | 2.43  | 1.48        | 1.42     |
| 22  | b     | 610 | CLA  | C1D-C2D | 2.43  | 1.48        | 1.42     |
| 22  | A     | 402 | CLA  | C1D-C2D | 2.43  | 1.48        | 1.42     |
| 22  | A     | 404 | CLA  | CMB-C2B | -2.43 | 1.46        | 1.51     |
| 22  | c     | 507 | CLA  | C4D-C3D | 2.43  | 1.48        | 1.42     |
| 32  | B     | 628 | LMT  | O3'-C3' | -2.43 | 1.37        | 1.43     |
| 22  | C     | 506 | CLA  | CMB-C2B | -2.43 | 1.46        | 1.51     |
| 22  | C     | 507 | CLA  | C1D-C2D | 2.42  | 1.48        | 1.42     |
| 22  | c     | 512 | CLA  | C4D-C3D | 2.42  | 1.48        | 1.42     |
| 22  | D     | 404 | CLA  | C4D-C3D | 2.42  | 1.48        | 1.42     |
| 34  | v     | 201 | HEM  | C1D-ND  | 2.42  | 1.39        | 1.33     |
| 22  | c     | 503 | CLA  | C4D-C3D | 2.42  | 1.48        | 1.42     |
| 22  | B     | 602 | CLA  | CMB-C2B | -2.42 | 1.46        | 1.51     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | B     | 608 | CLA  | C4D-C3D | 2.42  | 1.48        | 1.42     |
| 22  | c     | 506 | CLA  | C4D-C3D | 2.42  | 1.48        | 1.42     |
| 22  | B     | 614 | CLA  | CMB-C2B | -2.42 | 1.46        | 1.51     |
| 22  | a     | 405 | CLA  | CMB-C2B | -2.42 | 1.46        | 1.51     |
| 22  | c     | 501 | CLA  | C4D-C3D | 2.41  | 1.48        | 1.42     |
| 22  | c     | 502 | CLA  | C4D-C3D | 2.41  | 1.48        | 1.42     |
| 22  | C     | 519 | CLA  | C4D-C3D | 2.41  | 1.48        | 1.42     |
| 22  | b     | 608 | CLA  | C4D-C3D | 2.41  | 1.48        | 1.42     |
| 22  | C     | 507 | CLA  | C4D-C3D | 2.41  | 1.48        | 1.42     |
| 22  | B     | 614 | CLA  | C1D-C2D | 2.41  | 1.48        | 1.42     |
| 22  | H     | 101 | CLA  | CHC-C1C | 2.41  | 1.43        | 1.35     |
| 22  | d     | 406 | CLA  | C1D-C2D | 2.41  | 1.48        | 1.42     |
| 22  | B     | 605 | CLA  | C1D-C2D | 2.41  | 1.48        | 1.42     |
| 32  | i     | 103 | LMT  | O3'-C3' | -2.41 | 1.37        | 1.43     |
| 22  | c     | 512 | CLA  | CHC-C1C | 2.41  | 1.43        | 1.35     |
| 22  | b     | 605 | CLA  | C4D-C3D | 2.41  | 1.48        | 1.42     |
| 22  | c     | 506 | CLA  | CMB-C2B | -2.41 | 1.46        | 1.51     |
| 22  | C     | 510 | CLA  | CMB-C2B | -2.41 | 1.46        | 1.51     |
| 22  | C     | 509 | CLA  | CMD-C2D | -2.41 | 1.46        | 1.51     |
| 23  | D     | 401 | PHO  | CMD-C2D | -2.41 | 1.46        | 1.51     |
| 22  | b     | 612 | CLA  | CMD-C2D | -2.41 | 1.46        | 1.51     |
| 22  | B     | 607 | CLA  | CHC-C1C | 2.41  | 1.43        | 1.35     |
| 22  | c     | 520 | CLA  | C4D-C3D | 2.41  | 1.48        | 1.42     |
| 22  | C     | 506 | CLA  | C4D-C3D | 2.41  | 1.48        | 1.42     |
| 22  | b     | 614 | CLA  | C4D-C3D | 2.41  | 1.48        | 1.42     |
| 22  | a     | 405 | CLA  | C1D-C2D | 2.41  | 1.48        | 1.42     |
| 22  | C     | 511 | CLA  | CMB-C2B | -2.40 | 1.46        | 1.51     |
| 22  | b     | 615 | CLA  | C4D-C3D | 2.40  | 1.48        | 1.42     |
| 22  | d     | 406 | CLA  | C4D-C3D | 2.40  | 1.48        | 1.42     |
| 22  | c     | 507 | CLA  | C1D-C2D | 2.40  | 1.48        | 1.42     |
| 22  | H     | 101 | CLA  | C4D-C3D | 2.40  | 1.48        | 1.42     |
| 22  | b     | 607 | CLA  | CHC-C1C | 2.40  | 1.43        | 1.35     |
| 22  | B     | 601 | CLA  | C4D-C3D | 2.40  | 1.48        | 1.42     |
| 22  | b     | 607 | CLA  | CMB-C2B | -2.40 | 1.46        | 1.51     |
| 22  | b     | 617 | CLA  | CMB-C2B | -2.40 | 1.46        | 1.51     |
| 22  | b     | 620 | CLA  | C1D-C2D | 2.40  | 1.48        | 1.42     |
| 22  | c     | 510 | CLA  | CMB-C2B | -2.40 | 1.46        | 1.51     |
| 22  | B     | 602 | CLA  | C4D-C3D | 2.40  | 1.48        | 1.42     |
| 22  | b     | 610 | CLA  | CMB-C2B | -2.40 | 1.46        | 1.51     |
| 22  | b     | 619 | CLA  | C4D-C3D | 2.40  | 1.48        | 1.42     |
| 23  | d     | 401 | PHO  | CMD-C2D | -2.40 | 1.46        | 1.51     |
| 22  | c     | 506 | CLA  | C1D-C2D | 2.39  | 1.48        | 1.42     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | a     | 404 | CLA  | C1D-C2D | 2.39  | 1.48        | 1.42     |
| 22  | c     | 509 | CLA  | C1D-C2D | 2.39  | 1.48        | 1.42     |
| 22  | B     | 615 | CLA  | C1D-C2D | 2.39  | 1.48        | 1.42     |
| 22  | B     | 607 | CLA  | CMD-C2D | -2.39 | 1.46        | 1.51     |
| 22  | C     | 506 | CLA  | C1D-C2D | 2.39  | 1.48        | 1.42     |
| 22  | B     | 615 | CLA  | CMB-C2B | -2.39 | 1.46        | 1.51     |
| 22  | A     | 406 | CLA  | C1D-C2D | 2.39  | 1.48        | 1.42     |
| 22  | B     | 604 | CLA  | C4D-C3D | 2.39  | 1.48        | 1.42     |
| 22  | c     | 502 | CLA  | CHC-C1C | 2.39  | 1.43        | 1.35     |
| 22  | b     | 605 | CLA  | C1D-C2D | 2.38  | 1.48        | 1.42     |
| 22  | d     | 406 | CLA  | CHC-C1C | 2.39  | 1.43        | 1.35     |
| 22  | C     | 502 | CLA  | C4D-C3D | 2.38  | 1.48        | 1.42     |
| 22  | C     | 508 | CLA  | C1D-C2D | 2.38  | 1.48        | 1.42     |
| 23  | A     | 405 | PHO  | CMD-C2D | -2.38 | 1.46        | 1.51     |
| 22  | c     | 508 | CLA  | C1D-C2D | 2.38  | 1.48        | 1.42     |
| 22  | b     | 619 | CLA  | C1D-C2D | 2.38  | 1.48        | 1.42     |
| 22  | B     | 611 | CLA  | CMB-C2B | -2.38 | 1.46        | 1.51     |
| 22  | B     | 603 | CLA  | C4D-C3D | 2.38  | 1.48        | 1.42     |
| 22  | B     | 612 | CLA  | CMB-C2B | -2.38 | 1.46        | 1.51     |
| 22  | A     | 406 | CLA  | C4D-C3D | 2.38  | 1.48        | 1.42     |
| 22  | c     | 505 | CLA  | C4D-C3D | 2.38  | 1.48        | 1.42     |
| 22  | b     | 618 | CLA  | CHC-C1C | 2.38  | 1.43        | 1.35     |
| 22  | d     | 405 | CLA  | CMB-C2B | -2.38 | 1.46        | 1.51     |
| 22  | b     | 619 | CLA  | CMB-C2B | -2.38 | 1.46        | 1.51     |
| 22  | B     | 612 | CLA  | C4D-C3D | 2.38  | 1.48        | 1.42     |
| 22  | H     | 101 | CLA  | C1D-C2D | 2.38  | 1.48        | 1.42     |
| 23  | d     | 402 | PHO  | CMD-C2D | -2.38 | 1.46        | 1.51     |
| 22  | C     | 511 | CLA  | CHC-C1C | 2.38  | 1.43        | 1.35     |
| 23  | A     | 405 | PHO  | CHD-C4C | 2.38  | 1.36        | 1.35     |
| 22  | b     | 606 | CLA  | C4D-C3D | 2.38  | 1.48        | 1.42     |
| 22  | D     | 403 | CLA  | CMB-C2B | -2.38 | 1.46        | 1.51     |
| 22  | c     | 511 | CLA  | CHC-C1C | 2.37  | 1.43        | 1.35     |
| 22  | B     | 609 | CLA  | C4D-C3D | 2.37  | 1.48        | 1.42     |
| 22  | D     | 404 | CLA  | C1D-C2D | 2.37  | 1.48        | 1.42     |
| 22  | b     | 617 | CLA  | C1D-C2D | 2.37  | 1.48        | 1.42     |
| 22  | B     | 602 | CLA  | C1D-C2D | 2.37  | 1.48        | 1.42     |
| 22  | c     | 511 | CLA  | CMB-C2B | -2.37 | 1.46        | 1.51     |
| 22  | b     | 610 | CLA  | C4D-C3D | 2.37  | 1.48        | 1.42     |
| 22  | b     | 618 | CLA  | C1D-C2D | 2.37  | 1.48        | 1.42     |
| 22  | B     | 603 | CLA  | CMD-C2D | -2.37 | 1.46        | 1.51     |
| 22  | C     | 508 | CLA  | C4D-C3D | 2.36  | 1.48        | 1.42     |
| 22  | a     | 406 | CLA  | C1D-C2D | 2.36  | 1.48        | 1.42     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | b     | 618 | CLA  | C4D-C3D | 2.36  | 1.48        | 1.42     |
| 22  | a     | 405 | CLA  | CHC-C1C | 2.36  | 1.43        | 1.35     |
| 31  | b     | 626 | LMG  | C4-C5   | 2.36  | 1.58        | 1.53     |
| 26  | B     | 626 | DGD  | C4D-C5D | 2.36  | 1.58        | 1.53     |
| 34  | V     | 201 | HEM  | C4D-ND  | 2.36  | 1.39        | 1.33     |
| 22  | D     | 403 | CLA  | CMD-C2D | -2.36 | 1.46        | 1.51     |
| 22  | c     | 509 | CLA  | CHC-C1C | 2.36  | 1.43        | 1.35     |
| 22  | b     | 607 | CLA  | C1D-C2D | 2.35  | 1.48        | 1.42     |
| 22  | C     | 504 | CLA  | C4D-C3D | 2.36  | 1.48        | 1.42     |
| 22  | b     | 613 | CLA  | C4D-C3D | 2.36  | 1.48        | 1.42     |
| 22  | b     | 616 | CLA  | CMB-C2B | -2.36 | 1.46        | 1.51     |
| 22  | B     | 607 | CLA  | C4D-C3D | 2.35  | 1.48        | 1.42     |
| 22  | B     | 606 | CLA  | C1D-C2D | 2.35  | 1.48        | 1.42     |
| 22  | B     | 603 | CLA  | CHC-C1C | 2.35  | 1.43        | 1.35     |
| 22  | D     | 403 | CLA  | C4D-C3D | 2.35  | 1.48        | 1.42     |
| 22  | b     | 607 | CLA  | C4D-C3D | 2.35  | 1.48        | 1.42     |
| 22  | B     | 615 | CLA  | C4D-C3D | 2.35  | 1.48        | 1.42     |
| 26  | B     | 626 | DGD  | C3G-C2G | 2.35  | 1.57        | 1.50     |
| 22  | b     | 620 | CLA  | C4D-C3D | 2.35  | 1.48        | 1.42     |
| 22  | B     | 613 | CLA  | C1D-C2D | 2.35  | 1.48        | 1.42     |
| 22  | C     | 505 | CLA  | C4D-C3D | 2.35  | 1.48        | 1.42     |
| 22  | B     | 605 | CLA  | C4D-C3D | 2.35  | 1.48        | 1.42     |
| 22  | C     | 519 | CLA  | C1D-C2D | 2.34  | 1.48        | 1.42     |
| 22  | B     | 601 | CLA  | C1D-C2D | 2.35  | 1.48        | 1.42     |
| 22  | d     | 405 | CLA  | CMD-C2D | -2.35 | 1.46        | 1.51     |
| 22  | b     | 615 | CLA  | C1D-C2D | 2.34  | 1.48        | 1.42     |
| 22  | B     | 614 | CLA  | C4D-C3D | 2.34  | 1.48        | 1.42     |
| 22  | C     | 505 | CLA  | C1D-C2D | 2.34  | 1.48        | 1.42     |
| 22  | A     | 404 | CLA  | C1D-C2D | 2.34  | 1.48        | 1.42     |
| 22  | b     | 608 | CLA  | CHC-C1C | 2.34  | 1.43        | 1.35     |
| 22  | d     | 405 | CLA  | C4D-C3D | 2.34  | 1.48        | 1.42     |
| 22  | c     | 506 | CLA  | CHC-C1C | 2.34  | 1.43        | 1.35     |
| 22  | c     | 507 | CLA  | CHC-C1C | 2.34  | 1.43        | 1.35     |
| 34  | f     | 101 | HEM  | C1D-ND  | 2.34  | 1.39        | 1.33     |
| 22  | c     | 505 | CLA  | CHC-C1C | 2.34  | 1.43        | 1.35     |
| 22  | B     | 602 | CLA  | CHC-C1C | 2.33  | 1.43        | 1.35     |
| 22  | c     | 505 | CLA  | C1D-C2D | 2.33  | 1.48        | 1.42     |
| 22  | B     | 610 | CLA  | C3B-C2B | -2.33 | 1.37        | 1.40     |
| 22  | C     | 509 | CLA  | C1D-C2D | 2.33  | 1.48        | 1.42     |
| 22  | D     | 404 | CLA  | CHC-C1C | 2.33  | 1.43        | 1.35     |
| 32  | B     | 629 | LMT  | O3'-C3' | -2.33 | 1.37        | 1.43     |
| 22  | A     | 404 | CLA  | CMD-C2D | -2.33 | 1.46        | 1.51     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | b     | 620 | CLA  | CMB-C2B | -2.33 | 1.46        | 1.51     |
| 22  | d     | 405 | CLA  | CHC-C1C | 2.33  | 1.43        | 1.35     |
| 22  | A     | 403 | CLA  | C4D-C3D | 2.33  | 1.48        | 1.42     |
| 22  | a     | 403 | CLA  | CMD-C2D | -2.33 | 1.46        | 1.51     |
| 22  | B     | 610 | CLA  | C4D-C3D | 2.33  | 1.48        | 1.42     |
| 32  | b     | 604 | LMT  | O3'-C3' | -2.33 | 1.37        | 1.43     |
| 22  | b     | 612 | CLA  | C4D-C3D | 2.33  | 1.48        | 1.42     |
| 22  | C     | 503 | CLA  | C1D-C2D | 2.33  | 1.48        | 1.42     |
| 22  | B     | 613 | CLA  | CMB-C2B | -2.32 | 1.46        | 1.51     |
| 22  | C     | 502 | CLA  | CHC-C1C | 2.32  | 1.43        | 1.35     |
| 22  | c     | 504 | CLA  | C4D-C3D | 2.33  | 1.48        | 1.42     |
| 22  | a     | 406 | CLA  | CHC-C1C | 2.32  | 1.43        | 1.35     |
| 22  | C     | 512 | CLA  | CHC-C1C | 2.32  | 1.43        | 1.35     |
| 22  | B     | 612 | CLA  | CHC-C1C | 2.32  | 1.43        | 1.35     |
| 22  | b     | 608 | CLA  | CMD-C2D | -2.32 | 1.46        | 1.51     |
| 22  | c     | 503 | CLA  | CHC-C1C | 2.32  | 1.43        | 1.35     |
| 34  | F     | 101 | HEM  | C4D-ND  | 2.32  | 1.39        | 1.33     |
| 22  | b     | 617 | CLA  | C4D-C3D | 2.32  | 1.48        | 1.42     |
| 22  | c     | 510 | CLA  | CHC-C1C | 2.32  | 1.43        | 1.35     |
| 22  | B     | 613 | CLA  | C4D-C3D | 2.32  | 1.48        | 1.42     |
| 22  | c     | 503 | CLA  | C1D-C2D | 2.32  | 1.48        | 1.42     |
| 24  | A     | 407 | PL9  | C3-C4   | -2.32 | 1.45        | 1.49     |
| 22  | C     | 509 | CLA  | CHC-C1C | 2.32  | 1.43        | 1.35     |
| 26  | b     | 601 | DGD  | C3G-C2G | 2.31  | 1.57        | 1.50     |
| 34  | V     | 201 | HEM  | C1D-ND  | 2.31  | 1.39        | 1.33     |
| 22  | c     | 509 | CLA  | C4D-C3D | 2.31  | 1.48        | 1.42     |
| 22  | A     | 404 | CLA  | CHC-C1C | 2.31  | 1.43        | 1.35     |
| 32  | I     | 102 | LMT  | O2'-C2' | -2.31 | 1.37        | 1.43     |
| 22  | c     | 508 | CLA  | CHC-C1C | 2.31  | 1.43        | 1.35     |
| 31  | l     | 101 | LMG  | C7-C8   | 2.31  | 1.57        | 1.50     |
| 22  | b     | 617 | CLA  | CHC-C1C | 2.31  | 1.43        | 1.35     |
| 34  | F     | 101 | HEM  | C1D-ND  | 2.31  | 1.39        | 1.33     |
| 22  | B     | 604 | CLA  | CHC-C1C | 2.31  | 1.43        | 1.35     |
| 22  | A     | 403 | CLA  | CHC-C1C | 2.31  | 1.43        | 1.35     |
| 22  | b     | 615 | CLA  | C3B-C2B | -2.31 | 1.37        | 1.40     |
| 22  | C     | 502 | CLA  | C1D-C2D | 2.31  | 1.48        | 1.42     |
| 22  | B     | 614 | CLA  | CHC-C1C | 2.31  | 1.43        | 1.35     |
| 23  | d     | 402 | PHO  | C4C-C3C | 2.30  | 1.49        | 1.45     |
| 22  | A     | 404 | CLA  | C4D-C3D | 2.31  | 1.48        | 1.42     |
| 22  | A     | 402 | CLA  | CMD-C2D | -2.31 | 1.46        | 1.51     |
| 22  | c     | 501 | CLA  | CHC-C1C | 2.31  | 1.43        | 1.35     |
| 22  | B     | 612 | CLA  | C1D-C2D | 2.31  | 1.48        | 1.42     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | a     | 407 | PL9  | C3-C4   | -2.30 | 1.45        | 1.49     |
| 22  | c     | 511 | CLA  | C1D-C2D | 2.30  | 1.48        | 1.42     |
| 22  | C     | 509 | CLA  | C4D-C3D | 2.30  | 1.48        | 1.42     |
| 22  | a     | 405 | CLA  | CMD-C2D | -2.30 | 1.46        | 1.51     |
| 22  | C     | 511 | CLA  | C1D-C2D | 2.30  | 1.48        | 1.42     |
| 22  | B     | 606 | CLA  | C4D-C3D | 2.30  | 1.48        | 1.42     |
| 22  | b     | 616 | CLA  | CHC-C1C | 2.30  | 1.43        | 1.35     |
| 22  | C     | 508 | CLA  | CMD-C2D | -2.30 | 1.46        | 1.51     |
| 22  | C     | 519 | CLA  | CHC-C1C | 2.30  | 1.43        | 1.35     |
| 22  | C     | 505 | CLA  | CHC-C1C | 2.30  | 1.43        | 1.35     |
| 22  | B     | 609 | CLA  | CHC-C1C | 2.30  | 1.43        | 1.35     |
| 34  | f     | 101 | HEM  | C4D-ND  | 2.30  | 1.39        | 1.33     |
| 22  | B     | 605 | CLA  | CHC-C1C | 2.30  | 1.43        | 1.35     |
| 22  | a     | 404 | CLA  | CMD-C2D | -2.30 | 1.46        | 1.51     |
| 22  | b     | 620 | CLA  | CMD-C2D | -2.30 | 1.46        | 1.51     |
| 22  | b     | 619 | CLA  | CHC-C1C | 2.30  | 1.43        | 1.35     |
| 22  | B     | 606 | CLA  | CMD-C2D | -2.29 | 1.46        | 1.51     |
| 22  | D     | 403 | CLA  | CHC-C1C | 2.29  | 1.43        | 1.35     |
| 26  | D     | 407 | DGD  | C1G-C2G | 2.29  | 1.57        | 1.50     |
| 22  | a     | 405 | CLA  | C4D-C3D | 2.29  | 1.48        | 1.42     |
| 22  | b     | 605 | CLA  | CMD-C2D | -2.29 | 1.46        | 1.51     |
| 22  | A     | 402 | CLA  | C4D-C3D | 2.29  | 1.48        | 1.42     |
| 22  | b     | 611 | CLA  | C4D-C3D | 2.29  | 1.48        | 1.42     |
| 22  | B     | 608 | CLA  | C1D-C2D | 2.29  | 1.48        | 1.42     |
| 22  | a     | 403 | CLA  | CHC-C1C | 2.29  | 1.42        | 1.35     |
| 22  | a     | 403 | CLA  | C4D-C3D | 2.29  | 1.48        | 1.42     |
| 22  | B     | 601 | CLA  | CMD-C2D | -2.29 | 1.46        | 1.51     |
| 22  | b     | 616 | CLA  | C4D-C3D | 2.28  | 1.48        | 1.42     |
| 22  | B     | 606 | CLA  | CHC-C1C | 2.28  | 1.42        | 1.35     |
| 22  | A     | 406 | CLA  | CHC-C1C | 2.28  | 1.42        | 1.35     |
| 22  | c     | 503 | CLA  | CMD-C2D | -2.28 | 1.46        | 1.51     |
| 22  | B     | 614 | CLA  | CMD-C2D | -2.28 | 1.46        | 1.51     |
| 22  | B     | 615 | CLA  | CMD-C2D | -2.28 | 1.46        | 1.51     |
| 22  | C     | 501 | CLA  | CHC-C1C | 2.28  | 1.42        | 1.35     |
| 22  | b     | 612 | CLA  | C1D-C2D | 2.28  | 1.48        | 1.42     |
| 22  | b     | 614 | CLA  | CHC-C1C | 2.28  | 1.42        | 1.35     |
| 22  | b     | 610 | CLA  | CHC-C1C | 2.27  | 1.42        | 1.35     |
| 22  | C     | 508 | CLA  | CHC-C1C | 2.27  | 1.42        | 1.35     |
| 22  | B     | 604 | CLA  | CMD-C2D | -2.27 | 1.46        | 1.51     |
| 22  | a     | 404 | CLA  | C4D-C3D | 2.27  | 1.48        | 1.42     |
| 22  | C     | 510 | CLA  | CHC-C1C | 2.27  | 1.42        | 1.35     |
| 31  | D     | 409 | LMG  | O7-C8   | -2.27 | 1.40        | 1.46     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | A     | 403 | CLA  | CMD-C2D | -2.27 | 1.46        | 1.51     |
| 22  | B     | 602 | CLA  | CMD-C2D | -2.27 | 1.46        | 1.51     |
| 22  | b     | 613 | CLA  | CMD-C2D | -2.27 | 1.46        | 1.51     |
| 22  | C     | 503 | CLA  | CHC-C1C | 2.27  | 1.42        | 1.35     |
| 26  | b     | 601 | DGD  | C1G-C2G | 2.26  | 1.57        | 1.50     |
| 22  | b     | 617 | CLA  | CMD-C2D | -2.27 | 1.46        | 1.51     |
| 22  | b     | 605 | CLA  | CHC-C1C | 2.26  | 1.42        | 1.35     |
| 22  | b     | 611 | CLA  | CMD-C2D | -2.26 | 1.46        | 1.51     |
| 22  | c     | 508 | CLA  | CMD-C2D | -2.26 | 1.46        | 1.51     |
| 22  | c     | 520 | CLA  | CHC-C1C | 2.26  | 1.42        | 1.35     |
| 22  | c     | 505 | CLA  | CMD-C2D | -2.26 | 1.46        | 1.51     |
| 22  | C     | 507 | CLA  | CHC-C1C | 2.26  | 1.42        | 1.35     |
| 22  | A     | 402 | CLA  | CHC-C1C | 2.26  | 1.42        | 1.35     |
| 22  | b     | 611 | CLA  | CHC-C1C | 2.25  | 1.42        | 1.35     |
| 32  | B     | 629 | LMT  | O3B-C3B | -2.25 | 1.37        | 1.43     |
| 23  | d     | 401 | PHO  | CMB-C2B | -2.25 | 1.46        | 1.51     |
| 22  | C     | 506 | CLA  | CHC-C1C | 2.25  | 1.42        | 1.35     |
| 22  | B     | 601 | CLA  | CHC-C1C | 2.25  | 1.42        | 1.35     |
| 22  | c     | 507 | CLA  | CMD-C2D | -2.25 | 1.46        | 1.51     |
| 22  | C     | 505 | CLA  | CMD-C2D | -2.25 | 1.46        | 1.51     |
| 26  | c     | 517 | DGD  | C1G-C2G | 2.25  | 1.57        | 1.50     |
| 22  | b     | 608 | CLA  | C1D-C2D | 2.25  | 1.48        | 1.42     |
| 22  | C     | 511 | CLA  | CMD-C2D | -2.25 | 1.46        | 1.51     |
| 22  | b     | 609 | CLA  | CHC-C1C | 2.25  | 1.42        | 1.35     |
| 22  | B     | 608 | CLA  | CMD-C2D | -2.24 | 1.46        | 1.51     |
| 23  | A     | 405 | PHO  | C4C-C3C | 2.25  | 1.49        | 1.45     |
| 24  | a     | 407 | PL9  | C53-C6  | -2.25 | 1.46        | 1.50     |
| 22  | B     | 607 | CLA  | C1D-C2D | 2.24  | 1.48        | 1.42     |
| 22  | c     | 502 | CLA  | CMD-C2D | -2.24 | 1.46        | 1.51     |
| 22  | c     | 504 | CLA  | CHC-C1C | 2.24  | 1.42        | 1.35     |
| 22  | c     | 511 | CLA  | CMD-C2D | -2.24 | 1.46        | 1.51     |
| 22  | C     | 502 | CLA  | CMD-C2D | -2.24 | 1.46        | 1.51     |
| 22  | C     | 504 | CLA  | CHC-C1C | 2.24  | 1.42        | 1.35     |
| 22  | b     | 619 | CLA  | CMD-C2D | -2.24 | 1.46        | 1.51     |
| 31  | B     | 621 | LMG  | C4-C5   | 2.24  | 1.57        | 1.53     |
| 32  | D     | 408 | LMT  | O3B-C3B | -2.23 | 1.37        | 1.43     |
| 32  | b     | 604 | LMT  | O3B-C3B | -2.23 | 1.37        | 1.43     |
| 22  | B     | 615 | CLA  | CHC-C1C | 2.23  | 1.42        | 1.35     |
| 22  | B     | 605 | CLA  | CMD-C2D | -2.23 | 1.46        | 1.51     |
| 31  | L     | 101 | LMG  | C7-C8   | 2.23  | 1.57        | 1.50     |
| 22  | C     | 503 | CLA  | CMD-C2D | -2.23 | 1.46        | 1.51     |
| 32  | M     | 103 | LMT  | O3B-C3B | -2.23 | 1.37        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | b     | 610 | CLA  | CMD-C2D | -2.23 | 1.46        | 1.51     |
| 22  | A     | 406 | CLA  | CMD-C2D | -2.23 | 1.46        | 1.51     |
| 32  | b     | 629 | LMT  | O3B-C3B | -2.23 | 1.37        | 1.43     |
| 22  | b     | 606 | CLA  | CMD-C2D | -2.23 | 1.46        | 1.51     |
| 22  | c     | 520 | CLA  | CMD-C2D | -2.23 | 1.46        | 1.51     |
| 22  | c     | 502 | CLA  | C1D-C2D | 2.23  | 1.48        | 1.42     |
| 22  | C     | 507 | CLA  | CMD-C2D | -2.23 | 1.46        | 1.51     |
| 32  | i     | 103 | LMT  | O2'-C2' | -2.23 | 1.37        | 1.43     |
| 22  | a     | 406 | CLA  | CMD-C2D | -2.22 | 1.46        | 1.51     |
| 22  | B     | 613 | CLA  | CMD-C2D | -2.22 | 1.46        | 1.51     |
| 22  | H     | 101 | CLA  | CMD-C2D | -2.22 | 1.46        | 1.51     |
| 22  | c     | 512 | CLA  | CMD-C2D | -2.22 | 1.46        | 1.51     |
| 22  | B     | 611 | CLA  | C4D-C3D | 2.22  | 1.47        | 1.42     |
| 22  | b     | 609 | CLA  | CMD-C2D | -2.22 | 1.46        | 1.51     |
| 32  | B     | 623 | LMT  | O2'-C2' | -2.21 | 1.37        | 1.43     |
| 22  | b     | 607 | CLA  | CMD-C2D | -2.22 | 1.46        | 1.51     |
| 22  | b     | 620 | CLA  | CHC-C1C | 2.22  | 1.42        | 1.35     |
| 22  | B     | 603 | CLA  | C1D-C2D | 2.22  | 1.48        | 1.42     |
| 22  | D     | 403 | CLA  | C1D-C2D | 2.22  | 1.48        | 1.42     |
| 22  | b     | 606 | CLA  | C1D-C2D | 2.21  | 1.48        | 1.42     |
| 22  | C     | 519 | CLA  | CMD-C2D | -2.21 | 1.46        | 1.51     |
| 22  | b     | 614 | CLA  | CMD-C2D | -2.21 | 1.46        | 1.51     |
| 22  | B     | 612 | CLA  | CMD-C2D | -2.21 | 1.46        | 1.51     |
| 32  | b     | 603 | LMT  | O3B-C3B | -2.21 | 1.37        | 1.43     |
| 31  | I     | 101 | LMG  | C4-C5   | 2.21  | 1.57        | 1.53     |
| 23  | A     | 405 | PHO  | CMB-C2B | -2.21 | 1.46        | 1.51     |
| 22  | B     | 611 | CLA  | CHC-C1C | 2.21  | 1.42        | 1.35     |
| 31  | m     | 101 | LMG  | C7-C8   | 2.21  | 1.56        | 1.50     |
| 32  | B     | 629 | LMT  | O2'-C2' | -2.21 | 1.37        | 1.43     |
| 22  | b     | 613 | CLA  | C1D-C2D | 2.21  | 1.48        | 1.42     |
| 24  | j     | 101 | PL9  | C3-C4   | -2.20 | 1.45        | 1.49     |
| 23  | A     | 405 | PHO  | C1A-NA  | 2.20  | 1.42        | 1.37     |
| 31  | b     | 627 | LMG  | C4-C5   | 2.20  | 1.57        | 1.53     |
| 32  | B     | 628 | LMT  | O2B-C2B | -2.20 | 1.37        | 1.43     |
| 26  | b     | 601 | DGD  | C4D-C5D | 2.20  | 1.57        | 1.53     |
| 22  | c     | 506 | CLA  | CMD-C2D | -2.20 | 1.46        | 1.51     |
| 32  | b     | 628 | LMT  | O3B-C3B | -2.19 | 1.37        | 1.43     |
| 22  | d     | 406 | CLA  | CMD-C2D | -2.19 | 1.46        | 1.51     |
| 22  | B     | 609 | CLA  | CMD-C2D | -2.19 | 1.46        | 1.51     |
| 26  | c     | 517 | DGD  | C3G-C2G | 2.19  | 1.56        | 1.50     |
| 22  | C     | 506 | CLA  | CMD-C2D | -2.19 | 1.46        | 1.51     |
| 22  | b     | 616 | CLA  | C1D-C2D | 2.19  | 1.48        | 1.42     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | d     | 405 | CLA  | C1D-C2D | 2.19  | 1.48        | 1.42     |
| 32  | I     | 102 | LMT  | O3B-C3B | -2.19 | 1.37        | 1.43     |
| 32  | B     | 624 | LMT  | O3B-C3B | -2.19 | 1.37        | 1.43     |
| 22  | c     | 501 | CLA  | CMD-C2D | -2.19 | 1.46        | 1.51     |
| 23  | D     | 401 | PHO  | C1A-NA  | 2.19  | 1.42        | 1.37     |
| 32  | b     | 603 | LMT  | O2'-C2' | -2.18 | 1.37        | 1.43     |
| 32  | d     | 411 | LMT  | O3B-C3B | -2.18 | 1.37        | 1.43     |
| 23  | d     | 402 | PHO  | CMB-C2B | -2.18 | 1.46        | 1.51     |
| 32  | b     | 628 | LMT  | O2'-C2' | -2.18 | 1.37        | 1.43     |
| 31  | D     | 409 | LMG  | C7-C8   | 2.18  | 1.56        | 1.50     |
| 32  | M     | 102 | LMT  | O3B-C3B | -2.18 | 1.37        | 1.43     |
| 25  | g     | 101 | BCR  | C33-C5  | -2.18 | 1.47        | 1.51     |
| 32  | B     | 628 | LMT  | O3B-C3B | -2.17 | 1.37        | 1.43     |
| 32  | i     | 103 | LMT  | O2B-C2B | -2.17 | 1.37        | 1.43     |
| 22  | b     | 618 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.51     |
| 23  | D     | 401 | PHO  | CMB-C2B | -2.17 | 1.46        | 1.51     |
| 22  | c     | 510 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.51     |
| 22  | C     | 510 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.51     |
| 24  | A     | 407 | PL9  | C53-C6  | -2.17 | 1.46        | 1.50     |
| 32  | i     | 103 | LMT  | O3B-C3B | -2.17 | 1.37        | 1.43     |
| 23  | d     | 402 | PHO  | C1A-NA  | 2.16  | 1.42        | 1.37     |
| 22  | D     | 404 | CLA  | CMD-C2D | -2.16 | 1.46        | 1.51     |
| 22  | C     | 512 | CLA  | CMD-C2D | -2.16 | 1.46        | 1.51     |
| 23  | d     | 401 | PHO  | C1A-NA  | 2.16  | 1.42        | 1.37     |
| 22  | B     | 610 | CLA  | CMD-C2D | -2.16 | 1.46        | 1.51     |
| 32  | I     | 102 | LMT  | O2B-C2B | -2.15 | 1.37        | 1.43     |
| 32  | b     | 628 | LMT  | O2B-C2B | -2.15 | 1.37        | 1.43     |
| 22  | C     | 501 | CLA  | CMD-C2D | -2.15 | 1.46        | 1.51     |
| 22  | a     | 404 | CLA  | CHC-C1C | 2.15  | 1.42        | 1.35     |
| 27  | a     | 409 | LHG  | O7-C5   | -2.15 | 1.41        | 1.46     |
| 26  | C     | 516 | DGD  | C1G-C2G | 2.15  | 1.56        | 1.50     |
| 32  | M     | 102 | LMT  | O2'-C2' | -2.15 | 1.37        | 1.43     |
| 32  | B     | 624 | LMT  | O2'-C2' | -2.15 | 1.37        | 1.43     |
| 32  | b     | 629 | LMT  | O2'-C2' | -2.15 | 1.37        | 1.43     |
| 26  | C     | 516 | DGD  | C3G-C2G | 2.14  | 1.56        | 1.50     |
| 32  | b     | 604 | LMT  | O2'-C2' | -2.14 | 1.37        | 1.43     |
| 31  | e     | 101 | LMG  | C7-C8   | 2.14  | 1.56        | 1.50     |
| 32  | B     | 623 | LMT  | O3B-C3B | -2.14 | 1.37        | 1.43     |
| 22  | c     | 504 | CLA  | C1D-C2D | 2.14  | 1.48        | 1.42     |
| 26  | B     | 626 | DGD  | C1G-C2G | 2.13  | 1.56        | 1.50     |
| 32  | D     | 408 | LMT  | O2B-C2B | -2.13 | 1.37        | 1.43     |
| 31  | d     | 412 | LMG  | C7-C8   | 2.13  | 1.56        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 27  | c     | 519 | LHG  | O7-C5   | -2.13 | 1.41        | 1.46     |
| 22  | b     | 615 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.51     |
| 32  | M     | 103 | LMT  | O2'-C2' | -2.13 | 1.37        | 1.43     |
| 32  | B     | 629 | LMT  | O2B-C2B | -2.12 | 1.37        | 1.43     |
| 22  | B     | 611 | CLA  | C1D-C2D | 2.12  | 1.48        | 1.42     |
| 32  | b     | 603 | LMT  | O2B-C2B | -2.12 | 1.37        | 1.43     |
| 23  | d     | 401 | PHO  | C3B-C2B | -2.12 | 1.37        | 1.40     |
| 25  | y     | 101 | BCR  | C33-C5  | -2.11 | 1.47        | 1.51     |
| 32  | B     | 628 | LMT  | O2'-C2' | -2.11 | 1.37        | 1.43     |
| 24  | D     | 405 | PL9  | C6-C1   | -2.11 | 1.44        | 1.48     |
| 26  | c     | 515 | DGD  | O2G-C2G | -2.11 | 1.41        | 1.46     |
| 30  | b     | 602 | SQD  | O2-C2   | -2.11 | 1.37        | 1.43     |
