



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 02:46 PM EDT

PDB ID : 3KZI / pdb\_00003kzi  
Title : Crystal Structure of Monomeric Form of Cyanobacterial Photosystem II  
Authors : Gabdulkhakov, A.; Guskov, A.; Broser, M.; Kern, J.; Zouni, A.; Saenger, W.  
Deposited on : 2009-12-08  
Resolution : 3.60 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

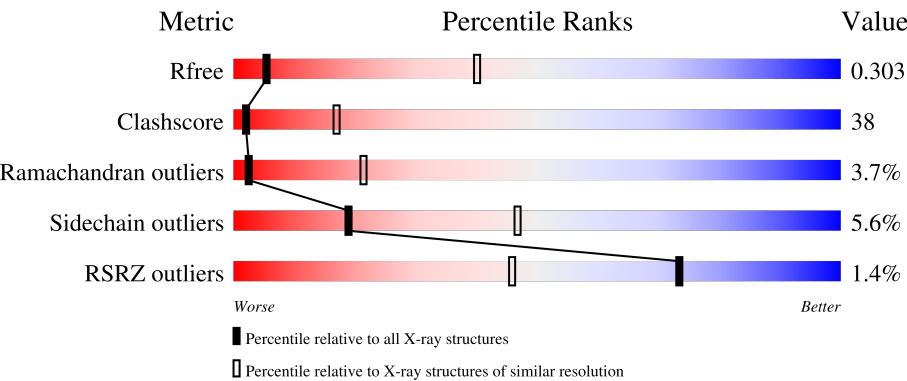
MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.015 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.50

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 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.



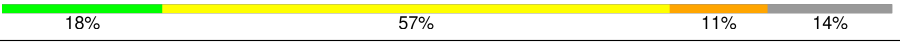
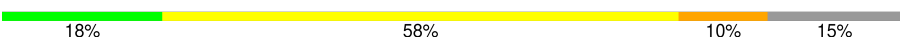
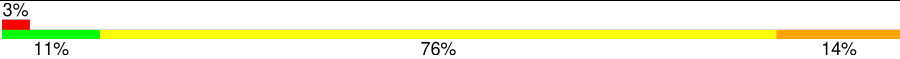
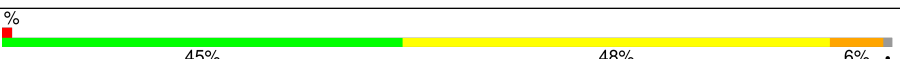
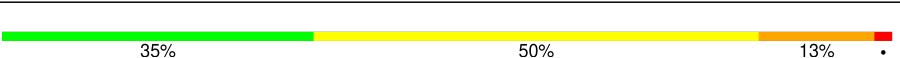
| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| R <sub>free</sub>     | 180053                      | 1747 (3.70-3.50)                                      |
| Clashscore            | 190562                      | 1827 (3.70-3.50)                                      |
| Ramachandran outliers | 187476                      | 1773 (3.70-3.50)                                      |
| Sidechain outliers    | 187428                      | 1772 (3.70-3.50)                                      |
| RSRZ outliers         | 180081                      | 1745 (3.70-3.50)                                      |

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                                               |
|-----|-------|--------|--------------------------------------------------------------------------------|
| 1   | A     | 344    | <div><div>2%</div><div>41%</div><div>50%</div><div>6%</div><div></div></div>   |
| 2   | B     | 510    | <div><div>2%</div><div>49%</div><div>40%</div><div>6%</div><div>5%</div></div> |
| 3   | C     | 461    | <div><div>%</div><div>37%</div><div>53%</div><div>7%</div><div></div></div>    |
| 4   | D     | 352    | <div><div>3%</div><div>48%</div><div>41%</div><div>8%</div><div></div></div>   |
| 5   | E     | 83     | <div><div></div><div>24%</div><div>54%</div><div>12%</div><div>7%</div></div>  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 6   | F     | 44     |    |
| 7   | H     | 65     |    |
| 8   | I     | 38     |    |
| 9   | J     | 40     |    |
| 10  | K     | 37     |    |
| 11  | L     | 37     |    |
| 12  | M     | 36     |    |
| 13  | O     | 246    |    |
| 14  | T     | 32     |    |
| 15  | U     | 104    |    |
| 16  | V     | 137    |    |
| 17  | y     | 46     |   |
| 18  | X     | 40     |  |
| 19  | Z     | 62     |  |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 21  | CLA  | A     | 362 | X         | -        | -       | -                |
| 21  | CLA  | A     | 363 | X         | -        | -       | -                |
| 21  | CLA  | A     | 364 | X         | -        | -       | -                |
| 21  | CLA  | A     | 366 | X         | -        | -       | -                |
| 21  | CLA  | B     | 511 | X         | -        | -       | -                |
| 21  | CLA  | B     | 512 | X         | -        | -       | -                |
| 21  | CLA  | B     | 513 | X         | -        | X       | -                |
| 21  | CLA  | B     | 514 | X         | -        | -       | -                |
| 21  | CLA  | B     | 515 | X         | -        | -       | -                |
| 21  | CLA  | B     | 516 | X         | -        | -       | -                |
| 21  | CLA  | B     | 517 | X         | -        | -       | -                |
| 21  | CLA  | B     | 518 | X         | -        | -       | -                |
| 21  | CLA  | B     | 519 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 21  | CLA  | B     | 520 | X         | -        | -       | -                |
| 21  | CLA  | B     | 521 | X         | -        | -       | -                |
| 21  | CLA  | B     | 522 | X         | -        | -       | -                |
| 21  | CLA  | B     | 523 | X         | -        | -       | -                |
| 21  | CLA  | B     | 524 | X         | -        | -       | -                |
| 21  | CLA  | B     | 525 | X         | -        | -       | -                |
| 21  | CLA  | B     | 526 | X         | -        | -       | -                |
| 21  | CLA  | C     | 477 | X         | -        | -       | -                |
| 21  | CLA  | C     | 478 | X         | -        | -       | -                |
| 21  | CLA  | C     | 479 | X         | -        | -       | -                |
| 21  | CLA  | C     | 480 | X         | -        | -       | -                |
| 21  | CLA  | C     | 481 | X         | -        | -       | -                |
| 21  | CLA  | C     | 482 | X         | -        | -       | -                |
| 21  | CLA  | C     | 483 | X         | -        | -       | -                |
| 21  | CLA  | C     | 484 | X         | -        | -       | -                |
| 21  | CLA  | C     | 485 | X         | -        | -       | -                |
| 21  | CLA  | C     | 486 | X         | -        | X       | -                |
| 21  | CLA  | C     | 487 | X         | -        | -       | -                |
| 21  | CLA  | C     | 488 | X         | -        | -       | -                |
| 21  | CLA  | D     | 354 | X         | -        | -       | -                |
| 21  | CLA  | D     | 356 | X         | -        | -       | -                |
| 21  | CLA  | K     | 483 | X         | -        | -       | -                |
| 22  | PHO  | A     | 365 | X         | -        | -       | -                |
| 22  | PHO  | D     | 355 | X         | -        | -       | -                |
| 23  | MES  | A     | 367 | -         | -        | X       | -                |
| 27  | LMG  | A     | 373 | -         | -        | X       | -                |
| 27  | LMG  | D     | 360 | -         | -        | X       | -                |
| 28  | DGD  | B     | 528 | -         | -        | X       | -                |
| 28  | DGD  | C     | 492 | X         | -        | -       | -                |
| 28  | DGD  | C     | 493 | X         | -        | X       | -                |
| 32  | PL9  | D     | 357 | -         | -        | X       | -                |



## 2 Entry composition [i](#)

There are 34 unique types of molecules in this entry. The entry contains 24678 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 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     | 485      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3812  | 2505 | 635 | 659 | 13 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3   | C     | 448      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3455  | 2262 | 580 | 600 | 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 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 5   | E     | 77       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 635   | 417 | 103 | 115 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 6   | F     | 38       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 307   | 207 | 50 | 49 | 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 |         |         |       |

- 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 |         |         |       |

- 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 |         |         |       |

- 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 |         |         |       |

- 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 |         |         |       |

- 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 |         |         |       |