| 26  | d     | 410 | DGD  | C1D-C2D | 2.11  | 1.58        | 1.52     |
| 26  | c     | 516 | DGD  | O2G-C2G | -2.10 | 1.41        | 1.46     |
| 26  | C     | 514 | DGD  | O1G-C1G | -2.10 | 1.40        | 1.45     |
| 31  | a     | 402 | LMG  | C4-C5   | 2.10  | 1.57        | 1.53     |
| 32  | M     | 103 | LMT  | O2B-C2B | -2.10 | 1.37        | 1.43     |
| 32  | B     | 623 | LMT  | O2B-C2B | -2.10 | 1.37        | 1.43     |
| 23  | D     | 401 | PHO  | CHD-C4C | 2.10  | 1.36        | 1.35     |
| 32  | d     | 411 | LMT  | O2B-C2B | -2.08 | 1.37        | 1.43     |
| 30  | B     | 627 | SQD  | O2-C2   | -2.08 | 1.37        | 1.43     |
| 31  | E     | 101 | LMG  | C7-C8   | 2.08  | 1.56        | 1.50     |
| 23  | D     | 401 | PHO  | C4C-C3C | 2.08  | 1.49        | 1.45     |
| 30  | a     | 412 | SQD  | O2-C2   | -2.07 | 1.38        | 1.43     |
| 30  | A     | 413 | SQD  | O2-C2   | -2.07 | 1.38        | 1.43     |
| 31  | a     | 402 | LMG  | O7-C8   | -2.07 | 1.41        | 1.46     |
| 32  | b     | 604 | LMT  | O2B-C2B | -2.07 | 1.38        | 1.43     |
| 22  | C     | 504 | CLA  | C1D-C2D | 2.06  | 1.47        | 1.42     |
| 22  | B     | 615 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 22  | C     | 501 | CLA  | C3B-C2B | -2.06 | 1.37        | 1.40     |
| 32  | d     | 411 | LMT  | O4'-C4B | -2.06 | 1.38        | 1.43     |
| 22  | C     | 504 | CLA  | C3B-C2B | -2.06 | 1.37        | 1.40     |
| 32  | d     | 411 | LMT  | O2'-C2' | -2.06 | 1.38        | 1.43     |
| 31  | d     | 409 | LMG  | C7-C8   | 2.06  | 1.56        | 1.50     |
| 30  | A     | 414 | SQD  | O3-C3   | -2.05 | 1.38        | 1.43     |
| 22  | b     | 615 | CLA  | CHC-C1C | 2.05  | 1.42        | 1.35     |
| 23  | d     | 401 | PHO  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 31  | m     | 101 | LMG  | C4-C5   | 2.05  | 1.57        | 1.53     |
| 31  | M     | 101 | LMG  | C7-C8   | 2.05  | 1.56        | 1.50     |
| 32  | D     | 408 | LMT  | O4'-C4B | -2.05 | 1.38        | 1.43     |
| 32  | b     | 629 | LMT  | O4'-C4B | -2.05 | 1.38        | 1.43     |
| 22  | b     | 620 | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 23  | D     | 401 | PHO  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 32  | M     | 102 | LMT  | O2B-C2B | -2.05 | 1.38        | 1.43     |
| 32  | I     | 102 | LMT  | O4'-C4B | -2.05 | 1.38        | 1.43     |
| 24  | d     | 407 | PL9  | C53-C6  | -2.04 | 1.46        | 1.50     |
| 23  | d     | 401 | PHO  | C4C-C3C | 2.04  | 1.49        | 1.45     |
| 31  | c     | 522 | LMG  | C7-C8   | 2.04  | 1.56        | 1.50     |
| 26  | C     | 515 | DGD  | O2G-C2G | -2.04 | 1.41        | 1.46     |
| 23  | A     | 405 | PHO  | C4C-NC  | 2.04  | 1.42        | 1.38     |
| 30  | a     | 401 | SQD  | O3-C3   | -2.04 | 1.38        | 1.43     |
| 23  | d     | 402 | PHO  | C4C-NC  | 2.03  | 1.42        | 1.38     |
| 22  | A     | 403 | CLA  | C3B-C2B | -2.03 | 1.37        | 1.40     |
| 22  | C     | 502 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 23  | A     | 405 | PHO  | C3B-C2B | -2.03 | 1.37        | 1.40     |
| 34  | F     | 101 | HEM  | FE-NC   | 2.03  | 2.03        | 1.95     |
| 31  | B     | 621 | LMG  | C7-C8   | 2.03  | 1.56        | 1.50     |
| 26  | D     | 407 | DGD  | O5D-C6D | -2.03 | 1.39        | 1.43     |
| 34  | v     | 201 | HEM  | C4C-NC  | 2.03  | 1.38        | 1.33     |
| 30  | F     | 103 | SQD  | O2-C2   | -2.03 | 1.38        | 1.43     |
| 32  | b     | 629 | LMT  | O2B-C2B | -2.03 | 1.38        | 1.43     |
| 32  | B     | 628 | LMT  | O4'-C4B | -2.02 | 1.38        | 1.43     |
| 32  | b     | 604 | LMT  | O4'-C4B | -2.02 | 1.38        | 1.43     |
| 23  | d     | 402 | PHO  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 32  | b     | 603 | LMT  | O4'-C4B | -2.02 | 1.38        | 1.43     |
| 32  | D     | 408 | LMT  | O2'-C2' | -2.02 | 1.38        | 1.43     |
| 22  | b     | 606 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 31  | D     | 406 | LMG  | C7-C8   | 2.02  | 1.56        | 1.50     |
| 31  | d     | 412 | LMG  | O7-C8   | -2.01 | 1.41        | 1.46     |
| 27  | A     | 410 | LHG  | O7-C5   | -2.01 | 1.41        | 1.46     |
| 22  | B     | 610 | CLA  | CHC-C1C | 2.01  | 1.42        | 1.35     |
| 22  | c     | 501 | CLA  | C3B-C2B | -2.01 | 1.37        | 1.40     |
| 22  | c     | 510 | CLA  | C1D-ND  | 2.00  | 1.42        | 1.38     |
| 32  | M     | 103 | LMT  | O4'-C4B | -2.00 | 1.38        | 1.43     |
| 22  | b     | 605 | CLA  | CMC-C2C | -2.00 | 1.46        | 1.50     |

All (1649) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 30  | b     | 602 | SQD  | O6-C1-C2 | 7.58 | 117.87      | 108.15   |
| 30  | B     | 627 | SQD  | O6-C1-C2 | 7.26 | 117.45      | 108.15   |
| 30  | A     | 413 | SQD  | O9-S-C6  | 7.14 | 113.14      | 106.83   |
| 30  | A     | 413 | SQD  | O6-C1-C2 | 6.80 | 116.86      | 108.15   |
| 30  | a     | 412 | SQD  | O6-C1-C2 | 6.80 | 116.86      | 108.15   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | a     | 412 | SQD  | O9-S-C6     | 6.54  | 112.61      | 106.83   |
| 30  | B     | 622 | SQD  | O7-S-C6     | 6.49  | 112.56      | 106.83   |
| 30  | f     | 103 | SQD  | O7-S-C6     | 6.27  | 112.37      | 106.83   |
| 24  | J     | 101 | PL9  | C7-C3-C2    | -6.06 | 118.23      | 123.75   |
| 30  | a     | 401 | SQD  | O7-S-C6     | 6.03  | 112.16      | 106.83   |
| 24  | J     | 101 | PL9  | C7-C3-C4    | 5.92  | 121.66      | 116.92   |
| 24  | j     | 101 | PL9  | C7-C3-C2    | -5.91 | 118.37      | 123.75   |
| 30  | F     | 103 | SQD  | O7-S-C6     | 5.85  | 112.00      | 106.83   |
| 30  | A     | 414 | SQD  | O7-S-C6     | 5.75  | 111.91      | 106.83   |
| 24  | d     | 407 | PL9  | C7-C3-C2    | -5.72 | 118.54      | 123.75   |
| 30  | B     | 627 | SQD  | O9-S-C6     | 5.71  | 111.87      | 106.83   |
| 24  | D     | 405 | PL9  | C7-C3-C2    | -5.63 | 118.62      | 123.75   |
| 24  | a     | 407 | PL9  | C7-C3-C2    | -5.62 | 118.64      | 123.75   |
| 30  | b     | 602 | SQD  | O7-S-C6     | 5.60  | 111.78      | 106.83   |
| 30  | d     | 403 | SQD  | O7-S-C6     | 5.56  | 111.74      | 106.83   |
| 30  | b     | 602 | SQD  | O9-S-C6     | 5.54  | 111.73      | 106.83   |
| 22  | B     | 610 | CLA  | CMB-C2B-C1B | -5.52 | 119.98      | 128.46   |
| 24  | j     | 101 | PL9  | C7-C3-C4    | 5.50  | 121.32      | 116.92   |
| 24  | A     | 407 | PL9  | C7-C3-C2    | -5.47 | 118.78      | 123.75   |
| 24  | a     | 407 | PL9  | C7-C3-C4    | 5.46  | 121.28      | 116.92   |
| 24  | A     | 407 | PL9  | C7-C3-C4    | 5.42  | 121.26      | 116.92   |
| 24  | d     | 407 | PL9  | C7-C3-C4    | 5.38  | 121.22      | 116.92   |
| 22  | b     | 615 | CLA  | CMB-C2B-C1B | -5.37 | 120.20      | 128.46   |
| 24  | D     | 405 | PL9  | C7-C3-C4    | 5.25  | 121.12      | 116.92   |
| 30  | B     | 627 | SQD  | O7-S-C6     | 5.24  | 111.46      | 106.83   |
| 30  | a     | 412 | SQD  | O7-S-C6     | 5.12  | 111.36      | 106.83   |
| 23  | A     | 405 | PHO  | C4D-CHA-C1A | -5.12 | 123.47      | 129.57   |
| 23  | d     | 401 | PHO  | C4D-CHA-C1A | -5.10 | 123.50      | 129.57   |
| 30  | B     | 622 | SQD  | O6-C1-C2    | 5.08  | 114.67      | 108.15   |
| 23  | d     | 402 | PHO  | C4D-CHA-C1A | -5.04 | 123.57      | 129.57   |
| 30  | d     | 403 | SQD  | O9-S-C6     | 5.00  | 111.25      | 106.83   |
| 26  | A     | 409 | DGD  | CDB-CCB-CBB | -5.00 | 98.65       | 112.94   |
| 30  | A     | 413 | SQD  | O7-S-C6     | 5.00  | 111.25      | 106.83   |
| 30  | F     | 103 | SQD  | O9-S-C6     | 4.92  | 111.18      | 106.83   |
| 26  | a     | 408 | DGD  | CDB-CCB-CBB | -4.92 | 98.89       | 112.94   |
| 30  | F     | 103 | SQD  | O8-S-C6     | 4.83  | 111.64      | 105.89   |
| 30  | A     | 414 | SQD  | O9-S-C6     | 4.83  | 111.10      | 106.83   |
| 30  | f     | 103 | SQD  | O8-S-C6     | 4.83  | 111.64      | 105.89   |
| 23  | D     | 401 | PHO  | C4D-CHA-C1A | -4.79 | 123.87      | 129.57   |
| 30  | a     | 401 | SQD  | O9-S-C6     | 4.75  | 111.03      | 106.83   |
| 30  | d     | 403 | SQD  | O6-C1-C2    | 4.72  | 114.20      | 108.15   |
| 26  | A     | 409 | DGD  | O3G-C3G-C2G | -4.70 | 99.80       | 110.99   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | f     | 103 | SQD  | O9-S-C6     | 4.62  | 110.91      | 106.83   |
| 26  | b     | 625 | DGD  | CDB-CCB-CBB | -4.59 | 99.83       | 112.94   |
| 26  | a     | 408 | DGD  | O3G-C3G-C2G | -4.55 | 100.16      | 110.99   |
| 26  | B     | 620 | DGD  | CDB-CCB-CBB | -4.52 | 100.03      | 112.94   |
| 26  | b     | 601 | DGD  | CDB-CCB-CBB | -4.50 | 100.09      | 112.94   |
| 30  | B     | 622 | SQD  | O9-S-C6     | 4.47  | 110.78      | 106.83   |
| 30  | d     | 403 | SQD  | O8-S-C6     | 4.45  | 111.18      | 105.89   |
| 26  | C     | 516 | DGD  | O3G-C3G-C2G | -4.43 | 100.45      | 110.99   |
| 26  | B     | 626 | DGD  | CDB-CCB-CBB | -4.41 | 100.33      | 112.94   |
| 31  | d     | 409 | LMG  | C1-C2-C3    | -4.40 | 101.46      | 109.99   |
| 31  | D     | 406 | LMG  | C1-C2-C3    | -4.36 | 101.54      | 109.99   |
| 30  | F     | 103 | SQD  | O6-C1-C2    | 4.35  | 113.72      | 108.15   |
| 22  | c     | 507 | CLA  | CMB-C2B-C1B | -4.18 | 122.04      | 128.46   |
| 30  | d     | 403 | SQD  | O5-C5-C4    | 4.17  | 117.49      | 109.73   |
| 30  | f     | 103 | SQD  | O6-C1-C2    | 4.17  | 113.50      | 108.15   |
| 30  | B     | 622 | SQD  | O5-C5-C4    | 4.15  | 117.45      | 109.73   |
| 26  | c     | 517 | DGD  | O3G-C3G-C2G | -4.13 | 101.16      | 110.99   |
| 22  | B     | 612 | CLA  | CMB-C2B-C1B | -4.13 | 122.11      | 128.46   |
| 30  | B     | 622 | SQD  | O8-S-C6     | 4.12  | 110.80      | 105.89   |
| 30  | a     | 401 | SQD  | O8-S-C6     | 4.12  | 110.79      | 105.89   |
| 22  | C     | 507 | CLA  | CMB-C2B-C1B | -4.09 | 122.17      | 128.46   |
| 22  | b     | 617 | CLA  | CMB-C2B-C1B | -4.09 | 122.17      | 128.46   |
| 30  | B     | 627 | SQD  | O8-S-C6     | 4.08  | 110.75      | 105.89   |
| 31  | C     | 517 | LMG  | C40-C39-C38 | -3.92 | 101.74      | 112.94   |
| 22  | B     | 607 | CLA  | CMB-C2B-C1B | -3.92 | 122.44      | 128.46   |
| 30  | A     | 413 | SQD  | O47-C7-C8   | 3.89  | 119.83      | 111.54   |
| 22  | b     | 612 | CLA  | CMB-C2B-C1B | -3.88 | 122.49      | 128.46   |
| 30  | a     | 412 | SQD  | O8-S-C6     | 3.88  | 110.51      | 105.89   |
| 30  | b     | 602 | SQD  | O47-C7-C8   | 3.85  | 119.75      | 111.54   |
| 22  | B     | 609 | CLA  | CMB-C2B-C1B | -3.84 | 122.56      | 128.46   |
| 22  | b     | 614 | CLA  | CMB-C2B-C1B | -3.83 | 122.57      | 128.46   |
| 26  | c     | 516 | DGD  | O5D-C6D-C5D | -3.83 | 102.32      | 108.96   |
| 31  | D     | 406 | LMG  | C40-C39-C38 | -3.83 | 101.99      | 112.94   |
| 31  | c     | 518 | LMG  | C40-C39-C38 | -3.82 | 102.02      | 112.94   |
| 27  | C     | 518 | LHG  | O4-P-O5     | 3.81  | 133.25      | 112.14   |
| 27  | A     | 410 | LHG  | O6-P-O3     | -3.81 | 93.81       | 104.68   |
| 31  | d     | 409 | LMG  | C40-C39-C38 | -3.81 | 102.05      | 112.94   |
| 30  | A     | 413 | SQD  | O8-S-C6     | 3.80  | 110.42      | 105.89   |
| 27  | a     | 409 | LHG  | O4-P-O5     | 3.80  | 133.17      | 112.14   |
| 27  | c     | 519 | LHG  | O4-P-O5     | 3.79  | 133.13      | 112.14   |
| 27  | A     | 410 | LHG  | O4-P-O5     | 3.78  | 133.06      | 112.14   |
| 30  | a     | 412 | SQD  | O47-C7-C8   | 3.77  | 119.57      | 111.54   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | i     | 103 | LMT  | O1'-C1'-C2' | 3.76  | 112.97      | 108.15   |
| 30  | A     | 414 | SQD  | O5-C5-C4    | 3.76  | 116.72      | 109.73   |
| 25  | J     | 102 | BCR  | C11-C10-C9  | -3.76 | 121.86      | 127.29   |
| 30  | b     | 602 | SQD  | O8-S-C6     | 3.75  | 110.36      | 105.89   |
| 30  | A     | 414 | SQD  | O8-S-C6     | 3.75  | 110.35      | 105.89   |
| 30  | B     | 627 | SQD  | O47-C7-C8   | 3.75  | 119.53      | 111.54   |
| 27  | a     | 409 | LHG  | O6-P-O3     | -3.74 | 94.00       | 104.68   |
| 26  | C     | 515 | DGD  | O5D-C6D-C5D | -3.74 | 102.47      | 108.96   |
| 22  | B     | 613 | CLA  | CMB-C2B-C1B | -3.74 | 122.72      | 128.46   |
| 30  | f     | 103 | SQD  | O9-S-O7     | -3.74 | 100.46      | 113.45   |
| 25  | j     | 102 | BCR  | C2-C1-C6    | 3.74  | 116.33      | 110.37   |
| 25  | c     | 513 | BCR  | C2-C1-C6    | 3.73  | 116.32      | 110.37   |
| 25  | K     | 101 | BCR  | C2-C1-C6    | 3.72  | 116.31      | 110.37   |
| 30  | d     | 403 | SQD  | O9-S-O7     | -3.72 | 100.50      | 113.45   |
| 22  | B     | 611 | CLA  | CMB-C2B-C1B | -3.72 | 122.74      | 128.46   |
| 26  | c     | 516 | DGD  | O3G-C3G-C2G | -3.72 | 102.14      | 110.99   |
| 22  | c     | 505 | CLA  | CMB-C2B-C1B | -3.72 | 122.74      | 128.46   |
| 26  | C     | 515 | DGD  | O3G-C3G-C2G | -3.72 | 102.15      | 110.99   |
| 30  | F     | 103 | SQD  | O5-C5-C4    | 3.71  | 116.62      | 109.73   |
| 30  | F     | 103 | SQD  | O9-S-O7     | -3.69 | 100.61      | 113.45   |
| 26  | B     | 626 | DGD  | O5D-C1E-C2E | 3.69  | 112.88      | 108.15   |
| 22  | c     | 506 | CLA  | CMB-C2B-C1B | -3.68 | 122.80      | 128.46   |
| 22  | B     | 601 | CLA  | CMB-C2B-C1B | -3.67 | 122.82      | 128.46   |
| 30  | f     | 103 | SQD  | O5-C5-C4    | 3.67  | 116.56      | 109.73   |
| 30  | B     | 627 | SQD  | O5-C5-C4    | 3.66  | 116.55      | 109.73   |
| 30  | B     | 622 | SQD  | O9-S-O7     | -3.66 | 100.72      | 113.45   |
| 22  | b     | 618 | CLA  | CMB-C2B-C1B | -3.66 | 122.85      | 128.46   |
| 22  | B     | 602 | CLA  | CMB-C2B-C1B | -3.64 | 122.86      | 128.46   |
| 25  | J     | 102 | BCR  | C2-C1-C6    | 3.64  | 116.18      | 110.37   |
| 22  | C     | 505 | CLA  | CMB-C2B-C1B | -3.64 | 122.86      | 128.46   |
| 30  | a     | 412 | SQD  | O9-S-O7     | -3.64 | 100.80      | 113.45   |
| 22  | c     | 508 | CLA  | CMB-C2B-C1B | -3.64 | 122.87      | 128.46   |
| 22  | b     | 605 | CLA  | CMB-C2B-C1B | -3.64 | 122.88      | 128.46   |
| 22  | c     | 512 | CLA  | CMB-C2B-C1B | -3.64 | 122.88      | 128.46   |
| 32  | I     | 102 | LMT  | O1'-C1'-C2' | 3.63  | 112.80      | 108.15   |
| 30  | b     | 602 | SQD  | O5-C5-C4    | 3.63  | 116.48      | 109.73   |
| 22  | c     | 510 | CLA  | CMB-C2B-C1B | -3.62 | 122.90      | 128.46   |
| 22  | b     | 616 | CLA  | CMB-C2B-C1B | -3.62 | 122.90      | 128.46   |
| 22  | A     | 406 | CLA  | CMB-C2B-C1B | -3.62 | 122.90      | 128.46   |
| 26  | b     | 601 | DGD  | O5D-C1E-C2E | 3.62  | 112.79      | 108.15   |
| 26  | d     | 410 | DGD  | O6D-C1D-O3G | -3.61 | 101.32      | 109.93   |
| 30  | A     | 413 | SQD  | O9-S-O7     | -3.61 | 100.90      | 113.45   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | a     | 401 | SQD  | O5-C5-C4    | 3.61  | 116.44      | 109.73   |
| 26  | b     | 625 | DGD  | O3G-C3G-C2G | -3.61 | 102.40      | 110.99   |
| 22  | C     | 510 | CLA  | CMB-C2B-C1B | -3.61 | 122.92      | 128.46   |
| 22  | C     | 508 | CLA  | CMB-C2B-C1B | -3.60 | 122.93      | 128.46   |
| 30  | a     | 401 | SQD  | O9-S-O7     | -3.60 | 100.95      | 113.45   |
| 30  | a     | 412 | SQD  | O5-C5-C4    | 3.59  | 116.41      | 109.73   |
| 22  | C     | 512 | CLA  | CMB-C2B-C1B | -3.58 | 122.96      | 128.46   |
| 22  | c     | 502 | CLA  | CMB-C2B-C1B | -3.57 | 122.97      | 128.46   |
| 30  | b     | 602 | SQD  | O9-S-O7     | -3.57 | 101.04      | 113.45   |
| 22  | b     | 607 | CLA  | CMB-C2B-C1B | -3.57 | 122.98      | 128.46   |
| 30  | A     | 413 | SQD  | O5-C5-C4    | 3.56  | 116.35      | 109.73   |
| 22  | c     | 503 | CLA  | CMB-C2B-C1B | -3.55 | 123.01      | 128.46   |
| 30  | a     | 401 | SQD  | C44-O6-C1   | 3.55  | 120.92      | 113.80   |
| 22  | C     | 502 | CLA  | CMB-C2B-C1B | -3.54 | 123.02      | 128.46   |
| 22  | c     | 509 | CLA  | CMB-C2B-C1B | -3.54 | 123.02      | 128.46   |
| 30  | B     | 627 | SQD  | O9-S-O7     | -3.54 | 101.15      | 113.45   |
| 26  | c     | 515 | DGD  | O3G-C3G-C2G | -3.54 | 102.58      | 110.99   |
| 30  | A     | 414 | SQD  | O9-S-O7     | -3.53 | 101.17      | 113.45   |
| 26  | D     | 407 | DGD  | O6D-C1D-O3G | -3.53 | 101.52      | 109.93   |
| 22  | C     | 503 | CLA  | CMB-C2B-C1B | -3.53 | 123.04      | 128.46   |
| 22  | B     | 605 | CLA  | CMB-C2B-C1B | -3.53 | 123.05      | 128.46   |
| 22  | C     | 509 | CLA  | CMB-C2B-C1B | -3.52 | 123.05      | 128.46   |
| 26  | B     | 620 | DGD  | O3G-C3G-C2G | -3.52 | 102.61      | 110.99   |
| 22  | c     | 520 | CLA  | CMB-C2B-C1B | -3.52 | 123.05      | 128.46   |
| 30  | B     | 622 | SQD  | O47-C7-C8   | 3.52  | 119.04      | 111.54   |
| 22  | a     | 404 | CLA  | CMB-C2B-C1B | -3.51 | 123.07      | 128.46   |
| 22  | C     | 519 | CLA  | CMB-C2B-C1B | -3.51 | 123.08      | 128.46   |
| 31  | c     | 522 | LMG  | C42-C41-C40 | -3.51 | 102.92      | 112.94   |
| 22  | C     | 506 | CLA  | CMB-C2B-C1B | -3.50 | 123.08      | 128.46   |
| 22  | D     | 404 | CLA  | CMB-C2B-C1B | -3.50 | 123.09      | 128.46   |
| 22  | b     | 606 | CLA  | CMB-C2B-C1B | -3.48 | 123.11      | 128.46   |
| 25  | j     | 102 | BCR  | C11-C10-C9  | -3.48 | 122.26      | 127.29   |
| 22  | b     | 609 | CLA  | CMB-C2B-C1B | -3.48 | 123.12      | 128.46   |
| 22  | a     | 406 | CLA  | CMB-C2B-C1B | -3.48 | 123.12      | 128.46   |
| 31  | C     | 521 | LMG  | C42-C41-C40 | -3.47 | 103.02      | 112.94   |
| 22  | C     | 511 | CLA  | CMB-C2B-C1B | -3.46 | 123.15      | 128.46   |
| 30  | d     | 403 | SQD  | O47-C7-C8   | 3.45  | 118.90      | 111.54   |
| 22  | A     | 402 | CLA  | CMB-C2B-C1B | -3.45 | 123.16      | 128.46   |
| 22  | a     | 403 | CLA  | CMB-C2B-C1B | -3.45 | 123.17      | 128.46   |
| 30  | F     | 103 | SQD  | O47-C7-C8   | 3.43  | 118.85      | 111.54   |
| 22  | c     | 511 | CLA  | CMB-C2B-C1B | -3.43 | 123.19      | 128.46   |
| 22  | B     | 604 | CLA  | CMB-C2B-C1B | -3.42 | 123.20      | 128.46   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 26  | C     | 514 | DGD  | O3G-C3G-C2G | -3.40 | 102.89      | 110.99   |
| 27  | c     | 519 | LHG  | O6-P-O3     | -3.39 | 95.01       | 104.68   |
| 22  | B     | 614 | CLA  | CMB-C2B-C1B | -3.39 | 123.25      | 128.46   |
| 22  | D     | 403 | CLA  | CMB-C2B-C1B | -3.38 | 123.28      | 128.46   |
| 30  | A     | 414 | SQD  | O47-C7-C8   | 3.37  | 118.72      | 111.54   |
| 22  | d     | 406 | CLA  | CMB-C2B-C1B | -3.36 | 123.29      | 128.46   |
| 22  | b     | 619 | CLA  | CMB-C2B-C1B | -3.36 | 123.30      | 128.46   |
| 22  | B     | 606 | CLA  | CMB-C2B-C1B | -3.35 | 123.31      | 128.46   |
| 22  | A     | 403 | CLA  | CMB-C2B-C1B | -3.34 | 123.34      | 128.46   |
| 22  | B     | 603 | CLA  | CMB-C2B-C1B | -3.33 | 123.34      | 128.46   |
| 22  | B     | 603 | CLA  | CBD-CHA-C1A | 3.33  | 133.12      | 128.77   |
| 22  | b     | 608 | CLA  | CMB-C2B-C1B | -3.32 | 123.36      | 128.46   |
| 22  | a     | 405 | CLA  | CMB-C2B-C1B | -3.32 | 123.37      | 128.46   |
| 22  | A     | 404 | CLA  | CMB-C2B-C1B | -3.31 | 123.38      | 128.46   |
| 26  | b     | 625 | DGD  | O6D-C1D-O3G | -3.30 | 102.06      | 109.93   |
| 27  | C     | 518 | LHG  | O6-P-O3     | -3.30 | 95.27       | 104.68   |
| 25  | j     | 102 | BCR  | C7-C8-C9    | -3.30 | 121.28      | 126.22   |
| 22  | B     | 615 | CLA  | CMB-C2B-C1B | -3.30 | 123.40      | 128.46   |
| 22  | d     | 405 | CLA  | CMB-C2B-C1B | -3.30 | 123.40      | 128.46   |
| 22  | c     | 503 | CLA  | O2D-CGD-O1D | -3.30 | 117.17      | 123.79   |
| 22  | b     | 611 | CLA  | CMB-C2B-C1B | -3.29 | 123.41      | 128.46   |
| 30  | A     | 414 | SQD  | C44-O6-C1   | 3.28  | 120.39      | 113.80   |
| 25  | A     | 408 | BCR  | C2-C1-C6    | 3.28  | 115.61      | 110.37   |
| 22  | b     | 610 | CLA  | CMB-C2B-C1B | -3.28 | 123.43      | 128.46   |
| 22  | b     | 618 | CLA  | O2D-CGD-O1D | -3.27 | 117.22      | 123.79   |
| 30  | B     | 627 | SQD  | C3-C4-C5    | 3.25  | 116.00      | 110.17   |
| 22  | B     | 612 | CLA  | CMB-C2B-C3B | 3.24  | 131.28      | 125.16   |
| 34  | f     | 101 | HEM  | CBD-CAD-C3D | -3.23 | 107.49      | 114.51   |
| 22  | H     | 101 | CLA  | CMB-C2B-C1B | -3.22 | 123.51      | 128.46   |
| 26  | B     | 620 | DGD  | O6D-C1D-O3G | -3.22 | 102.26      | 109.93   |
| 24  | J     | 101 | PL9  | C7-C8-C9    | -3.21 | 121.33      | 126.76   |
| 27  | A     | 410 | LHG  | C9-C10-C11  | -3.21 | 100.82      | 113.73   |
| 30  | a     | 401 | SQD  | O47-C7-C8   | 3.21  | 118.38      | 111.54   |
| 26  | c     | 517 | DGD  | O5D-C6D-C5D | -3.21 | 103.40      | 108.96   |
| 22  | B     | 608 | CLA  | CMB-C2B-C1B | -3.21 | 123.54      | 128.46   |
| 30  | f     | 103 | SQD  | O47-C7-C8   | 3.20  | 118.37      | 111.54   |
| 22  | b     | 620 | CLA  | CMB-C2B-C1B | -3.20 | 123.55      | 128.46   |
| 32  | b     | 604 | LMT  | C1'-O5'-C5' | -3.19 | 107.55      | 113.73   |
| 22  | B     | 610 | CLA  | CMB-C2B-C3B | 3.19  | 131.17      | 125.16   |
| 25  | J     | 102 | BCR  | C7-C8-C9    | -3.18 | 121.45      | 126.22   |
| 25  | J     | 102 | BCR  | C24-C23-C22 | -3.18 | 121.46      | 126.22   |
| 32  | B     | 629 | LMT  | C1'-O5'-C5' | -3.17 | 107.60      | 113.73   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | b     | 613 | CLA  | CMB-C2B-C1B | -3.17 | 123.59      | 128.46   |
| 26  | c     | 516 | DGD  | O6D-C1D-O3G | -3.16 | 102.42      | 109.93   |
| 22  | C     | 503 | CLA  | O2D-CGD-O1D | -3.16 | 117.45      | 123.79   |
| 27  | a     | 409 | LHG  | C9-C10-C11  | -3.15 | 101.06      | 113.73   |
| 24  | d     | 407 | PL9  | C40-C39-C41 | 3.15  | 120.17      | 115.39   |
| 24  | j     | 101 | PL9  | C7-C8-C9    | -3.14 | 121.45      | 126.76   |
| 22  | B     | 603 | CLA  | O2D-CGD-O1D | -3.14 | 117.48      | 123.79   |
| 22  | b     | 608 | CLA  | CBD-CHA-C1A | 3.14  | 132.87      | 128.77   |
| 22  | B     | 613 | CLA  | O2D-CGD-O1D | -3.14 | 117.49      | 123.79   |
| 26  | C     | 516 | DGD  | O5D-C6D-C5D | -3.12 | 103.55      | 108.96   |
| 26  | d     | 410 | DGD  | O3G-C3G-C2G | -3.12 | 103.56      | 110.99   |
| 22  | c     | 504 | CLA  | O2D-CGD-O1D | -3.12 | 117.53      | 123.79   |
| 25  | b     | 623 | BCR  | C24-C23-C22 | -3.12 | 121.55      | 126.22   |
| 31  | D     | 409 | LMG  | C38-C39-C40 | -3.11 | 101.20      | 113.73   |
| 25  | B     | 618 | BCR  | C2-C1-C6    | 3.11  | 115.33      | 110.37   |
| 24  | A     | 407 | PL9  | C22-C23-C24 | -3.11 | 121.09      | 127.81   |
| 25  | B     | 617 | BCR  | C15-C16-C17 | -3.11 | 116.61      | 123.45   |
| 30  | d     | 403 | SQD  | C3-C4-C5    | 3.10  | 115.73      | 110.17   |
| 22  | B     | 604 | CLA  | CHD-C4C-NC  | 3.10  | 126.45      | 124.28   |
| 22  | b     | 617 | CLA  | CMB-C2B-C3B | 3.10  | 130.99      | 125.16   |
| 27  | C     | 518 | LHG  | C18-C17-C16 | -3.08 | 104.12      | 112.94   |
| 31  | d     | 412 | LMG  | C38-C39-C40 | -3.08 | 101.32      | 113.73   |
| 24  | j     | 101 | PL9  | C27-C28-C29 | -3.07 | 121.20      | 128.69   |
| 24  | a     | 407 | PL9  | C22-C23-C24 | -3.07 | 121.17      | 127.81   |
| 22  | b     | 615 | CLA  | CMB-C2B-C3B | 3.07  | 130.95      | 125.16   |
| 22  | C     | 510 | CLA  | CBD-CHA-C1A | 3.07  | 132.78      | 128.77   |
| 31  | d     | 408 | LMG  | C38-C39-C40 | -3.07 | 101.39      | 113.73   |
| 27  | c     | 519 | LHG  | C18-C17-C16 | -3.07 | 104.18      | 112.94   |
| 30  | B     | 622 | SQD  | C3-C4-C5    | 3.06  | 115.66      | 110.17   |
| 22  | C     | 502 | CLA  | O2D-CGD-O1D | -3.05 | 117.67      | 123.79   |
| 22  | c     | 504 | CLA  | CMB-C2B-C1B | -3.05 | 123.78      | 128.46   |
| 26  | D     | 407 | DGD  | O3G-C3G-C2G | -3.04 | 103.75      | 110.99   |
| 22  | c     | 507 | CLA  | CMB-C2B-C3B | 3.04  | 130.90      | 125.16   |
| 31  | B     | 625 | LMG  | C38-C39-C40 | -3.04 | 101.49      | 113.73   |
| 25  | J     | 102 | BCR  | C27-C26-C25 | 3.04  | 126.88      | 122.86   |
| 25  | B     | 617 | BCR  | C33-C5-C6   | -3.04 | 121.06      | 124.50   |
| 25  | i     | 101 | BCR  | C2-C1-C6    | 3.04  | 115.22      | 110.37   |
| 26  | A     | 409 | DGD  | O6D-C1D-O3G | -3.04 | 102.69      | 109.93   |
| 26  | A     | 409 | DGD  | O5D-C6D-C5D | -3.04 | 103.69      | 108.96   |
| 26  | b     | 601 | DGD  | O3G-C3G-C2G | -3.04 | 103.77      | 110.99   |
| 26  | C     | 516 | DGD  | C1D-C2D-C3D | -3.03 | 104.12      | 109.99   |
| 24  | J     | 101 | PL9  | C27-C28-C29 | -3.03 | 121.31      | 128.69   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | b     | 610 | CLA  | CHD-C4C-NC  | 3.02  | 126.40      | 124.28   |
| 22  | B     | 613 | CLA  | CMB-C2B-C3B | 3.02  | 130.86      | 125.16   |
| 25  | j     | 102 | BCR  | C27-C26-C25 | 3.02  | 126.85      | 122.86   |
| 22  | C     | 507 | CLA  | O2D-CGD-O1D | -3.02 | 117.73      | 123.79   |
| 25  | b     | 622 | BCR  | C33-C5-C6   | -3.02 | 121.09      | 124.50   |
| 31  | B     | 625 | LMG  | O6-C1-O1    | -3.02 | 102.75      | 109.93   |
| 30  | B     | 622 | SQD  | C44-O6-C1   | 3.01  | 119.85      | 113.80   |
| 30  | f     | 103 | SQD  | C44-O6-C1   | 3.01  | 119.85      | 113.80   |
| 30  | F     | 103 | SQD  | C44-O6-C1   | 3.01  | 119.84      | 113.80   |
| 22  | B     | 607 | CLA  | CMB-C2B-C3B | 3.01  | 130.83      | 125.16   |
| 25  | x     | 101 | BCR  | C33-C5-C6   | -3.00 | 121.11      | 124.50   |
| 22  | B     | 604 | CLA  | O2D-CGD-O1D | -3.00 | 117.77      | 123.79   |
| 31  | e     | 101 | LMG  | C36-C37-C38 | -3.00 | 101.67      | 113.73   |
| 25  | j     | 102 | BCR  | C24-C23-C22 | -2.99 | 121.74      | 126.22   |
| 22  | C     | 504 | CLA  | O2D-CGD-O1D | -2.99 | 117.78      | 123.79   |
| 27  | c     | 519 | LHG  | O3-C3-C2    | -2.99 | 98.89       | 108.54   |
| 32  | M     | 102 | LMT  | C1'-O5'-C5' | -2.99 | 107.95      | 113.73   |
| 25  | b     | 623 | BCR  | C2-C1-C6    | 2.99  | 115.14      | 110.37   |
| 25  | b     | 622 | BCR  | C15-C16-C17 | -2.99 | 116.87      | 123.45   |
| 30  | a     | 412 | SQD  | C3-C4-C5    | 2.99  | 115.53      | 110.17   |
| 22  | a     | 403 | CLA  | O2D-CGD-O1D | -2.99 | 117.80      | 123.79   |
| 22  | B     | 605 | CLA  | O2D-CGD-O1D | -2.99 | 117.80      | 123.79   |
| 25  | J     | 102 | BCR  | C35-C13-C14 | -2.98 | 118.67      | 122.92   |
| 25  | g     | 101 | BCR  | C27-C26-C25 | 2.98  | 126.79      | 122.86   |
| 22  | b     | 617 | CLA  | C4B-C3B-CAB | -2.98 | 121.15      | 127.18   |