- 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 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 14  | T     | 30       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 256   | 180 | 36 | 38 | 2 |         |         |       |

- 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   | S | 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 |         |         |       |

- 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 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 18  | X     | 35       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 254   | 172 | 38 | 44 |   |         |         |       |

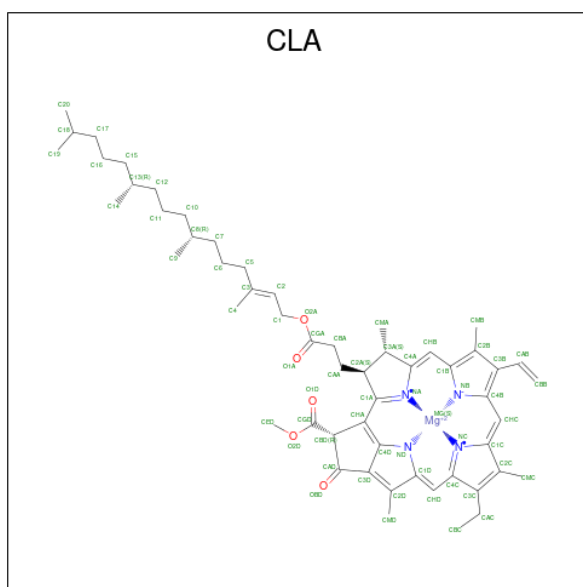
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

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

- Molecule 20 is FE (II) ION (CCD ID: FE2) (formula: Fe).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 20  | A     | 1        | Total | Fe | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 21 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).

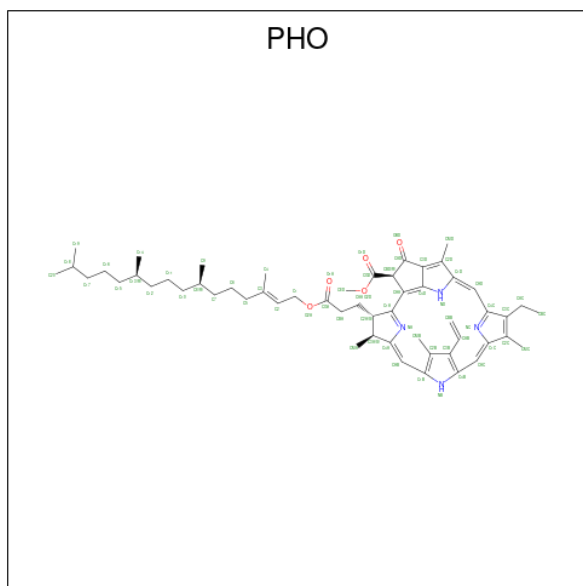
[illegible]

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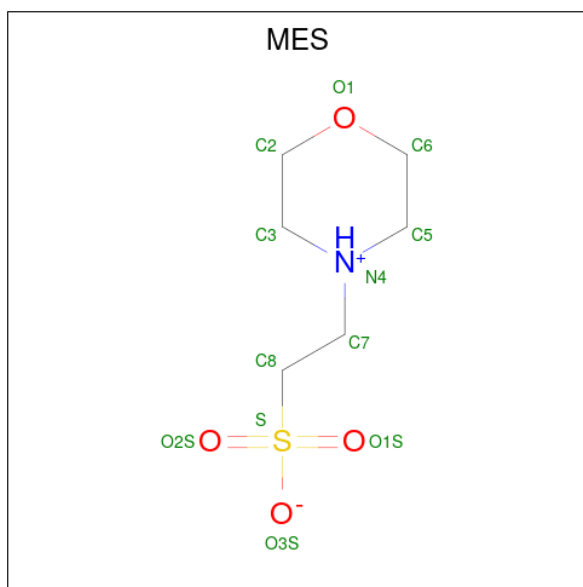
| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 21  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 21  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 21  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 21  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 21  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 21  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 21  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 21  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 21  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 21  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 21  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 21  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 21  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 21  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 21  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 21  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 21  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 21  | C     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 21  | D     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 21  | D     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 21  | K     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |

- Molecule 22 is PHEOPHYTIN A (CCD ID: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ).



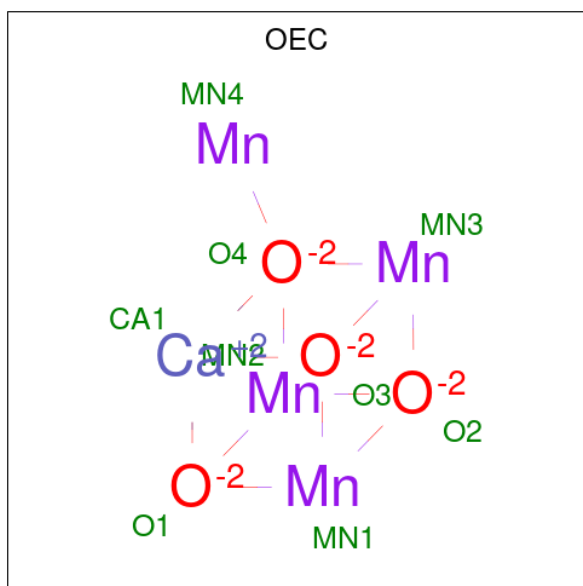
| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 22  | A     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |         |
| 22  | D     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |         |

- Molecule 23 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula:  $C_6H_{13}NO_4S$ ).



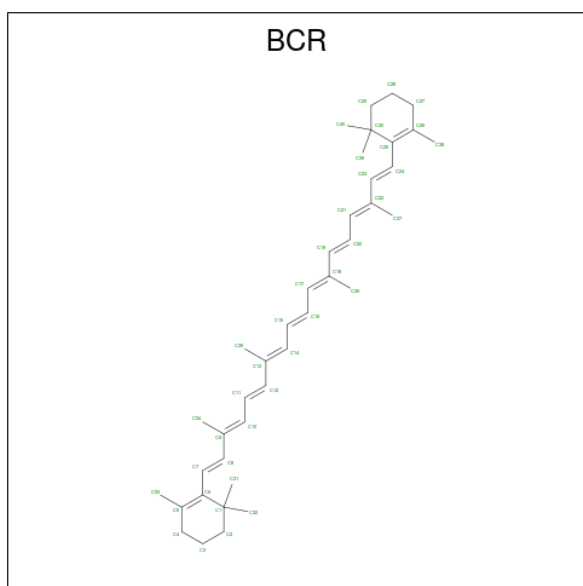
| Mol | Chain | Residues | Atoms |   |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|---------|
| 23  | A     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 12    | 6 | 1 | 4 | 1 |         |         |

- Molecule 24 is OXYGEN EVOLVING SYSTEM (CCD ID: OEC) (formula:  $\text{CaMn}_4\text{O}_4$ ).



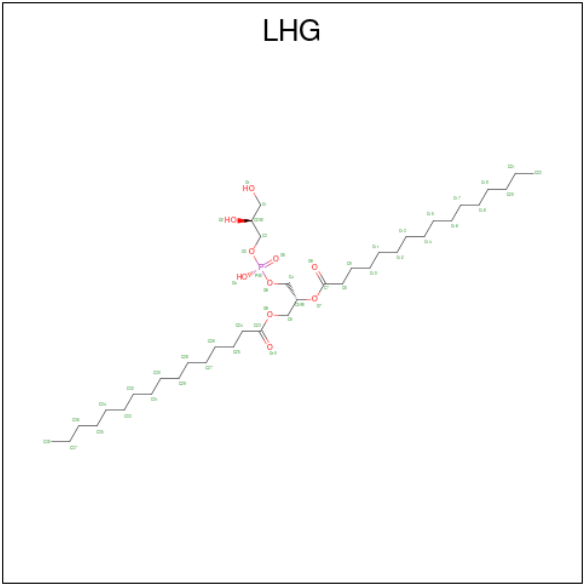
| Mol | Chain | Residues | Atoms |       | ZeroOcc | AltConf |
|-----|-------|----------|-------|-------|---------|---------|
| 24  | A     | 1        | Total | Ca Mn | 0       | 0       |
|     |       |          | 5     | 1 4   |         |         |

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula:  $\text{C}_{40}\text{H}_{56}$ ).