| 26  | C     | 515 | DGD  | O6D-C1D-O3G | -2.98 | 102.84      | 109.93   |
| 22  | B     | 612 | CLA  | C4B-C3B-CAB | -2.97 | 121.15      | 127.18   |
| 31  | E     | 101 | LMG  | C36-C37-C38 | -2.97 | 101.77      | 113.73   |
| 26  | c     | 515 | DGD  | O6D-C1D-O3G | -2.97 | 102.86      | 109.93   |
| 26  | B     | 626 | DGD  | O3G-C3G-C2G | -2.96 | 103.95      | 110.99   |
| 22  | B     | 608 | CLA  | O2D-CGD-O1D | -2.96 | 117.85      | 123.79   |
| 25  | F     | 102 | BCR  | C33-C5-C6   | -2.96 | 121.16      | 124.50   |
| 25  | y     | 101 | BCR  | C27-C26-C25 | 2.96  | 126.76      | 122.86   |
| 22  | B     | 606 | CLA  | O2D-CGD-O1D | -2.95 | 117.86      | 123.79   |
| 25  | B     | 618 | BCR  | C24-C23-C22 | -2.95 | 121.79      | 126.22   |
| 25  | H     | 102 | BCR  | C33-C5-C6   | -2.95 | 121.16      | 124.50   |
| 22  | C     | 509 | CLA  | CHD-C4C-NC  | 2.95  | 126.34      | 124.28   |
| 22  | c     | 506 | CLA  | CMB-C2B-C3B | 2.94  | 130.71      | 125.16   |
| 22  | c     | 507 | CLA  | O2D-CGD-O1D | -2.94 | 117.89      | 123.79   |
| 24  | d     | 407 | PL9  | C22-C23-C24 | -2.94 | 121.45      | 127.81   |
| 22  | b     | 612 | CLA  | CMB-C2B-C3B | 2.94  | 130.70      | 125.16   |
| 22  | B     | 609 | CLA  | CMB-C2B-C3B | 2.93  | 130.69      | 125.16   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | b     | 624 | BCR  | C7-C8-C9    | -2.93 | 121.83      | 126.22   |
| 24  | D     | 405 | PL9  | C22-C23-C24 | -2.93 | 121.47      | 127.81   |
| 22  | a     | 405 | CLA  | O2D-CGD-O1D | -2.93 | 117.90      | 123.79   |
| 25  | b     | 624 | BCR  | C3-C4-C5    | -2.93 | 109.00      | 113.81   |
| 24  | D     | 405 | PL9  | C40-C39-C41 | 2.93  | 119.83      | 115.39   |
| 22  | b     | 607 | CLA  | O2D-CGD-O1D | -2.93 | 117.91      | 123.79   |
| 24  | d     | 407 | PL9  | C7-C8-C9    | -2.93 | 121.81      | 126.76   |
| 32  | b     | 629 | LMT  | C3'-C4'-C5' | -2.92 | 104.32      | 110.86   |
| 22  | B     | 610 | CLA  | CBD-CHA-C1A | 2.93  | 132.59      | 128.77   |
| 22  | c     | 510 | CLA  | O2D-CGD-O1D | -2.92 | 117.92      | 123.79   |
| 32  | B     | 624 | LMT  | C3'-C4'-C5' | -2.92 | 104.33      | 110.86   |
| 22  | c     | 502 | CLA  | CBD-CHA-C1A | 2.92  | 132.58      | 128.77   |
| 25  | f     | 102 | BCR  | C33-C5-C6   | -2.92 | 121.20      | 124.50   |
| 22  | C     | 511 | CLA  | C3D-C4D-CHA | 2.91  | 112.84      | 108.16   |
| 25  | g     | 101 | BCR  | C38-C26-C25 | -2.91 | 121.21      | 124.50   |
| 22  | B     | 603 | CLA  | C3D-C4D-CHA | 2.91  | 112.83      | 108.16   |
| 31  | d     | 408 | LMG  | O6-C1-O1    | -2.91 | 103.00      | 109.93   |
| 27  | a     | 409 | LHG  | O8-C23-C24  | 2.91  | 120.81      | 111.90   |
| 22  | c     | 506 | CLA  | C3D-C4D-CHA | 2.91  | 112.83      | 108.16   |
| 22  | b     | 614 | CLA  | O2D-CGD-O1D | -2.90 | 117.96      | 123.79   |
| 22  | B     | 602 | CLA  | CMB-C2B-C3B | 2.90  | 130.63      | 125.16   |
| 22  | C     | 504 | CLA  | CMB-C2B-C1B | -2.90 | 124.00      | 128.46   |
| 22  | b     | 609 | CLA  | CHB-C4A-NA  | 2.90  | 128.42      | 124.38   |
| 22  | b     | 613 | CLA  | O2D-CGD-O1D | -2.89 | 117.98      | 123.79   |
| 24  | J     | 101 | PL9  | C22-C23-C24 | -2.89 | 121.55      | 127.81   |
| 22  | B     | 612 | CLA  | C3D-C4D-CHA | 2.89  | 112.80      | 108.16   |
| 22  | B     | 602 | CLA  | O2D-CGD-O1D | -2.89 | 117.99      | 123.79   |
| 22  | b     | 612 | CLA  | O2D-CGD-O1D | -2.89 | 117.99      | 123.79   |
| 22  | A     | 403 | CLA  | O2D-CGD-O1D | -2.89 | 118.00      | 123.79   |
| 22  | C     | 511 | CLA  | CBD-CHA-C1A | 2.89  | 132.54      | 128.77   |
| 24  | j     | 101 | PL9  | C22-C23-C24 | -2.89 | 121.57      | 127.81   |
| 22  | A     | 402 | CLA  | CHD-C4C-NC  | 2.89  | 126.30      | 124.28   |
| 27  | a     | 409 | LHG  | O3-C3-C2    | -2.89 | 99.22       | 108.54   |
| 22  | b     | 608 | CLA  | C3D-C4D-CHA | 2.88  | 112.79      | 108.16   |
| 22  | C     | 505 | CLA  | O2D-CGD-O1D | -2.88 | 118.00      | 123.79   |
| 22  | c     | 511 | CLA  | C3D-C4D-CHA | 2.88  | 112.79      | 108.16   |
| 22  | C     | 501 | CLA  | O2D-CGD-O1D | -2.88 | 118.00      | 123.79   |
| 22  | C     | 507 | CLA  | CMB-C2B-C3B | 2.88  | 130.59      | 125.16   |
| 22  | B     | 605 | CLA  | CHD-C4C-NC  | 2.88  | 126.30      | 124.28   |
| 26  | C     | 516 | DGD  | CDB-CCB-CBB | -2.88 | 99.27       | 114.56   |
| 22  | b     | 605 | CLA  | O2D-CGD-O1D | -2.88 | 118.01      | 123.79   |
| 22  | B     | 611 | CLA  | C2D-C3D-CAD | 2.88  | 146.68      | 134.94   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 27  | A     | 410 | LHG  | O8-C23-C24  | 2.88  | 120.71      | 111.90   |
| 22  | b     | 609 | CLA  | CBD-CHA-C1A | 2.88  | 132.53      | 128.77   |
| 22  | b     | 615 | CLA  | CBD-CHA-C1A | 2.87  | 132.53      | 128.77   |
| 22  | b     | 610 | CLA  | CBD-CHA-C1A | 2.87  | 132.53      | 128.77   |
| 22  | c     | 520 | CLA  | O2D-CGD-O1D | -2.87 | 118.02      | 123.79   |
| 22  | C     | 506 | CLA  | C3D-C4D-CHA | 2.87  | 112.77      | 108.16   |
| 26  | c     | 517 | DGD  | C1D-O6D-C5D | -2.87 | 108.18      | 113.73   |
| 26  | b     | 601 | DGD  | C1D-C2D-C3D | -2.87 | 104.44      | 109.99   |
| 22  | b     | 607 | CLA  | CMB-C2B-C3B | 2.87  | 130.56      | 125.16   |
| 30  | b     | 602 | SQD  | C3-C4-C5    | 2.87  | 115.32      | 110.17   |
| 22  | A     | 402 | CLA  | O2D-CGD-O1D | -2.87 | 118.03      | 123.79   |
| 22  | c     | 505 | CLA  | O2D-CGD-O1D | -2.87 | 118.03      | 123.79   |
| 22  | c     | 505 | CLA  | C3D-C4D-CHA | 2.87  | 112.76      | 108.16   |
| 22  | b     | 606 | CLA  | C3D-C4D-CHA | 2.87  | 112.76      | 108.16   |
| 26  | d     | 410 | DGD  | C3D-C4D-C5D | -2.86 | 105.03      | 110.17   |
| 32  | B     | 628 | LMT  | C1'-O5'-C5' | -2.86 | 108.20      | 113.73   |
| 26  | a     | 408 | DGD  | O6D-C1D-O3G | -2.86 | 103.12      | 109.93   |
| 22  | C     | 506 | CLA  | CBD-CHA-C1A | 2.86  | 132.51      | 128.77   |
| 22  | b     | 608 | CLA  | O2D-CGD-O1D | -2.86 | 118.05      | 123.79   |
| 25  | B     | 617 | BCR  | C28-C27-C26 | -2.86 | 109.11      | 113.81   |
| 22  | b     | 610 | CLA  | O2D-CGD-O1D | -2.86 | 118.05      | 123.79   |
| 22  | c     | 505 | CLA  | CMB-C2B-C3B | 2.86  | 130.55      | 125.16   |
| 22  | b     | 614 | CLA  | CMB-C2B-C3B | 2.86  | 130.54      | 125.16   |
| 22  | D     | 403 | CLA  | C3D-C4D-CHA | 2.86  | 112.74      | 108.16   |
| 27  | A     | 410 | LHG  | O3-C3-C2    | -2.86 | 99.32       | 108.54   |
| 26  | c     | 517 | DGD  | CDB-CCB-CBB | -2.86 | 99.40       | 114.56   |
| 22  | B     | 601 | CLA  | C3D-C4D-CHA | 2.85  | 112.74      | 108.16   |
| 22  | c     | 508 | CLA  | CBD-CHA-C1A | 2.85  | 132.49      | 128.77   |
| 26  | C     | 514 | DGD  | O6D-C1D-O3G | -2.85 | 103.14      | 109.93   |
| 22  | c     | 502 | CLA  | O2D-CGD-O1D | -2.85 | 118.07      | 123.79   |
| 22  | B     | 608 | CLA  | C3D-C4D-CHA | 2.85  | 112.73      | 108.16   |
| 22  | b     | 613 | CLA  | C3D-C4D-CHA | 2.85  | 112.73      | 108.16   |
| 25  | B     | 619 | BCR  | C3-C4-C5    | -2.84 | 109.14      | 113.81   |
| 26  | c     | 517 | DGD  | C1D-C2D-C3D | -2.85 | 104.48      | 109.99   |
| 22  | C     | 510 | CLA  | C3D-C4D-CHA | 2.84  | 112.72      | 108.16   |
| 22  | B     | 601 | CLA  | O2D-CGD-O1D | -2.84 | 118.08      | 123.79   |
| 22  | b     | 608 | CLA  | CHB-C4A-NA  | 2.84  | 128.34      | 124.38   |
| 22  | B     | 602 | CLA  | C3D-C4D-CHA | 2.84  | 112.71      | 108.16   |
| 22  | c     | 512 | CLA  | O2D-CGD-O1D | -2.84 | 118.09      | 123.79   |
| 24  | d     | 407 | PL9  | C37-C38-C39 | -2.84 | 121.67      | 127.81   |
| 25  | B     | 619 | BCR  | C7-C8-C9    | -2.84 | 121.97      | 126.22   |
| 31  | m     | 101 | LMG  | C22-C21-C20 | -2.84 | 104.83      | 112.94   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | C     | 510 | CLA  | CHB-C4A-NA  | 2.83  | 128.34      | 124.38   |
| 30  | d     | 403 | SQD  | C44-O6-C1   | 2.83  | 119.49      | 113.80   |
| 22  | A     | 404 | CLA  | O2D-CGD-O1D | -2.83 | 118.11      | 123.79   |
| 25  | b     | 622 | BCR  | C28-C27-C26 | -2.83 | 109.16      | 113.81   |
| 22  | C     | 505 | CLA  | CMB-C2B-C3B | 2.83  | 130.50      | 125.16   |
| 25  | J     | 102 | BCR  | C15-C14-C13 | -2.83 | 123.20      | 127.29   |
| 27  | C     | 518 | LHG  | O3-C3-C2    | -2.83 | 99.41       | 108.54   |
| 22  | c     | 510 | CLA  | C3D-C4D-CHA | 2.83  | 112.70      | 108.16   |
| 22  | C     | 519 | CLA  | C3D-C4D-CHA | 2.83  | 112.69      | 108.16   |
| 22  | b     | 616 | CLA  | C2D-C3D-CAD | 2.83  | 146.46      | 134.94   |
| 22  | C     | 503 | CLA  | CHD-C4C-NC  | 2.83  | 126.26      | 124.28   |
| 22  | c     | 507 | CLA  | C3D-C4D-CHA | 2.82  | 112.69      | 108.16   |
| 22  | c     | 509 | CLA  | CHD-C4C-NC  | 2.82  | 126.25      | 124.28   |
| 25  | b     | 624 | BCR  | C2-C1-C6    | 2.82  | 114.86      | 110.37   |
| 24  | D     | 405 | PL9  | C7-C8-C9    | -2.81 | 122.00      | 126.76   |
| 22  | B     | 602 | CLA  | C4B-C3B-CAB | -2.81 | 121.49      | 127.18   |
| 22  | b     | 607 | CLA  | C3D-C4D-CHA | 2.81  | 112.67      | 108.16   |
| 22  | C     | 507 | CLA  | CBD-CHA-C1A | 2.81  | 132.45      | 128.77   |
| 22  | C     | 505 | CLA  | C3D-C4D-CHA | 2.81  | 112.67      | 108.16   |
| 30  | b     | 602 | SQD  | C4-C3-C2    | 2.81  | 115.98      | 110.80   |
| 22  | c     | 503 | CLA  | CBD-CHA-C1A | 2.81  | 132.44      | 128.77   |
| 25  | B     | 619 | BCR  | C2-C1-C6    | 2.81  | 114.85      | 110.37   |
| 25  | F     | 102 | BCR  | C29-C30-C25 | 2.81  | 114.85      | 110.37   |
| 22  | B     | 604 | CLA  | CHB-C4A-NA  | 2.81  | 128.29      | 124.38   |
| 22  | b     | 609 | CLA  | CHD-C4C-NC  | 2.81  | 126.24      | 124.28   |
| 25  | c     | 521 | BCR  | C15-C16-C17 | -2.80 | 117.27      | 123.45   |
| 22  | D     | 404 | CLA  | C2D-C3D-CAD | 2.80  | 146.37      | 134.94   |
| 22  | B     | 605 | CLA  | CHB-C4A-NA  | 2.80  | 128.29      | 124.38   |
| 22  | c     | 502 | CLA  | C3D-C4D-CHA | 2.80  | 112.65      | 108.16   |
| 22  | c     | 504 | CLA  | C2D-C3D-CAD | 2.80  | 146.36      | 134.94   |
| 22  | B     | 609 | CLA  | O2D-CGD-O1D | -2.80 | 118.17      | 123.79   |
| 31  | a     | 402 | LMG  | C22-C21-C20 | -2.80 | 104.94      | 112.94   |
| 22  | c     | 501 | CLA  | O2D-CGD-O1D | -2.80 | 118.17      | 123.79   |
| 22  | c     | 508 | CLA  | C3D-C4D-CHA | 2.80  | 112.65      | 108.16   |
| 22  | a     | 406 | CLA  | C3D-C4D-CHA | 2.79  | 112.64      | 108.16   |
| 22  | B     | 615 | CLA  | C3D-C4D-CHA | 2.79  | 112.64      | 108.16   |
| 22  | b     | 614 | CLA  | C2D-C3D-CAD | 2.79  | 146.32      | 134.94   |
| 22  | b     | 611 | CLA  | C2D-C3D-CAD | 2.79  | 146.32      | 134.94   |
| 27  | C     | 518 | LHG  | C27-C28-C29 | -2.79 | 102.50      | 113.73   |
| 32  | b     | 628 | LMT  | C1'-O5'-C5' | -2.79 | 108.34      | 113.73   |
| 22  | a     | 403 | CLA  | C2D-C3D-CAD | 2.79  | 146.31      | 134.94   |
| 22  | C     | 503 | CLA  | C3D-C4D-CHA | 2.79  | 112.63      | 108.16   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | C     | 504 | CLA  | C3D-C4D-CHA | 2.79  | 112.63      | 108.16   |
| 22  | B     | 606 | CLA  | C2D-C3D-CAD | 2.79  | 146.30      | 134.94   |
| 30  | A     | 413 | SQD  | C3-C4-C5    | 2.79  | 115.17      | 110.17   |
| 22  | b     | 605 | CLA  | C3D-C4D-CHA | 2.79  | 112.63      | 108.16   |
| 25  | g     | 101 | BCR  | C7-C8-C9    | -2.79 | 122.05      | 126.22   |
| 22  | b     | 620 | CLA  | CHD-C4C-NC  | 2.79  | 126.23      | 124.28   |
| 22  | b     | 619 | CLA  | CBD-CHA-C1A | 2.78  | 132.41      | 128.77   |
| 26  | B     | 626 | DGD  | C3G-C2G-C1G | -2.78 | 105.47      | 111.86   |
| 25  | f     | 102 | BCR  | C29-C30-C25 | 2.78  | 114.81      | 110.37   |
| 31  | d     | 412 | LMG  | C22-C21-C20 | -2.78 | 104.99      | 112.94   |
| 25  | K     | 101 | BCR  | C24-C23-C22 | -2.78 | 122.05      | 126.22   |
| 22  | B     | 610 | CLA  | O2D-CGD-O1D | -2.78 | 118.20      | 123.79   |
| 31  | e     | 101 | LMG  | C22-C21-C20 | -2.78 | 104.99      | 112.94   |
| 31  | E     | 101 | LMG  | C22-C21-C20 | -2.78 | 104.99      | 112.94   |
| 25  | y     | 101 | BCR  | C38-C26-C25 | -2.78 | 121.36      | 124.50   |
| 26  | b     | 601 | DGD  | C3G-C2G-C1G | -2.78 | 105.48      | 111.86   |
| 22  | b     | 609 | CLA  | O2D-CGD-O1D | -2.78 | 118.21      | 123.79   |
| 22  | c     | 511 | CLA  | CBD-CHA-C1A | 2.78  | 132.40      | 128.77   |
| 22  | C     | 510 | CLA  | O2D-CGD-O1D | -2.78 | 118.21      | 123.79   |
| 22  | C     | 507 | CLA  | C3D-C4D-CHA | 2.78  | 112.62      | 108.16   |
| 22  | b     | 610 | CLA  | C3D-C4D-CHA | 2.78  | 112.61      | 108.16   |
| 22  | c     | 520 | CLA  | C2D-C3D-CAD | 2.78  | 146.26      | 134.94   |
| 22  | b     | 618 | CLA  | CBD-CHA-C1A | 2.78  | 132.40      | 128.77   |
| 22  | a     | 405 | CLA  | C2D-C3D-CAD | 2.78  | 146.26      | 134.94   |
| 22  | C     | 506 | CLA  | CMB-C2B-C3B | 2.78  | 130.39      | 125.16   |
| 22  | b     | 615 | CLA  | C3D-C4D-CHA | 2.78  | 112.61      | 108.16   |
| 22  | B     | 611 | CLA  | CMB-C2B-C3B | 2.77  | 130.39      | 125.16   |
| 25  | C     | 513 | BCR  | C15-C16-C17 | -2.77 | 117.34      | 123.45   |
| 22  | C     | 505 | CLA  | C2D-C3D-CAD | 2.77  | 146.25      | 134.94   |
| 22  | b     | 605 | CLA  | C2D-C3D-CAD | 2.77  | 146.25      | 134.94   |
| 22  | A     | 403 | CLA  | CHB-C4A-NA  | 2.77  | 128.25      | 124.38   |
| 22  | C     | 502 | CLA  | C3D-C4D-CHA | 2.77  | 112.61      | 108.16   |
| 22  | c     | 511 | CLA  | O2D-CGD-O1D | -2.77 | 118.22      | 123.79   |
| 22  | b     | 618 | CLA  | CMB-C2B-C3B | 2.77  | 130.38      | 125.16   |
| 31  | M     | 101 | LMG  | C22-C21-C20 | -2.77 | 105.02      | 112.94   |
| 22  | B     | 613 | CLA  | C4B-C3B-CAB | -2.77 | 121.57      | 127.18   |
| 22  | d     | 406 | CLA  | C2D-C3D-CAD | 2.77  | 146.23      | 134.94   |
| 22  | A     | 402 | CLA  | C2D-C3D-CAD | 2.77  | 146.24      | 134.94   |
| 22  | C     | 506 | CLA  | O2D-CGD-O1D | -2.77 | 118.23      | 123.79   |
| 22  | B     | 602 | CLA  | CBD-CHA-C1A | 2.77  | 132.39      | 128.77   |
| 22  | c     | 504 | CLA  | C3D-C4D-CHA | 2.77  | 112.60      | 108.16   |
| 22  | B     | 614 | CLA  | C2D-C3D-CAD | 2.77  | 146.23      | 134.94   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | b     | 620 | CLA  | C2D-C3D-CAD | 2.77  | 146.22      | 134.94   |
| 22  | C     | 510 | CLA  | CMB-C2B-C3B | 2.77  | 130.38      | 125.16   |
| 22  | c     | 510 | CLA  | CBD-CHA-C1A | 2.77  | 132.38      | 128.77   |
| 22  | B     | 608 | CLA  | CBD-CHA-C1A | 2.77  | 132.39      | 128.77   |
| 22  | B     | 601 | CLA  | C2D-C3D-CAD | 2.77  | 146.22      | 134.94   |
| 22  | B     | 613 | CLA  | C3D-C4D-CHA | 2.77  | 112.60      | 108.16   |
| 22  | c     | 507 | CLA  | C2D-C3D-CAD | 2.77  | 146.22      | 134.94   |
| 25  | J     | 102 | BCR  | C3-C4-C5    | -2.76 | 109.27      | 113.81   |
| 22  | b     | 606 | CLA  | CMB-C2B-C3B | 2.76  | 130.37      | 125.16   |
| 22  | b     | 611 | CLA  | O2D-CGD-O1D | -2.76 | 118.24      | 123.79   |
| 22  | c     | 506 | CLA  | O2D-CGD-O1D | -2.76 | 118.25      | 123.79   |
| 31  | i     | 102 | LMG  | O6-C1-O1    | -2.76 | 103.36      | 109.93   |
| 22  | C     | 501 | CLA  | CHB-C4A-NA  | 2.76  | 128.23      | 124.38   |
| 22  | c     | 508 | CLA  | CHB-C4A-NA  | 2.76  | 128.23      | 124.38   |
| 22  | A     | 404 | CLA  | C2D-C3D-CAD | 2.76  | 146.19      | 134.94   |
| 25  | B     | 618 | BCR  | C11-C10-C9  | -2.76 | 123.30      | 127.29   |
| 22  | C     | 501 | CLA  | C2D-C3D-CAD | 2.76  | 146.17      | 134.94   |
| 22  | C     | 511 | CLA  | CHB-C4A-NA  | 2.76  | 128.22      | 124.38   |
| 22  | C     | 506 | CLA  | CHB-C4A-NA  | 2.75  | 128.22      | 124.38   |
| 26  | c     | 516 | DGD  | CDB-CCB-CBB | -2.75 | 99.94       | 114.56   |
| 22  | B     | 610 | CLA  | C2D-C3D-CAD | 2.75  | 146.16      | 134.94   |
| 22  | C     | 509 | CLA  | C2D-C3D-CAD | 2.75  | 146.16      | 134.94   |
| 22  | b     | 614 | CLA  | C3D-C4D-CHA | 2.75  | 112.57      | 108.16   |
| 22  | B     | 607 | CLA  | C2D-C3D-CAD | 2.75  | 146.16      | 134.94   |
| 22  | c     | 501 | CLA  | C2D-C3D-CAD | 2.75  | 146.16      | 134.94   |
| 26  | B     | 626 | DGD  | C1D-C2D-C3D | -2.75 | 104.66      | 109.99   |
| 22  | A     | 406 | CLA  | C2D-C3D-CAD | 2.75  | 146.15      | 134.94   |
| 22  | d     | 405 | CLA  | C3D-C4D-CHA | 2.75  | 112.57      | 108.16   |
| 22  | B     | 609 | CLA  | C2D-C3D-CAD | 2.75  | 146.15      | 134.94   |
| 22  | c     | 505 | CLA  | C2D-C3D-CAD | 2.75  | 146.14      | 134.94   |
| 22  | B     | 607 | CLA  | O2D-CGD-O1D | -2.75 | 118.27      | 123.79   |
| 22  | B     | 604 | CLA  | C2D-C3D-CAD | 2.75  | 146.14      | 134.94   |
| 22  | H     | 101 | CLA  | CBD-CHA-C1A | 2.75  | 132.36      | 128.77   |
| 22  | H     | 101 | CLA  | C3D-C4D-CHA | 2.75  | 112.57      | 108.16   |
| 22  | B     | 605 | CLA  | C3D-C4D-CHA | 2.75  | 112.57      | 108.16   |
| 22  | C     | 508 | CLA  | CHD-C4C-NC  | 2.74  | 126.20      | 124.28   |
| 22  | b     | 617 | CLA  | C3D-C4D-CHA | 2.74  | 112.56      | 108.16   |
| 25  | b     | 621 | BCR  | C33-C5-C6   | -2.75 | 121.40      | 124.50   |
| 22  | C     | 504 | CLA  | C2D-C3D-CAD | 2.74  | 146.13      | 134.94   |
| 22  | b     | 610 | CLA  | CHB-C4A-NA  | 2.74  | 128.21      | 124.38   |
| 22  | B     | 603 | CLA  | CHB-C4A-NA  | 2.74  | 128.21      | 124.38   |
| 22  | d     | 405 | CLA  | C2D-C3D-CAD | 2.74  | 146.12      | 134.94   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | c     | 501 | CLA  | CMB-C2B-C1B | -2.74 | 124.25      | 128.46   |
| 22  | b     | 619 | CLA  | C3D-C4D-CHA | 2.74  | 112.56      | 108.16   |
| 26  | d     | 410 | DGD  | CDB-CCB-CBB | -2.74 | 100.02      | 114.56   |
| 22  | b     | 615 | CLA  | C2D-C3D-CAD | 2.74  | 146.10      | 134.94   |
| 22  | c     | 511 | CLA  | C2D-C3D-CAD | 2.74  | 146.10      | 134.94   |
| 22  | b     | 612 | CLA  | C2D-C3D-CAD | 2.73  | 146.09      | 134.94   |
| 22  | C     | 502 | CLA  | C2D-C3D-CAD | 2.74  | 146.09      | 134.94   |
| 31  | b     | 627 | LMG  | C22-C21-C20 | -2.73 | 105.12      | 112.94   |
| 22  | C     | 508 | CLA  | C2D-C3D-CAD | 2.73  | 146.08      | 134.94   |
| 22  | c     | 502 | CLA  | C2D-C3D-CAD | 2.73  | 146.09      | 134.94   |
| 22  | D     | 403 | CLA  | C2D-C3D-CAD | 2.73  | 146.09      | 134.94   |
| 32  | B     | 623 | LMT  | C1'-O5'-C5' | -2.73 | 108.45      | 113.73   |
| 22  | d     | 406 | CLA  | CHD-C4C-NC  | 2.73  | 126.19      | 124.28   |
| 22  | b     | 607 | CLA  | C4B-C3B-CAB | -2.73 | 121.65      | 127.18   |
| 22  | d     | 406 | CLA  | O2D-CGD-O1D | -2.73 | 118.31      | 123.79   |
| 22  | B     | 615 | CLA  | C2D-C3D-CAD | 2.73  | 146.06      | 134.94   |
| 22  | b     | 620 | CLA  | C3D-C4D-CHA | 2.73  | 112.54      | 108.16   |
| 22  | b     | 619 | CLA  | O2D-CGD-O1D | -2.73 | 118.31      | 123.79   |
| 25  | c     | 521 | BCR  | C2-C1-C6    | 2.73  | 114.72      | 110.37   |
| 22  | c     | 512 | CLA  | C3D-C4D-CHA | 2.73  | 112.54      | 108.16   |
| 22  | B     | 606 | CLA  | C3D-C4D-CHA | 2.73  | 112.54      | 108.16   |
| 22  | c     | 507 | CLA  | CBD-CHA-C1A | 2.73  | 132.34      | 128.77   |
| 27  | c     | 519 | LHG  | C27-C28-C29 | -2.73 | 102.76      | 113.73   |
| 22  | b     | 619 | CLA  | C2D-C3D-CAD | 2.72  | 146.05      | 134.94   |
| 22  | B     | 607 | CLA  | C3D-C4D-CHA | 2.73  | 112.53      | 108.16   |
| 22  | c     | 501 | CLA  | CHB-C4A-NA  | 2.73  | 128.18      | 124.38   |
| 22  | a     | 406 | CLA  | CMB-C2B-C3B | 2.72  | 130.29      | 125.16   |
| 24  | D     | 405 | PL9  | C37-C38-C39 | -2.72 | 121.92      | 127.81   |
| 22  | C     | 512 | CLA  | C3D-C4D-CHA | 2.72  | 112.53      | 108.16   |
| 31  | C     | 517 | LMG  | O6-C1-O1    | -2.72 | 103.45      | 109.93   |
| 22  | c     | 506 | CLA  | CHB-C4A-NA  | 2.72  | 128.18      | 124.38   |
| 22  | c     | 511 | CLA  | CHB-C4A-NA  | 2.72  | 128.17      | 124.38   |
| 25  | j     | 102 | BCR  | C35-C13-C14 | -2.71 | 119.05      | 122.92   |
| 22  | a     | 406 | CLA  | C2D-C3D-CAD | 2.72  | 146.01      | 134.94   |
| 26  | D     | 407 | DGD  | CDB-CCB-CBB | -2.72 | 100.14      | 114.56   |
| 22  | C     | 512 | CLA  | C2D-C3D-CAD | 2.72  | 146.01      | 134.94   |
| 22  | c     | 503 | CLA  | C3D-C4D-CHA | 2.71  | 112.52      | 108.16   |
| 22  | C     | 503 | CLA  | CBD-CHA-C1A | 2.71  | 132.32      | 128.77   |
| 26  | C     | 515 | DGD  | CDB-CCB-CBB | -2.72 | 100.14      | 114.56   |
| 22  | A     | 406 | CLA  | CMB-C2B-C3B | 2.71  | 130.28      | 125.16   |
| 22  | B     | 613 | CLA  | C2D-C3D-CAD | 2.71  | 146.00      | 134.94   |
| 22  | b     | 617 | CLA  | CBD-CHA-C1A | 2.71  | 132.31      | 128.77   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | C     | 519 | CLA  | O2D-CGD-O1D | -2.71 | 118.35      | 123.79   |
| 22  | C     | 511 | CLA  | C2D-C3D-CAD | 2.71  | 145.99      | 134.94   |
| 22  | b     | 612 | CLA  | C3D-C4D-CHA | 2.71  | 112.51      | 108.16   |
| 22  | c     | 512 | CLA  | CMB-C2B-C3B | 2.71  | 130.27      | 125.16   |
| 22  | c     | 510 | CLA  | CMB-C2B-C3B | 2.71  | 130.27      | 125.16   |
| 22  | c     | 509 | CLA  | C2D-C3D-CAD | 2.71  | 145.99      | 134.94   |
| 25  | B     | 617 | BCR  | C15-C14-C13 | -2.71 | 123.37      | 127.29   |
| 22  | b     | 609 | CLA  | C2D-C3D-CAD | 2.71  | 145.98      | 134.94   |
| 22  | b     | 608 | CLA  | C1-C2-C3    | -2.71 | 121.53      | 126.23   |
| 22  | B     | 613 | CLA  | CHB-C4A-NA  | 2.71  | 128.16      | 124.38   |
| 22  | A     | 404 | CLA  | C3D-C4D-CHA | 2.71  | 112.50      | 108.16   |
| 25  | C     | 520 | BCR  | C27-C26-C25 | 2.71  | 126.43      | 122.86   |
| 25  | B     | 616 | BCR  | C33-C5-C6   | -2.71 | 121.44      | 124.50   |
| 22  | B     | 602 | CLA  | C2D-C3D-CAD | 2.71  | 145.97      | 134.94   |
| 25  | y     | 101 | BCR  | C7-C8-C9    | -2.70 | 122.17      | 126.22   |
| 22  | b     | 613 | CLA  | C2D-C3D-CAD | 2.71  | 145.97      | 134.94   |
| 22  | B     | 611 | CLA  | C3D-C4D-CHA | 2.70  | 112.50      | 108.16   |
| 30  | a     | 412 | SQD  | C5-C6-S     | -2.70 | 110.62      | 114.40   |
| 22  | b     | 616 | CLA  | CMB-C2B-C3B | 2.70  | 130.25      | 125.16   |
| 31  | c     | 518 | LMG  | O6-C1-O1    | -2.70 | 103.49      | 109.93   |
| 23  | d     | 402 | PHO  | CMB-C2B-C3B | 2.70  | 130.25      | 125.16   |
| 22  | C     | 507 | CLA  | C2D-C3D-CAD | 2.70  | 145.95      | 134.94   |
| 24  | D     | 405 | PL9  | C20-C19-C21 | 2.70  | 119.49      | 115.39   |
| 22  | c     | 508 | CLA  | C2D-C3D-CAD | 2.70  | 145.94      | 134.94   |
| 22  | c     | 512 | CLA  | C2D-C3D-CAD | 2.70  | 145.95      | 134.94   |
| 22  | c     | 503 | CLA  | C2D-C3D-CAD | 2.70  | 145.95      | 134.94   |
| 22  | C     | 508 | CLA  | C3D-C4D-CHA | 2.70  | 112.49      | 108.16   |
| 22  | C     | 511 | CLA  | O2D-CGD-O1D | -2.70 | 118.37      | 123.79   |
| 22  | a     | 404 | CLA  | C2D-C3D-CAD | 2.70  | 145.94      | 134.94   |
| 22  | b     | 617 | CLA  | O2D-CGD-O1D | -2.70 | 118.37      | 123.79   |
| 22  | d     | 406 | CLA  | C3D-C4D-CHA | 2.70  | 112.49      | 108.16   |
| 22  | B     | 605 | CLA  | CBD-CHA-C1A | 2.70  | 132.30      | 128.77   |
| 24  | a     | 407 | PL9  | C37-C38-C39 | -2.70 | 122.12      | 128.69   |
| 22  | A     | 403 | CLA  | C2D-C3D-CAD | 2.70  | 145.93      | 134.94   |
| 22  | B     | 614 | CLA  | C3D-C4D-CHA | 2.70  | 112.49      | 108.16   |
| 24  | d     | 407 | PL9  | C32-C33-C34 | -2.69 | 121.98      | 127.81   |
| 22  | B     | 614 | CLA  | O2D-CGD-O1D | -2.69 | 118.38      | 123.79   |
| 22  | b     | 616 | CLA  | C3D-C4D-CHA | 2.69  | 112.48      | 108.16   |
| 22  | b     | 606 | CLA  | C2D-C3D-CAD | 2.69  | 145.92      | 134.94   |
| 22  | c     | 501 | CLA  | C3D-C4D-CHA | 2.69  | 112.48      | 108.16   |
| 31  | b     | 626 | LMG  | C40-C41-C42 | -2.69 | 102.89      | 113.73   |
| 22  | D     | 404 | CLA  | CMB-C2B-C3B | 2.69  | 130.23      | 125.16   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | D     | 404 | CLA  | CHD-C4C-NC  | 2.69  | 126.16      | 124.28   |
| 30  | B     | 627 | SQD  | C4-C3-C2    | 2.69  | 115.76      | 110.80   |
| 31  | D     | 409 | LMG  | C22-C21-C20 | -2.69 | 105.25      | 112.94   |
| 22  | C     | 512 | CLA  | CBD-CHA-C1A | 2.69  | 132.28      | 128.77   |
| 22  | b     | 619 | CLA  | CHB-C4A-NA  | 2.69  | 128.13      | 124.38   |
| 22  | B     | 605 | CLA  | CMB-C2B-C3B | 2.69  | 130.23      | 125.16   |
| 22  | c     | 502 | CLA  | CMB-C2B-C3B | 2.69  | 130.23      | 125.16   |
| 22  | c     | 506 | CLA  | C4B-C3B-CAB | -2.69 | 121.74      | 127.18   |
| 22  | b     | 606 | CLA  | C1B-CHB-C4A | -2.69 | 124.80      | 130.12   |
| 22  | c     | 520 | CLA  | C3D-C4D-CHA | 2.69  | 112.47      | 108.16   |
| 22  | a     | 405 | CLA  | C3D-C4D-CHA | 2.69  | 112.47      | 108.16   |
| 24  | a     | 407 | PL9  | C27-C28-C29 | -2.68 | 122.00      | 127.81   |
| 22  | B     | 612 | CLA  | CHB-C4A-NA  | 2.69  | 128.13      | 124.38   |
| 22  | a     | 406 | CLA  | CHB-C4A-NA  | 2.68  | 128.12      | 124.38   |
| 22  | c     | 512 | CLA  | CHB-C4A-NA  | 2.68  | 128.12      | 124.38   |
| 22  | b     | 607 | CLA  | C2D-C3D-CAD | 2.68  | 145.88      | 134.94   |
| 22  | b     | 618 | CLA  | C4B-C3B-CAB | -2.68 | 121.75      | 127.18   |
| 23  | D     | 401 | PHO  | O2D-CGD-O1D | -2.68 | 118.41      | 123.79   |
| 22  | C     | 504 | CLA  | CHB-C4A-NA  | 2.68  | 128.12      | 124.38   |
| 22  | c     | 506 | CLA  | C2D-C3D-CAD | 2.68  | 145.87      | 134.94   |
| 22  | C     | 519 | CLA  | C2D-C3D-CAD | 2.68  | 145.85      | 134.94   |
| 22  | B     | 608 | CLA  | C2D-C3D-CAD | 2.68  | 145.86      | 134.94   |
| 22  | b     | 618 | CLA  | C3D-C4D-CHA | 2.68  | 112.46      | 108.16   |
| 22  | c     | 508 | CLA  | CHD-C4C-NC  | 2.68  | 126.15      | 124.28   |
| 22  | b     | 606 | CLA  | CHB-C4A-NA  | 2.68  | 128.12      | 124.38   |
| 22  | b     | 617 | CLA  | C2D-C3D-CAD | 2.68  | 145.85      | 134.94   |
| 22  | b     | 618 | CLA  | C2D-C3D-CAD | 2.68  | 145.85      | 134.94   |
| 22  | H     | 101 | CLA  | C2D-C3D-CAD | 2.67  | 145.85      | 134.94   |
| 22  | c     | 520 | CLA  | CBD-CHA-C1A | 2.67  | 132.27      | 128.77   |
| 23  | D     | 401 | PHO  | CMB-C2B-C3B | 2.68  | 130.20      | 125.16   |
| 22  | C     | 512 | CLA  | CMB-C2B-C3B | 2.67  | 130.20      | 125.16   |