| 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  | C     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | C     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | D     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | J     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | J     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | X     | 1        | Total C<br>40 40 | 0       | 0       |
| 25  | Z     | 1        | Total C<br>40 40 | 0       | 0       |

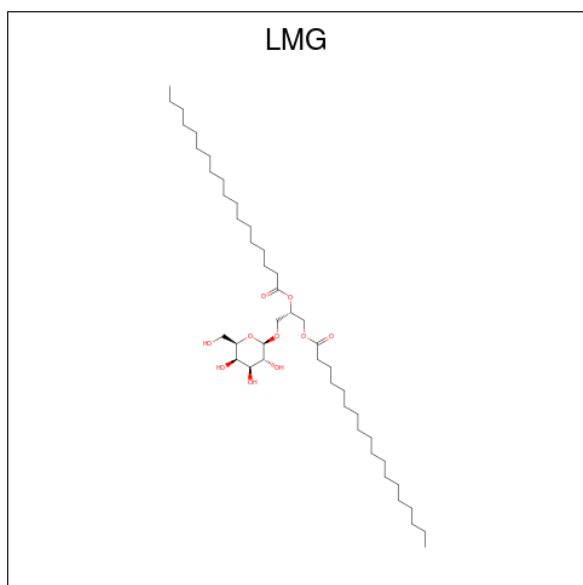
- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).





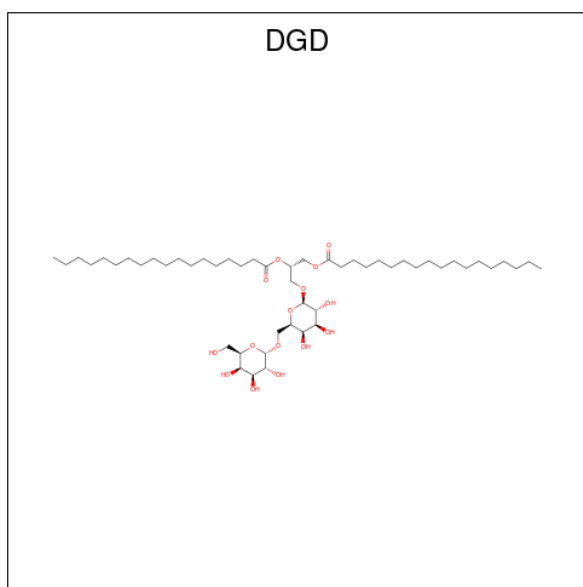
| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 26  | A     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 39    | 28 | 10 | 1 |         |         |
| 26  | C     | 1       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

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



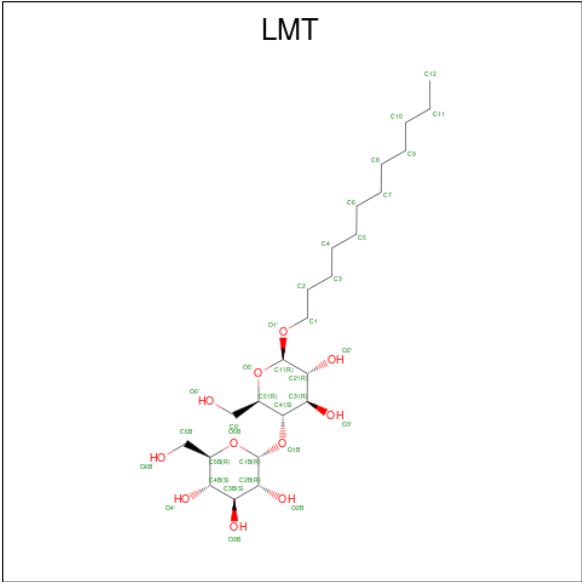
| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 27  | A     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 51    | 41 | 10 |         |         |
| 27  | B     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 49    | 39 | 10 |         |         |
| 27  | C     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 45    | 35 | 10 |         |         |
| 27  | D     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 46    | 36 | 10 |         |         |
| 27  | D     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 48    | 38 | 10 |         |         |
| 27  | I     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 43    | 33 | 10 |         |         |
| 27  | J     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 48    | 38 | 10 |         |         |
| 27  | M     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 42    | 32 | 10 |         |         |

- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



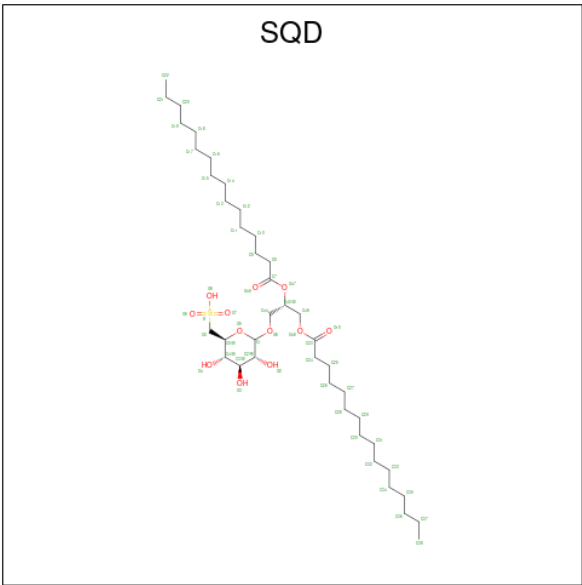
| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 28  | A     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 52    | 37 | 15 |         |         |
| 28  | B     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 66    | 51 | 15 |         |         |
| 28  | B     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 58    | 43 | 15 |         |         |
| 28  | C     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 56    | 41 | 15 |         |         |
| 28  | C     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 53    | 38 | 15 |         |         |
| 28  | C     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 62    | 47 | 15 |         |         |
| 28  | C     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 66    | 51 | 15 |         |         |
| 28  | D     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 63    | 48 | 15 |         |         |

- Molecule 29 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



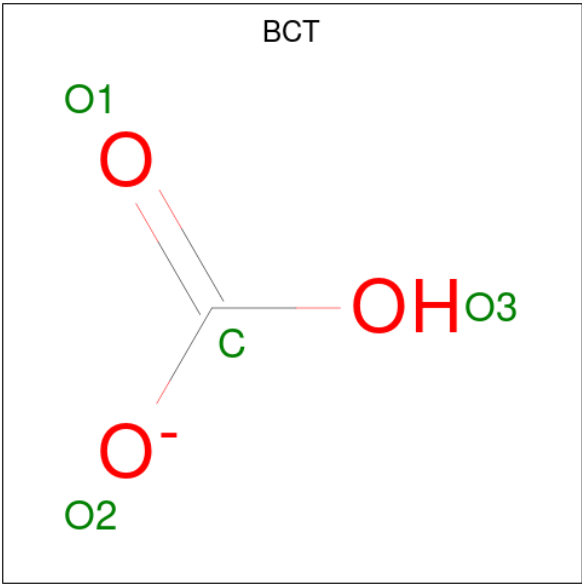
| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 29  | A     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 29  | B     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 29  | D     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 29  | D     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 31    | 20 | 11 |         |         |
| 29  | I     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 29  | O     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 29  | T     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |

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



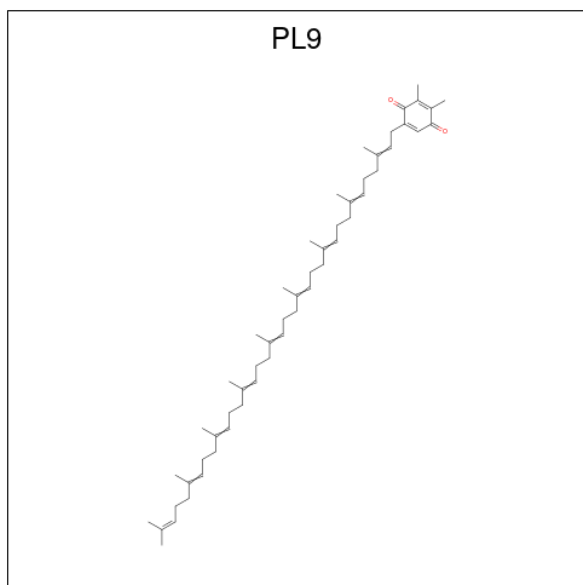
| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 30  | C     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 51    | 38 | 12 | 1 |         |         |
| 30  | D     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 43    | 30 | 12 | 1 |         |         |
| 30  | F     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 45    | 32 | 12 | 1 |         |         |
| 30  | L     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 47    | 34 | 12 | 1 |         |         |

- Molecule 31 is BICARBONATE ION (CCD ID: BCT) (formula:  $\text{CHO}_3^-$ ).



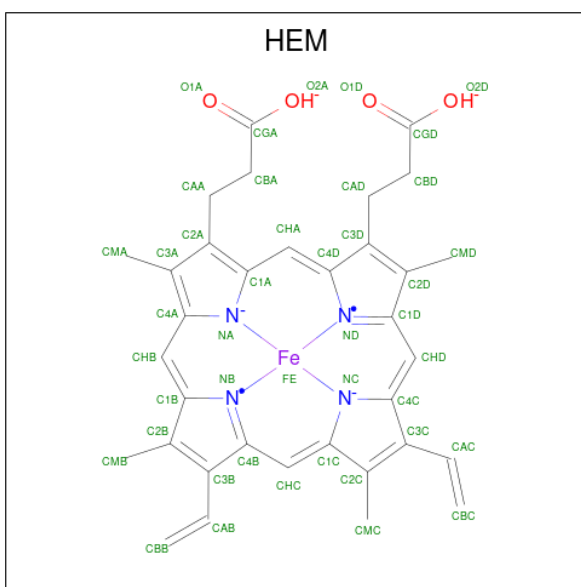
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 31  | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 1 | 3 |         |         |

- Molecule 32 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula:  $C_{53}H_{80}O_2$ ).



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

- Molecule 33 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).

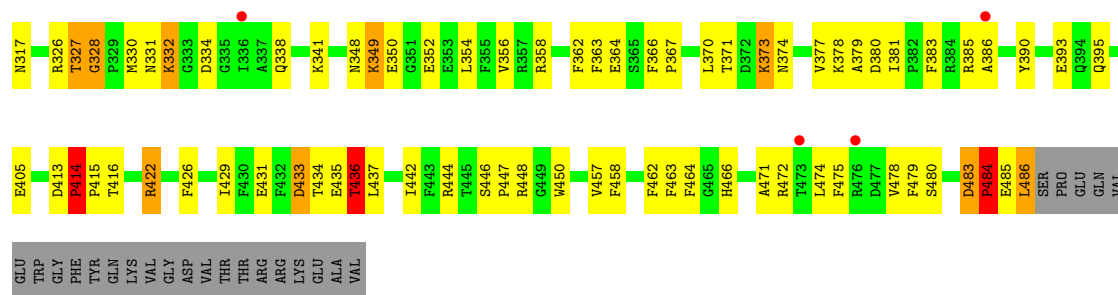


| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 33  | F     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 33  | V     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |

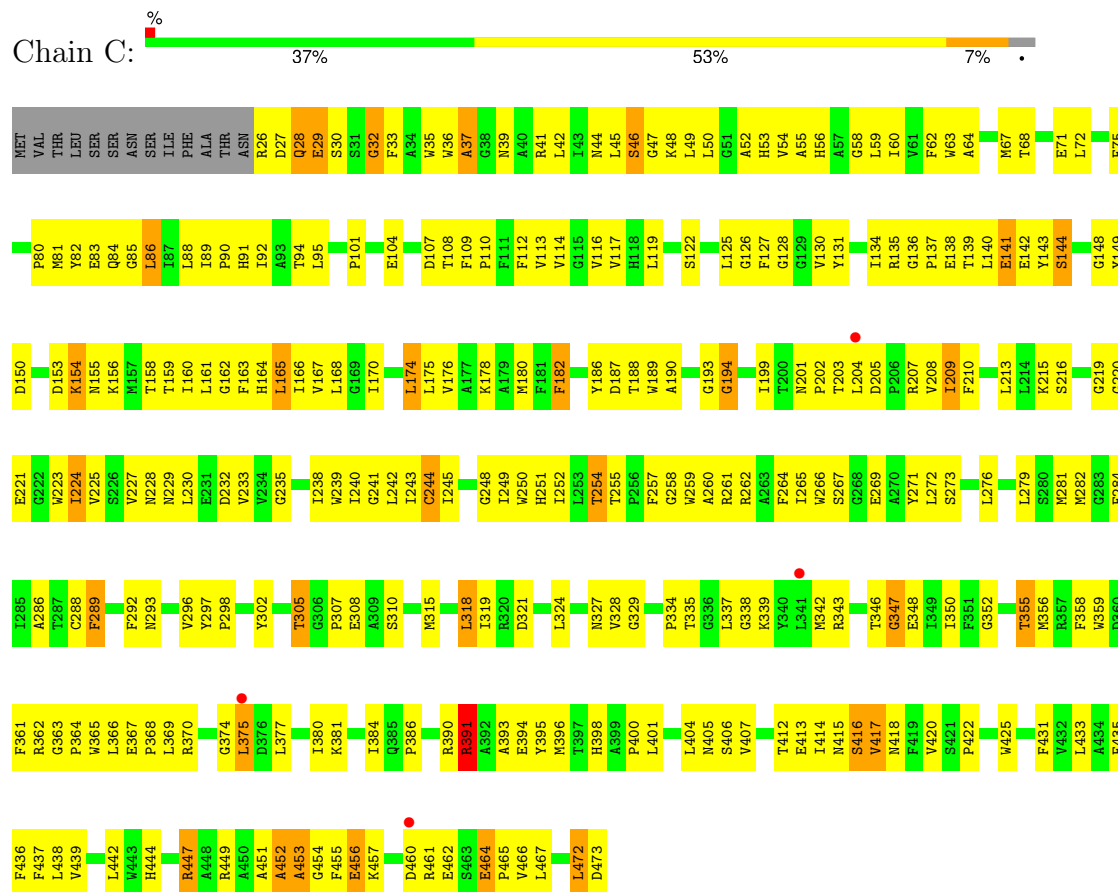
- Molecule 34 is CALCIUM ION (CCD ID: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 34  | F     | 1        | Total Ca<br>1 1 | 0       | 0       |
| 34  | K     | 1        | Total Ca<br>1 1 | 0       | 0       |
| 34  | O     | 1        | Total Ca<br>1 1 | 0       | 0       |

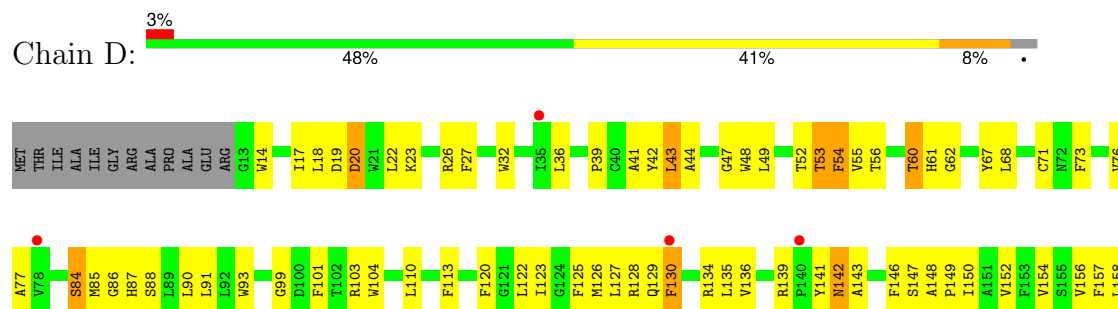




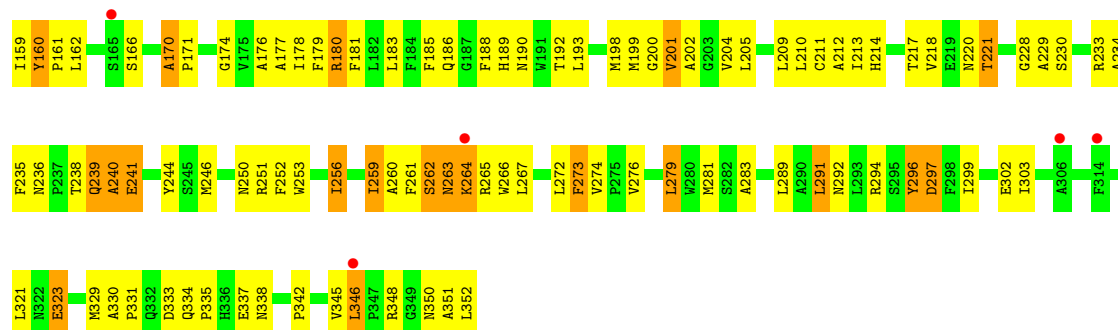
• Molecule 3: Photosystem II CP43 protein