| 31  | E     | 101 | LMG  | C1-C2-C3    | -2.67 | 104.81      | 109.99   |
| 22  | B     | 605 | CLA  | C2D-C3D-CAD | 2.67  | 145.84      | 134.94   |
| 22  | C     | 512 | CLA  | O2D-CGD-O1D | -2.67 | 118.43      | 123.79   |
| 22  | B     | 612 | CLA  | C2D-C3D-CAD | 2.67  | 145.83      | 134.94   |
| 22  | B     | 612 | CLA  | O2D-CGD-O1D | -2.67 | 118.43      | 123.79   |
| 22  | C     | 506 | CLA  | C4B-C3B-CAB | -2.67 | 121.77      | 127.18   |
| 24  | D     | 405 | PL9  | C32-C33-C34 | -2.67 | 122.04      | 127.81   |
| 22  | C     | 503 | CLA  | CHB-C4A-NA  | 2.67  | 128.10      | 124.38   |
| 22  | C     | 503 | CLA  | C2D-C3D-CAD | 2.67  | 145.82      | 134.94   |
| 22  | c     | 510 | CLA  | C2D-C3D-CAD | 2.67  | 145.81      | 134.94   |
| 22  | C     | 519 | CLA  | CHB-C4A-NA  | 2.66  | 128.10      | 124.38   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | C     | 502 | CLA  | CBD-CHA-C1A | 2.66  | 132.25      | 128.77   |
| 22  | A     | 406 | CLA  | C3D-C4D-CHA | 2.66  | 112.44      | 108.16   |
| 23  | d     | 401 | PHO  | O2D-CGD-O1D | -2.67 | 118.44      | 123.79   |
| 27  | c     | 519 | LHG  | O8-C23-C24  | 2.66  | 120.05      | 111.90   |
| 22  | D     | 403 | CLA  | CMB-C2B-C3B | 2.66  | 130.18      | 125.16   |
| 22  | C     | 501 | CLA  | CMB-C2B-C1B | -2.66 | 124.37      | 128.46   |
| 25  | b     | 623 | BCR  | C29-C30-C25 | 2.66  | 114.61      | 110.37   |
| 24  | D     | 405 | PL9  | C27-C28-C29 | -2.66 | 122.06      | 127.81   |
| 22  | C     | 502 | CLA  | CMB-C2B-C3B | 2.66  | 130.17      | 125.16   |
| 22  | d     | 406 | CLA  | CHB-C4A-NA  | 2.66  | 128.09      | 124.38   |
| 22  | c     | 505 | CLA  | CHB-C4A-NA  | 2.66  | 128.09      | 124.38   |
| 22  | c     | 509 | CLA  | C3D-C4D-CHA | 2.66  | 112.43      | 108.16   |
| 32  | d     | 411 | LMT  | C3'-C4'-C5' | -2.66 | 104.92      | 110.86   |
| 22  | b     | 615 | CLA  | O2D-CGD-O1D | -2.66 | 118.46      | 123.79   |
| 22  | c     | 503 | CLA  | CHD-C4C-NC  | 2.66  | 126.14      | 124.28   |
| 25  | C     | 520 | BCR  | C2-C1-C6    | 2.66  | 114.61      | 110.37   |
| 22  | B     | 612 | CLA  | CBD-CHA-C1A | 2.66  | 132.24      | 128.77   |
| 31  | I     | 101 | LMG  | O6-C1-O1    | -2.66 | 103.61      | 109.93   |
| 22  | C     | 504 | CLA  | C4A-NA-C1A  | 2.65  | 110.12      | 106.38   |
| 25  | c     | 514 | BCR  | C28-C27-C26 | -2.65 | 109.45      | 113.81   |
| 22  | a     | 404 | CLA  | C3D-C4D-CHA | 2.65  | 112.42      | 108.16   |
| 22  | a     | 404 | CLA  | O2D-CGD-O1D | -2.65 | 118.47      | 123.79   |
| 22  | B     | 608 | CLA  | CHB-C4A-NA  | 2.65  | 128.07      | 124.38   |
| 22  | C     | 506 | CLA  | C2D-C3D-CAD | 2.65  | 145.73      | 134.94   |
| 22  | c     | 503 | CLA  | CMB-C2B-C3B | 2.65  | 130.15      | 125.16   |
| 22  | C     | 511 | CLA  | CMB-C2B-C3B | 2.64  | 130.14      | 125.16   |
| 22  | A     | 404 | CLA  | CHB-C4A-NA  | 2.64  | 128.07      | 124.38   |
| 22  | B     | 603 | CLA  | C4B-C3B-CAB | -2.65 | 121.82      | 127.18   |
| 22  | c     | 505 | CLA  | CBD-CHA-C1A | 2.65  | 132.23      | 128.77   |
| 22  | C     | 503 | CLA  | CMB-C2B-C3B | 2.64  | 130.14      | 125.16   |
| 22  | c     | 509 | CLA  | CBD-CHA-C1A | 2.64  | 132.23      | 128.77   |
| 22  | D     | 404 | CLA  | C3D-C4D-CHA | 2.64  | 112.40      | 108.16   |
| 32  | D     | 408 | LMT  | C3'-C4'-C5' | -2.64 | 104.95      | 110.86   |
| 31  | L     | 101 | LMG  | C40-C41-C42 | -2.64 | 103.10      | 113.73   |
| 22  | H     | 101 | CLA  | O2D-CGD-O1D | -2.64 | 118.49      | 123.79   |
| 22  | b     | 609 | CLA  | CMB-C2B-C3B | 2.64  | 130.13      | 125.16   |
| 22  | C     | 519 | CLA  | CMB-C2B-C3B | 2.64  | 130.13      | 125.16   |
| 22  | b     | 615 | CLA  | C1-C2-C3    | -2.64 | 121.65      | 126.23   |
| 22  | c     | 508 | CLA  | CMB-C2B-C3B | 2.64  | 130.13      | 125.16   |
| 22  | B     | 611 | CLA  | C4A-NA-C1A  | 2.64  | 110.10      | 106.38   |
| 22  | a     | 404 | CLA  | CHB-C4A-NA  | 2.64  | 128.06      | 124.38   |
| 22  | C     | 510 | CLA  | C2D-C3D-CAD | 2.64  | 145.70      | 134.94   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 27  | C     | 518 | LHG  | O8-C23-C24  | 2.64  | 119.97      | 111.90   |
| 22  | c     | 502 | CLA  | C4B-C3B-CAB | -2.63 | 121.84      | 127.18   |
| 22  | B     | 609 | CLA  | CBD-CHA-C1A | 2.63  | 132.21      | 128.77   |
| 26  | C     | 516 | DGD  | C1D-O6D-C5D | -2.63 | 108.64      | 113.73   |
| 22  | c     | 506 | CLA  | CBD-CHA-C1A | 2.63  | 132.21      | 128.77   |
| 31  | B     | 621 | LMG  | C40-C41-C42 | -2.63 | 103.14      | 113.73   |
| 22  | C     | 509 | CLA  | C3D-C4D-CHA | 2.63  | 112.38      | 108.16   |
| 25  | C     | 513 | BCR  | C28-C27-C26 | -2.63 | 109.49      | 113.81   |
| 22  | c     | 507 | CLA  | CHB-C4A-NA  | 2.63  | 128.05      | 124.38   |
| 25  | c     | 514 | BCR  | C11-C10-C9  | -2.63 | 123.49      | 127.29   |
| 22  | c     | 520 | CLA  | CHB-C4A-NA  | 2.63  | 128.05      | 124.38   |
| 22  | C     | 504 | CLA  | CMD-C2D-C3D | 2.62  | 130.11      | 125.16   |
| 22  | c     | 512 | CLA  | CBD-CHA-C1A | 2.63  | 132.20      | 128.77   |
| 31  | c     | 518 | LMG  | C22-C21-C20 | -2.63 | 105.44      | 112.94   |
| 22  | b     | 608 | CLA  | C4B-C3B-CAB | -2.62 | 121.86      | 127.18   |
| 23  | A     | 405 | PHO  | O2D-CGD-O1D | -2.62 | 118.52      | 123.79   |
| 30  | A     | 413 | SQD  | C44-O6-C1   | 2.62  | 119.07      | 113.80   |
| 22  | B     | 601 | CLA  | CMB-C2B-C3B | 2.62  | 130.10      | 125.16   |
| 22  | B     | 610 | CLA  | C3D-C4D-CHA | 2.62  | 112.37      | 108.16   |
| 22  | C     | 508 | CLA  | CHB-C4A-NA  | 2.62  | 128.04      | 124.38   |
| 22  | C     | 501 | CLA  | C3D-C4D-CHA | 2.62  | 112.36      | 108.16   |
| 22  | B     | 604 | CLA  | CMB-C2B-C3B | 2.62  | 130.10      | 125.16   |
| 22  | b     | 609 | CLA  | C3D-C4D-CHA | 2.62  | 112.36      | 108.16   |
| 26  | c     | 516 | DGD  | C3G-C2G-C1G | -2.62 | 105.84      | 111.86   |
| 22  | b     | 613 | CLA  | CBD-CHA-C1A | 2.62  | 132.20      | 128.77   |
| 24  | d     | 407 | PL9  | C27-C28-C29 | -2.62 | 122.14      | 127.81   |
| 25  | b     | 623 | BCR  | C11-C10-C9  | -2.62 | 123.50      | 127.29   |
| 22  | C     | 519 | CLA  | CBD-CHA-C1A | 2.62  | 132.19      | 128.77   |
| 22  | a     | 406 | CLA  | CBD-CHA-C1A | 2.62  | 132.19      | 128.77   |
| 25  | b     | 622 | BCR  | C15-C14-C13 | -2.61 | 123.51      | 127.29   |
| 22  | B     | 609 | CLA  | C3D-C4D-CHA | 2.61  | 112.36      | 108.16   |
| 31  | d     | 408 | LMG  | C22-C23-C24 | -2.61 | 103.22      | 113.73   |
| 25  | b     | 623 | BCR  | C15-C16-C17 | -2.61 | 117.70      | 123.45   |
| 22  | b     | 608 | CLA  | C2D-C3D-CAD | 2.61  | 145.58      | 134.94   |
| 25  | c     | 521 | BCR  | C27-C26-C25 | 2.61  | 126.31      | 122.86   |
| 22  | B     | 606 | CLA  | CMB-C2B-C3B | 2.61  | 130.08      | 125.16   |
| 22  | D     | 403 | CLA  | C4B-C3B-CAB | -2.61 | 121.89      | 127.18   |
| 22  | b     | 610 | CLA  | C2D-C3D-CAD | 2.61  | 145.58      | 134.94   |
| 22  | D     | 404 | CLA  | O2D-CGD-O1D | -2.61 | 118.55      | 123.79   |
| 22  | B     | 609 | CLA  | CHB-C4A-NA  | 2.61  | 128.02      | 124.38   |
| 22  | a     | 406 | CLA  | CHD-C4C-NC  | 2.61  | 126.10      | 124.28   |
| 22  | C     | 512 | CLA  | CHB-C4A-NA  | 2.61  | 128.02      | 124.38   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | d     | 405 | CLA  | C4B-C3B-CAB | -2.61 | 121.90      | 127.18   |
| 22  | A     | 403 | CLA  | C3D-C4D-CHA | 2.60  | 112.34      | 108.16   |
| 22  | c     | 503 | CLA  | CHB-C4A-NA  | 2.60  | 128.01      | 124.38   |
| 22  | D     | 404 | CLA  | CHB-C4A-NA  | 2.60  | 128.01      | 124.38   |
| 31  | B     | 625 | LMG  | C22-C23-C24 | -2.60 | 103.25      | 113.73   |
| 22  | B     | 603 | CLA  | C1-C2-C3    | -2.60 | 121.72      | 126.23   |
| 22  | B     | 607 | CLA  | CHB-C4A-NA  | 2.60  | 128.01      | 124.38   |
| 22  | a     | 404 | CLA  | CMB-C2B-C3B | 2.60  | 130.06      | 125.16   |
| 22  | B     | 603 | CLA  | C2D-C3D-CAD | 2.60  | 145.53      | 134.94   |
| 22  | c     | 509 | CLA  | O2D-CGD-O1D | -2.60 | 118.57      | 123.79   |
| 22  | B     | 615 | CLA  | CHD-C4C-NC  | 2.60  | 126.10      | 124.28   |
| 22  | c     | 509 | CLA  | CHB-C4A-NA  | 2.59  | 128.00      | 124.38   |
| 22  | C     | 507 | CLA  | CHD-C4C-NC  | 2.59  | 126.09      | 124.28   |
| 22  | c     | 504 | CLA  | C4B-C3B-CAB | -2.59 | 121.94      | 127.18   |
| 22  | C     | 507 | CLA  | CHB-C4A-NA  | 2.59  | 127.99      | 124.38   |
| 22  | B     | 611 | CLA  | CHB-C4A-NA  | 2.59  | 127.99      | 124.38   |
| 22  | B     | 605 | CLA  | C4A-NA-C1A  | 2.59  | 110.03      | 106.38   |
| 25  | j     | 102 | BCR  | C3-C4-C5    | -2.59 | 109.56      | 113.81   |
| 31  | l     | 101 | LMG  | C40-C41-C42 | -2.59 | 103.33      | 113.73   |
| 22  | c     | 509 | CLA  | CMB-C2B-C3B | 2.59  | 130.03      | 125.16   |
| 22  | c     | 511 | CLA  | CMB-C2B-C3B | 2.58  | 130.03      | 125.16   |
| 22  | b     | 616 | CLA  | CHB-C4A-NA  | 2.58  | 127.98      | 124.38   |
| 22  | B     | 615 | CLA  | CBD-CHA-C1A | 2.58  | 132.15      | 128.77   |
| 22  | b     | 618 | CLA  | CHB-C4A-NA  | 2.58  | 127.98      | 124.38   |
| 22  | b     | 611 | CLA  | C3D-C4D-CHA | 2.58  | 112.30      | 108.16   |
| 25  | B     | 619 | BCR  | C27-C26-C25 | 2.58  | 126.27      | 122.86   |
| 22  | b     | 619 | CLA  | CMB-C2B-C3B | 2.58  | 130.02      | 125.16   |
| 22  | B     | 604 | CLA  | C3D-C4D-CHA | 2.58  | 112.30      | 108.16   |
| 25  | b     | 624 | BCR  | C27-C26-C25 | 2.58  | 126.26      | 122.86   |
| 22  | B     | 606 | CLA  | C1B-CHB-C4A | -2.58 | 125.01      | 130.12   |
| 25  | C     | 513 | BCR  | C29-C30-C25 | 2.58  | 114.48      | 110.37   |
| 31  | C     | 517 | LMG  | C22-C21-C20 | -2.57 | 105.58      | 112.94   |
| 26  | C     | 515 | DGD  | C3G-C2G-C1G | -2.58 | 105.95      | 111.86   |
| 22  | c     | 502 | CLA  | CHB-C4A-NA  | 2.57  | 127.97      | 124.38   |
| 22  | b     | 608 | CLA  | C4A-NA-C1A  | 2.57  | 110.01      | 106.38   |
| 34  | F     | 101 | HEM  | CBD-CAD-C3D | -2.57 | 108.93      | 114.51   |
| 22  | C     | 504 | CLA  | C4B-C3B-CAB | -2.57 | 121.97      | 127.18   |
| 22  | C     | 508 | CLA  | CMB-C2B-C3B | 2.57  | 130.00      | 125.16   |
| 24  | d     | 407 | PL9  | C20-C19-C21 | 2.57  | 119.29      | 115.39   |
| 25  | c     | 513 | BCR  | C24-C23-C22 | -2.57 | 122.37      | 126.22   |
| 25  | B     | 618 | BCR  | C15-C14-C13 | -2.57 | 123.57      | 127.29   |
| 22  | C     | 509 | CLA  | CMB-C2B-C3B | 2.57  | 130.00      | 125.16   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | B     | 614 | CLA  | CBD-CHA-C1A | 2.57  | 132.12      | 128.77   |
| 22  | d     | 406 | CLA  | CMB-C2B-C3B | 2.57  | 130.00      | 125.16   |
| 25  | i     | 101 | BCR  | C27-C26-C25 | 2.57  | 126.25      | 122.86   |
| 22  | b     | 606 | CLA  | O2D-CGD-O1D | -2.57 | 118.64      | 123.79   |
| 22  | A     | 402 | CLA  | C3D-C4D-CHA | 2.56  | 112.27      | 108.16   |
| 30  | a     | 412 | SQD  | O48-C23-C24 | 2.56  | 119.74      | 111.90   |
| 22  | B     | 610 | CLA  | C1-C2-C3    | -2.56 | 121.78      | 126.23   |
| 22  | C     | 502 | CLA  | C4B-C3B-CAB | -2.56 | 121.99      | 127.18   |
| 22  | b     | 613 | CLA  | CHB-C4A-NA  | 2.56  | 127.95      | 124.38   |
| 22  | b     | 606 | CLA  | C4B-C3B-CAB | -2.56 | 121.99      | 127.18   |
| 22  | a     | 403 | CLA  | CHB-C4A-NA  | 2.56  | 127.95      | 124.38   |
| 22  | D     | 403 | CLA  | O2D-CGD-O1D | -2.56 | 118.65      | 123.79   |
| 22  | b     | 605 | CLA  | CMB-C2B-C3B | 2.56  | 129.98      | 125.16   |
| 22  | b     | 612 | CLA  | CHB-C4A-NA  | 2.56  | 127.95      | 124.38   |
| 22  | c     | 503 | CLA  | C4B-C3B-CAB | -2.56 | 122.00      | 127.18   |
| 22  | B     | 606 | CLA  | CHB-C4A-NA  | 2.56  | 127.95      | 124.38   |
| 22  | C     | 505 | CLA  | CHB-C4A-NA  | 2.56  | 127.95      | 124.38   |
| 22  | c     | 504 | CLA  | CMD-C2D-C3D | 2.56  | 129.98      | 125.16   |
| 31  | d     | 408 | LMG  | O2-C2-C1    | -2.56 | 104.48      | 110.03   |
| 22  | c     | 501 | CLA  | CBD-CHA-C1A | 2.56  | 132.11      | 128.77   |
| 22  | B     | 614 | CLA  | CHB-C4A-NA  | 2.56  | 127.94      | 124.38   |
| 22  | H     | 101 | CLA  | CHB-C4A-NA  | 2.55  | 127.94      | 124.38   |
| 22  | C     | 501 | CLA  | CBD-CHA-C1A | 2.55  | 132.11      | 128.77   |
| 22  | B     | 602 | CLA  | CHB-C4A-NA  | 2.55  | 127.94      | 124.38   |
| 25  | A     | 408 | BCR  | C27-C26-C25 | 2.55  | 126.23      | 122.86   |
| 32  | M     | 103 | LMT  | C1'-O5'-C5' | -2.55 | 108.81      | 113.73   |
| 25  | c     | 513 | BCR  | C7-C8-C9    | -2.55 | 122.40      | 126.22   |
| 22  | c     | 502 | CLA  | CMD-C2D-C3D | 2.55  | 129.96      | 125.16   |
| 25  | J     | 102 | BCR  | C38-C26-C25 | -2.55 | 121.62      | 124.50   |
| 23  | d     | 401 | PHO  | CMB-C2B-C3B | 2.55  | 129.96      | 125.16   |
| 22  | b     | 607 | CLA  | CBD-CHA-C1A | 2.54  | 132.09      | 128.77   |
| 22  | C     | 512 | CLA  | C4B-C3B-CAB | -2.54 | 122.03      | 127.18   |
| 32  | b     | 603 | LMT  | C1'-O5'-C5' | -2.54 | 108.82      | 113.73   |
| 22  | c     | 505 | CLA  | CHD-C4C-NC  | 2.54  | 126.06      | 124.28   |
| 26  | d     | 410 | DGD  | CFB-CEB-CDB | -2.54 | 101.08      | 114.56   |
| 22  | C     | 501 | CLA  | C4A-NA-C1A  | 2.54  | 109.96      | 106.38   |
| 25  | c     | 521 | BCR  | C15-C14-C13 | -2.54 | 123.62      | 127.29   |
| 22  | b     | 610 | CLA  | C4A-NA-C1A  | 2.54  | 109.95      | 106.38   |
| 22  | d     | 405 | CLA  | CMB-C2B-C3B | 2.54  | 129.94      | 125.16   |
| 32  | i     | 103 | LMT  | C1'-O5'-C5' | -2.54 | 108.83      | 113.73   |
| 25  | j     | 102 | BCR  | C38-C26-C25 | -2.53 | 121.64      | 124.50   |
| 22  | C     | 503 | CLA  | C4A-NA-C1A  | 2.53  | 109.95      | 106.38   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | A     | 406 | CLA  | C4B-C3B-CAB | -2.53 | 122.05      | 127.18   |
| 22  | b     | 608 | CLA  | CMB-C2B-C3B | 2.53  | 129.93      | 125.16   |
| 26  | D     | 407 | DGD  | CFB-CEB-CDB | -2.53 | 101.13      | 114.56   |
| 25  | B     | 616 | BCR  | C7-C8-C9    | -2.53 | 122.43      | 126.22   |
| 22  | b     | 616 | CLA  | C4A-NA-C1A  | 2.53  | 109.94      | 106.38   |
| 22  | C     | 512 | CLA  | CHD-C4C-NC  | 2.53  | 126.05      | 124.28   |
| 22  | C     | 511 | CLA  | C4A-NA-C1A  | 2.53  | 109.94      | 106.38   |
| 25  | c     | 514 | BCR  | C15-C16-C17 | -2.53 | 117.89      | 123.45   |
| 22  | C     | 504 | CLA  | CBD-CHA-C1A | 2.52  | 132.07      | 128.77   |
| 22  | B     | 615 | CLA  | CHB-C4A-NA  | 2.52  | 127.90      | 124.38   |
| 24  | a     | 407 | PL9  | C20-C19-C21 | 2.52  | 119.22      | 115.39   |
| 22  | B     | 603 | CLA  | C4A-NA-C1A  | 2.52  | 109.94      | 106.38   |
| 22  | c     | 503 | CLA  | C4A-NA-C1A  | 2.52  | 109.94      | 106.38   |
| 22  | A     | 404 | CLA  | CMB-C2B-C3B | 2.52  | 129.91      | 125.16   |
| 22  | B     | 605 | CLA  | C4B-C3B-CAB | -2.52 | 122.07      | 127.18   |
| 31  | D     | 409 | LMG  | C38-C37-C36 | -2.52 | 101.18      | 114.56   |
| 22  | a     | 403 | CLA  | CHD-C4C-NC  | 2.52  | 126.04      | 124.28   |
| 31  | B     | 625 | LMG  | O2-C2-C1    | -2.52 | 104.56      | 110.03   |
| 25  | b     | 622 | BCR  | C35-C13-C14 | -2.52 | 119.33      | 122.92   |
| 25  | c     | 514 | BCR  | C29-C30-C25 | 2.52  | 114.38      | 110.37   |
| 26  | A     | 409 | DGD  | CBB-CAB-C9B | -2.52 | 101.20      | 114.56   |
| 22  | c     | 504 | CLA  | CBA-CAA-C2A | 2.51  | 120.10      | 113.95   |
| 22  | b     | 613 | CLA  | CMB-C2B-C3B | 2.52  | 129.90      | 125.16   |
| 31  | L     | 101 | LMG  | C1-C2-C3    | -2.51 | 105.12      | 109.99   |
| 22  | a     | 406 | CLA  | O2D-CGD-O1D | -2.51 | 118.75      | 123.79   |
| 24  | A     | 407 | PL9  | C37-C38-C39 | -2.51 | 122.58      | 128.69   |
| 22  | C     | 510 | CLA  | C4A-NA-C1A  | 2.51  | 109.92      | 106.38   |
| 22  | c     | 520 | CLA  | CMB-C2B-C3B | 2.51  | 129.89      | 125.16   |
| 22  | c     | 504 | CLA  | CBD-CHA-C1A | 2.51  | 132.05      | 128.77   |
| 22  | C     | 510 | CLA  | C4B-C3B-CAB | -2.51 | 122.10      | 127.18   |
| 22  | b     | 611 | CLA  | CMB-C2B-C3B | 2.51  | 129.89      | 125.16   |
| 22  | c     | 501 | CLA  | C4A-NA-C1A  | 2.51  | 109.91      | 106.38   |
| 24  | J     | 101 | PL9  | C20-C19-C21 | 2.51  | 119.20      | 115.39   |
| 25  | B     | 616 | BCR  | C11-C10-C9  | -2.51 | 123.66      | 127.29   |
| 25  | B     | 618 | BCR  | C29-C30-C25 | 2.51  | 114.37      | 110.37   |
| 22  | B     | 615 | CLA  | C4A-NA-C1A  | 2.51  | 109.91      | 106.38   |
| 22  | c     | 510 | CLA  | CHB-C4A-NA  | 2.50  | 127.87      | 124.38   |
| 26  | c     | 515 | DGD  | C3G-C2G-C1G | -2.50 | 106.11      | 111.86   |
| 22  | D     | 404 | CLA  | C1-C2-C3    | -2.50 | 121.89      | 126.23   |
| 22  | B     | 610 | CLA  | C4B-CHC-C1C | -2.50 | 124.18      | 127.47   |
| 22  | b     | 620 | CLA  | CHB-C4A-NA  | 2.50  | 127.87      | 124.38   |
| 25  | c     | 514 | BCR  | C15-C14-C13 | -2.50 | 123.68      | 127.29   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | b     | 629 | LMT  | C1'-O5'-C5' | -2.50 | 108.90      | 113.73   |
| 22  | a     | 405 | CLA  | CHB-C4A-NA  | 2.50  | 127.86      | 124.38   |
| 22  | b     | 613 | CLA  | C1B-CHB-C4A | -2.49 | 125.18      | 130.12   |
| 22  | C     | 504 | CLA  | C1B-CHB-C4A | -2.49 | 125.18      | 130.12   |
| 31  | D     | 409 | LMG  | C1-C2-C3    | -2.49 | 105.16      | 109.99   |
| 22  | A     | 406 | CLA  | O2D-CGD-O1D | -2.49 | 118.79      | 123.79   |
| 22  | b     | 610 | CLA  | CMB-C2B-C3B | 2.49  | 129.85      | 125.16   |
| 22  | c     | 505 | CLA  | C1B-CHB-C4A | -2.49 | 125.19      | 130.12   |
| 22  | C     | 503 | CLA  | C4B-C3B-CAB | -2.49 | 122.14      | 127.18   |
| 22  | d     | 405 | CLA  | CBD-CHA-C1A | 2.49  | 132.02      | 128.77   |
| 30  | d     | 403 | SQD  | O48-C23-C24 | 2.49  | 119.52      | 111.90   |
| 26  | d     | 410 | DGD  | C3G-C2G-C1G | -2.49 | 106.14      | 111.86   |
| 22  | C     | 508 | CLA  | CBD-CHA-C1A | 2.49  | 132.02      | 128.77   |
| 22  | a     | 406 | CLA  | C4B-C3B-CAB | -2.49 | 122.14      | 127.18   |
| 22  | b     | 611 | CLA  | CHB-C4A-NA  | 2.49  | 127.85      | 124.38   |
| 25  | B     | 618 | BCR  | C15-C16-C17 | -2.49 | 117.97      | 123.45   |
| 22  | B     | 613 | CLA  | CHD-C4C-NC  | 2.48  | 126.02      | 124.28   |
| 22  | C     | 507 | CLA  | C4A-NA-C1A  | 2.48  | 109.88      | 106.38   |
| 22  | a     | 404 | CLA  | C1B-CHB-C4A | -2.48 | 125.20      | 130.12   |
| 31  | m     | 101 | LMG  | O2-C2-C1    | -2.48 | 104.64      | 110.03   |
| 22  | b     | 606 | CLA  | CBD-CHA-C1A | 2.48  | 132.02      | 128.77   |
| 26  | C     | 515 | DGD  | O6E-C1E-O5D | -2.48 | 104.02      | 109.93   |
| 25  | c     | 514 | BCR  | C33-C5-C6   | -2.48 | 121.70      | 124.50   |
| 22  | a     | 405 | CLA  | CMB-C2B-C3B | 2.48  | 129.83      | 125.16   |
| 23  | d     | 401 | PHO  | CBD-CHA-C1A | 2.48  | 130.97      | 126.67   |
| 31  | b     | 626 | LMG  | O2-C2-C1    | -2.48 | 104.65      | 110.03   |
| 22  | B     | 604 | CLA  | C4A-NA-C1A  | 2.48  | 109.87      | 106.38   |
| 22  | B     | 608 | CLA  | CMB-C2B-C3B | 2.48  | 129.83      | 125.16   |
| 25  | C     | 520 | BCR  | C15-C16-C17 | -2.48 | 117.99      | 123.45   |
| 22  | C     | 509 | CLA  | CBD-CHA-C1A | 2.48  | 132.01      | 128.77   |
| 23  | d     | 402 | PHO  | O2D-CGD-O1D | -2.47 | 118.82      | 123.79   |
| 22  | B     | 611 | CLA  | CBD-CHA-C1A | 2.47  | 132.00      | 128.77   |
| 31  | d     | 412 | LMG  | C38-C37-C36 | -2.47 | 101.42      | 114.56   |
| 22  | c     | 504 | CLA  | C4A-NA-C1A  | 2.47  | 109.87      | 106.38   |
| 24  | A     | 407 | PL9  | C20-C19-C21 | 2.47  | 119.15      | 115.39   |
| 22  | A     | 402 | CLA  | CHB-C4A-NA  | 2.47  | 127.83      | 124.38   |
| 30  | A     | 413 | SQD  | O48-C23-C24 | 2.47  | 119.47      | 111.90   |
| 22  | B     | 614 | CLA  | CMB-C2B-C3B | 2.47  | 129.81      | 125.16   |
| 22  | B     | 604 | CLA  | CBD-CHA-C1A | 2.47  | 132.00      | 128.77   |
| 22  | b     | 617 | CLA  | CHB-C4A-NA  | 2.47  | 127.83      | 124.38   |
| 22  | c     | 510 | CLA  | C4B-C3B-CAB | -2.47 | 122.18      | 127.18   |
| 26  | B     | 620 | DGD  | C3G-C2G-C1G | -2.47 | 106.20      | 111.86   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | A     | 407 | PL9  | C27-C28-C29 | -2.47 | 122.48      | 127.81   |
| 26  | b     | 625 | DGD  | C3G-C2G-C1G | -2.47 | 106.20      | 111.86   |
| 22  | C     | 512 | CLA  | C4A-NA-C1A  | 2.46  | 109.85      | 106.38   |
| 22  | C     | 507 | CLA  | C4B-C3B-CAB | -2.46 | 122.19      | 127.18   |
| 31  | b     | 627 | LMG  | O6-C1-O1    | -2.46 | 104.07      | 109.93   |
| 26  | b     | 625 | DGD  | CBB-CAB-C9B | -2.46 | 101.49      | 114.56   |
| 23  | d     | 402 | PHO  | O1D-CGD-CBD | 2.46  | 129.48      | 124.45   |
| 22  | c     | 504 | CLA  | CHB-C4A-NA  | 2.46  | 127.81      | 124.38   |
| 22  | c     | 507 | CLA  | CHD-C4C-NC  | 2.46  | 126.00      | 124.28   |
| 22  | A     | 406 | CLA  | CHB-C4A-NA  | 2.46  | 127.81      | 124.38   |
| 22  | B     | 612 | CLA  | C1B-CHB-C4A | -2.46 | 125.24      | 130.12   |
| 22  | b     | 615 | CLA  | CMD-C2D-C3D | 2.46  | 129.79      | 125.16   |
| 31  | a     | 402 | LMG  | O6-C1-O1    | -2.46 | 104.07      | 109.93   |
| 22  | B     | 611 | CLA  | C4B-C3B-CAB | -2.46 | 122.20      | 127.18   |
| 22  | c     | 511 | CLA  | CMD-C2D-C3D | 2.46  | 129.79      | 125.16   |
| 31  | d     | 408 | LMG  | C38-C37-C36 | -2.46 | 101.52      | 114.56   |
| 22  | c     | 507 | CLA  | C4B-C3B-CAB | -2.46 | 122.20      | 127.18   |
| 30  | B     | 627 | SQD  | O48-C23-C24 | 2.46  | 119.42      | 111.90   |
| 31  | B     | 621 | LMG  | C1-C2-C3    | -2.46 | 105.23      | 109.99   |
| 25  | C     | 513 | BCR  | C33-C5-C6   | -2.45 | 121.73      | 124.50   |
| 25  | C     | 513 | BCR  | C15-C14-C13 | -2.45 | 123.74      | 127.29   |
| 26  | C     | 516 | DGD  | CFB-CEB-CDB | -2.45 | 101.53      | 114.56   |
| 25  | K     | 101 | BCR  | C11-C10-C9  | -2.45 | 123.74      | 127.29   |
| 22  | d     | 405 | CLA  | O2D-CGD-O1D | -2.45 | 118.86      | 123.79   |
| 22  | B     | 607 | CLA  | C1B-CHB-C4A | -2.45 | 125.26      | 130.12   |
| 22  | B     | 613 | CLA  | C1B-CHB-C4A | -2.45 | 125.26      | 130.12   |
| 22  | A     | 403 | CLA  | C4A-NA-C1A  | 2.45  | 109.84      | 106.38   |
| 22  | C     | 509 | CLA  | CHB-C4A-NA  | 2.45  | 127.80      | 124.38   |
| 22  | a     | 403 | CLA  | C3D-C4D-CHA | 2.45  | 112.09      | 108.16   |
| 31  | B     | 625 | LMG  | O3-C3-C2    | -2.45 | 104.89      | 110.36   |
| 22  | C     | 505 | CLA  | C1B-CHB-C4A | -2.45 | 125.27      | 130.12   |
| 22  | C     | 506 | CLA  | C4A-NA-C1A  | 2.44  | 109.83      | 106.38   |
| 23  | A     | 405 | PHO  | CMB-C2B-C3B | 2.44  | 129.76      | 125.16   |
| 22  | c     | 506 | CLA  | C1B-CHB-C4A | -2.44 | 125.28      | 130.12   |
| 22  | B     | 614 | CLA  | C4A-NA-C1A  | 2.44  | 109.82      | 106.38   |
| 26  | a     | 408 | DGD  | CBB-CAB-C9B | -2.44 | 101.60      | 114.56   |
| 22  | b     | 607 | CLA  | CHB-C4A-NA  | 2.44  | 127.79      | 124.38   |
| 22  | B     | 602 | CLA  | C1B-CHB-C4A | -2.44 | 125.28      | 130.12   |
| 22  | A     | 403 | CLA  | CBD-CHA-C1A | 2.44  | 131.96      | 128.77   |
| 22  | C     | 511 | CLA  | C4B-C3B-CAB | -2.44 | 122.24      | 127.18   |
| 22  | b     | 609 | CLA  | C4A-NA-C1A  | 2.44  | 109.82      | 106.38   |
| 22  | B     | 601 | CLA  | CBD-CHA-C1A | 2.44  | 131.96      | 128.77   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | a     | 401 | SQD  | C1-O5-C5    | 2.44  | 118.45      | 113.73   |
| 22  | C     | 502 | CLA  | CHB-C4A-NA  | 2.44  | 127.78      | 124.38   |
| 26  | c     | 516 | DGD  | O6E-C1E-O5D | -2.44 | 104.13      | 109.93   |
| 30  | F     | 103 | SQD  | C1-O5-C5    | 2.44  | 118.45      | 113.73   |
| 31  | d     | 409 | LMG  | C38-C37-C36 | -2.44 | 101.62      | 114.56   |
| 31  | b     | 626 | LMG  | C1-C2-C3    | -2.44 | 105.27      | 109.99   |
| 22  | C     | 509 | CLA  | O2D-CGD-O1D | -2.43 | 118.90      | 123.79   |
| 30  | A     | 414 | SQD  | C5-C6-S     | -2.43 | 111.00      | 114.40   |
| 22  | C     | 505 | CLA  | CHD-C4C-NC  | 2.43  | 125.98      | 124.28   |
| 22  | B     | 603 | CLA  | CMB-C2B-C3B | 2.43  | 129.74      | 125.16   |
| 22  | A     | 403 | CLA  | CMB-C2B-C3B | 2.43  | 129.74      | 125.16   |
| 31  | C     | 521 | LMG  | O2-C2-C1    | -2.43 | 104.75      | 110.03   |
| 25  | J     | 102 | BCR  | C15-C16-C17 | -2.43 | 118.09      | 123.45   |
| 22  | b     | 611 | CLA  | C1B-CHB-C4A | -2.43 | 125.30      | 130.12   |
| 22  | c     | 520 | CLA  | C4A-NA-C1A  | 2.43  | 109.81      | 106.38   |
| 25  | B     | 616 | BCR  | C27-C26-C25 | 2.43  | 126.07      | 122.86   |
| 24  | a     | 407 | PL9  | C7-C8-C9    | -2.43 | 122.65      | 126.76   |
| 22  | b     | 620 | CLA  | O2D-CGD-O1D | -2.43 | 118.92      | 123.79   |
| 31  | d     | 409 | LMG  | C22-C23-C24 | -2.43 | 103.96      | 113.73   |
| 22  | c     | 508 | CLA  | O2D-CGD-O1D | -2.43 | 118.92      | 123.79   |
| 31  | c     | 518 | LMG  | O2-C2-C1    | -2.43 | 104.76      | 110.03   |
| 22  | a     | 406 | CLA  | C4A-NA-C1A  | 2.42  | 109.80      | 106.38   |
| 31  | I     | 101 | LMG  | O2-C2-C1    | -2.42 | 104.77      | 110.03   |
| 22  | c     | 511 | CLA  | C4A-NA-C1A  | 2.42  | 109.80      | 106.38   |
| 31  | d     | 408 | LMG  | O1-C1-C2    | -2.42 | 105.05      | 108.15   |
| 22  | d     | 405 | CLA  | C4A-NA-C1A  | 2.42  | 109.79      | 106.38   |
| 24  | A     | 407 | PL9  | C7-C8-C9    | -2.42 | 122.67      | 126.76   |
| 22  | B     | 607 | CLA  | C4B-C3B-CAB | -2.42 | 122.28      | 127.18   |
| 22  | B     | 612 | CLA  | CHD-C4C-NC  | 2.42  | 125.97      | 124.28   |
| 22  | b     | 607 | CLA  | C1B-CHB-C4A | -2.42 | 125.33      | 130.12   |
| 22  | D     | 403 | CLA  | CBD-CHA-C1A | 2.42  | 131.93      | 128.77   |
| 25  | b     | 621 | BCR  | C27-C26-C25 | 2.42  | 126.05      | 122.86   |
| 22  | b     | 606 | CLA  | CMD-C2D-C3D | 2.42  | 129.71      | 125.16   |
| 27  | C     | 518 | LHG  | C11-C10-C9  | -2.42 | 101.73      | 114.56   |
| 22  | b     | 614 | CLA  | CHB-C4A-NA  | 2.41  | 127.75      | 124.38   |
| 26  | a     | 408 | DGD  | O5D-C6D-C5D | -2.41 | 104.78      | 108.96   |
| 22  | A     | 404 | CLA  | C1B-CHB-C4A | -2.41 | 125.34      | 130.12   |