• Molecule 4: Photosystem II D2 protein

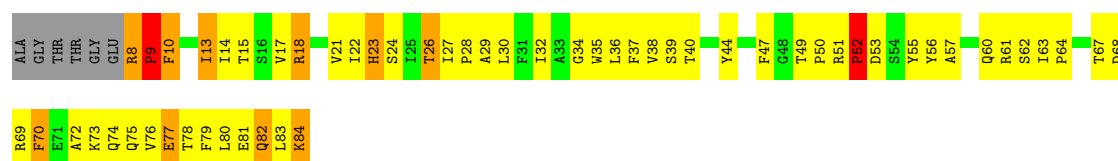






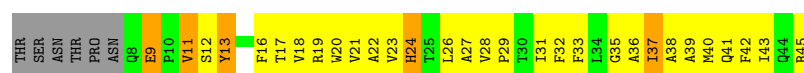
• Molecule 5: Cytochrome b559 subunit alpha

Chain E: 24% 54% 12% 7%



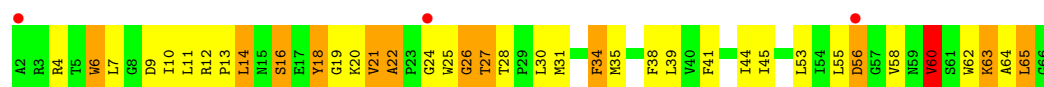
• Molecule 6: Cytochrome b559 subunit beta

Chain F: 18% 57% 11% 14%



• Molecule 7: Photosystem II reaction center protein H

Chain H: 5% 42% 38% 18%



• Molecule 8: Photosystem II reaction center protein I

Chain I: 29% 58% 5% 8%

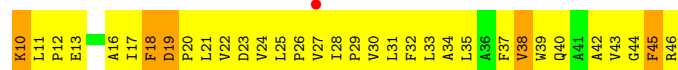


• Molecule 9: Photosystem II reaction center protein J

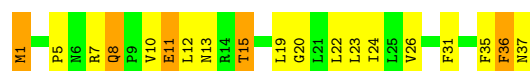
Chain J: 18% 58% 10% 15%



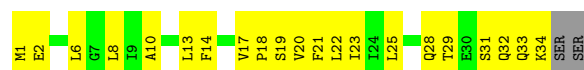
• Molecule 10: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein M



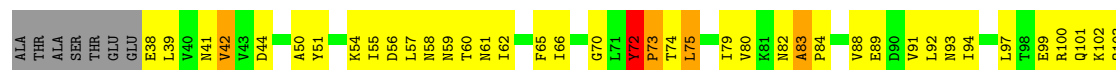
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



- Molecule 14: Photosystem II reaction center protein T



- Molecule 15: Photosystem II 12 kDa extrinsic protein





• Molecule 16: Cytochrome c-550



• Molecule 17: Photosystem II reaction center protein ycf12



• Molecule 18: Photosystem II reaction center X protein



• Molecule 19: Photosystem II reaction center protein Z



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | C 2 2 21                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 119.89Å 224.69Å 337.28Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 29.87 – 3.60<br>29.87 – 3.60                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 89.2 (29.87-3.60)<br>99.1 (29.87-3.60)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.11                                                        | Depositor        |
| $R_{sym}$                                                               | 0.07                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.24 (at 3.56Å)                                             | Xtriage          |
| Refinement program                                                      | CNS 1.2                                                     | Depositor        |
| R, $R_{free}$                                                           | 0.297 , 0.308<br>0.296 , 0.303                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 1054 reflections (2.00%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 153.9                                                       | Xtriage          |
| Anisotropy                                                              | 0.105                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.28 , 83.1                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.90                                                        | EDS              |
| Total number of atoms                                                   | 24678                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 163.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, FE2, LMG, LMT, BCR, BCT, MES, PL9, CA, OEC, CLA, HEM, DGD, SQD, PHO

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     | 0.55         | 0/2713  | 1.06        | 19/3700 (0.5%)   |
| 2   | B     | 0.54         | 0/3947  | 1.03        | 26/5379 (0.5%)   |
| 3   | C     | 0.50         | 0/3567  | 1.00        | 13/4856 (0.3%)   |
| 4   | D     | 0.58         | 0/2801  | 1.01        | 12/3818 (0.3%)   |
| 5   | E     | 0.50         | 0/654   | 1.17        | 9/891 (1.0%)     |
| 6   | F     | 0.80         | 0/317   | 0.99        | 0/433            |
| 7   | H     | 0.48         | 0/520   | 0.93        | 2/709 (0.3%)     |
| 8   | I     | 0.54         | 0/293   | 1.08        | 2/395 (0.5%)     |
| 9   | J     | 0.48         | 0/255   | 1.17        | 2/346 (0.6%)     |
| 10  | K     | 0.50         | 0/303   | 0.96        | 1/416 (0.2%)     |
| 11  | L     | 0.50         | 0/311   | 1.02        | 1/422 (0.2%)     |
| 12  | M     | 0.54         | 0/270   | 0.91        | 0/367            |
| 13  | O     | 0.53         | 0/1876  | 1.03        | 13/2548 (0.5%)   |
| 14  | T     | 0.56         | 0/265   | 0.97        | 0/359            |
| 15  | U     | 0.55         | 0/785   | 1.10        | 6/1064 (0.6%)    |
| 16  | V     | 0.51         | 0/1081  | 0.95        | 4/1468 (0.3%)    |
| 17  | y     | 0.66         | 0/202   | 1.23        | 1/272 (0.4%)     |
| 18  | X     | 0.48         | 0/257   | 0.90        | 0/348            |
| 19  | Z     | 0.48         | 0/490   | 1.12        | 4/669 (0.6%)     |
| All | All   | 0.54         | 0/20907 | 1.03        | 115/28460 (0.4%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 1                   |

There are no bond length outliers.