| 22  | H     | 101 | CLA  | CMB-C2B-C3B | 2.41  | 129.71      | 125.16   |
| 22  | c     | 507 | CLA  | C4A-NA-C1A  | 2.41  | 109.78      | 106.38   |
| 26  | c     | 517 | DGD  | CFB-CEB-CDB | -2.41 | 101.76      | 114.56   |
| 22  | C     | 511 | CLA  | CMD-C2D-C3D | 2.41  | 129.70      | 125.16   |
| 25  | b     | 623 | BCR  | C15-C14-C13 | -2.41 | 123.81      | 127.29   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | M     | 103 | LMT  | C3'-C4'-C5' | -2.41 | 105.48      | 110.86   |
| 23  | d     | 402 | PHO  | CBD-CHA-C1A | 2.41  | 130.85      | 126.67   |
| 25  | b     | 624 | BCR  | C11-C10-C9  | -2.41 | 123.81      | 127.29   |
| 31  | B     | 625 | LMG  | C38-C37-C36 | -2.41 | 101.77      | 114.56   |
| 22  | b     | 619 | CLA  | C4A-NA-C1A  | 2.41  | 109.78      | 106.38   |
| 31  | c     | 522 | LMG  | O2-C2-C1    | -2.41 | 104.80      | 110.03   |
| 22  | b     | 620 | CLA  | C4A-NA-C1A  | 2.41  | 109.77      | 106.38   |
| 22  | A     | 406 | CLA  | CBD-CHA-C1A | 2.41  | 131.91      | 128.77   |
| 22  | A     | 406 | CLA  | CHD-C4C-NC  | 2.41  | 125.96      | 124.28   |
| 23  | D     | 401 | PHO  | O1D-CGD-CBD | 2.41  | 129.37      | 124.45   |
| 22  | b     | 605 | CLA  | CBD-CHA-C1A | 2.40  | 131.91      | 128.77   |
| 22  | b     | 610 | CLA  | C4B-C3B-CAB | -2.40 | 122.31      | 127.18   |
| 22  | b     | 616 | CLA  | CBD-CHA-C1A | 2.40  | 131.91      | 128.77   |
| 22  | a     | 403 | CLA  | CBD-CHA-C1A | 2.40  | 131.91      | 128.77   |
| 25  | K     | 101 | BCR  | C7-C8-C9    | -2.40 | 122.62      | 126.22   |
| 22  | a     | 405 | CLA  | C1B-CHB-C4A | -2.40 | 125.36      | 130.12   |
| 26  | a     | 408 | DGD  | C3G-C2G-C1G | -2.40 | 106.35      | 111.86   |
| 25  | C     | 513 | BCR  | C11-C10-C9  | -2.40 | 123.82      | 127.29   |
| 22  | a     | 406 | CLA  | C1B-CHB-C4A | -2.40 | 125.36      | 130.12   |
| 22  | B     | 611 | CLA  | CHD-C4C-NC  | 2.40  | 125.96      | 124.28   |
| 22  | B     | 611 | CLA  | CMD-C2D-C3D | 2.40  | 129.69      | 125.16   |
| 22  | B     | 603 | CLA  | O1D-CGD-CBD | 2.40  | 129.36      | 124.45   |
| 22  | C     | 505 | CLA  | C4B-C3B-CAB | -2.40 | 122.31      | 127.18   |
| 25  | b     | 621 | BCR  | C2-C1-C6    | 2.40  | 114.20      | 110.37   |
| 22  | C     | 519 | CLA  | C1B-CHB-C4A | -2.40 | 125.36      | 130.12   |
| 22  | A     | 403 | CLA  | CHD-C4C-NC  | 2.40  | 125.96      | 124.28   |
| 31  | L     | 101 | LMG  | C40-C39-C38 | -2.40 | 101.83      | 114.56   |
| 31  | l     | 101 | LMG  | C1-C2-C3    | -2.40 | 105.34      | 109.99   |
| 22  | b     | 616 | CLA  | C4B-C3B-CAB | -2.40 | 122.32      | 127.18   |
| 31  | l     | 101 | LMG  | C22-C23-C24 | -2.40 | 104.09      | 113.73   |
| 22  | B     | 608 | CLA  | C1-C2-C3    | -2.40 | 122.07      | 126.23   |
| 22  | B     | 609 | CLA  | C4B-C3B-CAB | -2.40 | 122.33      | 127.18   |
| 31  | m     | 101 | LMG  | C1-C2-C3    | -2.39 | 105.35      | 109.99   |
| 22  | b     | 612 | CLA  | C1B-CHB-C4A | -2.39 | 125.38      | 130.12   |
| 22  | b     | 614 | CLA  | CBD-CHA-C1A | 2.39  | 131.89      | 128.77   |
| 25  | b     | 621 | BCR  | C15-C14-C13 | -2.39 | 123.83      | 127.29   |
| 25  | B     | 617 | BCR  | C29-C30-C25 | 2.39  | 114.18      | 110.37   |
| 32  | I     | 102 | LMT  | C1'-O5'-C5' | -2.39 | 109.11      | 113.73   |
| 31  | D     | 406 | LMG  | C38-C37-C36 | -2.39 | 101.88      | 114.56   |
| 23  | A     | 405 | PHO  | CBD-CHA-C1A | 2.39  | 130.81      | 126.67   |
| 30  | B     | 622 | SQD  | O48-C23-C24 | 2.39  | 119.20      | 111.90   |
| 22  | d     | 406 | CLA  | C4A-NA-C1A  | 2.39  | 109.74      | 106.38   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | B     | 615 | CLA  | CMB-C2B-C3B | 2.39  | 129.66      | 125.16   |
| 23  | d     | 401 | PHO  | O1D-CGD-CBD | 2.39  | 129.32      | 124.45   |
| 31  | D     | 409 | LMG  | O3-C3-C2    | -2.38 | 105.03      | 110.36   |
| 22  | C     | 511 | CLA  | CHD-C4C-NC  | 2.38  | 125.95      | 124.28   |
| 22  | c     | 506 | CLA  | C3A-C4A-CHB | -2.38 | 119.38      | 124.33   |
| 22  | D     | 403 | CLA  | C1B-CHB-C4A | -2.38 | 125.40      | 130.12   |
| 22  | B     | 604 | CLA  | C1B-CHB-C4A | -2.38 | 125.40      | 130.12   |
| 25  | B     | 618 | BCR  | C7-C8-C9    | -2.38 | 122.66      | 126.22   |
| 25  | B     | 616 | BCR  | C2-C1-C6    | 2.38  | 114.16      | 110.37   |
| 31  | M     | 101 | LMG  | O2-C2-C1    | -2.38 | 104.86      | 110.03   |
| 22  | B     | 604 | CLA  | C4B-C3B-CAB | -2.38 | 122.36      | 127.18   |
| 22  | c     | 512 | CLA  | CHD-C4C-NC  | 2.38  | 125.94      | 124.28   |
| 26  | B     | 620 | DGD  | CBB-CAB-C9B | -2.38 | 101.94      | 114.56   |
| 26  | c     | 515 | DGD  | C6B-C7B-C8B | -2.38 | 104.17      | 113.73   |
| 22  | b     | 617 | CLA  | C4A-NA-C1A  | 2.38  | 109.73      | 106.38   |
| 22  | H     | 101 | CLA  | C4B-C3B-CAB | -2.38 | 122.37      | 127.18   |
| 22  | b     | 613 | CLA  | CMD-C2D-C3D | 2.37  | 129.63      | 125.16   |
| 34  | V     | 201 | HEM  | C3A-C4A-NA  | -2.37 | 107.91      | 109.50   |
| 22  | d     | 405 | CLA  | CMD-C2D-C3D | 2.37  | 129.63      | 125.16   |
| 31  | i     | 102 | LMG  | O2-C2-C1    | -2.37 | 104.88      | 110.03   |
| 22  | A     | 403 | CLA  | C1B-CHB-C4A | -2.37 | 125.43      | 130.12   |
| 31  | c     | 522 | LMG  | C40-C39-C38 | -2.37 | 101.98      | 114.56   |
| 31  | d     | 408 | LMG  | O3-C3-C2    | -2.37 | 105.06      | 110.36   |
| 26  | C     | 514 | DGD  | C6B-C7B-C8B | -2.37 | 104.20      | 113.73   |
| 22  | B     | 613 | CLA  | C4A-NA-C1A  | 2.37  | 109.72      | 106.38   |
| 24  | j     | 101 | PL9  | C20-C19-C21 | 2.37  | 118.98      | 115.39   |
| 22  | B     | 601 | CLA  | C1B-CHB-C4A | -2.37 | 125.43      | 130.12   |
| 22  | B     | 608 | CLA  | C1B-CHB-C4A | -2.36 | 125.43      | 130.12   |
| 22  | c     | 508 | CLA  | C1B-CHB-C4A | -2.36 | 125.43      | 130.12   |
| 22  | A     | 404 | CLA  | CBD-CHA-C1A | 2.37  | 131.86      | 128.77   |
| 22  | b     | 620 | CLA  | CBD-CHA-C1A | 2.36  | 131.86      | 128.77   |
| 25  | b     | 623 | BCR  | C7-C8-C9    | -2.36 | 122.68      | 126.22   |
| 22  | C     | 506 | CLA  | C1B-CHB-C4A | -2.36 | 125.43      | 130.12   |
| 31  | B     | 621 | LMG  | O2-C2-C1    | -2.36 | 104.90      | 110.03   |
| 22  | c     | 512 | CLA  | C4A-NA-C1A  | 2.36  | 109.71      | 106.38   |
| 22  | A     | 406 | CLA  | C4A-NA-C1A  | 2.36  | 109.71      | 106.38   |
| 25  | c     | 513 | BCR  | C11-C10-C9  | -2.36 | 123.87      | 127.29   |
| 30  | a     | 412 | SQD  | C44-O6-C1   | 2.36  | 118.54      | 113.80   |
| 31  | D     | 406 | LMG  | O6-C1-C2    | -2.36 | 105.47      | 110.30   |
| 31  | e     | 101 | LMG  | C1-C2-C3    | -2.36 | 105.42      | 109.99   |
| 22  | H     | 101 | CLA  | C4A-NA-C1A  | 2.36  | 109.71      | 106.38   |
| 30  | A     | 414 | SQD  | O48-C23-C24 | 2.36  | 119.11      | 111.90   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 23  | A     | 405 | PHO  | C2D-C3D-CAD | 2.36  | 144.55      | 134.94   |
| 22  | B     | 606 | CLA  | C1-C2-C3    | -2.36 | 122.14      | 126.23   |
| 23  | D     | 401 | PHO  | C2D-C3D-CAD | 2.36  | 144.54      | 134.94   |
| 31  | b     | 626 | LMG  | C40-C39-C38 | -2.36 | 102.05      | 114.56   |
| 22  | C     | 508 | CLA  | O2D-CGD-O1D | -2.35 | 119.06      | 123.79   |
| 22  | a     | 404 | CLA  | CHD-C4C-NC  | 2.35  | 125.93      | 124.28   |
| 31  | d     | 412 | LMG  | O3-C3-C2    | -2.35 | 105.10      | 110.36   |
| 31  | C     | 517 | LMG  | O2-C2-C1    | -2.35 | 104.92      | 110.03   |
| 22  | b     | 612 | CLA  | C4B-C3B-CAB | -2.35 | 122.41      | 127.18   |
| 31  | m     | 101 | LMG  | C1-O6-C5    | -2.35 | 109.18      | 113.73   |
| 23  | d     | 402 | PHO  | C2D-C3D-CAD | 2.35  | 144.52      | 134.94   |
| 22  | b     | 616 | CLA  | CHD-C4C-NC  | 2.35  | 125.92      | 124.28   |
| 22  | b     | 620 | CLA  | CMB-C2B-C3B | 2.35  | 129.59      | 125.16   |
| 31  | L     | 101 | LMG  | O3-C3-C2    | -2.35 | 105.11      | 110.36   |
| 22  | C     | 505 | CLA  | CBD-CHA-C1A | 2.35  | 131.84      | 128.77   |
| 25  | i     | 101 | BCR  | C33-C5-C6   | -2.35 | 121.84      | 124.50   |
| 22  | D     | 403 | CLA  | CHB-C4A-NA  | 2.35  | 127.65      | 124.38   |
| 25  | B     | 617 | BCR  | C35-C13-C14 | -2.35 | 119.58      | 122.92   |
| 22  | b     | 609 | CLA  | C4B-C3B-CAB | -2.35 | 122.43      | 127.18   |
| 22  | b     | 614 | CLA  | C4B-C3B-CAB | -2.35 | 122.43      | 127.18   |
| 25  | A     | 408 | BCR  | C15-C14-C13 | -2.35 | 123.90      | 127.29   |
| 22  | C     | 501 | CLA  | CHD-C4C-NC  | 2.34  | 125.92      | 124.28   |
| 25  | b     | 622 | BCR  | C29-C30-C25 | 2.34  | 114.11      | 110.37   |
| 22  | H     | 101 | CLA  | C1B-CHB-C4A | -2.34 | 125.47      | 130.12   |
| 22  | d     | 406 | CLA  | CBD-CHA-C1A | 2.34  | 131.83      | 128.77   |
| 31  | D     | 406 | LMG  | C22-C23-C24 | -2.34 | 104.31      | 113.73   |
| 22  | c     | 505 | CLA  | C4A-NA-C1A  | 2.34  | 109.68      | 106.38   |
| 22  | D     | 404 | CLA  | CMD-C2D-C3D | 2.34  | 129.57      | 125.16   |
| 31  | l     | 101 | LMG  | C40-C39-C38 | -2.34 | 102.14      | 114.56   |
| 27  | c     | 519 | LHG  | C11-C10-C9  | -2.34 | 102.14      | 114.56   |
| 22  | B     | 612 | CLA  | C4A-NA-C1A  | 2.34  | 109.68      | 106.38   |
| 25  | A     | 408 | BCR  | C33-C5-C6   | -2.34 | 121.86      | 124.50   |
| 22  | A     | 402 | CLA  | CMB-C2B-C3B | 2.34  | 129.57      | 125.16   |
| 31  | l     | 101 | LMG  | O3-C3-C2    | -2.34 | 105.13      | 110.36   |
| 23  | A     | 405 | PHO  | O1D-CGD-CBD | 2.34  | 129.22      | 124.45   |
| 30  | a     | 401 | SQD  | O48-C23-C24 | 2.34  | 119.05      | 111.90   |
| 30  | F     | 103 | SQD  | C3-C4-C5    | 2.34  | 114.37      | 110.17   |
| 31  | M     | 101 | LMG  | C1-O6-C5    | -2.34 | 109.21      | 113.73   |
| 22  | c     | 508 | CLA  | C4A-NA-C1A  | 2.34  | 109.67      | 106.38   |
| 22  | B     | 606 | CLA  | CBD-CHA-C1A | 2.33  | 131.82      | 128.77   |
| 22  | b     | 617 | CLA  | C2B-C3B-CAB | 2.33  | 132.10      | 127.33   |
| 22  | A     | 406 | CLA  | C1B-CHB-C4A | -2.33 | 125.50      | 130.12   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | B     | 607 | CLA  | CHD-C4C-NC  | 2.33  | 125.91      | 124.28   |
| 22  | c     | 504 | CLA  | C1B-CHB-C4A | -2.33 | 125.51      | 130.12   |
| 31  | d     | 409 | LMG  | O6-C1-C2    | -2.33 | 105.54      | 110.30   |
| 22  | b     | 611 | CLA  | C4B-C3B-CAB | -2.33 | 122.47      | 127.18   |
| 22  | B     | 605 | CLA  | C1B-CHB-C4A | -2.33 | 125.51      | 130.12   |
| 22  | B     | 606 | CLA  | C4B-C3B-CAB | -2.33 | 122.47      | 127.18   |
| 22  | C     | 519 | CLA  | C4A-NA-C1A  | 2.32  | 109.66      | 106.38   |
| 25  | j     | 102 | BCR  | C15-C14-C13 | -2.33 | 123.93      | 127.29   |
| 23  | d     | 401 | PHO  | C2D-C3D-CAD | 2.33  | 144.42      | 134.94   |
| 31  | M     | 101 | LMG  | C1-C2-C3    | -2.33 | 105.48      | 109.99   |
| 22  | B     | 613 | CLA  | CBD-CHA-C1A | 2.32  | 131.81      | 128.77   |
| 22  | c     | 504 | CLA  | CMB-C2B-C3B | 2.32  | 129.54      | 125.16   |
| 22  | a     | 404 | CLA  | C4A-NA-C1A  | 2.32  | 109.66      | 106.38   |
| 32  | D     | 408 | LMT  | C1'-O5'-C5' | -2.32 | 109.24      | 113.73   |
| 22  | C     | 510 | CLA  | C3A-C4A-CHB | -2.32 | 119.50      | 124.33   |
| 22  | C     | 511 | CLA  | O2A-CGA-O1A | -2.32 | 117.42      | 123.48   |
| 22  | C     | 502 | CLA  | CMD-C2D-C3D | 2.32  | 129.53      | 125.16   |
| 22  | b     | 616 | CLA  | CMD-C2D-C3D | 2.32  | 129.53      | 125.16   |
| 22  | c     | 505 | CLA  | C4B-C3B-CAB | -2.32 | 122.48      | 127.18   |
| 22  | B     | 607 | CLA  | CMD-C2D-C3D | 2.32  | 129.53      | 125.16   |
| 26  | A     | 409 | DGD  | C3G-C2G-C1G | -2.32 | 106.54      | 111.86   |
| 22  | c     | 508 | CLA  | C3A-C4A-CHB | -2.32 | 119.52      | 124.33   |
| 31  | C     | 521 | LMG  | C40-C39-C38 | -2.32 | 102.26      | 114.56   |
| 31  | L     | 101 | LMG  | C22-C23-C24 | -2.32 | 104.41      | 113.73   |
| 30  | F     | 103 | SQD  | C5-C6-S     | -2.32 | 111.16      | 114.40   |
| 22  | b     | 619 | CLA  | C4B-C3B-CAB | -2.32 | 122.49      | 127.18   |
| 22  | B     | 601 | CLA  | CHB-C4A-NA  | 2.31  | 127.61      | 124.38   |
| 22  | c     | 501 | CLA  | CHD-C4C-NC  | 2.31  | 125.90      | 124.28   |
| 22  | D     | 403 | CLA  | CMD-C2D-C3D | 2.32  | 129.52      | 125.16   |
| 30  | A     | 414 | SQD  | C1-O5-C5    | 2.31  | 118.21      | 113.73   |
| 22  | b     | 618 | CLA  | C4A-NA-C1A  | 2.31  | 109.64      | 106.38   |
| 25  | c     | 513 | BCR  | C27-C26-C25 | 2.31  | 125.91      | 122.86   |
| 31  | b     | 626 | LMG  | O6-C1-O1    | -2.31 | 104.42      | 109.93   |
| 22  | c     | 509 | CLA  | C4A-NA-C1A  | 2.31  | 109.64      | 106.38   |
| 22  | c     | 502 | CLA  | C4A-NA-C1A  | 2.31  | 109.64      | 106.38   |
| 26  | c     | 515 | DGD  | C9B-C8B-C7B | -2.31 | 106.34      | 112.94   |
| 25  | i     | 101 | BCR  | C15-C16-C17 | -2.31 | 118.36      | 123.45   |
| 22  | C     | 504 | CLA  | CBA-CAA-C2A | 2.31  | 119.59      | 113.95   |
| 22  | B     | 608 | CLA  | CMD-C2D-C3D | 2.31  | 129.51      | 125.16   |
| 25  | b     | 624 | BCR  | C38-C26-C25 | -2.31 | 121.89      | 124.50   |
| 31  | d     | 412 | LMG  | O6-C1-O1    | -2.31 | 104.44      | 109.93   |
| 22  | B     | 609 | CLA  | C1B-CHB-C4A | -2.31 | 125.55      | 130.12   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | a     | 403 | CLA  | CMB-C2B-C3B | 2.30  | 129.50      | 125.16   |
| 22  | b     | 612 | CLA  | CHD-C4C-NC  | 2.30  | 125.89      | 124.28   |
| 22  | a     | 405 | CLA  | CBD-CHA-C1A | 2.30  | 131.78      | 128.77   |
| 30  | f     | 103 | SQD  | C3-C4-C5    | 2.30  | 114.30      | 110.17   |
| 22  | c     | 507 | CLA  | C1B-CHB-C4A | -2.30 | 125.56      | 130.12   |
| 22  | C     | 506 | CLA  | C3A-C4A-CHB | -2.30 | 119.55      | 124.33   |
| 26  | c     | 516 | DGD  | CFB-CEB-CDB | -2.30 | 102.36      | 114.56   |
| 22  | A     | 402 | CLA  | CBD-CHA-C1A | 2.30  | 131.78      | 128.77   |
| 25  | y     | 101 | BCR  | C1-C6-C5    | -2.30 | 119.26      | 122.59   |
| 22  | B     | 606 | CLA  | C4A-NA-C1A  | 2.30  | 109.62      | 106.38   |
| 22  | c     | 511 | CLA  | C4B-C3B-CAB | -2.30 | 122.53      | 127.18   |
| 22  | c     | 505 | CLA  | C3A-C4A-CHB | -2.30 | 119.55      | 124.33   |
| 31  | L     | 101 | LMG  | C38-C37-C36 | -2.29 | 102.38      | 114.56   |
| 22  | C     | 504 | CLA  | CMB-C2B-C3B | 2.29  | 129.48      | 125.16   |
| 25  | c     | 513 | BCR  | C15-C16-C17 | -2.29 | 118.40      | 123.45   |
| 22  | b     | 608 | CLA  | O1D-CGD-CBD | 2.29  | 129.13      | 124.45   |
| 22  | D     | 404 | CLA  | C1B-CHB-C4A | -2.29 | 125.58      | 130.12   |
| 22  | d     | 406 | CLA  | C1B-CHB-C4A | -2.29 | 125.58      | 130.12   |
| 26  | c     | 516 | DGD  | O3D-C3D-C4D | -2.29 | 105.24      | 110.36   |
| 22  | c     | 511 | CLA  | O2A-CGA-O1A | -2.29 | 117.50      | 123.48   |
| 26  | c     | 515 | DGD  | C1D-C2D-C3D | -2.29 | 105.55      | 109.99   |
| 31  | C     | 517 | LMG  | C38-C37-C36 | -2.29 | 102.40      | 114.56   |
| 25  | C     | 520 | BCR  | C11-C10-C9  | -2.29 | 123.98      | 127.29   |
| 31  | B     | 625 | LMG  | O1-C1-C2    | -2.29 | 105.22      | 108.15   |
| 25  | B     | 619 | BCR  | C38-C26-C25 | -2.29 | 121.92      | 124.50   |
| 31  | e     | 101 | LMG  | O3-C3-C2    | -2.29 | 105.25      | 110.36   |
| 22  | b     | 609 | CLA  | C1B-CHB-C4A | -2.28 | 125.59      | 130.12   |
| 22  | b     | 616 | CLA  | O2D-CGD-O1D | -2.28 | 119.20      | 123.79   |
| 22  | B     | 615 | CLA  | O2D-CGD-O1D | -2.28 | 119.20      | 123.79   |
| 22  | b     | 614 | CLA  | C1B-CHB-C4A | -2.28 | 125.59      | 130.12   |
| 31  | c     | 518 | LMG  | O1-C7-C8    | -2.28 | 105.56      | 110.99   |
| 22  | b     | 605 | CLA  | C1B-CHB-C4A | -2.28 | 125.60      | 130.12   |
| 32  | B     | 624 | LMT  | C1'-O5'-C5' | -2.28 | 109.32      | 113.73   |
| 22  | D     | 404 | CLA  | CBD-CHA-C1A | 2.28  | 131.75      | 128.77   |
| 31  | B     | 621 | LMG  | O3-C3-C2    | -2.28 | 105.26      | 110.36   |
| 22  | C     | 508 | CLA  | C4A-NA-C1A  | 2.28  | 109.59      | 106.38   |
| 24  | j     | 101 | PL9  | C12-C13-C14 | -2.28 | 122.88      | 127.81   |
| 26  | b     | 625 | DGD  | C1D-C2D-C3D | -2.28 | 105.58      | 109.99   |
| 22  | C     | 510 | CLA  | CHD-C4C-NC  | 2.28  | 125.88      | 124.28   |
| 31  | e     | 101 | LMG  | O6-C1-O1    | -2.28 | 104.50      | 109.93   |
| 22  | A     | 404 | CLA  | C4A-NA-C1A  | 2.28  | 109.59      | 106.38   |
| 26  | b     | 601 | DGD  | O6D-C1D-O3G | -2.28 | 104.51      | 109.93   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | b     | 623 | BCR  | C27-C26-C25 | 2.28  | 125.86      | 122.86   |
| 22  | B     | 605 | CLA  | O1D-CGD-CBD | 2.28  | 129.10      | 124.45   |
| 22  | b     | 612 | CLA  | C4A-NA-C1A  | 2.27  | 109.59      | 106.38   |
| 22  | D     | 403 | CLA  | C4A-NA-C1A  | 2.27  | 109.59      | 106.38   |
| 22  | a     | 403 | CLA  | C4A-NA-C1A  | 2.27  | 109.58      | 106.38   |
| 25  | C     | 520 | BCR  | C24-C23-C22 | -2.27 | 122.82      | 126.22   |
| 22  | b     | 606 | CLA  | C4A-NA-C1A  | 2.27  | 109.58      | 106.38   |
| 22  | c     | 510 | CLA  | C4A-NA-C1A  | 2.27  | 109.58      | 106.38   |
| 22  | B     | 601 | CLA  | CMD-C2D-C3D | 2.27  | 129.44      | 125.16   |
| 31  | d     | 412 | LMG  | C1-C2-C3    | -2.27 | 105.59      | 109.99   |
| 25  | C     | 513 | BCR  | C24-C23-C22 | -2.27 | 122.82      | 126.22   |
| 22  | b     | 605 | CLA  | CHB-C4A-NA  | 2.27  | 127.55      | 124.38   |
| 22  | a     | 406 | CLA  | CMD-C2D-C3D | 2.27  | 129.44      | 125.16   |
| 22  | c     | 511 | CLA  | CHD-C4C-NC  | 2.27  | 125.87      | 124.28   |
| 25  | x     | 101 | BCR  | C29-C30-C25 | 2.27  | 113.99      | 110.37   |
| 24  | a     | 407 | PL9  | C32-C33-C34 | -2.27 | 122.90      | 127.81   |
| 22  | b     | 613 | CLA  | C1-C2-C3    | -2.27 | 122.30      | 126.23   |
| 31  | C     | 521 | LMG  | O3-C3-C2    | -2.27 | 105.29      | 110.36   |
| 24  | J     | 101 | PL9  | C12-C13-C14 | -2.27 | 122.91      | 127.81   |
| 22  | b     | 606 | CLA  | C3A-C4A-CHB | -2.27 | 119.62      | 124.33   |
| 22  | C     | 501 | CLA  | C4B-C3B-CAB | -2.26 | 122.59      | 127.18   |
| 22  | B     | 608 | CLA  | C4A-NA-C1A  | 2.26  | 109.57      | 106.38   |
| 22  | b     | 615 | CLA  | CHD-C4C-NC  | 2.26  | 125.86      | 124.28   |
| 25  | K     | 101 | BCR  | C27-C26-C25 | 2.26  | 125.85      | 122.86   |
| 22  | B     | 603 | CLA  | C1B-CHB-C4A | -2.26 | 125.63      | 130.12   |
| 22  | B     | 612 | CLA  | C2B-C3B-CAB | 2.26  | 131.96      | 127.33   |
| 31  | C     | 521 | LMG  | C23-C22-C21 | -2.26 | 106.47      | 112.94   |
| 22  | D     | 404 | CLA  | C3A-C4A-CHB | -2.26 | 119.62      | 124.33   |
| 25  | K     | 101 | BCR  | C15-C16-C17 | -2.26 | 118.47      | 123.45   |
| 30  | f     | 103 | SQD  | C1-O5-C5    | 2.26  | 118.11      | 113.73   |
| 25  | c     | 513 | BCR  | C15-C14-C13 | -2.26 | 124.02      | 127.29   |
| 25  | b     | 624 | BCR  | C24-C23-C22 | -2.26 | 122.83      | 126.22   |
| 31  | B     | 621 | LMG  | C40-C39-C38 | -2.26 | 102.56      | 114.56   |
| 26  | B     | 626 | DGD  | O6D-C1D-O3G | -2.26 | 104.55      | 109.93   |
| 31  | a     | 402 | LMG  | O3-C3-C2    | -2.26 | 105.31      | 110.36   |
| 22  | B     | 607 | CLA  | C4A-NA-C1A  | 2.26  | 109.56      | 106.38   |
| 25  | F     | 102 | BCR  | C27-C26-C25 | 2.26  | 125.84      | 122.86   |
| 22  | c     | 509 | CLA  | C1B-CHB-C4A | -2.26 | 125.65      | 130.12   |
| 22  | b     | 605 | CLA  | CMD-C2D-C3D | 2.25  | 129.41      | 125.16   |
| 25  | j     | 102 | BCR  | C15-C16-C17 | -2.25 | 118.48      | 123.45   |
| 22  | C     | 502 | CLA  | C1B-CHB-C4A | -2.25 | 125.65      | 130.12   |
| 22  | c     | 506 | CLA  | C4A-NA-C1A  | 2.25  | 109.56      | 106.38   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | i     | 102 | LMG  | O3-C3-C2    | -2.25 | 105.32      | 110.36   |
| 22  | C     | 509 | CLA  | C4A-NA-C1A  | 2.25  | 109.56      | 106.38   |
| 22  | c     | 512 | CLA  | C4B-C3B-CAB | -2.25 | 122.61      | 127.18   |
| 22  | B     | 611 | CLA  | O2D-CGD-O1D | -2.25 | 119.27      | 123.79   |
| 22  | B     | 612 | CLA  | CMD-C2D-C3D | 2.25  | 129.41      | 125.16   |
| 24  | D     | 405 | PL9  | C42-C43-C44 | -2.25 | 122.94      | 127.81   |
| 22  | d     | 406 | CLA  | C4B-C3B-CAB | -2.25 | 122.62      | 127.18   |
| 22  | A     | 402 | CLA  | C4A-NA-C1A  | 2.25  | 109.55      | 106.38   |
| 22  | D     | 404 | CLA  | C4B-C3B-CAB | -2.25 | 122.62      | 127.18   |
| 22  | B     | 602 | CLA  | C4A-NA-C1A  | 2.25  | 109.55      | 106.38   |
| 22  | b     | 617 | CLA  | C1B-CHB-C4A | -2.25 | 125.66      | 130.12   |
| 22  | b     | 618 | CLA  | CHD-C4C-NC  | 2.25  | 125.85      | 124.28   |
| 22  | c     | 504 | CLA  | O1D-CGD-CBD | 2.24  | 129.04      | 124.45   |
| 26  | B     | 620 | DGD  | C4E-C3E-C2E | -2.25 | 106.66      | 110.80   |
| 31  | l     | 101 | LMG  | C38-C37-C36 | -2.25 | 102.64      | 114.56   |
| 22  | B     | 610 | CLA  | CMD-C2D-C3D | 2.25  | 129.39      | 125.16   |
| 22  | b     | 613 | CLA  | C4B-C3B-CAB | -2.24 | 122.64      | 127.18   |
| 22  | B     | 611 | CLA  | C1B-CHB-C4A | -2.24 | 125.68      | 130.12   |
| 22  | a     | 405 | CLA  | C4A-NA-C1A  | 2.24  | 109.54      | 106.38   |
| 22  | C     | 506 | CLA  | CHD-C4C-NC  | 2.24  | 125.85      | 124.28   |
| 25  | g     | 101 | BCR  | C1-C6-C5    | -2.24 | 119.35      | 122.59   |
| 22  | C     | 519 | CLA  | CMD-C2D-C3D | 2.24  | 129.38      | 125.16   |
| 34  | v     | 201 | HEM  | C3A-C4A-NA  | -2.24 | 108.00      | 109.50   |
| 25  | C     | 513 | BCR  | C38-C26-C25 | -2.24 | 121.97      | 124.50   |
| 26  | C     | 515 | DGD  | CFB-CEB-CDB | -2.24 | 102.68      | 114.56   |
| 31  | b     | 626 | LMG  | O3-C3-C2    | -2.24 | 105.36      | 110.36   |
| 31  | c     | 522 | LMG  | C38-C37-C36 | -2.24 | 102.69      | 114.56   |
| 22  | C     | 508 | CLA  | C1B-CHB-C4A | -2.23 | 125.69      | 130.12   |
| 25  | y     | 101 | BCR  | C33-C5-C6   | -2.24 | 121.97      | 124.50   |
| 31  | c     | 518 | LMG  | C38-C37-C36 | -2.24 | 102.69      | 114.56   |
| 26  | d     | 410 | DGD  | O5D-C1E-C2E | 2.24  | 111.02      | 108.15   |
| 22  | C     | 511 | CLA  | C1B-CHB-C4A | -2.23 | 125.69      | 130.12   |
| 22  | b     | 615 | CLA  | C4B-CHC-C1C | -2.23 | 124.53      | 127.47   |
| 22  | B     | 609 | CLA  | C4A-NA-C1A  | 2.23  | 109.53      | 106.38   |
| 22  | b     | 615 | CLA  | CBA-CAA-C2A | -2.23 | 108.49      | 113.95   |
| 22  | A     | 402 | CLA  | C1B-CHB-C4A | -2.23 | 125.69      | 130.12   |
| 22  | B     | 607 | CLA  | C3A-C4A-CHB | -2.23 | 119.69      | 124.33   |
| 22  | b     | 608 | CLA  | C1B-CHB-C4A | -2.23 | 125.70      | 130.12   |
| 31  | L     | 101 | LMG  | O1-C1-C2    | -2.23 | 105.29      | 108.15   |
| 25  | c     | 514 | BCR  | C38-C26-C25 | -2.23 | 121.98      | 124.50   |
| 31  | b     | 626 | LMG  | C38-C37-C36 | -2.23 | 102.72      | 114.56   |
| 23  | d     | 402 | PHO  | CMB-C2B-C1B | -2.23 | 121.71      | 125.68   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | b     | 611 | CLA  | C4A-NA-C1A  | 2.23  | 109.52      | 106.38   |
| 30  | b     | 602 | SQD  | O48-C23-C24 | 2.23  | 118.72      | 111.90   |
| 22  | B     | 614 | CLA  | C4B-C3B-CAB | -2.23 | 122.67      | 127.18   |
| 31  | a     | 402 | LMG  | O1-C7-C8    | -2.23 | 105.69      | 110.99   |
| 31  | I     | 101 | LMG  | C23-C22-C21 | -2.23 | 106.58      | 112.94   |
| 22  | d     | 406 | CLA  | C3A-C4A-CHB | -2.23 | 119.70      | 124.33   |
| 22  | C     | 505 | CLA  | CMD-C2D-C3D | 2.23  | 129.35      | 125.16   |
| 32  | B     | 628 | LMT  | O1'-C1'-C2' | 2.23  | 111.00      | 108.15   |
| 23  | D     | 401 | PHO  | CMB-C2B-C1B | -2.23 | 121.72      | 125.68   |
| 24  | D     | 405 | PL9  | C31-C32-C33 | -2.22 | 105.32      | 111.64   |
| 31  | D     | 409 | LMG  | O2-C2-C1    | -2.22 | 105.20      | 110.03   |
| 23  | d     | 402 | PHO  | C3D-C4D-ND  | 2.22  | 109.61      | 106.81   |
| 25  | c     | 521 | BCR  | C24-C23-C22 | -2.22 | 122.89      | 126.22   |
| 24  | d     | 407 | PL9  | C31-C32-C33 | -2.22 | 105.32      | 111.64   |
| 22  | a     | 403 | CLA  | C1B-CHB-C4A | -2.22 | 125.71      | 130.12   |
| 22  | B     | 609 | CLA  | C3A-C4A-CHB | -2.22 | 119.71      | 124.33   |
| 31  | C     | 517 | LMG  | O3-C3-C2    | -2.22 | 105.39      | 110.36   |
| 30  | B     | 622 | SQD  | C4-C3-C2    | 2.22  | 114.90      | 110.80   |
| 31  | c     | 518 | LMG  | O3-C3-C2    | -2.22 | 105.39      | 110.36   |
| 26  | c     | 516 | DGD  | C3D-C4D-C5D | -2.22 | 106.19      | 110.17   |
| 22  | b     | 617 | CLA  | CHD-C4C-NC  | 2.22  | 125.83      | 124.28   |
| 22  | c     | 507 | CLA  | C1-C2-C3    | -2.22 | 122.38      | 126.23   |
| 22  | C     | 503 | CLA  | CMD-C2D-C3D | 2.22  | 129.34      | 125.16   |
| 24  | a     | 407 | PL9  | C31-C32-C33 | -2.22 | 105.33      | 111.64   |
| 22  | b     | 608 | CLA  | CHD-C4C-NC  | 2.22  | 125.83      | 124.28   |
| 31  | I     | 101 | LMG  | C20-C21-C22 | -2.22 | 104.81      | 113.73   |
| 22  | C     | 504 | CLA  | O1D-CGD-CBD | 2.22  | 128.98      | 124.45   |
| 22  | c     | 507 | CLA  | CMD-C2D-C3D | 2.22  | 129.34      | 125.16   |
| 22  | C     | 509 | CLA  | C1B-CHB-C4A | -2.22 | 125.72      | 130.12   |
| 22  | b     | 610 | CLA  | C1B-CHB-C4A | -2.22 | 125.73      | 130.12   |
| 22  | C     | 505 | CLA  | C4A-NA-C1A  | 2.22  | 109.50      | 106.38   |
| 31  | B     | 621 | LMG  | O6-C1-O1    | -2.22 | 104.65      | 109.93   |
| 31  | I     | 101 | LMG  | O3-C3-C2    | -2.21 | 105.41      | 110.36   |
| 31  | c     | 522 | LMG  | O3-C3-C2    | -2.21 | 105.41      | 110.36   |
| 22  | D     | 404 | CLA  | C4A-NA-C1A  | 2.22  | 109.50      | 106.38   |
| 31  | b     | 627 | LMG  | O1-C7-C8    | -2.21 | 105.72      | 110.99   |
| 32  | d     | 411 | LMT  | C1'-O5'-C5' | -2.21 | 109.45      | 113.73   |
| 31  | i     | 102 | LMG  | C20-C21-C22 | -2.21 | 104.83      | 113.73   |
| 23  | d     | 402 | PHO  | CHD-C4C-NC  | -2.21 | 124.73      | 128.68   |
| 22  | B     | 615 | CLA  | C1B-CHB-C4A | -2.21 | 125.74      | 130.12   |
| 22  | d     | 405 | CLA  | CHB-C4A-NA  | 2.21  | 127.46      | 124.38   |
| 31  | E     | 101 | LMG  | O6-C1-O1    | -2.21 | 104.67      | 109.93   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | b     | 612 | CLA  | CMD-C2D-C3D | 2.21  | 129.32      | 125.16   |
| 22  | C     | 510 | CLA  | C1B-CHB-C4A | -2.21 | 125.74      | 130.12   |
| 23  | D     | 401 | PHO  | CBD-CHA-C1A | 2.21  | 130.50      | 126.67   |
| 24  | D     | 405 | PL9  | C12-C13-C14 | -2.21 | 123.04      | 127.81   |
| 22  | C     | 501 | CLA  | CMD-C2D-C3D | 2.20  | 129.31      | 125.16   |
| 26  | C     | 514 | DGD  | C9B-C8B-C7B | -2.20 | 106.64      | 112.94   |
| 25  | c     | 521 | BCR  | C33-C5-C6   | -2.20 | 122.01      | 124.50   |
| 31  | l     | 101 | LMG  | O2-C2-C1    | -2.20 | 105.25      | 110.03   |
| 31  | D     | 406 | LMG  | O6-C1-O1    | -2.20 | 104.69      | 109.93   |
| 25  | F     | 102 | BCR  | C11-C10-C9  | -2.20 | 124.11      | 127.29   |
| 31  | C     | 521 | LMG  | O6-C1-O1    | -2.20 | 104.69      | 109.93   |
| 31  | C     | 517 | LMG  | O1-C7-C8    | -2.20 | 105.76      | 110.99   |
| 31  | E     | 101 | LMG  | O2-C2-C1    | -2.20 | 105.26      | 110.03   |
| 22  | c     | 502 | CLA  | C1B-CHB-C4A | -2.20 | 125.77      | 130.12   |
| 25  | H     | 102 | BCR  | C29-C30-C25 | 2.20  | 113.87      | 110.37   |
| 22  | b     | 612 | CLA  | C3A-C4A-CHB | -2.20 | 119.76      | 124.33   |
| 22  | c     | 503 | CLA  | CMD-C2D-C3D | 2.20  | 129.30      | 125.16   |
| 22  | b     | 618 | CLA  | CMD-C2D-C3D | 2.20  | 129.30      | 125.16   |
| 25  | C     | 520 | BCR  | C33-C5-C6   | -2.20 | 122.02      | 124.50   |
| 22  | B     | 614 | CLA  | CHD-C4C-NC  | 2.20  | 125.82      | 124.28   |
| 25  | A     | 408 | BCR  | C38-C26-C25 | -2.20 | 122.02      | 124.50   |
| 31  | C     | 521 | LMG  | C20-C21-C22 | -2.20 | 104.90      | 113.73   |
| 34  | f     | 101 | HEM  | CAD-CBD-CGD | -2.19 | 109.39      | 113.53   |
| 30  | f     | 103 | SQD  | C5-C6-S     | -2.19 | 111.33      | 114.40   |
| 22  | B     | 612 | CLA  | C3A-C4A-CHB | -2.19 | 119.77      | 124.33   |
| 31  | c     | 522 | LMG  | O6-C1-O1    | -2.19 | 104.70      | 109.93   |
| 22  | c     | 512 | CLA  | C1B-CHB-C4A | -2.19 | 125.77      | 130.12   |
| 25  | F     | 102 | BCR  | C7-C8-C9    | -2.19 | 122.93      | 126.22   |
| 31  | E     | 101 | LMG  | O3-C3-C2    | -2.19 | 105.47      | 110.36   |
| 31  | C     | 521 | LMG  | C38-C37-C36 | -2.19 | 102.94      | 114.56   |
| 22  | A     | 406 | CLA  | CMD-C2D-C3D | 2.19  | 129.29      | 125.16   |
| 25  | C     | 520 | BCR  | C7-C8-C9    | -2.19 | 122.94      | 126.22   |
| 24  | A     | 407 | PL9  | C32-C33-C34 | -2.19 | 123.08      | 127.81   |
| 22  | b     | 608 | CLA  | C3A-C4A-CHB | -2.19 | 119.78      | 124.33   |
| 22  | c     | 520 | CLA  | C1B-CHB-C4A | -2.19 | 125.78      | 130.12   |
| 25  | F     | 102 | BCR  | C15-C16-C17 | -2.19 | 118.63      | 123.45   |
| 22  | B     | 608 | CLA  | C4B-C3B-CAB | -2.19 | 122.75      | 127.18   |
| 25  | H     | 102 | BCR  | C27-C26-C25 | 2.18  | 125.74      | 122.86   |
| 26  | C     | 514 | DGD  | C3G-C2G-C1G | -2.19 | 106.84      | 111.86   |
| 22  | b     | 618 | CLA  | C1B-CHB-C4A | -2.19 | 125.79      | 130.12   |
| 22  | b     | 619 | CLA  | C1B-CHB-C4A | -2.19 | 125.79      | 130.12   |
| 22  | C     | 519 | CLA  | C3A-C4A-CHB | -2.18 | 119.79      | 124.33   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | C     | 502 | CLA  | C4A-NA-C1A  | 2.18  | 109.46      | 106.38   |
| 22  | b     | 619 | CLA  | C3A-C4A-CHB | -2.18 | 119.79      | 124.33   |
| 22  | b     | 610 | CLA  | O1D-CGD-CBD | 2.18  | 128.91      | 124.45   |
| 22  | C     | 512 | CLA  | C1B-CHB-C4A | -2.18 | 125.79      | 130.12   |
| 25  | f     | 102 | BCR  | C27-C26-C25 | 2.18  | 125.74      | 122.86   |
| 32  | M     | 102 | LMT  | C3'-C4'-C5' | -2.18 | 105.99      | 110.86   |
| 22  | b     | 611 | CLA  | CBD-CHA-C1A | 2.18  | 131.62      | 128.77   |
| 22  | A     | 403 | CLA  | C3A-C4A-CHB | -2.18 | 119.80      | 124.33   |
| 31  | b     | 627 | LMG  | O3-C3-C2    | -2.18 | 105.49      | 110.36   |
| 26  | a     | 408 | DGD  | C1D-C2D-C3D | -2.18 | 105.77      | 109.99   |
| 22  | b     | 620 | CLA  | C1B-CHB-C4A | -2.18 | 125.81      | 130.12   |
| 25  | B     | 619 | BCR  | C24-C23-C22 | -2.18 | 122.96      | 126.22   |
| 31  | B     | 621 | LMG  | C38-C37-C36 | -2.18 | 103.00      | 114.56   |
| 26  | C     | 515 | DGD  | O3D-C3D-C4D | -2.18 | 105.50      | 110.36   |
| 22  | c     | 501 | CLA  | C4B-C3B-CAB | -2.17 | 122.77      | 127.18   |
| 22  | c     | 505 | CLA  | CMD-C2D-C3D | 2.17  | 129.25      | 125.16   |
| 30  | d     | 403 | SQD  | C4-C3-C2    | 2.17  | 114.81      | 110.80   |
| 22  | B     | 610 | CLA  | CHB-C4A-NA  | 2.17  | 127.41      | 124.38   |
| 26  | b     | 601 | DGD  | CBB-CAB-C9B | -2.17 | 103.04      | 114.56   |
| 22  | b     | 605 | CLA  | C4A-NA-C1A  | 2.17  | 109.44      | 106.38   |
| 22  | b     | 605 | CLA  | C1-C2-C3    | -2.17 | 122.46      | 126.23   |
| 22  | A     | 404 | CLA  | C4B-C3B-CAB | -2.17 | 122.78      | 127.18   |
| 22  | d     | 406 | CLA  | CMD-C2D-C3D | 2.17  | 129.25      | 125.16   |
| 25  | J     | 102 | BCR  | C20-C21-C22 | -2.17 | 124.15      | 127.29   |
| 31  | c     | 522 | LMG  | C23-C22-C21 | -2.17 | 106.75      | 112.94   |
| 22  | B     | 613 | CLA  | CMD-C2D-C3D | 2.17  | 129.24      | 125.16   |
| 32  | b     | 628 | LMT  | O1'-C1'-C2' | 2.17  | 110.93      | 108.15   |
| 22  | a     | 404 | CLA  | CBD-CHA-C1A | 2.17  | 131.60      | 128.77   |
| 22  | C     | 507 | CLA  | C1-C2-C3    | -2.17 | 122.47      | 126.23   |
| 31  | i     | 102 | LMG  | C23-C22-C21 | -2.16 | 106.75      | 112.94   |
| 22  | C     | 511 | CLA  | C3A-C4A-CHB | -2.16 | 119.83      | 124.33   |
| 31  | C     | 517 | LMG  | O1-C1-C2    | -2.16 | 105.38      | 108.15   |
| 25  | i     | 101 | BCR  | C38-C26-C25 | -2.16 | 122.05      | 124.50   |
| 31  | c     | 522 | LMG  | C20-C21-C22 | -2.16 | 105.04      | 113.73   |
| 22  | b     | 614 | CLA  | CMD-C2D-C3D | 2.16  | 129.23      | 125.16   |
| 25  | B     | 617 | BCR  | C24-C23-C22 | -2.16 | 122.98      | 126.22   |
| 26  | b     | 601 | DGD  | CAB-C9B-C8B | -2.16 | 103.10      | 114.56   |
| 23  | A     | 405 | PHO  | C3D-C4D-ND  | 2.16  | 109.53      | 106.81   |
| 22  | C     | 505 | CLA  | CBA-CAA-C2A | -2.16 | 108.67      | 113.95   |
| 22  | B     | 607 | CLA  | CBD-CHA-C1A | 2.16  | 131.59      | 128.77   |
| 31  | e     | 101 | LMG  | O2-C2-C1    | -2.16 | 105.34      | 110.03   |
| 22  | b     | 614 | CLA  | C3A-C4A-CHB | -2.16 | 119.84      | 124.33   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | a     | 404 | CLA  | C3A-C4A-CHB | -2.16 | 119.84      | 124.33   |
| 26  | a     | 408 | DGD  | CAB-C9B-C8B | -2.16 | 103.12      | 114.56   |
| 22  | b     | 609 | CLA  | C3A-C4A-CHB | -2.16 | 119.85      | 124.33   |
| 22  | B     | 601 | CLA  | C4A-NA-C1A  | 2.16  | 109.42      | 106.38   |
| 22  | d     | 405 | CLA  | C1B-CHB-C4A | -2.16 | 125.85      | 130.12   |
| 22  | B     | 602 | CLA  | CMD-C2D-C3D | 2.15  | 129.22      | 125.16   |
| 22  | c     | 506 | CLA  | CMD-C2D-C3D | 2.15  | 129.22      | 125.16   |
| 31  | d     | 409 | LMG  | O6-C1-O1    | -2.15 | 104.80      | 109.93   |
| 23  | D     | 401 | PHO  | C3D-C4D-ND  | 2.15  | 109.52      | 106.81   |
| 23  | d     | 401 | PHO  | C4D-CHA-CBD | -2.15 | 105.53      | 107.88   |
| 25  | B     | 618 | BCR  | C27-C26-C25 | 2.15  | 125.70      | 122.86   |
| 22  | b     | 608 | CLA  | CMD-C2D-C3D | 2.15  | 129.22      | 125.16   |
| 24  | d     | 407 | PL9  | C36-C34-C33 | -2.15 | 116.92      | 121.06   |
| 22  | c     | 511 | CLA  | C1B-CHB-C4A | -2.15 | 125.86      | 130.12   |
| 25  | g     | 101 | BCR  | C33-C5-C6   | -2.15 | 122.07      | 124.50   |
| 25  | g     | 101 | BCR  | C15-C16-C17 | -2.15 | 118.71      | 123.45   |
| 26  | C     | 514 | DGD  | O5D-C6D-C5D | -2.15 | 105.23      | 108.96   |
| 22  | b     | 616 | CLA  | C1B-CHB-C4A | -2.15 | 125.86      | 130.12   |
| 22  | c     | 520 | CLA  | CMD-C2D-C3D | 2.15  | 129.21      | 125.16   |
| 31  | b     | 626 | LMG  | C20-C21-C22 | -2.15 | 105.07      | 113.73   |
| 24  | A     | 407 | PL9  | C12-C13-C14 | -2.15 | 123.16      | 127.81   |
| 22  | C     | 508 | CLA  | C3A-C4A-CHB | -2.15 | 119.87      | 124.33   |
| 22  | b     | 613 | CLA  | C4A-NA-C1A  | 2.15  | 109.41      | 106.38   |
| 22  | C     | 505 | CLA  | C3A-C4A-CHB | -2.15 | 119.86      | 124.33   |
| 31  | B     | 621 | LMG  | C20-C21-C22 | -2.15 | 105.09      | 113.73   |
| 22  | B     | 610 | CLA  | C1D-CHD-C4C | 2.15  | 125.93      | 122.60   |
| 22  | B     | 605 | CLA  | C3A-C4A-CHB | -2.15 | 119.87      | 124.33   |
| 22  | b     | 607 | CLA  | CMD-C2D-C3D | 2.14  | 129.20      | 125.16   |
| 25  | f     | 102 | BCR  | C11-C10-C9  | -2.14 | 124.19      | 127.29   |
| 30  | a     | 401 | SQD  | C5-C6-S     | -2.14 | 111.41      | 114.40   |
| 23  | d     | 401 | PHO  | C3D-C4D-ND  | 2.14  | 109.51      | 106.81   |
| 30  | F     | 103 | SQD  | O48-C23-C24 | 2.14  | 118.46      | 111.90   |
| 30  | f     | 103 | SQD  | O48-C23-C24 | 2.14  | 118.46      | 111.90   |
| 31  | M     | 101 | LMG  | O3-C3-C2    | -2.14 | 105.57      | 110.36   |
| 22  | B     | 606 | CLA  | CHD-C4C-NC  | 2.14  | 125.78      | 124.28   |
| 22  | c     | 501 | CLA  | CMD-C2D-C3D | 2.14  | 129.19      | 125.16   |
| 31  | d     | 412 | LMG  | O2-C2-C1    | -2.14 | 105.39      | 110.03   |
| 22  | B     | 603 | CLA  | CMD-C2D-C3D | 2.14  | 129.19      | 125.16   |
| 31  | B     | 621 | LMG  | C23-C22-C21 | -2.14 | 106.83      | 112.94   |
| 22  | a     | 406 | CLA  | C3A-C4A-CHB | -2.14 | 119.89      | 124.33   |
| 26  | c     | 516 | DGD  | CBB-CAB-C9B | -2.14 | 103.22      | 114.56   |
| 22  | A     | 404 | CLA  | CHD-C4C-NC  | 2.14  | 125.78      | 124.28   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | b     | 626 | LMG  | C23-C22-C21 | -2.14 | 106.83      | 112.94   |
| 22  | C     | 512 | CLA  | CMD-C2D-C3D | 2.14  | 129.18      | 125.16   |
| 25  | b     | 621 | BCR  | C15-C16-C17 | -2.13 | 118.75      | 123.45   |
| 31  | L     | 101 | LMG  | O2-C2-C1    | -2.13 | 105.40      | 110.03   |
| 32  | b     | 629 | LMT  | O1'-C1'-C2' | 2.13  | 110.89      | 108.15   |
| 22  | c     | 520 | CLA  | CHD-C4C-NC  | 2.13  | 125.77      | 124.28   |
| 22  | b     | 615 | CLA  | CHB-C4A-NA  | 2.13  | 127.36      | 124.38   |
| 22  | b     | 613 | CLA  | C3A-C4A-CHB | -2.13 | 119.89      | 124.33   |
| 26  | A     | 409 | DGD  | CAB-C9B-C8B | -2.13 | 103.25      | 114.56   |
| 30  | A     | 413 | SQD  | C5-C6-S     | -2.13 | 111.42      | 114.40   |
| 22  | C     | 506 | CLA  | CMD-C2D-C3D | 2.13  | 129.17      | 125.16   |
| 22  | B     | 606 | CLA  | CMD-C2D-C3D | 2.13  | 129.17      | 125.16   |
| 25  | K     | 101 | BCR  | C3-C4-C5    | -2.13 | 110.31      | 113.81   |
| 22  | c     | 509 | CLA  | O2A-CGA-O1A | -2.13 | 117.92      | 123.48   |
| 22  | C     | 519 | CLA  | CHD-C4C-NC  | 2.13  | 125.77      | 124.28   |
| 25  | b     | 622 | BCR  | C24-C23-C22 | -2.12 | 123.04      | 126.22   |
| 25  | K     | 101 | BCR  | C15-C14-C13 | -2.12 | 124.22      | 127.29   |
| 30  | A     | 414 | SQD  | C6-C5-C4    | -2.12 | 107.38      | 111.86   |
| 22  | C     | 504 | CLA  | C1-C2-C3    | -2.12 | 122.55      | 126.23   |
| 22  | b     | 619 | CLA  | CMD-C2D-C3D | 2.12  | 129.16      | 125.16   |
| 25  | b     | 623 | BCR  | C33-C5-C6   | -2.12 | 122.10      | 124.50   |
| 25  | g     | 101 | BCR  | C24-C23-C22 | -2.12 | 123.04      | 126.22   |
| 22  | c     | 511 | CLA  | C3A-C4A-CHB | -2.12 | 119.93      | 124.33   |
| 22  | c     | 512 | CLA  | C3A-C4A-CHB | -2.12 | 119.93      | 124.33   |
| 24  | D     | 405 | PL9  | C46-C47-C48 | -2.11 | 105.63      | 111.64   |
| 25  | g     | 101 | BCR  | C3-C2-C1    | -2.12 | 106.71      | 114.77   |
| 25  | B     | 616 | BCR  | C38-C26-C25 | -2.12 | 122.11      | 124.50   |
| 25  | H     | 102 | BCR  | C16-C15-C14 | -2.11 | 118.80      | 123.45   |
| 26  | B     | 626 | DGD  | CAB-C9B-C8B | -2.11 | 103.35      | 114.56   |
| 22  | c     | 510 | CLA  | C1B-CHB-C4A | -2.11 | 125.93      | 130.12   |
| 22  | D     | 404 | CLA  | CBA-CAA-C2A | -2.11 | 108.78      | 113.95   |
| 26  | C     | 514 | DGD  | C1D-C2D-C3D | -2.11 | 105.90      | 109.99   |
| 22  | b     | 607 | CLA  | C4A-NA-C1A  | 2.11  | 109.36      | 106.38   |
| 26  | C     | 515 | DGD  | CBB-CAB-C9B | -2.11 | 103.35      | 114.56   |
| 23  | d     | 402 | PHO  | C4D-CHA-CBD | -2.11 | 105.58      | 107.88   |
| 22  | a     | 405 | CLA  | C4B-C3B-CAB | -2.11 | 122.91      | 127.18   |
| 22  | C     | 507 | CLA  | C1B-CHB-C4A | -2.11 | 125.94      | 130.12   |
| 25  | f     | 102 | BCR  | C15-C16-C17 | -2.11 | 118.81      | 123.45   |
| 22  | B     | 611 | CLA  | O2A-CGA-O1A | -2.11 | 117.97      | 123.48   |
| 22  | b     | 619 | CLA  | O2A-CGA-O1A | -2.11 | 117.97      | 123.48   |
| 25  | i     | 101 | BCR  | C15-C14-C13 | -2.11 | 124.25      | 127.29   |
| 31  | m     | 101 | LMG  | O3-C3-C2    | -2.11 | 105.65      | 110.36   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | C     | 501 | CLA  | C1B-CHB-C4A | -2.11 | 125.95      | 130.12   |
| 31  | b     | 626 | LMG  | O1-C7-C8    | -2.10 | 105.98      | 110.99   |
| 26  | C     | 516 | DGD  | CBB-CAB-C9B | -2.10 | 103.40      | 114.56   |
| 22  | B     | 613 | CLA  | C3A-C4A-CHB | -2.10 | 119.96      | 124.33   |
| 24  | D     | 405 | PL9  | O1-C4-C3    | -2.10 | 118.19      | 120.69   |
| 25  | A     | 408 | BCR  | C24-C23-C22 | -2.10 | 123.07      | 126.22   |
| 22  | c     | 510 | CLA  | C3A-C4A-CHB | -2.10 | 119.96      | 124.33   |
| 22  | b     | 611 | CLA  | CHD-C4C-NC  | 2.10  | 125.75      | 124.28   |
| 34  | V     | 201 | HEM  | CAD-CBD-CGD | -2.10 | 109.57      | 113.53   |
| 22  | b     | 619 | CLA  | CHD-C4C-NC  | 2.10  | 125.75      | 124.28   |
| 26  | C     | 515 | DGD  | O2D-C2D-C1D | -2.10 | 105.48      | 110.03   |
| 24  | D     | 405 | PL9  | C36-C34-C33 | -2.10 | 117.03      | 121.06   |
| 22  | C     | 503 | CLA  | C1B-CHB-C4A | -2.10 | 125.97      | 130.12   |
| 22  | b     | 616 | CLA  | O2A-CGA-O1A | -2.09 | 118.01      | 123.48   |
| 22  | B     | 603 | CLA  | C3A-C4A-CHB | -2.09 | 119.98      | 124.33   |
| 34  | f     | 101 | HEM  | C3A-C4A-NA  | -2.09 | 108.10      | 109.50   |
| 26  | a     | 408 | DGD  | CDA-CCA-CBA | -2.09 | 106.97      | 112.94   |
| 22  | C     | 507 | CLA  | CMD-C2D-C3D | 2.09  | 129.10      | 125.16   |
| 26  | c     | 515 | DGD  | O5D-C1E-C2E | 2.09  | 110.83      | 108.15   |
| 22  | c     | 509 | CLA  | C3A-C4A-CHB | -2.09 | 119.99      | 124.33   |
| 24  | d     | 407 | PL9  | C42-C43-C44 | -2.09 | 123.30      | 127.81   |
| 27  | a     | 409 | LHG  | C27-C26-C25 | -2.09 | 103.48      | 114.56   |
| 27  | A     | 410 | LHG  | C27-C26-C25 | -2.09 | 103.48      | 114.56   |
| 24  | a     | 407 | PL9  | C12-C13-C14 | -2.09 | 123.30      | 127.81   |
| 26  | B     | 626 | DGD  | C9A-C8A-C7A | -2.08 | 106.98      | 112.94   |
| 25  | J     | 102 | BCR  | C33-C5-C6   | -2.09 | 122.14      | 124.50   |
| 24  | j     | 101 | PL9  | O2-C1-C2    | -2.08 | 116.86      | 121.82   |
| 22  | b     | 614 | CLA  | C4A-NA-C1A  | 2.08  | 109.32      | 106.38   |
| 26  | c     | 515 | DGD  | O5D-C6D-C5D | -2.08 | 105.35      | 108.96   |
| 22  | A     | 402 | CLA  | O1D-CGD-CBD | 2.08  | 128.71      | 124.45   |
| 22  | b     | 610 | CLA  | C3A-C4A-CHB | -2.08 | 120.00      | 124.33   |
| 22  | b     | 615 | CLA  | C1B-CHB-C4A | -2.08 | 126.00      | 130.12   |
| 23  | d     | 401 | PHO  | CMB-C2B-C1B | -2.08 | 121.98      | 125.68   |
| 25  | j     | 102 | BCR  | C29-C30-C25 | 2.08  | 113.68      | 110.37   |
| 22  | c     | 501 | CLA  | C3A-C4A-CHB | -2.08 | 120.01      | 124.33   |
| 24  | d     | 407 | PL9  | O2-C1-C2    | -2.07 | 116.88      | 121.82   |
| 25  | B     | 619 | BCR  | C11-C10-C9  | -2.08 | 124.29      | 127.29   |
| 22  | H     | 101 | CLA  | C1-C2-C3    | -2.08 | 122.63      | 126.23   |
| 31  | c     | 518 | LMG  | O1-C1-C2    | -2.07 | 105.49      | 108.15   |
| 31  | I     | 101 | LMG  | O1-C7-C8    | -2.07 | 106.06      | 110.99   |
| 25  | J     | 102 | BCR  | C29-C30-C25 | 2.07  | 113.67      | 110.37   |
| 25  | C     | 520 | BCR  | C38-C26-C25 | -2.07 | 122.16      | 124.50   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 26  | c     | 516 | DGD  | O2D-C2D-C1D | -2.07 | 105.53      | 110.03   |
| 24  | A     | 407 | PL9  | C11-C12-C13 | -2.07 | 105.75      | 111.64   |
| 26  | A     | 409 | DGD  | CDA-CCA-CBA | -2.07 | 107.02      | 112.94   |
| 26  | b     | 601 | DGD  | O3E-C3E-C2E | -2.07 | 105.73      | 110.36   |
| 22  | b     | 620 | CLA  | C4B-C3B-CAB | -2.07 | 122.99      | 127.18   |
| 26  | d     | 410 | DGD  | CAB-C9B-C8B | -2.07 | 103.57      | 114.56   |
| 22  | A     | 404 | CLA  | CMD-C2D-C3D | 2.07  | 129.06      | 125.16   |
| 26  | B     | 626 | DGD  | CBB-CAB-C9B | -2.07 | 103.58      | 114.56   |
| 22  | c     | 510 | CLA  | CHD-C4C-NC  | 2.07  | 125.73      | 124.28   |
| 22  | d     | 405 | CLA  | O2A-CGA-O1A | -2.07 | 118.07      | 123.48   |
| 25  | B     | 619 | BCR  | C33-C5-C6   | -2.07 | 122.16      | 124.50   |
| 26  | C     | 514 | DGD  | C5B-C4B-C3B | -2.07 | 103.59      | 114.56   |
| 22  | B     | 610 | CLA  | CBA-CAA-C2A | -2.07 | 108.89      | 113.95   |
| 24  | d     | 407 | PL9  | C46-C47-C48 | -2.07 | 105.77      | 111.64   |
| 22  | C     | 501 | CLA  | C3A-C4A-CHB | -2.06 | 120.04      | 124.33   |
| 25  | j     | 102 | BCR  | C20-C21-C22 | -2.06 | 124.31      | 127.29   |
| 25  | b     | 624 | BCR  | C15-C16-C17 | -2.06 | 118.91      | 123.45   |
| 24  | D     | 405 | PL9  | O2-C1-C2    | -2.06 | 116.90      | 121.82   |
| 25  | c     | 513 | BCR  | C3-C4-C5    | -2.06 | 110.42      | 113.81   |
| 23  | D     | 401 | PHO  | C4D-CHA-CBD | -2.06 | 105.63      | 107.88   |
| 32  | B     | 623 | LMT  | O1'-C1'-C2' | 2.06  | 110.79      | 108.15   |
| 22  | c     | 510 | CLA  | CMD-C2D-C3D | 2.06  | 129.04      | 125.16   |
| 22  | B     | 608 | CLA  | C3A-C4A-CHB | -2.06 | 120.05      | 124.33   |
| 26  | c     | 516 | DGD  | CAB-C9B-C8B | -2.06 | 103.62      | 114.56   |
| 22  | H     | 101 | CLA  | CMD-C2D-C3D | 2.06  | 129.04      | 125.16   |
| 26  | D     | 407 | DGD  | C3D-C4D-C5D | -2.06 | 106.47      | 110.17   |
| 22  | C     | 512 | CLA  | O1D-CGD-CBD | 2.06  | 128.66      | 124.45   |
| 22  | d     | 405 | CLA  | CHD-C4C-NC  | 2.06  | 125.72      | 124.28   |
| 22  | c     | 501 | CLA  | C1B-CHB-C4A | -2.06 | 126.04      | 130.12   |
| 22  | c     | 501 | CLA  | CMB-C2B-C3B | 2.06  | 129.04      | 125.16   |
| 26  | b     | 625 | DGD  | CAB-C9B-C8B | -2.06 | 103.63      | 114.56   |
| 24  | a     | 407 | PL9  | C11-C12-C13 | -2.06 | 105.79      | 111.64   |
| 31  | c     | 522 | LMG  | C1-C2-C3    | -2.06 | 106.01      | 109.99   |
| 26  | C     | 516 | DGD  | C3G-O3G-C1D | 2.05  | 117.92      | 113.80   |
| 26  | B     | 626 | DGD  | O3E-C3E-C2E | -2.05 | 105.77      | 110.36   |
| 22  | B     | 614 | CLA  | C1B-CHB-C4A | -2.06 | 126.05      | 130.12   |
| 31  | d     | 408 | LMG  | O1-C7-C8    | -2.06 | 106.10      | 110.99   |
| 25  | b     | 623 | BCR  | C20-C21-C22 | -2.05 | 124.32      | 127.29   |
| 31  | b     | 627 | LMG  | O2-C2-C1    | -2.05 | 105.57      | 110.03   |
| 22  | b     | 617 | CLA  | C1-C2-C3    | -2.05 | 122.67      | 126.23   |
| 24  | A     | 407 | PL9  | C31-C32-C33 | -2.05 | 105.81      | 111.64   |
| 31  | I     | 101 | LMG  | O1-C1-C2    | -2.05 | 105.53      | 108.15   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | l     | 101 | LMG  | O1-C1-C2    | -2.05 | 105.52      | 108.15   |
| 24  | a     | 407 | PL9  | O2-C1-C2    | -2.05 | 116.94      | 121.82   |
| 22  | c     | 512 | CLA  | CMD-C2D-C3D | 2.05  | 129.02      | 125.16   |
| 22  | C     | 504 | CLA  | C3A-C4A-CHB | -2.05 | 120.08      | 124.33   |
| 22  | B     | 611 | CLA  | C1-C2-C3    | -2.05 | 122.68      | 126.23   |
| 22  | B     | 601 | CLA  | C3A-C4A-CHB | -2.05 | 120.07      | 124.33   |
| 25  | A     | 408 | BCR  | C15-C16-C17 | -2.05 | 118.94      | 123.45   |
| 25  | x     | 101 | BCR  | C15-C16-C17 | -2.05 | 118.94      | 123.45   |
| 26  | B     | 620 | DGD  | C1D-C2D-C3D | -2.05 | 106.02      | 109.99   |
| 26  | D     | 407 | DGD  | C3G-C2G-C1G | -2.05 | 107.16      | 111.86   |
| 26  | c     | 515 | DGD  | O3E-C3E-C2E | -2.05 | 105.79      | 110.36   |
| 22  | B     | 604 | CLA  | CMD-C2D-C3D | 2.04  | 129.01      | 125.16   |
| 22  | b     | 615 | CLA  | C4A-NA-C1A  | 2.04  | 109.26      | 106.38   |
| 22  | c     | 503 | CLA  | O2D-CGD-CBD | 2.04  | 115.47      | 111.34   |
| 26  | c     | 515 | DGD  | C5B-C4B-C3B | -2.04 | 103.71      | 114.56   |
| 22  | C     | 509 | CLA  | C4B-C3B-CAB | -2.04 | 123.04      | 127.18   |
| 26  | A     | 409 | DGD  | C1D-C2D-C3D | -2.04 | 106.03      | 109.99   |
| 31  | D     | 406 | LMG  | O3-C3-C2    | -2.04 | 105.79      | 110.36   |
| 22  | H     | 101 | CLA  | C3A-C4A-CHB | -2.04 | 120.08      | 124.33   |
| 22  | c     | 502 | CLA  | C3A-C4A-CHB | -2.04 | 120.09      | 124.33   |
| 24  | J     | 101 | PL9  | O2-C1-C2    | -2.04 | 116.95      | 121.82   |
| 26  | b     | 601 | DGD  | C9A-C8A-C7A | -2.04 | 107.11      | 112.94   |
| 24  | d     | 407 | PL9  | C12-C13-C14 | -2.04 | 123.40      | 127.81   |
| 22  | a     | 403 | CLA  | O1D-CGD-CBD | 2.04  | 128.62      | 124.45   |
| 25  | C     | 520 | BCR  | C15-C14-C13 | -2.04 | 124.34      | 127.29   |
| 22  | B     | 615 | CLA  | C4B-C3B-CAB | -2.04 | 123.05      | 127.18   |
| 26  | C     | 515 | DGD  | CAB-C9B-C8B | -2.04 | 103.74      | 114.56   |
| 26  | C     | 514 | DGD  | O3E-C3E-C2E | -2.04 | 105.80      | 110.36   |
| 25  | b     | 621 | BCR  | C11-C10-C9  | -2.04 | 124.34      | 127.29   |
| 26  | c     | 517 | DGD  | CBB-CAB-C9B | -2.04 | 103.74      | 114.56   |
| 22  | B     | 604 | CLA  | C3A-C4A-CHB | -2.04 | 120.10      | 124.33   |
| 25  | b     | 624 | BCR  | C33-C5-C6   | -2.03 | 122.20      | 124.50   |
| 25  | b     | 622 | BCR  | C7-C8-C9    | -2.04 | 123.17      | 126.22   |
| 22  | c     | 507 | CLA  | C3A-C4A-CHB | -2.03 | 120.10      | 124.33   |
| 25  | c     | 513 | BCR  | C8-C7-C6    | -2.04 | 121.23      | 127.23   |
| 23  | A     | 405 | PHO  | CHD-C4C-NC  | -2.03 | 125.05      | 128.68   |
| 31  | C     | 521 | LMG  | C1-C2-C3    | -2.03 | 106.05      | 109.99   |
| 24  | a     | 407 | PL9  | C36-C34-C33 | -2.03 | 117.15      | 121.06   |
| 24  | A     | 407 | PL9  | O2-C1-C2    | -2.03 | 116.97      | 121.82   |
| 22  | B     | 614 | CLA  | C3A-C4A-CHB | -2.03 | 120.11      | 124.33   |
| 22  | B     | 614 | CLA  | CMD-C2D-C3D | 2.03  | 128.99      | 125.16   |
| 31  | a     | 402 | LMG  | O2-C2-C1    | -2.03 | 105.62      | 110.03   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | B     | 610 | CLA  | C4B-C3B-CAB | -2.03 | 123.06      | 127.18   |
| 25  | B     | 616 | BCR  | C15-C14-C13 | -2.03 | 124.35      | 127.29   |
| 22  | B     | 602 | CLA  | C1-C2-C3    | -2.03 | 122.71      | 126.23   |
| 23  | D     | 401 | PHO  | CHD-C4C-NC  | -2.03 | 125.06      | 128.68   |
| 22  | b     | 615 | CLA  | C2B-C3B-CAB | 2.03  | 131.47      | 127.33   |
| 22  | b     | 615 | CLA  | C4B-C3B-CAB | -2.03 | 123.07      | 127.18   |
| 25  | c     | 521 | BCR  | C11-C10-C9  | -2.03 | 124.36      | 127.29   |
| 22  | c     | 503 | CLA  | C1B-CHB-C4A | -2.03 | 126.10      | 130.12   |
| 25  | f     | 102 | BCR  | C24-C23-C22 | -2.03 | 123.18      | 126.22   |
| 25  | B     | 618 | BCR  | C33-C5-C6   | -2.03 | 122.21      | 124.50   |
| 22  | A     | 404 | CLA  | C3A-C4A-CHB | -2.03 | 120.11      | 124.33   |
| 22  | b     | 617 | CLA  | CMD-C2D-C3D | 2.03  | 128.98      | 125.16   |
| 22  | B     | 609 | CLA  | CMD-C2D-C3D | 2.03  | 128.98      | 125.16   |
| 26  | D     | 407 | DGD  | CAB-C9B-C8B | -2.02 | 103.81      | 114.56   |
| 22  | B     | 615 | CLA  | C3A-C4A-CHB | -2.02 | 120.12      | 124.33   |
| 26  | c     | 517 | DGD  | O2D-C2D-C1D | -2.02 | 105.64      | 110.03   |
| 22  | B     | 602 | CLA  | O2A-CGA-O1A | -2.02 | 118.19      | 123.48   |
| 22  | c     | 508 | CLA  | CMD-C2D-C3D | 2.02  | 128.97      | 125.16   |
| 22  | a     | 405 | CLA  | CMD-C2D-C3D | 2.02  | 128.97      | 125.16   |
| 22  | D     | 403 | CLA  | O2A-CGA-O1A | -2.02 | 118.20      | 123.48   |
| 26  | C     | 516 | DGD  | C3G-C2G-C1G | -2.02 | 107.23      | 111.86   |
| 25  | x     | 101 | BCR  | C27-C26-C25 | 2.02  | 125.52      | 122.86   |
| 26  | C     | 516 | DGD  | O2D-C2D-C1D | -2.02 | 105.65      | 110.03   |
| 22  | B     | 602 | CLA  | C3A-C4A-CHB | -2.02 | 120.14      | 124.33   |
| 25  | c     | 514 | BCR  | C24-C23-C22 | -2.02 | 123.20      | 126.22   |
| 22  | C     | 503 | CLA  | C3A-C4A-CHB | -2.02 | 120.14      | 124.33   |
| 22  | b     | 607 | CLA  | O2A-CGA-O1A | -2.02 | 118.21      | 123.48   |
| 31  | e     | 101 | LMG  | O1-C7-C8    | -2.02 | 106.19      | 110.99   |
| 26  | C     | 514 | DGD  | O2D-C2D-C1D | -2.02 | 105.65      | 110.03   |
| 22  | B     | 610 | CLA  | C2B-C3B-CAB | 2.02  | 131.45      | 127.33   |
| 26  | C     | 515 | DGD  | C5B-C4B-C3B | -2.01 | 103.86      | 114.56   |
| 22  | c     | 508 | CLA  | O2A-CGA-O1A | -2.01 | 118.22      | 123.48   |
| 22  | B     | 607 | CLA  | O1D-CGD-CBD | 2.01  | 128.56      | 124.45   |
| 22  | C     | 505 | CLA  | C1-C2-C3    | -2.01 | 122.74      | 126.23   |
| 27  | c     | 519 | LHG  | C27-C26-C25 | -2.01 | 103.89      | 114.56   |
| 26  | C     | 516 | DGD  | CAB-C9B-C8B | -2.01 | 103.90      | 114.56   |
| 31  | B     | 625 | LMG  | O1-C7-C8    | -2.01 | 106.21      | 110.99   |
| 22  | C     | 510 | CLA  | CMD-C2D-C3D | 2.01  | 128.94      | 125.16   |
| 30  | A     | 414 | SQD  | O6-C1-C2    | 2.01  | 110.72      | 108.15   |
| 26  | C     | 516 | DGD  | O3E-C3E-C2E | -2.00 | 105.88      | 110.36   |
| 30  | a     | 412 | SQD  | C4-C3-C2    | 2.00  | 114.50      | 110.80   |
| 30  | B     | 627 | SQD  | O5-C5-C6    | 2.00  | 110.19      | 105.91   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | M     | 103 | LMT  | O1'-C1'-C2' | 2.00  | 110.72      | 108.15   |
| 22  | c     | 506 | CLA  | CHD-C4C-NC  | 2.00  | 125.68      | 124.28   |
| 26  | c     | 517 | DGD  | C3G-C2G-C1G | -2.00 | 107.26      | 111.86   |
| 26  | d     | 410 | DGD  | C5B-C4B-C3B | -2.00 | 103.93      | 114.56   |
| 31  | i     | 102 | LMG  | O1-C7-C8    | -2.00 | 106.23      | 110.99   |
| 22  | c     | 520 | CLA  | C3A-C4A-CHB | -2.00 | 120.17      | 124.33   |

There are no chirality outliers.