All (115) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 19  | Z     | 34  | ASP  | N-CA-C | -9.30 | 101.71      | 113.43   |
| 17  | y     | 22  | LEU  | N-CA-C | -9.06 | 101.48      | 112.54   |
| 3   | C     | 182 | PHE  | N-CA-C | 8.82  | 123.87      | 113.20   |
| 13  | O     | 102 | THR  | N-CA-C | 8.79  | 120.94      | 111.36   |
| 5   | E     | 57  | ALA  | N-CA-C | -8.68 | 99.34       | 110.53   |
| 15  | U     | 51  | TYR  | N-CA-C | -8.63 | 97.72       | 110.23   |
| 3   | C     | 439 | VAL  | N-CA-C | -8.45 | 102.63      | 110.82   |
| 2   | B     | 483 | ASP  | CA-C-N | 8.38  | 130.31      | 119.84   |
| 2   | B     | 483 | ASP  | C-N-CA | 8.38  | 130.31      | 119.84   |
| 9   | J     | 36  | LEU  | N-CA-C | -8.34 | 103.24      | 113.41   |
| 15  | U     | 74  | THR  | N-CA-C | 8.15  | 119.86      | 110.97   |
| 3   | C     | 318 | LEU  | N-CA-C | -8.07 | 102.56      | 111.36   |
| 13  | O     | 103 | SER  | N-CA-C | 7.89  | 121.67      | 110.23   |
| 8   | I     | 2   | GLU  | N-CA-C | -7.63 | 103.42      | 112.89   |
| 5   | E     | 24  | SER  | N-CA-C | -7.57 | 103.30      | 112.54   |
| 2   | B     | 328 | GLY  | CA-C-N | 7.55  | 127.46      | 120.21   |
| 2   | B     | 328 | GLY  | C-N-CA | 7.55  | 127.46      | 120.21   |
| 5   | E     | 70  | PHE  | N-CA-C | 7.46  | 119.05      | 111.07   |
| 2   | B     | 327 | THR  | N-CA-C | 7.42  | 119.54      | 110.41   |
| 3   | C     | 347 | GLY  | N-CA-C | 7.33  | 123.41      | 114.69   |
| 4   | D     | 54  | PHE  | N-CA-C | 7.16  | 121.89      | 112.72   |
| 2   | B     | 236 | THR  | N-CA-C | -7.08 | 105.18      | 114.31   |
| 10  | K     | 38  | VAL  | N-CA-C | -6.99 | 103.70      | 110.42   |
| 4   | D     | 296 | TYR  | N-CA-C | 6.96  | 118.66      | 111.14   |
| 2   | B     | 363 | PHE  | N-CA-C | 6.87  | 119.89      | 108.96   |
| 9   | J     | 39  | SER  | N-CA-C | -6.86 | 104.01      | 114.16   |
| 3   | C     | 254 | THR  | N-CA-C | 6.82  | 117.58      | 108.38   |
| 4   | D     | 156 | VAL  | N-CA-C | 6.75  | 117.36      | 110.82   |
| 15  | U     | 72  | TYR  | N-CA-C | 6.71  | 124.64      | 109.81   |
| 5   | E     | 67  | THR  | N-CA-C | 6.62  | 122.17      | 113.30   |
| 19  | Z     | 37  | LYS  | N-CA-C | -6.60 | 104.95      | 112.87   |
| 13  | O     | 200 | LEU  | CA-C-N | 6.60  | 128.09      | 119.84   |
| 13  | O     | 200 | LEU  | C-N-CA | 6.60  | 128.09      | 119.84   |
| 1   | A     | 87  | ASN  | N-CA-C | -6.58 | 105.07      | 113.23   |
| 3   | C     | 37  | ALA  | N-CA-C | -6.56 | 103.38      | 112.30   |
| 15  | U     | 62  | ILE  | N-CA-C | 6.53  | 118.07      | 110.62   |
| 16  | V     | 104 | ASN  | CA-C-N | 6.43  | 126.19      | 119.76   |
| 16  | V     | 104 | ASN  | C-N-CA | 6.43  | 126.19      | 119.76   |
| 1   | A     | 36  | ILE  | N-CA-C | -6.42 | 106.29      | 111.81   |
| 4   | D     | 272 | LEU  | N-CA-C | -6.30 | 103.72      | 111.40   |
| 2   | B     | 37  | MET  | N-CA-C | -6.29 | 104.52      | 111.82   |
| 4   | D     | 142 | ASN  | N-CA-C | -6.27 | 105.46      | 113.23   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | B     | 381 | ILE  | CA-C-N  | 6.22  | 126.19      | 119.78   |
| 2   | B     | 381 | ILE  | C-N-CA  | 6.22  | 126.19      | 119.78   |
| 2   | B     | 332 | LYS  | N-CA-C  | -6.20 | 105.68      | 113.18   |
| 13  | O     | 40  | GLY  | N-CA-C  | -6.13 | 107.24      | 115.21   |
| 1   | A     | 142 | TRP  | N-CA-C  | 6.12  | 123.83      | 110.80   |
| 13  | O     | 249 | ASP  | N-CA-C  | -6.01 | 105.59      | 113.17   |
| 2   | B     | 484 | PRO  | N-CA-C  | 6.00  | 124.82      | 112.47   |
| 4   | D     | 147 | SER  | N-CA-C  | -5.94 | 104.89      | 111.36   |
| 4   | D     | 273 | PHE  | N-CA-C  | 5.92  | 118.24      | 111.02   |
| 1   | A     | 32  | TRP  | N-CA-C  | -5.91 | 104.42      | 111.69   |
| 13  | O     | 196 | SER  | N-CA-C  | 5.91  | 116.04      | 108.24   |
| 3   | C     | 32  | GLY  | N-CA-C  | -5.89 | 99.23       | 113.18   |
| 2   | B     | 163 | GLY  | CA-C-N  | 5.84  | 127.14      | 119.84   |
| 2   | B     | 163 | GLY  | C-N-CA  | 5.84  | 127.14      | 119.84   |
| 2   | B     | 174 | LEU  | N-CA-C  | -5.79 | 108.02      | 114.62   |
| 1   | A     | 78  | ILE  | N-CA-C  | 5.79  | 116.57      | 110.72   |
| 5   | E     | 8   | ARG  | CA-C-N  | 5.74  | 127.02      | 119.84   |
| 5   | E     | 8   | ARG  | C-N-CA  | 5.74  | 127.02      | 119.84   |
| 16  | V     | 75  | ASN  | CA-C-N  | 5.73  | 125.44      | 119.82   |
| 16  | V     | 75  | ASN  | C-N-CA  | 5.73  | 125.44      | 119.82   |
| 3   | C     | 224 | ILE  | CB-CA-C | -5.64 | 104.64      | 112.04   |
| 13  | O     | 128 | ASP  | N-CA-C  | 5.62  | 119.23      | 112.93   |
| 3   | C     | 302 | TYR  | N-CA-C  | -5.60 | 101.36      | 109.31   |
| 4   | D     | 297 | ASP  | N-CA-C  | 5.59  | 117.91      | 109.41   |
| 1   | A     | 261 | GLN  | N-CA-C  | 5.57  | 122.66      | 110.80   |
| 2   | B     | 80  | ILE  | N-CA-C  | 5.55  | 116.94      | 110.62   |
| 2   | B     | 49  | ASP  | CA-C-N  | 5.53  | 126.01      | 120.04   |
| 2   | B     | 49  | ASP  | C-N-CA  | 5.53  | 126.01      | 120.04   |
| 5   | E     | 26  | THR  | N-CA-C  | 5.51  | 116.97      | 111.07   |
| 5   | E     | 23  | HIS  | N-CA-C  | 5.50  | 119.25      | 112.54   |
| 7   | H     | 34  | PHE  | N-CA-C  | -5.50 | 105.28      | 111.28   |
| 1   | A     | 146 | ALA  | N-CA-C  | -5.50 | 105.37      | 111.36   |
| 1   | A     | 339 | PHE  | CA-C-N  | 5.49  | 126.71      | 119.84   |
| 1   | A     | 339 | PHE  | C-N-CA  | 5.49  | 126.71      | 119.84   |
| 1   | A     | 88  | ALA  | N-CA-C  | -5.49 | 105.45      | 111.82   |
| 4   | D     | 170 | ALA  | N-CA-C  | -5.46 | 103.04      | 110.36   |
| 5   | E     | 13  | ILE  | N-CA-C  | 5.42  | 115.62      | 110.42   |
| 7   | H     | 22  | ALA  | N-CA-C  | -5.41 | 102.28      | 110.39   |
| 4   | D     | 181 | PHE  | N-CA-C  | -5.40 | 105.48      | 111.36   |
| 2   | B     | 247 | PHE  | N-CA-C  | -5.39 | 105.31      | 111.14   |
| 1   | A     | 83  | VAL  | CA-C-N  | 5.37  | 125.31      | 119.78   |
| 1   | A     | 83  | VAL  | C-N-CA  | 5.37  | 125.31      | 119.78   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3   | C     | 228 | ASN  | N-CA-C | 5.37  | 119.61      | 112.30   |
| 2   | B     | 77  | GLY  | N-CA-C | 5.34  | 120.04      | 113.79   |
| 15  | U     | 70  | GLY  | N-CA-C | 5.34  | 122.16      | 114.10   |
| 8   | I     | 17  | LEU  | N-CA-C | -5.33 | 105.11      | 111.03   |
| 11  | L     | 36  | PHE  | N-CA-C | -5.32 | 106.29      | 112.89   |
| 13  | O     | 205 | GLU  | N-CA-C | 5.29  | 120.01      | 113.50   |
| 2   | B     | 19  | LEU  | N-CA-C | -5.28 | 105.20      | 111.69   |
| 1   | A     | 56  | PRO  | CA-C-N | 5.25  | 125.26      | 119.90   |
| 1   | A     | 56  | PRO  | C-N-CA | 5.25  | 125.26      | 119.90   |
| 3   | C     | 464 | GLU  | CA-C-N | 5.23  | 126.38      | 119.84   |
| 3   | C     | 464 | GLU  | C-N-CA | 5.23  | 126.38      | 119.84   |
| 19  | Z     | 35  | ARG  | N-CA-C | -5.21 | 105.67      | 112.23   |
| 3   | C     | 391 | ARG  | N-CA-C | -5.18 | 105.54      | 111.14   |
| 1   | A     | 33  | PHE  | N-CA-C | -5.17 | 105.82      | 111.82   |
| 2   | B     | 57  | ARG  | N-CA-C | -5.17 | 107.14      | 113.50   |
| 2   | B     | 237 | VAL  | N-CA-C | -5.17 | 104.59      | 111.05   |
| 13  | O     | 181 | ASN  | N-CA-C | 5.14  | 119.40      | 113.18   |
| 13  | O     | 194 | TYR  | N-CA-C | 5.14  | 117.75      | 110.50   |
| 2   | B     | 165 | GLY  | N-CA-C | -5.14 | 105.87      | 111.21   |
| 15  | U     | 75  | LEU  | N-CA-C | 5.12  | 116.67      | 111.14   |
| 2   | B     | 120 | LEU  | N-CA-C | -5.12 | 103.28      | 110.50   |
| 19  | Z     | 33  | TRP  | N-CA-C | -5.11 | 106.13      | 112.47   |
| 13  | O     | 81  | GLU  | CA-C-N | 5.09  | 124.75      | 119.56   |
| 13  | O     | 81  | GLU  | C-N-CA | 5.09  | 124.75      | 119.56   |
| 1   | A     | 266 | ASN  | N-CA-C | -5.07 | 107.03      | 114.39   |
| 2   | B     | 317 | ASN  | N-CA-C | -5.07 | 105.89      | 113.89   |
| 1   | A     | 296 | ASN  | N-CA-C | 5.05  | 118.70      | 112.24   |
| 1   | A     | 195 | HIS  | CA-C-N | 5.01  | 124.45      | 119.24   |
| 1   | A     | 195 | HIS  | C-N-CA | 5.01  | 124.45      | 119.24   |
| 4   | D     | 235 | PHE  | N-CA-C | 5.01  | 117.13      | 109.07   |
| 4   | D     | 299 | ILE  | N-CA-C | 5.00  | 115.72      | 110.62   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 161 | TYR  | Sidechain |



## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2628  | 0        | 2524     | 258     | 0            |
| 2   | B     | 3812  | 0        | 3683     | 274     | 0            |
| 3   | C     | 3455  | 0        | 3378     | 387     | 0            |
| 4   | D     | 2706  | 0        | 2608     | 244     | 0            |
| 5   | E     | 635   | 0        | 625      | 82      | 0            |
| 6   | F     | 307   | 0        | 312      | 52      | 0            |
| 7   | H     | 507   | 0        | 521      | 69      | 0            |
| 8   | I     | 286   | 0        | 308      | 25      | 0            |
| 9   | J     | 249   | 0        | 262      | 52      | 0            |
| 10  | K     | 293   | 0        | 305      | 63      | 0            |
| 11  | L     | 304   | 0        | 316      | 29      | 0            |
| 12  | M     | 267   | 0        | 289      | 34      | 0            |
| 13  | O     | 1845  | 0        | 1801     | 127     | 0            |
| 14  | T     | 256   | 0        | 262      | 26      | 0            |
| 15  | U     | 774   | 0        | 773      | 51      | 0            |
| 16  | V     | 1060  | 0        | 1068     | 51      | 0            |
| 17  | y     | 201   | 0        | 226      | 32      | 0            |
| 18  | X     | 254   | 0        | 282      | 30      | 0            |
| 19  | Z     | 479   | 0        | 516      | 69      | 0            |
| 20  | A     | 1     | 0        | 0        | 0       | 0            |
| 21  | A     | 260   | 0        | 288      | 48      | 0            |
| 21  | B     | 1040  | 0        | 1152     | 131     | 0            |
| 21  | C     | 780   | 0        | 864      | 134     | 0            |
| 21  | D     | 130   | 0        | 144      | 18      | 0            |
| 21  | K     | 65    | 0        | 72       | 12      | 0            |
| 22  | A     | 64    | 0        | 74       | 6       | 0            |
| 22  | D     | 64    | 0        | 74       | 15      | 0            |
| 23  | A     | 12    | 0        | 13       | 13      | 0            |
| 24  | A     | 5     | 0        | 0        | 0       | 0            |
| 25  | A     | 40    | 0        | 56       | 9       | 0            |
| 25  | B     | 120   | 0        | 168      | 8       | 0            |
| 25  | C     | 80    | 0        | 112      | 24      | 0            |
| 25  | D     | 40    | 0        | 56       | 8       | 0            |
| 25  | J     | 80    | 0        | 112      | 19      | 0            |
| 25  | X     | 40    | 0        | 56       | 5       | 0            |
| 25  | Z     | 40    | 0        | 56       | 5       | 0            |
| 26  | A     | 39    | 0        | 51       | 7       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 26  | C     | 37    | 0        | 44       | 5       | 0            |
| 27  | A     | 51    | 0        | 72       | 40      | 0            |
| 27  | B     | 49    | 0        | 68       | 6       | 0            |
| 27  | C     | 45    | 0        | 60       | 6       | 0            |
| 27  | D     | 94    | 0        | 127      | 36      | 0            |
| 27  | I     | 43    | 0        | 56       | 0       | 0            |
| 27  | J     | 48    | 0        | 66       | 4       | 0            |
| 27  | M     | 42    | 0        | 54       | 3       | 0            |
| 28  | A     | 52    | 0        | 62       | 1       | 0            |
| 28  | B     | 124   | 0        | 170      | 41      | 0            |
| 28  | C     | 237   | 0        | 311      | 77      | 0            |
| 28  | D     | 63    | 0        | 87       | 0       | 0            |
| 29  | A     | 35    | 0        | 46       | 0       | 0            |
| 29  | B     | 35    | 0        | 46       | 2       | 0            |
| 29  | D     | 66    | 0        | 81       | 3       | 0            |
| 29  | I     | 35    | 0        | 46       | 2       | 0            |
| 29  | O     | 35    | 0        | 46       | 1       | 0            |
| 29  | T     | 35    | 0        | 46       | 1       | 0            |
| 30  | C     | 51    | 0        | 68       | 5       | 0            |
| 30  | D     | 43    | 0        | 49       | 9       | 0            |
| 30  | F     | 45    | 0        | 53       | 0       | 0            |
| 30  | L     | 47    | 0        | 60       | 2       | 0            |
| 31  | D     | 4     | 0        | 0        | 0       | 0            |
| 32  | D     | 55    | 0        | 80       | 30      | 0            |
| 33  | F     | 43    | 0        | 30       | 6       | 0            |
| 33  | V     | 43    | 0        | 30       | 5       | 0            |
| 34  | F     | 1     | 0        | 0        | 0       | 0            |
| 34  | K     | 1     | 0        | 0        | 0       | 0            |
| 34  | O     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 24678 | 0        | 25265    | 1891    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 38.