All (4) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 30  | d     | 403 | SQD  | C45-O47-C7-C8   |
| 30  | B     | 622 | SQD  | C45-O47-C7-C8   |
| 26  | C     | 515 | DGD  | C2G-O2G-C1B-C2B |
| 26  | c     | 516 | DGD  | C2G-O2G-C1B-C2B |

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed      | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|---------------|--------|---------------|-----------------------|-------|
| 1   | A     | 335/344 (97%) | 1.00   | 46 (13%) 4 8  | 206, 208, 208, 209    | 0     |
| 1   | a     | 335/344 (97%) | 1.07   | 72 (21%) 1 4  | 206, 208, 209, 209    | 0     |
| 2   | B     | 490/510 (96%) | 0.81   | 72 (14%) 3 7  | 206, 207, 209, 210    | 0     |
| 2   | b     | 490/510 (96%) | 0.95   | 82 (16%) 2 6  | 206, 208, 209, 210    | 0     |
| 3   | C     | 447/461 (96%) | 0.98   | 71 (15%) 3 7  | 206, 208, 209, 209    | 0     |
| 3   | c     | 447/461 (96%) | 0.89   | 76 (17%) 2 6  | 205, 208, 209, 210    | 0     |
| 4   | D     | 340/352 (96%) | 0.79   | 36 (10%) 7 13 | 205, 207, 208, 210    | 0     |
| 4   | d     | 340/352 (96%) | 0.85   | 49 (14%) 3 8  | 206, 208, 209, 209    | 0     |
| 5   | E     | 82/84 (97%)   | 0.95   | 15 (18%) 2 5  | 206, 208, 209, 209    | 0     |
| 5   | e     | 82/84 (97%)   | 0.67   | 10 (12%) 5 10 | 207, 208, 209, 209    | 0     |
| 6   | F     | 35/45 (77%)   | 0.53   | 5 (14%) 3 8   | 207, 207, 208, 209    | 0     |
| 6   | f     | 35/45 (77%)   | 0.47   | 3 (8%) 11 17  | 207, 208, 209, 209    | 0     |
| 7   | H     | 65/66 (98%)   | 1.35   | 20 (30%) 1 3  | 206, 208, 209, 209    | 0     |
| 7   | h     | 65/66 (98%)   | 1.66   | 26 (40%) 1 3  | 207, 208, 209, 209    | 0     |
| 8   | I     | 35/38 (92%)   | 1.18   | 8 (22%) 1 4   | 207, 208, 209, 209    | 0     |
| 8   | i     | 35/38 (92%)   | 0.55   | 2 (5%) 23 25  | 206, 207, 209, 210    | 0     |
| 9   | J     | 34/40 (85%)   | 0.84   | 3 (8%) 10 16  | 207, 208, 208, 209    | 0     |
| 9   | j     | 34/40 (85%)   | 0.10   | 0 100 100     | 206, 208, 209, 209    | 0     |
| 10  | K     | 37/46 (80%)   | 0.65   | 3 (8%) 12 18  | 207, 208, 209, 209    | 0     |
| 10  | k     | 37/46 (80%)   | 0.61   | 6 (16%) 2 6   | 207, 208, 209, 209    | 0     |
| 11  | L     | 37/37 (100%)  | 1.13   | 10 (27%) 1 4  | 207, 208, 209, 209    | 0     |
| 11  | l     | 37/37 (100%)  | 0.98   | 6 (16%) 2 6   | 206, 208, 209, 210    | 0     |
| 12  | M     | 34/36 (94%)   | 0.97   | 5 (14%) 3 7   | 206, 207, 208, 209    | 0     |
| 12  | m     | 34/36 (94%)   | 0.63   | 2 (5%) 22 24  | 207, 207, 208, 209    | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 13  | O     | 243/272 (89%)   | 1.28   | 62 (25%) 1 4  | 205, 208, 209, 210    | 0     |
| 13  | o     | 243/272 (89%)   | 1.09   | 42 (17%) 2 6  | 206, 208, 209, 210    | 0     |
| 14  | T     | 32/32 (100%)    | 0.86   | 7 (21%) 1 4   | 206, 208, 208, 209    | 0     |
| 14  | t     | 32/32 (100%)    | 0.99   | 3 (9%) 9 15   | 206, 207, 209, 209    | 0     |
| 15  | U     | 97/134 (72%)    | 1.71   | 32 (32%) 1 3  | 206, 207, 208, 209    | 0     |
| 15  | u     | 97/134 (72%)    | 1.91   | 45 (46%) 1 3  | 206, 207, 208, 209    | 0     |
| 16  | V     | 137/163 (84%)   | 0.62   | 14 (10%) 7 14 | 206, 207, 208, 209    | 0     |
| 16  | v     | 137/163 (84%)   | 1.16   | 33 (24%) 1 4  | 206, 208, 209, 209    | 0     |
| 17  | g     | 28/46 (60%)     | 1.37   | 8 (28%) 1 3   | 207, 208, 209, 209    | 0     |
| 17  | y     | 28/46 (60%)     | 0.82   | 6 (21%) 1 4   | 206, 208, 209, 209    | 0     |
| 18  | X     | 37/41 (90%)     | 1.24   | 8 (21%) 1 4   | 206, 208, 209, 210    | 0     |
| 18  | x     | 37/41 (90%)     | 1.70   | 18 (48%) 1 3  | 207, 208, 208, 209    | 0     |
| 19  | G     | 0/28            | -      | -             | -                     | -     |
| 19  | Y     | 0/28            | -      | -             | -                     | -     |
| 20  | Z     | 62/62 (100%)    | 0.55   | 5 (8%) 12 18  | 206, 207, 208, 209    | 0     |
| 20  | z     | 62/62 (100%)    | 1.01   | 10 (16%) 2 7  | 207, 208, 209, 210    | 0     |
| All | All   | 5214/5674 (91%) | 0.98   | 921 (17%) 2 6 | 205, 208, 209, 210    | 0     |

All (921) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 5   | E     | 84  | LYS  | 10.6 |
| 15  | U     | 38  | GLU  | 8.5  |
| 3   | C     | 149 | TYR  | 8.0  |
| 1   | A     | 11  | ALA  | 7.8  |
| 7   | h     | 66  | GLY  | 7.4  |
| 18  | X     | 47  | GLN  | 7.3  |
| 15  | U     | 39  | LEU  | 6.8  |
| 3   | c     | 149 | TYR  | 6.8  |
| 1   | A     | 190 | HIS  | 6.6  |
| 16  | v     | 111 | GLU  | 6.5  |
| 13  | o     | 171 | GLU  | 6.5  |
| 1   | a     | 299 | GLY  | 6.3  |
| 1   | A     | 299 | GLY  | 6.1  |
| 7   | h     | 56  | ASP  | 6.1  |
| 3   | C     | 147 | PHE  | 6.1  |
| 15  | U     | 40  | VAL  | 6.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 13  | o     | 54  | GLY  | 6.0  |
| 1   | A     | 10  | SER  | 6.0  |
| 13  | o     | 55  | ALA  | 6.0  |
| 2   | b     | 296 | ALA  | 5.9  |
| 4   | d     | 197 | HIS  | 5.8  |
| 2   | b     | 485 | GLU  | 5.8  |
| 18  | X     | 46  | VAL  | 5.8  |
| 14  | t     | 32  | LYS  | 5.7  |
| 13  | o     | 53  | ARG  | 5.7  |
| 6   | f     | 13  | TYR  | 5.7  |
| 2   | B     | 411 | PHE  | 5.6  |
| 13  | o     | 51  | THR  | 5.6  |
| 3   | C     | 148 | GLY  | 5.6  |
| 3   | c     | 209 | ILE  | 5.5  |
| 4   | D     | 227 | GLU  | 5.5  |
| 6   | f     | 11  | VAL  | 5.5  |
| 3   | C     | 143 | TYR  | 5.5  |
| 7   | H     | 4   | ARG  | 5.3  |
| 18  | X     | 12  | ILE  | 5.2  |
| 3   | c     | 202 | PRO  | 5.2  |
| 18  | x     | 13  | THR  | 5.2  |
| 1   | a     | 198 | HIS  | 5.2  |
| 14  | t     | 31  | LYS  | 5.1  |
| 1   | a     | 190 | HIS  | 5.1  |
| 18  | x     | 42  | GLN  | 5.1  |
| 4   | d     | 191 | TRP  | 5.0  |
| 17  | g     | 27  | MET  | 5.0  |
| 18  | X     | 45  | LYS  | 5.0  |
| 13  | O     | 206 | GLU  | 5.0  |
| 1   | A     | 165 | GLN  | 5.0  |
| 7   | H     | 55  | LEU  | 4.9  |
| 7   | H     | 64  | ALA  | 4.9  |
| 2   | b     | 305 | ILE  | 4.9  |
| 15  | u     | 71  | LEU  | 4.9  |
| 1   | A     | 195 | HIS  | 4.9  |
| 1   | A     | 293 | MET  | 4.9  |
| 3   | C     | 142 | GLU  | 4.9  |
| 17  | y     | 46  | LEU  | 4.8  |
| 5   | E     | 60  | GLN  | 4.8  |
| 2   | b     | 298 | LEU  | 4.8  |
| 7   | h     | 3   | ARG  | 4.8  |
| 3   | c     | 178 | LYS  | 4.8  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 15  | u     | 70  | GLY  | 4.8  |
| 3   | c     | 147 | PHE  | 4.7  |
| 2   | b     | 133 | LEU  | 4.7  |
| 7   | h     | 26  | GLY  | 4.7  |
| 1   | a     | 286 | THR  | 4.7  |
| 16  | V     | 28  | GLU  | 4.7  |
| 4   | D     | 197 | HIS  | 4.7  |
| 2   | b     | 490 | GLN  | 4.6  |
| 18  | X     | 11  | THR  | 4.6  |
| 13  | o     | 220 | LYS  | 4.6  |
| 7   | h     | 55  | LEU  | 4.5  |
| 12  | M     | 1   | MET  | 4.5  |
| 13  | o     | 124 | GLU  | 4.5  |
| 7   | H     | 3   | ARG  | 4.5  |
| 13  | O     | 220 | LYS  | 4.5  |
| 3   | C     | 325 | GLY  | 4.5  |
| 3   | c     | 199 | ILE  | 4.5  |
| 2   | B     | 420 | TYR  | 4.4  |
| 2   | b     | 402 | TYR  | 4.4  |
| 2   | B     | 84  | THR  | 4.4  |
| 13  | O     | 91  | PHE  | 4.4  |
| 7   | h     | 23  | PRO  | 4.4  |
| 16  | v     | 34  | LEU  | 4.4  |
| 2   | b     | 289 | GLN  | 4.4  |
| 4   | D     | 198 | MET  | 4.4  |
| 3   | c     | 210 | PHE  | 4.4  |
| 5   | E     | 56  | TYR  | 4.4  |
| 11  | l     | 1   | MET  | 4.4  |
| 2   | b     | 297 | THR  | 4.3  |
| 13  | O     | 222 | GLN  | 4.3  |
| 15  | u     | 69  | ARG  | 4.3  |
| 1   | a     | 11  | ALA  | 4.3  |
| 18  | x     | 16  | LEU  | 4.3  |
| 2   | b     | 299 | GLU  | 4.3  |
| 3   | C     | 332 | GLN  | 4.3  |
| 13  | O     | 170 | GLY  | 4.3  |
| 3   | C     | 140 | LEU  | 4.3  |
| 2   | B     | 378 | LYS  | 4.3  |
| 4   | d     | 227 | GLU  | 4.3  |
| 12  | m     | 33  | GLN  | 4.3  |
| 7   | H     | 66  | GLY  | 4.2  |
| 15  | u     | 74  | THR  | 4.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | b     | 482 | ILE  | 4.2  |
| 1   | A     | 15  | GLU  | 4.2  |
| 2   | B     | 185 | TRP  | 4.2  |
| 3   | c     | 204 | LEU  | 4.2  |
| 11  | l     | 8   | GLN  | 4.2  |
| 10  | K     | 42  | ALA  | 4.2  |
| 7   | h     | 25  | TRP  | 4.2  |
| 2   | b     | 288 | VAL  | 4.2  |
| 2   | b     | 167 | TRP  | 4.2  |
| 15  | u     | 72  | TYR  | 4.2  |
| 1   | A     | 137 | LEU  | 4.2  |
| 16  | V     | 47  | LEU  | 4.2  |
| 7   | H     | 63  | LYS  | 4.2  |
| 15  | u     | 57  | LEU  | 4.2  |
| 7   | h     | 27  | THR  | 4.2  |
| 3   | C     | 141 | GLU  | 4.1  |
| 3   | c     | 78  | GLU  | 4.1  |
| 2   | b     | 267 | LEU  | 4.1  |
| 3   | c     | 146 | PHE  | 4.1  |
| 15  | u     | 115 | THR  | 4.1  |
| 4   | D     | 192 | THR  | 4.1  |
| 1   | A     | 294 | ALA  | 4.1  |
| 7   | h     | 4   | ARG  | 4.1  |
| 13  | O     | 53  | ARG  | 4.1  |
| 4   | d     | 295 | SER  | 4.1  |
| 3   | c     | 180 | MET  | 4.1  |
| 15  | u     | 75  | LEU  | 4.1  |
| 13  | O     | 205 | GLU  | 4.1  |
| 4   | D     | 25  | ASP  | 4.1  |
| 16  | v     | 130 | MET  | 4.0  |
| 1   | A     | 175 | GLY  | 4.0  |
| 1   | a     | 328 | MET  | 4.0  |
| 2   | b     | 166 | MET  | 4.0  |
| 13  | o     | 215 | ARG  | 4.0  |
| 15  | u     | 65  | PHE  | 4.0  |
| 4   | d     | 239 | GLN  | 4.0  |
| 1   | a     | 287 | ALA  | 4.0  |
| 13  | O     | 175 | PRO  | 4.0  |
| 2   | b     | 304 | ALA  | 4.0  |
| 2   | B     | 218 | LEU  | 4.0  |
| 2   | b     | 302 | TRP  | 4.0  |
| 13  | o     | 190 | LEU  | 4.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | b     | 431 | GLU  | 4.0  |
| 13  | O     | 90  | GLU  | 4.0  |
| 4   | d     | 294 | ARG  | 3.9  |
| 3   | c     | 184 | GLY  | 3.9  |
| 13  | O     | 223 | ILE  | 3.9  |
| 15  | U     | 53  | GLU  | 3.9  |
| 2   | b     | 483 | ASP  | 3.9  |
| 3   | C     | 340 | TYR  | 3.9  |
| 13  | O     | 171 | GLU  | 3.9  |
| 13  | O     | 50  | ASP  | 3.9  |
| 13  | O     | 58  | ILE  | 3.9  |
| 15  | u     | 107 | GLU  | 3.9  |
| 2   | b     | 185 | TRP  | 3.9  |
| 1   | A     | 198 | HIS  | 3.9  |
| 3   | C     | 266 | TRP  | 3.9  |
| 18  | X     | 13  | THR  | 3.9  |
| 2   | b     | 300 | GLU  | 3.9  |
| 2   | b     | 120 | LEU  | 3.9  |
| 6   | f     | 12  | SER  | 3.9  |
| 18  | x     | 12  | ILE  | 3.9  |
| 1   | a     | 199 | GLN  | 3.9  |
| 4   | d     | 199 | MET  | 3.8  |
| 2   | b     | 484 | PRO  | 3.8  |
| 3   | C     | 453 | ALA  | 3.8  |
| 7   | H     | 6   | TRP  | 3.8  |
| 13  | O     | 218 | LEU  | 3.8  |
| 15  | U     | 118 | GLU  | 3.8  |
| 13  | O     | 169 | LYS  | 3.8  |
| 13  | o     | 52  | ALA  | 3.8  |
| 7   | h     | 11  | LEU  | 3.8  |
| 4   | d     | 139 | ARG  | 3.8  |
| 20  | z     | 1   | MET  | 3.8  |
| 3   | C     | 137 | PRO  | 3.8  |
| 13  | O     | 55  | ALA  | 3.8  |
| 3   | C     | 212 | TYR  | 3.8  |
| 8   | I     | 35  | LYS  | 3.8  |
| 13  | O     | 244 | GLU  | 3.8  |
| 3   | c     | 179 | ALA  | 3.8  |
| 2   | b     | 301 | ALA  | 3.8  |
| 3   | c     | 200 | THR  | 3.8  |
| 13  | o     | 151 | LEU  | 3.8  |
| 16  | V     | 29  | LEU  | 3.8  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3   | C     | 326 | ALA  | 3.7  |
| 3   | c     | 258 | GLY  | 3.7  |
| 13  | O     | 56  | TYR  | 3.7  |
| 8   | I     | 34  | ARG  | 3.7  |
| 3   | c     | 203 | THR  | 3.7  |
| 7   | h     | 2   | ALA  | 3.7  |
| 3   | C     | 45  | LEU  | 3.7  |
| 2   | b     | 295 | GLY  | 3.7  |
| 3   | C     | 151 | TRP  | 3.7  |
| 7   | h     | 14  | LEU  | 3.7  |
| 2   | B     | 219 | VAL  | 3.7  |
| 2   | B     | 347 | ARG  | 3.7  |
| 14  | t     | 30  | THR  | 3.7  |
| 18  | x     | 11  | THR  | 3.7  |
| 16  | v     | 47  | LEU  | 3.7  |
| 17  | y     | 42  | ARG  | 3.7  |
| 3   | c     | 372 | PRO  | 3.7  |
| 1   | a     | 236 | GLY  | 3.7  |
| 17  | g     | 46  | LEU  | 3.7  |
| 5   | e     | 3   | GLY  | 3.6  |
| 2   | B     | 356 | VAL  | 3.6  |
| 4   | D     | 295 | SER  | 3.6  |
| 4   | d     | 201 | VAL  | 3.6  |
| 20  | Z     | 1   | MET  | 3.6  |
| 1   | a     | 282 | GLY  | 3.6  |
| 5   | E     | 82  | GLN  | 3.6  |
| 5   | E     | 57  | ALA  | 3.6  |
| 15  | U     | 128 | TYR  | 3.6  |
| 10  | k     | 11  | LEU  | 3.6  |
| 3   | c     | 260 | ALA  | 3.6  |
| 3   | c     | 259 | TRP  | 3.6  |
| 13  | O     | 49  | ASP  | 3.6  |
| 4   | D     | 77  | ALA  | 3.6  |
| 13  | O     | 54  | GLY  | 3.6  |
| 7   | h     | 7   | LEU  | 3.6  |
| 3   | c     | 324 | LEU  | 3.6  |
| 2   | B     | 412 | THR  | 3.6  |
| 13  | O     | 190 | LEU  | 3.6  |
| 5   | e     | 82  | GLN  | 3.6  |
| 1   | A     | 14  | TRP  | 3.5  |
| 2   | b     | 287 | ARG  | 3.5  |
| 16  | v     | 49  | GLU  | 3.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | B     | 490 | GLN  | 3.5  |
| 2   | b     | 179 | GLN  | 3.5  |
| 7   | H     | 65  | LEU  | 3.5  |
| 2   | b     | 292 | LEU  | 3.5  |
| 15  | U     | 45  | GLU  | 3.5  |
| 3   | C     | 138 | GLU  | 3.5  |
| 1   | A     | 179 | THR  | 3.5  |
| 16  | v     | 44  | THR  | 3.5  |
| 16  | V     | 30  | THR  | 3.5  |
| 2   | B     | 370 | LEU  | 3.5  |
| 3   | C     | 150 | ASP  | 3.5  |
| 15  | u     | 39  | LEU  | 3.5  |
| 3   | C     | 402 | GLY  | 3.5  |
| 1   | A     | 286 | THR  | 3.5  |
| 3   | c     | 262 | ARG  | 3.5  |
| 2   | B     | 85  | GLY  | 3.5  |
| 16  | v     | 125 | ASP  | 3.5  |
| 16  | v     | 35  | THR  | 3.5  |
| 4   | d     | 240 | ALA  | 3.4  |
| 7   | H     | 27  | THR  | 3.4  |
| 15  | u     | 116 | GLU  | 3.4  |
| 1   | A     | 298 | ASN  | 3.4  |
| 15  | U     | 121 | LEU  | 3.4  |
| 2   | B     | 127 | ARG  | 3.4  |
| 13  | o     | 170 | GLY  | 3.4  |
| 4   | d     | 194 | ASN  | 3.4  |
| 1   | A     | 266 | ASN  | 3.4  |
| 15  | U     | 117 | VAL  | 3.4  |
| 4   | D     | 228 | GLY  | 3.4  |
| 1   | A     | 12  | ASN  | 3.4  |
| 13  | o     | 213 | VAL  | 3.4  |
| 13  | o     | 169 | LYS  | 3.4  |
| 1   | a     | 293 | MET  | 3.4  |
| 10  | K     | 46  | ARG  | 3.4  |
| 1   | A     | 301 | ASN  | 3.4  |
| 2   | B     | 83  | GLU  | 3.4  |
| 13  | o     | 221 | GLY  | 3.4  |
| 5   | e     | 84  | LYS  | 3.3  |
| 3   | c     | 191 | PRO  | 3.3  |
| 3   | c     | 197 | ARG  | 3.3  |
| 3   | C     | 152 | LYS  | 3.3  |
| 3   | c     | 148 | GLY  | 3.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | a     | 246 | TYR  | 3.3  |
| 3   | c     | 198 | VAL  | 3.3  |
| 16  | V     | 27  | ALA  | 3.3  |
| 6   | F     | 11  | VAL  | 3.3  |
| 15  | U     | 42  | VAL  | 3.3  |
| 1   | A     | 201 | GLY  | 3.3  |
| 16  | v     | 36  | VAL  | 3.3  |
| 2   | b     | 195 | PRO  | 3.3  |
| 3   | C     | 43  | ILE  | 3.3  |
| 13  | O     | 48  | LEU  | 3.3  |
| 11  | l     | 2   | GLU  | 3.3  |
| 4   | d     | 13  | GLY  | 3.3  |
| 4   | D     | 199 | MET  | 3.3  |
| 12  | M     | 33  | GLN  | 3.3  |
| 3   | C     | 146 | PHE  | 3.3  |
| 15  | u     | 68  | TYR  | 3.3  |
| 13  | o     | 84  | ASN  | 3.3  |
| 2   | b     | 229 | LEU  | 3.3  |
| 3   | c     | 261 | ARG  | 3.2  |
| 1   | A     | 78  | ILE  | 3.2  |
| 2   | b     | 122 | LEU  | 3.2  |
| 16  | V     | 130 | MET  | 3.2  |
| 1   | a     | 201 | GLY  | 3.2  |
| 4   | D     | 296 | TYR  | 3.2  |
| 15  | u     | 45  | GLU  | 3.2  |
| 1   | a     | 179 | THR  | 3.2  |
| 4   | d     | 195 | PRO  | 3.2  |
| 2   | B     | 353 | GLU  | 3.2  |
| 2   | B     | 293 | ALA  | 3.2  |
| 17  | g     | 23  | THR  | 3.2  |
| 16  | v     | 133 | LEU  | 3.2  |
| 1   | a     | 195 | HIS  | 3.2  |
| 3   | C     | 144 | SER  | 3.2  |
| 1   | a     | 149 | ALA  | 3.2  |
| 13  | O     | 57  | PRO  | 3.2  |
| 13  | o     | 62  | GLN  | 3.2  |
| 15  | u     | 121 | LEU  | 3.2  |
| 3   | C     | 28  | GLN  | 3.2  |
| 9   | J     | 8   | ILE  | 3.2  |
| 3   | C     | 204 | LEU  | 3.2  |
| 3   | c     | 183 | GLY  | 3.1  |
| 2   | b     | 218 | LEU  | 3.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 13  | O     | 215 | ARG  | 3.1  |
| 2   | b     | 70  | GLY  | 3.1  |
| 1   | a     | 15  | GLU  | 3.1  |
| 11  | L     | 33  | SER  | 3.1  |
| 4   | D     | 26  | ARG  | 3.1  |
| 2   | B     | 350 | GLU  | 3.1  |
| 1   | A     | 13  | LEU  | 3.1  |
| 4   | d     | 177 | ALA  | 3.1  |
| 13  | O     | 89  | ALA  | 3.1  |
| 1   | A     | 199 | GLN  | 3.1  |
| 13  | o     | 172 | PHE  | 3.1  |
| 16  | v     | 31  | PRO  | 3.1  |
| 2   | B     | 354 | LEU  | 3.1  |
| 4   | d     | 241 | GLU  | 3.1  |
| 7   | h     | 6   | TRP  | 3.1  |
| 2   | b     | 69  | LEU  | 3.1  |
| 4   | D     | 174 | GLY  | 3.1  |
| 4   | d     | 198 | MET  | 3.1  |
| 1   | A     | 16  | ARG  | 3.1  |
| 2   | B     | 379 | ALA  | 3.1  |
| 5   | e     | 42  | LEU  | 3.1  |
| 2   | b     | 408 | GLY  | 3.1  |
| 1   | a     | 223 | LEU  | 3.1  |
| 2   | b     | 491 | VAL  | 3.0  |
| 3   | c     | 430 | HIS  | 3.0  |
| 13  | O     | 225 | LEU  | 3.0  |
| 16  | v     | 78  | LEU  | 3.0  |
| 16  | v     | 131 | ARG  | 3.0  |
| 7   | H     | 2   | ALA  | 3.0  |
| 15  | u     | 50  | ALA  | 3.0  |
| 2   | B     | 214 | LEU  | 3.0  |
| 3   | C     | 411 | ALA  | 3.0  |
| 18  | x     | 45  | LYS  | 3.0  |
| 3   | c     | 201 | ASN  | 3.0  |
| 5   | E     | 83  | LEU  | 3.0  |
| 2   | b     | 183 | PRO  | 3.0  |
| 3   | C     | 139 | THR  | 3.0  |
| 16  | v     | 46  | THR  | 3.0  |
| 13  | O     | 219 | THR  | 3.0  |
| 2   | b     | 127 | ARG  | 3.0  |
| 2   | b     | 178 | VAL  | 3.0  |
| 13  | o     | 152 | VAL  | 3.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 15  | U     | 119 | THR  | 3.0  |
| 16  | v     | 126 | ILE  | 3.0  |
| 11  | L     | 7   | ARG  | 3.0  |
| 1   | a     | 235 | TYR  | 3.0  |
| 13  | O     | 261 | ILE  | 3.0  |
| 13  | o     | 216 | PHE  | 3.0  |
| 16  | v     | 45  | ILE  | 3.0  |
| 18  | X     | 42  | GLN  | 3.0  |
| 2   | b     | 219 | VAL  | 3.0  |
| 3   | c     | 151 | TRP  | 3.0  |
| 3   | C     | 265 | ILE  | 3.0  |
| 15  | u     | 58  | ASN  | 3.0  |
| 7   | H     | 14  | LEU  | 3.0  |
| 2   | B     | 295 | GLY  | 3.0  |
| 4   | d     | 200 | GLY  | 3.0  |
| 13  | O     | 79  | LYS  | 3.0  |
| 13  | o     | 214 | LYS  | 3.0  |
| 18  | x     | 43  | ILE  | 3.0  |
| 3   | C     | 191 | PRO  | 3.0  |
| 4   | d     | 265 | ARG  | 3.0  |
| 4   | d     | 203 | GLY  | 3.0  |
| 1   | a     | 327 | GLY  | 3.0  |
| 2   | B     | 183 | PRO  | 2.9  |
| 7   | H     | 56  | ASP  | 2.9  |
| 20  | z     | 4   | LEU  | 2.9  |
| 4   | d     | 14  | TRP  | 2.9  |
| 1   | a     | 152 | ALA  | 2.9  |
| 7   | H     | 54  | ILE  | 2.9  |
| 4   | D     | 24  | ARG  | 2.9  |
| 4   | D     | 177 | ALA  | 2.9  |
| 2   | B     | 352 | GLU  | 2.9  |
| 3   | C     | 324 | LEU  | 2.9  |
| 13  | O     | 125 | ASP  | 2.9  |
| 2   | B     | 180 | PRO  | 2.9  |
| 3   | C     | 181 | PHE  | 2.9  |
| 1   | a     | 175 | GLY  | 2.9  |
| 2   | B     | 417 | VAL  | 2.9  |
| 3   | C     | 97  | TRP  | 2.9  |
| 13  | o     | 173 | ASN  | 2.9  |
| 1   | A     | 289 | GLY  | 2.9  |
| 5   | e     | 4   | THR  | 2.9  |
| 7   | H     | 10  | ILE  | 2.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | a     | 319 | ASP  | 2.9  |
| 1   | A     | 138 | GLY  | 2.9  |
| 6   | F     | 15  | ILE  | 2.9  |
| 3   | c     | 182 | PHE  | 2.9  |
| 2   | B     | 402 | TYR  | 2.9  |
| 7   | h     | 65  | LEU  | 2.9  |
| 13  | O     | 51  | THR  | 2.9  |
| 15  | u     | 51  | TYR  | 2.9  |
| 2   | B     | 132 | ALA  | 2.9  |
| 3   | C     | 209 | ILE  | 2.9  |
| 13  | O     | 202 | GLN  | 2.9  |
| 4   | D     | 171 | PRO  | 2.9  |
| 4   | D     | 170 | ALA  | 2.9  |
| 7   | h     | 5   | THR  | 2.9  |
| 3   | C     | 331 | ALA  | 2.9  |
| 7   | h     | 22  | ALA  | 2.9  |
| 15  | u     | 47  | LEU  | 2.8  |
| 2   | b     | 373 | LYS  | 2.8  |
| 1   | A     | 191 | ASN  | 2.8  |
| 2   | B     | 410 | THR  | 2.8  |
| 3   | C     | 46  | SER  | 2.8  |
| 18  | x     | 40  | ILE  | 2.8  |
| 2   | b     | 168 | VAL  | 2.8  |
| 7   | H     | 5   | THR  | 2.8  |
| 11  | L     | 28  | ALA  | 2.8  |
| 15  | u     | 117 | VAL  | 2.8  |
| 2   | B     | 179 | GLN  | 2.8  |
| 1   | a     | 16  | ARG  | 2.8  |
| 1   | a     | 192 | ILE  | 2.8  |
| 2   | b     | 234 | ILE  | 2.8  |
| 3   | c     | 157 | MET  | 2.8  |
| 1   | A     | 178 | GLY  | 2.8  |
| 1   | a     | 224 | ILE  | 2.8  |
| 2   | B     | 298 | LEU  | 2.8  |
| 3   | C     | 27  | ASP  | 2.8  |
| 3   | C     | 263 | ALA  | 2.8  |
| 7   | H     | 62  | TRP  | 2.8  |
| 2   | b     | 385 | ARG  | 2.8  |
| 2   | B     | 322 | GLY  | 2.8  |
| 8   | I     | 1   | MET  | 2.8  |
| 3   | C     | 154 | LYS  | 2.8  |
| 4   | d     | 148 | ALA  | 2.8  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 20  | z     | 28  | ALA  | 2.8  |
| 2   | B     | 416 | THR  | 2.8  |
| 1   | a     | 324 | ALA  | 2.8  |
| 3   | c     | 266 | TRP  | 2.8  |
| 7   | h     | 13  | PRO  | 2.8  |
| 13  | O     | 46  | PRO  | 2.8  |
| 1   | a     | 202 | VAL  | 2.7  |
| 3   | c     | 196 | VAL  | 2.7  |
| 4   | d     | 206 | GLY  | 2.7  |
| 1   | A     | 196 | PRO  | 2.7  |
| 2   | B     | 131 | PRO  | 2.7  |
| 8   | I     | 32  | PRO  | 2.7  |
| 2   | B     | 128 | THR  | 2.7  |
| 16  | v     | 146 | LEU  | 2.7  |
| 5   | e     | 43  | ALA  | 2.7  |
| 2   | b     | 194 | ASN  | 2.7  |
| 4   | d     | 59  | TYR  | 2.7  |
| 1   | a     | 245 | THR  | 2.7  |
| 13  | O     | 168 | PHE  | 2.7  |
| 13  | O     | 204 | LYS  | 2.7  |
| 20  | z     | 24  | PRO  | 2.7  |
| 13  | O     | 234 | THR  | 2.7  |
| 14  | T     | 27  | PRO  | 2.7  |
| 2   | B     | 296 | ALA  | 2.7  |
| 3   | c     | 264 | PHE  | 2.7  |
| 2   | B     | 418 | LYS  | 2.7  |
| 3   | c     | 192 | GLY  | 2.7  |
| 4   | d     | 192 | THR  | 2.7  |
| 7   | H     | 11  | LEU  | 2.7  |
| 13  | O     | 76  | PHE  | 2.7  |
| 13  | O     | 216 | PHE  | 2.7  |
| 3   | C     | 210 | PHE  | 2.7  |
| 15  | U     | 47  | LEU  | 2.7  |
| 13  | o     | 222 | GLN  | 2.7  |
| 15  | U     | 122 | VAL  | 2.7  |
| 3   | c     | 373 | ASN  | 2.7  |
| 3   | c     | 405 | ASN  | 2.7  |
| 2   | b     | 489 | GLU  | 2.7  |
| 11  | L     | 34  | TYR  | 2.7  |
| 2   | b     | 181 | VAL  | 2.7  |
| 15  | u     | 82  | ASN  | 2.7  |
| 1   | A     | 177 | SER  | 2.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3   | c     | 143 | TYR  | 2.7  |
| 3   | c     | 27  | ASP  | 2.7  |
| 4   | D     | 190 | ASN  | 2.7  |
| 13  | o     | 122 | VAL  | 2.7  |
| 15  | u     | 42  | VAL  | 2.7  |
| 18  | x     | 14  | PRO  | 2.7  |
| 3   | c     | 365 | TRP  | 2.7  |
| 4   | d     | 141 | TYR  | 2.6  |
| 1   | A     | 18  | CYS  | 2.6  |
| 3   | C     | 42  | LEU  | 2.6  |
| 4   | D     | 78  | VAL  | 2.6  |
| 2   | B     | 120 | LEU  | 2.6  |
| 2   | b     | 266 | GLU  | 2.6  |
| 3   | C     | 261 | ARG  | 2.6  |
| 3   | c     | 156 | LYS  | 2.6  |
| 20  | z     | 25  | VAL  | 2.6  |
| 1   | a     | 301 | ASN  | 2.6  |
| 2   | B     | 393 | GLU  | 2.6  |
| 3   | c     | 257 | PHE  | 2.6  |
| 8   | I     | 3   | THR  | 2.6  |
| 20  | Z     | 27  | TYR  | 2.6  |
| 20  | z     | 17  | PHE  | 2.6  |
| 1   | a     | 187 | GLN  | 2.6  |
| 2   | B     | 171 | PRO  | 2.6  |
| 3   | C     | 105 | VAL  | 2.6  |
| 13  | O     | 195 | ASP  | 2.6  |
| 13  | o     | 50  | ASP  | 2.6  |
| 1   | a     | 303 | ASN  | 2.6  |
| 2   | B     | 414 | PRO  | 2.6  |
| 3   | C     | 44  | ASN  | 2.6  |
| 5   | E     | 17  | VAL  | 2.6  |
| 18  | x     | 46  | VAL  | 2.6  |
| 1   | A     | 192 | ILE  | 2.6  |
| 3   | c     | 213 | LEU  | 2.6  |
| 1   | A     | 282 | GLY  | 2.6  |
| 17  | y     | 44  | GLY  | 2.6  |
| 3   | C     | 157 | MET  | 2.6  |
| 4   | d     | 202 | ALA  | 2.6  |
| 4   | d     | 83  | ASN  | 2.6  |
| 4   | d     | 176 | ALA  | 2.6  |
| 4   | D     | 189 | HIS  | 2.6  |
| 16  | v     | 132 | ASN  | 2.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 4   | d     | 283 | ALA  | 2.6  |
| 11  | l     | 14  | ARG  | 2.6  |
| 1   | a     | 150 | PRO  | 2.6  |
| 1   | a     | 200 | LEU  | 2.6  |
| 3   | c     | 363 | GLY  | 2.6  |
| 4   | D     | 193 | LEU  | 2.6  |
| 12  | m     | 34  | LYS  | 2.6  |
| 1   | A     | 265 | PHE  | 2.6  |
| 2   | b     | 350 | GLU  | 2.6  |
| 13  | O     | 258 | GLU  | 2.6  |
| 13  | O     | 213 | VAL  | 2.6  |
| 2   | B     | 326 | ARG  | 2.6  |
| 4   | D     | 294 | ARG  | 2.6  |
| 16  | v     | 29  | LEU  | 2.6  |
| 2   | B     | 306 | PRO  | 2.6  |
| 1   | a     | 325 | ASN  | 2.6  |
| 3   | C     | 213 | LEU  | 2.6  |
| 4   | d     | 187 | GLY  | 2.6  |
| 7   | H     | 7   | LEU  | 2.6  |
| 2   | b     | 284 | ILE  | 2.6  |
| 1   | a     | 80  | GLY  | 2.6  |
| 3   | C     | 341 | LEU  | 2.6  |
| 4   | D     | 239 | GLN  | 2.6  |
| 2   | b     | 126 | PRO  | 2.5  |
| 5   | E     | 58  | GLN  | 2.5  |
| 5   | E     | 25  | ILE  | 2.5  |
| 15  | u     | 46  | LYS  | 2.5  |
| 15  | u     | 84  | PRO  | 2.5  |
| 4   | D     | 191 | TRP  | 2.5  |
| 15  | u     | 62  | ILE  | 2.5  |
| 18  | x     | 38  | ILE  | 2.5  |
| 17  | y     | 39  | LEU  | 2.5  |
| 3   | c     | 385 | GLN  | 2.5  |
| 15  | u     | 122 | VAL  | 2.5  |
| 1   | A     | 204 | GLY  | 2.5  |
| 2   | B     | 385 | ARG  | 2.5  |
| 13  | o     | 240 | THR  | 2.5  |
| 1   | a     | 12  | ASN  | 2.5  |
| 3   | c     | 206 | PRO  | 2.5  |
| 9   | J     | 11  | TRP  | 2.5  |
| 4   | D     | 194 | ASN  | 2.5  |
| 13  | O     | 162 | ILE  | 2.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | a     | 10  | SER  | 2.5  |
| 14  | T     | 26  | PRO  | 2.5  |
| 3   | C     | 134 | ILE  | 2.5  |
| 7   | h     | 10  | ILE  | 2.5  |
| 3   | c     | 256 | PRO  | 2.5  |
| 3   | c     | 283 | GLY  | 2.5  |
| 13  | o     | 189 | GLY  | 2.5  |
| 13  | o     | 228 | ALA  | 2.5  |
| 16  | V     | 49  | GLU  | 2.5  |
| 4   | D     | 211 | CYS  | 2.5  |
| 13  | o     | 88  | GLU  | 2.5  |
| 13  | O     | 242 | GLU  | 2.5  |
| 16  | v     | 113 | GLU  | 2.5  |
| 3   | c     | 228 | ASN  | 2.5  |
| 10  | K     | 43  | VAL  | 2.5  |
| 16  | v     | 138 | LEU  | 2.5  |
| 4   | d     | 189 | HIS  | 2.5  |
| 1   | A     | 290 | ILE  | 2.5  |
| 2   | b     | 294 | SER  | 2.5  |
| 15  | U     | 48  | GLY  | 2.5  |
| 17  | g     | 45  | ASN  | 2.5  |
| 20  | Z     | 30  | PRO  | 2.5  |
| 18  | X     | 44  | ASP  | 2.5  |
| 3   | c     | 427 | ALA  | 2.5  |
| 13  | O     | 52  | ALA  | 2.5  |
| 3   | c     | 97  | TRP  | 2.5  |
| 3   | c     | 207 | ARG  | 2.5  |
| 4   | D     | 226 | GLY  | 2.5  |
| 11  | l     | 9   | PRO  | 2.5  |
| 13  | O     | 151 | LEU  | 2.5  |
| 1   | A     | 212 | CYS  | 2.5  |
| 3   | C     | 78  | GLU  | 2.5  |
| 3   | C     | 104 | GLU  | 2.5  |
| 3   | c     | 185 | LEU  | 2.5  |
| 8   | i     | 35  | LYS  | 2.5  |
| 1   | a     | 289 | GLY  | 2.4  |
| 3   | C     | 403 | SER  | 2.4  |
| 2   | B     | 346 | PHE  | 2.4  |
| 7   | h     | 9   | ASP  | 2.4  |
| 2   | B     | 121 | GLU  | 2.4  |
| 18  | x     | 17  | LYS  | 2.4  |
| 8   | I     | 6   | ILE  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | B     | 122 | LEU  | 2.4  |
| 1   | a     | 194 | MET  | 2.4  |
| 7   | H     | 26  | GLY  | 2.4  |
| 15  | u     | 85  | TYR  | 2.4  |
| 1   | a     | 220 | THR  | 2.4  |
| 2   | b     | 78  | TRP  | 2.4  |
| 4   | D     | 195 | PRO  | 2.4  |
| 16  | V     | 131 | ARG  | 2.4  |
| 1   | A     | 203 | ALA  | 2.4  |
| 13  | O     | 203 | ALA  | 2.4  |
| 15  | U     | 123 | GLU  | 2.4  |
| 1   | A     | 194 | MET  | 2.4  |
| 4   | D     | 297 | ASP  | 2.4  |
| 13  | O     | 269 | ILE  | 2.4  |
| 1   | a     | 225 | ARG  | 2.4  |
| 13  | o     | 210 | ARG  | 2.4  |
| 16  | v     | 124 | ALA  | 2.4  |
| 1   | a     | 153 | SER  | 2.4  |
| 4   | d     | 165 | SER  | 2.4  |
| 4   | d     | 278 | GLY  | 2.4  |
| 3   | C     | 256 | PRO  | 2.4  |
| 3   | c     | 364 | PRO  | 2.4  |
| 4   | d     | 324 | GLY  | 2.4  |
| 1   | A     | 161 | TYR  | 2.4  |
| 2   | b     | 303 | SER  | 2.4  |
| 15  | U     | 96  | GLY  | 2.4  |
| 15  | u     | 104 | ILE  | 2.4  |
| 3   | C     | 135 | ARG  | 2.4  |
| 3   | C     | 377 | LEU  | 2.4  |
| 4   | d     | 204 | VAL  | 2.4  |
| 1   | a     | 139 | MET  | 2.4  |
| 4   | d     | 95  | PRO  | 2.4  |
| 10  | k     | 15  | TYR  | 2.4  |
| 15  | U     | 120 | ALA  | 2.4  |
| 5   | e     | 47  | PHE  | 2.4  |
| 5   | E     | 6   | GLY  | 2.4  |
| 13  | o     | 33  | TYR  | 2.4  |
| 5   | E     | 5   | THR  | 2.4  |
| 2   | B     | 351 | GLY  | 2.4  |
| 3   | C     | 262 | ARG  | 2.4  |
| 3   | C     | 182 | PHE  | 2.4  |
| 6   | F     | 16  | PHE  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | a     | 207 | GLY  | 2.4  |
| 4   | d     | 207 | GLY  | 2.4  |
| 13  | o     | 164 | THR  | 2.4  |
| 15  | u     | 38  | GLU  | 2.4  |
| 5   | E     | 21  | VAL  | 2.4  |
| 4   | d     | 172 | SER  | 2.4  |
| 10  | k     | 10  | LYS  | 2.4  |
| 15  | U     | 46  | LYS  | 2.4  |
| 2   | b     | 177 | SER  | 2.4  |
| 5   | e     | 44  | TYR  | 2.4  |
| 2   | B     | 130 | GLU  | 2.4  |
| 2   | B     | 373 | LYS  | 2.4  |
| 3   | C     | 145 | SER  | 2.4  |
| 6   | F     | 13  | TYR  | 2.4  |
| 15  | u     | 59  | ASN  | 2.4  |
| 11  | L     | 8   | GLN  | 2.4  |
| 15  | U     | 43  | VAL  | 2.4  |
| 17  | g     | 35  | ILE  | 2.4  |
| 2   | B     | 413 | ASP  | 2.4  |
| 2   | b     | 119 | ASP  | 2.4  |
| 15  | U     | 44  | ASP  | 2.4  |
| 1   | a     | 176 | ILE  | 2.4  |
| 4   | d     | 288 | GLY  | 2.4  |
| 15  | u     | 40  | VAL  | 2.4  |
| 3   | C     | 180 | MET  | 2.3  |
| 2   | B     | 399 | VAL  | 2.3  |
| 2   | b     | 347 | ARG  | 2.3  |
| 6   | F     | 14  | PRO  | 2.3  |
| 15  | u     | 66  | ILE  | 2.3  |
| 2   | B     | 161 | LEU  | 2.3  |
| 16  | V     | 34  | LEU  | 2.3  |
| 16  | V     | 38  | LEU  | 2.3  |
| 3   | C     | 369 | LEU  | 2.3  |
| 7   | h     | 54  | ILE  | 2.3  |
| 16  | V     | 151 | ILE  | 2.3  |
| 2   | B     | 309 | LEU  | 2.3  |
| 2   | b     | 351 | GLY  | 2.3  |
| 13  | o     | 168 | PHE  | 2.3  |
| 13  | o     | 31  | LEU  | 2.3  |
| 20  | z     | 3   | ILE  | 2.3  |
| 13  | o     | 86  | ARG  | 2.3  |
| 1   | a     | 229 | GLU  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | a     | 137 | LEU  | 2.3  |
| 2   | B     | 124 | ARG  | 2.3  |
| 3   | c     | 212 | TYR  | 2.3  |
| 5   | E     | 81  | GLU  | 2.3  |
| 2   | B     | 289 | GLN  | 2.3  |
| 2   | b     | 395 | GLN  | 2.3  |
| 8   | I     | 25  | SER  | 2.3  |
| 1   | a     | 244 | GLU  | 2.3  |
| 3   | C     | 200 | THR  | 2.3  |
| 13  | O     | 126 | GLY  | 2.3  |
| 1   | a     | 298 | ASN  | 2.3  |
| 3   | c     | 433 | LEU  | 2.3  |
| 2   | B     | 401 | PHE  | 2.3  |
| 4   | D     | 283 | ALA  | 2.3  |
| 12  | M     | 5   | GLN  | 2.3  |
| 13  | O     | 31  | LEU  | 2.3  |
| 3   | C     | 202 | PRO  | 2.3  |
| 2   | b     | 117 | TYR  | 2.3  |
| 17  | y     | 43  | ARG  | 2.3  |
| 13  | O     | 77  | LEU  | 2.3  |
| 1   | a     | 170 | ASP  | 2.3  |
| 7   | h     | 8   | GLY  | 2.3  |
| 13  | o     | 223 | ILE  | 2.3  |
| 2   | B     | 215 | PHE  | 2.3  |
| 1   | a     | 18  | CYS  | 2.3  |
| 15  | u     | 67  | GLN  | 2.3  |
| 15  | U     | 41  | ASN  | 2.3  |
| 17  | y     | 45  | ASN  | 2.3  |
| 1   | a     | 196 | PRO  | 2.3  |
| 1   | a     | 204 | GLY  | 2.3  |
| 2   | B     | 86  | ILE  | 2.3  |
| 5   | E     | 18  | ARG  | 2.3  |
| 13  | O     | 270 | GLU  | 2.3  |
| 4   | d     | 280 | TRP  | 2.3  |
| 2   | b     | 285 | ASN  | 2.3  |
| 15  | U     | 81  | LYS  | 2.3  |
| 11  | L     | 1   | MET  | 2.2  |
| 3   | c     | 181 | PHE  | 2.2  |
| 15  | U     | 75  | LEU  | 2.2  |
| 12  | M     | 4   | ASN  | 2.2  |
| 15  | U     | 116 | GLU  | 2.2  |
| 16  | v     | 129 | LYS  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 11  | L     | 6   | ASN  | 2.2  |
| 13  | o     | 89  | ALA  | 2.2  |
| 11  | l     | 3   | PRO  | 2.2  |
| 3   | c     | 434 | ALA  | 2.2  |
| 15  | U     | 77  | LYS  | 2.2  |
| 2   | B     | 50  | PRO  | 2.2  |
| 16  | v     | 37  | PRO  | 2.2  |
| 20  | z     | 23  | VAL  | 2.2  |
| 16  | v     | 50  | LYS  | 2.2  |
| 13  | O     | 224 | SER  | 2.2  |
| 2   | b     | 290 | ALA  | 2.2  |
| 15  | U     | 54  | LYS  | 2.2  |
| 15  | U     | 106 | ARG  | 2.2  |
| 1   | a     | 165 | GLN  | 2.2  |
| 15  | u     | 55  | ILE  | 2.2  |
| 2   | B     | 290 | ALA  | 2.2  |
| 2   | b     | 393 | GLU  | 2.2  |
| 15  | U     | 50  | ALA  | 2.2  |
| 18  | x     | 15  | SER  | 2.2  |
| 4   | D     | 176 | ALA  | 2.2  |
| 13  | O     | 260 | LYS  | 2.2  |
| 16  | V     | 43  | LYS  | 2.2  |
| 15  | U     | 51  | TYR  | 2.2  |
| 15  | U     | 55  | ILE  | 2.2  |
| 16  | V     | 44  | THR  | 2.2  |
| 16  | v     | 48  | THR  | 2.2  |
| 1   | a     | 333 | GLU  | 2.2  |
| 4   | d     | 282 | SER  | 2.2  |
| 18  | x     | 47  | GLN  | 2.2  |
| 2   | b     | 486 | LEU  | 2.2  |
| 4   | d     | 182 | LEU  | 2.2  |
| 11  | L     | 30  | LEU  | 2.2  |
| 7   | h     | 28  | THR  | 2.2  |
| 15  | u     | 128 | TYR  | 2.2  |
| 1   | A     | 76  | ASN  | 2.2  |
| 15  | u     | 76  | ALA  | 2.2  |
| 3   | C     | 407 | VAL  | 2.2  |
| 13  | O     | 129 | PHE  | 2.2  |
| 2   | b     | 359 | MET  | 2.2  |
| 2   | B     | 294 | SER  | 2.2  |
| 10  | k     | 13  | GLU  | 2.2  |
| 4   | D     | 200 | GLY  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | b     | 286 | ARG  | 2.2  |
| 16  | v     | 122 | ARG  | 2.2  |
| 2   | B     | 323 | GLY  | 2.2  |
| 3   | C     | 201 | ASN  | 2.2  |
| 13  | O     | 107 | ILE  | 2.2  |
| 15  | u     | 79  | ILE  | 2.2  |
| 15  | u     | 110 | GLU  | 2.2  |
| 4   | D     | 282 | SER  | 2.2  |
| 15  | U     | 78  | LEU  | 2.2  |
| 1   | A     | 80  | GLY  | 2.2  |
| 1   | a     | 203 | ALA  | 2.2  |
| 2   | B     | 355 | PHE  | 2.2  |
| 2   | b     | 67  | ALA  | 2.2  |
| 1   | a     | 238 | LYS  | 2.2  |
| 1   | a     | 178 | GLY  | 2.2  |
| 2   | b     | 80  | ILE  | 2.2  |
| 20  | Z     | 34  | ASP  | 2.2  |
| 4   | D     | 278 | GLY  | 2.2  |
| 18  | x     | 37  | LEU  | 2.2  |
| 5   | E     | 61  | ARG  | 2.2  |
| 2   | B     | 172 | TYR  | 2.2  |
| 2   | b     | 72  | THR  | 2.2  |
| 3   | c     | 95  | LEU  | 2.2  |
| 3   | c     | 388 | GLN  | 2.2  |
| 13  | O     | 152 | VAL  | 2.2  |
| 1   | a     | 186 | PHE  | 2.1  |
| 3   | C     | 47  | GLY  | 2.1  |
| 2   | b     | 265 | ILE  | 2.1  |
| 18  | x     | 44  | ASP  | 2.1  |
| 20  | Z     | 31  | GLN  | 2.1  |
| 1   | A     | 300 | PHE  | 2.1  |
| 4   | d     | 138 | VAL  | 2.1  |
| 16  | v     | 128 | PRO  | 2.1  |
| 1   | a     | 193 | LEU  | 2.1  |
| 14  | T     | 32  | LYS  | 2.1  |
| 17  | g     | 24  | MET  | 2.1  |
| 20  | z     | 21  | ILE  | 2.1  |
| 7   | h     | 18  | TYR  | 2.1  |
| 2   | B     | 415 | PRO  | 2.1  |
| 1   | a     | 13  | LEU  | 2.1  |
| 3   | c     | 175 | LEU  | 2.1  |
| 15  | u     | 109 | LEU  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | a     | 247 | ASN  | 2.1  |
| 4   | d     | 332 | GLN  | 2.1  |
| 13  | O     | 173 | ASN  | 2.1  |
| 9   | J     | 7   | ARG  | 2.1  |
| 12  | M     | 2   | GLU  | 2.1  |
| 13  | o     | 91  | PHE  | 2.1  |
| 2   | b     | 224 | ARG  | 2.1  |
| 1   | a     | 156 | ALA  | 2.1  |
| 3   | C     | 155 | ASN  | 2.1  |
| 4   | D     | 29  | PHE  | 2.1  |
| 2   | B     | 232 | GLY  | 2.1  |
| 13  | O     | 88  | GLU  | 2.1  |
| 14  | T     | 6   | TYR  | 2.1  |
| 15  | u     | 114 | VAL  | 2.1  |
| 17  | g     | 28  | ILE  | 2.1  |
| 3   | C     | 98  | GLY  | 2.1  |
| 3   | c     | 142 | GLU  | 2.1  |
| 7   | h     | 12  | ARG  | 2.1  |
| 5   | e     | 45  | ASP  | 2.1  |
| 15  | u     | 97  | LEU  | 2.1  |
| 1   | a     | 14  | TRP  | 2.1  |
| 1   | A     | 287 | ALA  | 2.1  |
| 3   | c     | 106 | VAL  | 2.1  |
| 3   | c     | 138 | GLU  | 2.1  |
| 3   | C     | 405 | ASN  | 2.1  |
| 11  | L     | 37  | ASN  | 2.1  |
| 2   | b     | 225 | LEU  | 2.1  |
| 7   | H     | 28  | THR  | 2.1  |
| 15  | u     | 81  | LYS  | 2.1  |
| 16  | v     | 43  | LYS  | 2.1  |
| 13  | O     | 209 | ALA  | 2.1  |
| 14  | T     | 28  | ARG  | 2.1  |
| 16  | v     | 112 | GLN  | 2.1  |
| 4   | d     | 15  | PHE  | 2.1  |
| 15  | U     | 97  | LEU  | 2.1  |
| 2   | b     | 261 | ALA  | 2.1  |
| 4   | d     | 285 | GLY  | 2.1  |
| 1   | a     | 283 | VAL  | 2.1  |
| 2   | b     | 121 | GLU  | 2.1  |
| 2   | b     | 411 | PHE  | 2.1  |
| 3   | C     | 197 | ARG  | 2.1  |
| 3   | C     | 409 | GLY  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3   | c     | 329 | GLY  | 2.1  |
| 13  | o     | 123 | GLU  | 2.1  |
| 2   | b     | 228 | ALA  | 2.1  |
| 2   | b     | 339 | ALA  | 2.1  |
| 11  | L     | 32  | SER  | 2.1  |
| 13  | o     | 230 | VAL  | 2.1  |
| 3   | c     | 45  | LEU  | 2.1  |
| 14  | T     | 30  | THR  | 2.1  |
| 2   | b     | 349 | LYS  | 2.1  |
| 1   | a     | 285 | PHE  | 2.1  |
| 13  | O     | 177 | TYR  | 2.1  |
| 2   | B     | 345 | VAL  | 2.1  |
| 16  | v     | 51  | GLN  | 2.1  |
| 3   | c     | 340 | TYR  | 2.1  |
| 5   | e     | 46  | VAL  | 2.1  |
| 15  | u     | 44  | ASP  | 2.1  |
| 1   | a     | 284 | TRP  | 2.1  |
| 14  | T     | 29  | ILE  | 2.1  |
| 3   | c     | 287 | THR  | 2.1  |
| 2   | b     | 123 | PHE  | 2.1  |
| 3   | C     | 258 | GLY  | 2.1  |
| 3   | c     | 341 | LEU  | 2.1  |
| 2   | B     | 212 | ALA  | 2.1  |
| 3   | c     | 229 | ASN  | 2.1  |
| 1   | a     | 172 | MET  | 2.1  |
| 16  | V     | 113 | GLU  | 2.1  |
| 13  | O     | 243 | SER  | 2.1  |
| 13  | o     | 229 | LYS  | 2.1  |
| 2   | b     | 293 | ALA  | 2.1  |
| 16  | v     | 142 | ALA  | 2.1  |
| 18  | x     | 39  | ALA  | 2.1  |
| 4   | d     | 289 | LEU  | 2.1  |
| 8   | i     | 24  | LEU  | 2.1  |
| 13  | O     | 93  | PRO  | 2.1  |
| 2   | B     | 320 | ALA  | 2.0  |
| 4   | d     | 155 | SER  | 2.0  |
| 15  | u     | 43  | VAL  | 2.0  |
| 18  | x     | 20  | PHE  | 2.0  |
| 4   | d     | 321 | LEU  | 2.0  |
| 3   | c     | 144 | SER  | 2.0  |
| 1   | a     | 191 | ASN  | 2.0  |
| 2   | b     | 306 | PRO  | 2.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3   | c     | 375 | LEU  | 2.0  |
| 1   | A     | 197 | PHE  | 2.0  |
| 1   | A     | 344 | ALA  | 2.0  |
| 20  | z     | 20  | VAL  | 2.0  |
| 3   | C     | 264 | PHE  | 2.0  |
| 4   | D     | 292 | ASN  | 2.0  |
| 13  | o     | 238 | ALA  | 2.0  |
| 15  | u     | 118 | GLU  | 2.0  |
| 2   | B     | 292 | LEU  | 2.0  |
| 17  | g     | 31  | ALA  | 2.0  |
| 16  | v     | 117 | VAL  | 2.0  |
| 2   | b     | 55  | MET  | 2.0  |
| 3   | c     | 403 | SER  | 2.0  |
| 10  | k     | 12  | PRO  | 2.0  |
| 3   | c     | 208 | VAL  | 2.0  |
| 10  | k     | 17  | ILE  | 2.0  |
| 1   | a     | 92  | HIS  | 2.0  |
| 3   | c     | 145 | SER  | 2.0  |
| 7   | h     | 16  | SER  | 2.0  |
| 4   | D     | 241 | GLU  | 2.0  |
| 8   | I     | 2   | GLU  | 2.0  |
| 1   | a     | 288 | LEU  | 2.0  |
| 2   | B     | 174 | LEU  | 2.0  |

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

| Mol | Type | Chain | Res | Atoms | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|-------|-----------------------------|-------|
| 35  | CA   | o     | 301 | 1/1   | 0.66 | 13.65 | 209,209,209,209             | 0     |
| 32  | LMT  | i     | 103 | 35/35 | 1.26 | 8.11  | 206,209,210,210             | 0     |
| 35  | CA   | K     | 102 | 1/1   | 0.67 | 6.01  | 210,210,210,210             | 0     |
| 22  | CLA  | a     | 406 | 65/65 | 0.69 | 5.67  | 206,208,208,209             | 0     |
| 25  | BCR  | i     | 101 | 40/40 | 0.74 | 5.64  | 206,207,208,208             | 0     |
| 25  | BCR  | B     | 619 | 40/40 | 1.05 | 5.29  | 205,207,208,208             | 0     |
| 31  | LMG  | i     | 102 | 43/55 | 0.77 | 4.97  | 205,207,209,210             | 0     |
| 30  | SQD  | a     | 401 | 54/54 | 0.70 | 4.87  | 205,208,210,213             | 0     |
| 25  | BCR  | c     | 521 | 40/40 | 1.56 | 4.69  | 206,208,209,209             | 0     |
| 31  | LMG  | C     | 517 | 45/55 | 1.13 | 4.44  | 206,207,209,210             | 0     |
| 32  | LMT  | I     | 102 | 35/35 | 1.26 | 4.32  | 206,208,210,210             | 0     |
| 25  | BCR  | b     | 624 | 40/40 | 0.74 | 4.06  | 205,206,207,208             | 0     |
| 26  | DGD  | D     | 407 | 63/66 | 0.66 | 4.01  | 206,208,209,210             | 0     |
| 24  | PL9  | j     | 101 | 35/55 | 0.39 | 3.95  | 205,208,209,210             | 0     |
| 26  | DGD  | B     | 626 | 52/66 | 0.56 | 3.61  | 206,208,210,211             | 0     |
| 22  | CLA  | b     | 605 | 65/65 | 1.41 | 3.50  | 206,208,210,210             | 0     |
| 25  | BCR  | c     | 513 | 40/40 | 0.76 | 3.20  | 206,207,208,209             | 0     |
| 25  | BCR  | y     | 101 | 40/40 | 0.77 | 3.13  | 206,207,208,208             | 0     |
| 25  | BCR  | K     | 101 | 40/40 | 0.54 | 2.98  | 206,207,208,209             | 0     |
| 22  | CLA  | A     | 406 | 65/65 | 0.64 | 2.96  | 206,208,209,209             | 0     |
| 22  | CLA  | B     | 604 | 65/65 | 0.54 | 2.84  | 206,207,208,209             | 0     |
| 31  | LMG  | c     | 518 | 45/55 | 0.80 | 2.82  | 206,208,209,210             | 0     |
| 31  | LMG  | I     | 101 | 43/55 | 0.96 | 2.80  | 205,208,210,211             | 0     |
| 22  | CLA  | B     | 603 | 65/65 | 0.53 | 2.46  | 205,207,208,208             | 0     |
| 25  | BCR  | g     | 101 | 40/40 | 0.76 | 2.38  | 205,207,208,209             | 0     |
| 22  | CLA  | c     | 512 | 65/65 | 1.05 | 2.37  | 206,207,209,210             | 0     |
| 25  | BCR  | f     | 102 | 40/40 | 0.34 | 2.33  | 206,207,208,209             | 0     |
| 25  | BCR  | C     | 520 | 40/40 | 1.05 | 2.24  | 206,207,209,210             | 0     |
| 26  | DGD  | b     | 601 | 52/66 | 0.44 | 2.21  | 204,208,209,210             | 0     |
| 30  | SQD  | B     | 627 | 47/54 | 0.78 | 2.21  | 206,208,210,212             | 0     |
| 32  | LMT  | B     | 623 | 35/35 | 0.66 | 2.13  | 206,208,210,210             | 0     |
| 32  | LMT  | D     | 408 | 31/35 | 0.45 | 2.10  | 207,208,210,210             | 0     |
| 22  | CLA  | B     | 609 | 65/65 | 0.63 | 2.08  | 206,207,209,210             | 0     |
| 25  | BCR  | c     | 514 | 40/40 | 1.18 | 2.06  | 206,208,208,209             | 0     |
| 25  | BCR  | H     | 102 | 40/40 | 1.22 | 2.04  | 206,207,209,210             | 0     |
| 32  | LMT  | d     | 411 | 31/35 | 0.63 | 2.02  | 206,209,210,211             | 0     |
| 22  | CLA  | B     | 601 | 65/65 | 1.05 | 2.02  | 205,208,209,209             | 0     |
| 32  | LMT  | b     | 629 | 35/35 | 0.96 | 2.00  | 206,208,209,210             | 0     |
| 22  | CLA  | B     | 605 | 65/65 | 0.53 | 1.96  | 206,207,208,209             | 0     |
| 22  | CLA  | B     | 614 | 65/65 | 0.86 | 1.93  | 205,207,208,209             | 0     |
| 22  | CLA  | D     | 404 | 65/65 | 0.48 | 1.93  | 205,207,208,208             | 0     |
| 31  | LMG  | e     | 101 | 44/55 | 0.48 | 1.89  | 205,208,209,211             | 0     |

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| Mol | Type | Chain | Res | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 22  | CLA  | d     | 406 | 65/65 | 0.47 | 1.89 | 206,207,209,209             | 0     |
| 24  | PL9  | J     | 101 | 35/55 | 0.44 | 1.89 | 206,207,210,210             | 0     |
| 22  | CLA  | c     | 501 | 65/65 | 0.67 | 1.86 | 206,207,209,209             | 0     |
| 26  | DGD  | d     | 410 | 63/66 | 0.81 | 1.85 | 206,208,210,211             | 0     |
| 31  | LMG  | b     | 627 | 42/55 | 0.53 | 1.83 | 204,207,211,211             | 0     |
| 30  | SQD  | d     | 403 | 43/54 | 0.76 | 1.77 | 205,208,209,209             | 0     |
| 22  | CLA  | B     | 608 | 65/65 | 0.80 | 1.75 | 205,207,209,210             | 0     |
| 25  | BCR  | C     | 513 | 40/40 | 0.91 | 1.74 | 205,207,208,208             | 0     |
| 22  | CLA  | B     | 602 | 65/65 | 0.48 | 1.69 | 205,207,208,209             | 0     |
| 25  | BCR  | A     | 408 | 40/40 | 0.48 | 1.61 | 206,207,208,208             | 0     |
| 30  | SQD  | f     | 103 | 45/54 | 0.69 | 1.59 | 205,208,210,210             | 0     |
| 22  | CLA  | B     | 615 | 65/65 | 0.86 | 1.56 | 206,207,209,209             | 0     |
| 35  | CA   | k     | 101 | 1/1   | 0.27 | 1.54 | 208,208,208,208             | 0     |
| 32  | LMT  | b     | 628 | 35/35 | 0.50 | 1.49 | 206,208,210,210             | 0     |
| 25  | BCR  | B     | 617 | 40/40 | 0.42 | 1.49 | 205,207,208,209             | 0     |
| 22  | CLA  | C     | 511 | 65/65 | 1.15 | 1.37 | 206,207,208,209             | 0     |
| 22  | CLA  | B     | 611 | 65/65 | 0.39 | 1.34 | 205,207,208,208             | 0     |
| 22  | CLA  | b     | 620 | 65/65 | 0.95 | 1.29 | 206,208,209,210             | 0     |
| 22  | CLA  | b     | 614 | 65/65 | 0.62 | 1.27 | 206,207,209,210             | 0     |
| 22  | CLA  | c     | 511 | 65/65 | 0.94 | 1.23 | 206,208,209,209             | 0     |
| 25  | BCR  | F     | 102 | 40/40 | 0.42 | 1.21 | 205,207,208,208             | 0     |
| 32  | LMT  | B     | 628 | 35/35 | 0.62 | 1.21 | 206,208,210,211             | 0     |
| 22  | CLA  | C     | 501 | 65/65 | 0.43 | 1.19 | 206,208,209,209             | 0     |
| 30  | SQD  | B     | 622 | 43/54 | 0.52 | 1.09 | 205,208,209,212             | 0     |
| 22  | CLA  | c     | 506 | 65/65 | 0.68 | 1.08 | 206,208,209,209             | 0     |
| 30  | SQD  | F     | 103 | 45/54 | 0.71 | 1.06 | 205,208,209,210             | 0     |
| 22  | CLA  | c     | 510 | 65/65 | 0.62 | 1.06 | 206,208,209,211             | 0     |
| 22  | CLA  | b     | 607 | 65/65 | 0.53 | 1.06 | 205,207,208,208             | 0     |
| 22  | CLA  | C     | 512 | 65/65 | 1.00 | 1.05 | 205,207,209,211             | 0     |
| 22  | CLA  | b     | 608 | 65/65 | 0.45 | 1.05 | 205,207,208,209             | 0     |
| 30  | SQD  | A     | 414 | 54/54 | 0.46 | 1.04 | 205,207,209,210             | 0     |
| 22  | CLA  | b     | 619 | 65/65 | 0.86 | 1.04 | 206,208,209,209             | 0     |
| 22  | CLA  | b     | 609 | 65/65 | 0.46 | 1.03 | 206,207,208,209             | 0     |
| 22  | CLA  | B     | 607 | 65/65 | 0.42 | 1.01 | 206,207,208,209             | 0     |
| 32  | LMT  | B     | 624 | 35/35 | 0.45 | 1.00 | 206,207,211,212             | 0     |
| 26  | DGD  | a     | 408 | 56/66 | 0.44 | 0.92 | 206,208,210,211             | 0     |
| 31  | LMG  | a     | 402 | 42/55 | 0.39 | 0.92 | 204,207,209,210             | 0     |
| 30  | SQD  | b     | 602 | 47/54 | 0.44 | 0.92 | 205,208,209,212             | 0     |
| 22  | CLA  | C     | 508 | 65/65 | 0.79 | 0.91 | 205,207,208,209             | 0     |
| 22  | CLA  | C     | 502 | 65/65 | 0.54 | 0.89 | 206,207,208,208             | 0     |
| 34  | HEM  | v     | 201 | 43/43 | 0.56 | 0.88 | 206,207,208,209             | 0     |
| 31  | LMG  | m     | 101 | 42/55 | 0.53 | 0.85 | 205,207,209,210             | 0     |

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| Mol | Type | Chain | Res | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 26  | DGD  | A     | 409 | 56/66 | 0.45 | 0.82 | 206,208,210,211             | 0     |
| 25  | BCR  | x     | 101 | 40/40 | 0.76 | 0.78 | 206,207,209,209             | 0     |
| 22  | CLA  | C     | 506 | 65/65 | 0.56 | 0.72 | 206,207,208,209             | 0     |
| 31  | LMG  | M     | 101 | 42/55 | 0.44 | 0.68 | 205,208,209,210             | 0     |
| 22  | CLA  | c     | 503 | 65/65 | 0.45 | 0.68 | 206,207,208,209             | 0     |
| 22  | CLA  | C     | 510 | 65/65 | 0.61 | 0.64 | 206,207,209,209             | 0     |
| 32  | LMT  | b     | 603 | 35/35 | 0.46 | 0.62 | 206,208,210,210             | 0     |
| 22  | CLA  | b     | 610 | 65/65 | 0.46 | 0.62 | 206,207,209,209             | 0     |
| 34  | HEM  | F     | 101 | 43/43 | 0.47 | 0.61 | 206,207,208,210             | 0     |
| 22  | CLA  | B     | 613 | 65/65 | 0.44 | 0.58 | 206,207,208,209             | 0     |
| 22  | CLA  | c     | 505 | 65/65 | 0.59 | 0.57 | 205,207,208,209             | 0     |
| 22  | CLA  | c     | 502 | 65/65 | 0.64 | 0.55 | 206,207,208,209             | 0     |
| 25  | BCR  | b     | 623 | 40/40 | 0.35 | 0.54 | 205,206,207,207             | 0     |
| 22  | CLA  | b     | 612 | 65/65 | 0.37 | 0.54 | 205,207,209,209             | 0     |
| 22  | CLA  | b     | 613 | 65/65 | 0.55 | 0.52 | 205,207,208,209             | 0     |
| 25  | BCR  | j     | 102 | 40/40 | 0.27 | 0.49 | 206,208,209,210             | 0     |
| 24  | PL9  | a     | 407 | 45/55 | 0.33 | 0.46 | 205,207,208,209             | 0     |
| 31  | LMG  | E     | 101 | 44/55 | 0.42 | 0.44 | 204,208,209,210             | 0     |
| 33  | BCT  | d     | 404 | 4/4   | 0.47 | 0.42 | 206,207,208,208             | 0     |
| 22  | CLA  | b     | 616 | 65/65 | 0.36 | 0.42 | 206,207,208,209             | 0     |
| 22  | CLA  | c     | 508 | 65/65 | 0.48 | 0.41 | 205,208,209,209             | 0     |
| 32  | LMT  | b     | 604 | 35/35 | 0.37 | 0.38 | 207,208,210,210             | 0     |
| 22  | CLA  | b     | 606 | 65/65 | 0.39 | 0.38 | 205,207,209,210             | 0     |
| 34  | HEM  | V     | 201 | 43/43 | 0.33 | 0.35 | 201,207,208,209             | 0     |
| 24  | PL9  | A     | 407 | 45/55 | 0.46 | 0.34 | 206,207,208,210             | 0     |
| 25  | BCR  | b     | 621 | 40/40 | 0.32 | 0.33 | 206,207,208,208             | 0     |
| 22  | CLA  | H     | 101 | 65/65 | 0.36 | 0.28 | 206,207,208,209             | 0     |
| 22  | CLA  | C     | 507 | 65/65 | 0.37 | 0.27 | 206,207,208,208             | 0     |
| 22  | CLA  | c     | 504 | 65/65 | 0.34 | 0.27 | 205,207,208,209             | 0     |
| 32  | LMT  | B     | 629 | 35/35 | 0.36 | 0.24 | 206,208,209,210             | 0     |
| 22  | CLA  | B     | 610 | 65/65 | 0.34 | 0.18 | 205,207,208,208             | 0     |
| 25  | BCR  | B     | 616 | 40/40 | 0.35 | 0.16 | 205,207,208,209             | 0     |
| 21  | FE2  | A     | 401 | 1/1   | 0.28 | 0.16 | 209,209,209,209             | 0     |
| 22  | CLA  | C     | 505 | 65/65 | 0.39 | 0.11 | 206,207,209,210             | 0     |
| 34  | HEM  | f     | 101 | 43/43 | 0.25 | 0.11 | 206,207,209,209             | 0     |
| 22  | CLA  | b     | 618 | 65/65 | 0.37 | 0.11 | 206,207,209,210             | 0     |
| 26  | DGD  | B     | 620 | 58/66 | 0.35 | 0.11 | 205,207,209,209             | 0     |
| 31  | LMG  | c     | 522 | 48/55 | 0.28 | 0.10 | 205,207,209,210             | 0     |
| 22  | CLA  | C     | 504 | 65/65 | 0.33 | 0.07 | 205,207,208,209             | 0     |
| 22  | CLA  | C     | 503 | 65/65 | 0.37 | 0.05 | 206,207,208,209             | 0     |
| 35  | CA   | O     | 301 | 1/1   | 0.36 | 0.05 | 208,208,208,208             | 0     |
| 25  | BCR  | B     | 618 | 40/40 | 0.28 | 0.05 | 205,206,208,208             | 0     |

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| Mol | Type | Chain | Res | Atoms | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|-------|-----------------------------|-------|
| 22  | CLA  | b     | 617 | 65/65 | 0.32 | 0.04  | 206,207,208,209             | 0     |
| 22  | CLA  | C     | 509 | 65/65 | 0.37 | 0.01  | 205,207,208,208             | 0     |
| 23  | PHO  | d     | 401 | 64/64 | 0.43 | 0.01  | 206,207,208,208             | 0     |
| 30  | SQD  | a     | 412 | 51/54 | 0.23 | -0.00 | 205,207,208,209             | 0     |
| 27  | LHG  | c     | 519 | 37/49 | 0.30 | -0.03 | 204,207,210,213             | 0     |
| 25  | BCR  | b     | 622 | 40/40 | 0.33 | -0.03 | 205,207,208,208             | 0     |
| 22  | CLA  | a     | 404 | 65/65 | 0.51 | -0.05 | 204,207,208,208             | 0     |
| 31  | LMG  | C     | 521 | 48/55 | 0.29 | -0.06 | 206,207,208,209             | 0     |
| 26  | DGD  | b     | 625 | 58/66 | 0.34 | -0.08 | 206,207,208,209             | 0     |
| 29  | OEX  | a     | 411 | 10/10 | 0.49 | -0.14 | 200,204,205,206             | 0     |
| 28  | CL   | A     | 411 | 1/1   | 0.36 | -0.18 | 204,204,204,204             | 0     |
| 33  | BCT  | D     | 402 | 4/4   | 0.27 | -0.23 | 208,208,208,208             | 0     |
| 22  | CLA  | B     | 612 | 65/65 | 0.30 | -0.29 | 203,207,208,209             | 0     |
| 31  | LMG  | l     | 101 | 51/55 | 0.27 | -0.29 | 206,207,209,209             | 0     |
| 22  | CLA  | c     | 507 | 65/65 | 0.27 | -0.31 | 206,207,209,209             | 0     |
| 31  | LMG  | d     | 409 | 48/55 | 0.26 | -0.32 | 206,207,209,210             | 0     |
| 31  | LMG  | D     | 406 | 48/55 | 0.26 | -0.33 | 204,207,208,209             | 0     |
| 25  | BCR  | J     | 102 | 40/40 | 0.29 | -0.34 | 205,207,209,209             | 0     |
| 27  | LHG  | A     | 410 | 39/49 | 0.28 | -0.39 | 206,207,209,210             | 0     |
| 24  | PL9  | d     | 407 | 55/55 | 0.29 | -0.42 | 205,207,208,208             | 0     |
| 29  | OEX  | A     | 412 | 10/10 | 0.45 | -0.42 | 197,202,205,206             | 0     |
| 22  | CLA  | c     | 509 | 65/65 | 0.26 | -0.43 | 206,207,209,209             | 0     |
| 27  | LHG  | a     | 409 | 39/49 | 0.26 | -0.49 | 206,207,209,209             | 0     |
| 23  | PHO  | D     | 401 | 64/64 | 0.34 | -0.51 | 205,207,208,209             | 0     |
| 22  | CLA  | a     | 403 | 65/65 | 0.51 | -0.51 | 205,207,208,210             | 0     |
| 22  | CLA  | b     | 615 | 65/65 | 0.25 | -0.56 | 205,207,208,209             | 0     |
| 30  | SQD  | A     | 413 | 51/54 | 0.22 | -0.57 | 204,207,209,209             | 0     |
| 22  | CLA  | d     | 405 | 65/65 | 0.44 | -0.58 | 205,207,208,208             | 0     |
| 31  | LMG  | D     | 409 | 46/55 | 0.29 | -0.58 | 205,207,208,209             | 0     |
| 31  | LMG  | d     | 412 | 46/55 | 0.19 | -0.59 | 205,207,208,209             | 0     |
| 26  | DGD  | C     | 514 | 53/66 | 0.28 | -0.65 | 205,206,208,209             | 0     |
| 23  | PHO  | A     | 405 | 64/64 | 0.29 | -0.68 | 205,207,208,209             | 0     |
| 31  | LMG  | B     | 625 | 49/55 | 0.28 | -0.69 | 205,207,208,208             | 0     |
| 26  | DGD  | c     | 515 | 53/66 | 0.30 | -0.71 | 205,207,209,210             | 0     |
| 32  | LMT  | M     | 102 | 35/35 | 0.36 | -0.71 | 205,208,209,209             | 0     |
| 22  | CLA  | A     | 402 | 65/65 | 0.32 | -0.73 | 206,207,208,209             | 0     |
| 22  | CLA  | c     | 520 | 65/65 | 0.26 | -0.78 | 206,207,208,209             | 0     |
| 22  | CLA  | a     | 405 | 65/65 | 0.32 | -0.79 | 205,207,209,209             | 0     |
| 22  | CLA  | A     | 403 | 65/65 | 0.31 | -0.80 | 205,207,208,208             | 0     |
| 26  | DGD  | C     | 516 | 66/66 | 0.31 | -0.80 | 205,207,208,208             | 0     |
| 23  | PHO  | d     | 402 | 64/64 | 0.24 | -0.82 | 206,207,209,209             | 0     |
| 24  | PL9  | D     | 405 | 55/55 | 0.25 | -0.83 | 205,207,208,208             | 0     |

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| Mol | Type | Chain | Res | Atoms | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|-------|-----------------------------|-------|
| 31  | LMG  | d     | 408 | 49/55 | 0.23 | -0.83 | 205,207,208,209             | 0     |
| 28  | CL   | a     | 410 | 1/1   | 0.40 | -0.90 | 205,205,205,205             | 0     |
| 22  | CLA  | b     | 611 | 65/65 | 0.25 | -0.93 | 206,207,208,209             | 0     |
| 26  | DGD  | C     | 515 | 62/66 | 0.24 | -1.00 | 205,207,209,210             | 0     |
| 26  | DGD  | c     | 517 | 66/66 | 0.22 | -1.02 | 206,207,209,209             | 0     |
| 22  | CLA  | C     | 519 | 65/65 | 0.24 | -1.04 | 205,207,209,209             | 0     |
| 22  | CLA  | B     | 606 | 65/65 | 0.29 | -1.07 | 205,207,208,209             | 0     |
| 22  | CLA  | D     | 403 | 65/65 | 0.31 | -1.10 | 205,207,208,208             | 0     |
| 31  | LMG  | L     | 101 | 51/55 | 0.22 | -1.12 | 205,207,208,209             | 0     |
| 32  | LMT  | M     | 103 | 35/35 | 0.28 | -1.13 | 206,208,209,209             | 0     |
| 31  | LMG  | b     | 626 | 49/55 | 0.27 | -1.19 | 205,207,209,209             | 0     |
| 27  | LHG  | C     | 518 | 37/49 | 0.29 | -1.19 | 205,208,210,211             | 0     |
| 22  | CLA  | A     | 404 | 65/65 | 0.26 | -1.37 | 204,207,208,209             | 0     |
| 26  | DGD  | c     | 516 | 62/66 | 0.21 | -1.45 | 206,208,208,209             | 0     |
| 31  | LMG  | B     | 621 | 49/55 | 0.24 | -1.47 | 206,207,208,209             | 0     |
| 21  | FE2  | a     | 413 | 1/1   | 0.12 | -2.88 | 206,206,206,206             | 0     |

## 6.5 Other polymers ⓘ

There are no such residues in this entry.