All (1891) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 30:C:475:SQD:C3   | 30:C:475:SQD:C4  | 1.74                     | 1.58              |
| 16:V:63:CYS:SG    | 33:V:164:HEM:HAB | 1.65                     | 1.35              |
| 27:A:373:LMG:H112 | 4:D:266:TRP:CH2  | 1.77                     | 1.19              |
| 1:A:271:LEU:HD11  | 23:A:367:MES:C8  | 1.73                     | 1.17              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:B:533:DGD:HAH1 | 12:M:17:VAL:HG21  | 1.21                     | 1.14              |
| 2:B:121:GLU:HG2   | 7:H:4:ARG:HG2     | 1.25                     | 1.13              |
| 9:J:15:THR:HG21   | 10:K:38:VAL:HG13  | 1.18                     | 1.13              |
| 2:B:327:THR:HA    | 21:B:517:CLA:O1A  | 1.49                     | 1.12              |
| 15:U:83:ALA:HB1   | 15:U:84:PRO:HD2   | 1.23                     | 1.11              |
| 1:A:271:LEU:CD1   | 23:A:367:MES:H82  | 1.80                     | 1.11              |
| 3:C:174:LEU:HD22  | 21:C:478:CLA:H161 | 1.21                     | 1.10              |
| 10:K:10:LYS:O     | 10:K:10:LYS:HG2   | 1.44                     | 1.10              |
| 3:C:293:ASN:HA    | 28:C:491:DGD:O2E  | 1.53                     | 1.09              |
| 27:A:373:LMG:H332 | 12:M:22:LEU:HD21  | 1.27                     | 1.08              |
| 3:C:174:LEU:CD2   | 21:C:478:CLA:H161 | 1.84                     | 1.07              |
| 17:y:35:ILE:HG22  | 19:Z:21:ILE:HG23  | 1.37                     | 1.06              |
| 21:B:518:CLA:H42  | 4:D:127:LEU:HD11  | 1.07                     | 1.05              |
| 5:E:15:THR:HG22   | 9:J:7:ARG:CG      | 1.85                     | 1.05              |
| 3:C:473:ASP:HB2   | 14:T:26:PRO:HB3   | 1.31                     | 1.05              |
| 28:B:528:DGD:O1B  | 28:B:528:DGD:HG12 | 1.57                     | 1.04              |
| 1:A:129:ARG:HH21  | 4:D:256:ILE:HD12  | 1.20                     | 1.04              |
| 5:E:15:THR:CG2    | 9:J:7:ARG:HG2     | 1.86                     | 1.04              |
| 3:C:254:THR:HG22  | 3:C:255:THR:H     | 1.18                     | 1.04              |
| 13:O:178:ARG:HH11 | 13:O:178:ARG:HG3  | 1.18                     | 1.04              |
| 1:A:214:MET:HE2   | 1:A:214:MET:HA    | 1.40                     | 1.03              |
| 28:B:528:DGD:O2D  | 4:D:87:HIS:HB2    | 1.58                     | 1.03              |
| 27:D:360:LMG:O6   | 11:L:15:THR:HG21  | 1.62                     | 1.00              |
| 27:A:373:LMG:H112 | 4:D:266:TRP:HH2   | 0.85                     | 1.00              |
| 2:B:250:PHE:HD1   | 28:B:528:DGD:HB92 | 1.22                     | 1.00              |
| 2:B:149:LEU:HG    | 21:B:513:CLA:HBC1 | 1.41                     | 1.00              |
| 27:A:373:LMG:H372 | 12:M:18:PRO:CB    | 1.91                     | 0.98              |
| 1:A:317:TRP:CZ3   | 4:D:180:ARG:HD3   | 2.00                     | 0.96              |
| 27:A:373:LMG:C37  | 12:M:18:PRO:HB3   | 1.93                     | 0.96              |
| 27:A:373:LMG:H372 | 12:M:18:PRO:HB3   | 0.97                     | 0.96              |
| 13:O:69:LEU:HB3   | 13:O:107:ILE:HB   | 1.49                     | 0.95              |
| 13:O:230:VAL:HG12 | 13:O:231:ASP:H    | 1.30                     | 0.94              |
| 14:T:29:ILE:H     | 14:T:29:ILE:HD12  | 1.33                     | 0.94              |
| 3:C:286:ALA:HB2   | 21:C:478:CLA:HMD1 | 1.50                     | 0.93              |
| 15:U:83:ALA:HB1   | 15:U:84:PRO:CD    | 1.98                     | 0.93              |
| 25:C:489:BCR:H312 | 19:Z:9:LEU:HD11   | 1.51                     | 0.93              |
| 1:A:11:ALA:O      | 1:A:12:ASN:HB2    | 1.67                     | 0.93              |
| 27:A:373:LMG:C11  | 4:D:266:TRP:HH2   | 1.80                     | 0.92              |
| 2:B:332:LYS:HE3   | 28:B:533:DGD:O4D  | 1.68                     | 0.92              |
| 11:L:1:MET:HG2    | 11:L:1:MET:O      | 1.70                     | 0.92              |
| 3:C:407:VAL:HA    | 28:C:493:DGD:O2E  | 1.70                     | 0.91              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:B:517:CLA:H202 | 4:D:281:MET:SD    | 2.11                     | 0.91              |
| 4:D:186:GLN:HB2   | 21:D:354:CLA:HBC1 | 1.52                     | 0.91              |
| 3:C:225:VAL:HG21  | 28:C:491:DGD:HG11 | 1.52                     | 0.90              |
| 1:A:286:THR:HG23  | 21:A:362:CLA:HED3 | 1.50                     | 0.90              |
| 27:D:360:LMG:O7   | 11:L:19:LEU:HD21  | 1.71                     | 0.89              |
| 27:D:360:LMG:H212 | 14:T:17:PHE:HZ    | 1.36                     | 0.89              |
| 21:B:524:CLA:H18  | 28:B:533:DGD:HAS1 | 1.53                     | 0.89              |
| 5:E:15:THR:CG2    | 9:J:7:ARG:CG      | 2.48                     | 0.89              |
| 28:B:528:DGD:HO2D | 4:D:87:HIS:CG     | 1.90                     | 0.89              |
| 3:C:224:ILE:O     | 3:C:227:VAL:HG23  | 1.73                     | 0.89              |
| 2:B:414:PRO:HB2   | 2:B:415:PRO:HD3   | 1.55                     | 0.88              |
| 2:B:434:THR:HG23  | 13:O:204:LYS:HE3  | 1.54                     | 0.88              |
| 21:B:514:CLA:H11  | 21:B:522:CLA:H152 | 1.54                     | 0.88              |
| 1:A:214:MET:HE1   | 4:D:142:ASN:ND2   | 1.89                     | 0.88              |
| 7:H:35:MET:HE2    | 25:X:107:BCR:HC21 | 1.55                     | 0.88              |
| 28:C:493:DGD:HE62 | 9:J:40:LEU:HD21   | 1.54                     | 0.88              |
| 2:B:271:THR:HG22  | 2:B:273:TYR:H     | 1.39                     | 0.88              |
| 5:E:15:THR:HG21   | 9:J:7:ARG:HG2     | 1.56                     | 0.87              |
| 3:C:305:THR:HG22  | 3:C:308:GLU:H     | 1.40                     | 0.87              |
| 13:O:218:LEU:HD22 | 15:U:119:THR:HG21 | 1.57                     | 0.87              |
| 18:X:12:ILE:HG12  | 18:X:16:LEU:HD12  | 1.56                     | 0.87              |
| 13:O:69:LEU:HD12  | 13:O:70:CYS:H     | 1.39                     | 0.87              |
| 27:A:373:LMG:H231 | 27:D:360:LMG:H202 | 1.54                     | 0.87              |
| 4:D:23:LYS:HZ1    | 30:D:361:SQD:H462 | 1.38                     | 0.87              |
| 3:C:155:ASN:HD21  | 3:C:255:THR:HB    | 1.40                     | 0.87              |
| 28:B:528:DGD:HBE1 | 4:D:159:ILE:HG23  | 1.57                     | 0.87              |
| 1:A:193:LEU:HD11  | 21:A:362:CLA:HMC2 | 1.56                     | 0.86              |
| 3:C:447:ARG:HG2   | 3:C:447:ARG:HH11  | 1.40                     | 0.86              |
| 2:B:250:PHE:HD1   | 28:B:528:DGD:C9B  | 1.88                     | 0.86              |
| 16:V:30:THR:HB    | 16:V:31:PRO:HD2   | 1.54                     | 0.86              |
| 4:D:259:ILE:HG12  | 27:D:360:LMG:H301 | 1.57                     | 0.86              |
| 11:L:5:PRO:HA     | 11:L:7:ARG:HH22   | 1.40                     | 0.86              |
| 25:C:489:BCR:H353 | 25:J:112:BCR:H321 | 1.56                     | 0.85              |
| 13:O:178:ARG:HH11 | 13:O:178:ARG:CG   | 1.88                     | 0.85              |
| 4:D:129:GLN:NE2   | 4:D:143:ALA:HA    | 1.92                     | 0.85              |
| 21:B:513:CLA:HBB1 | 21:B:515:CLA:H171 | 1.59                     | 0.85              |
| 7:H:12:ARG:O      | 7:H:12:ARG:HD3    | 1.76                     | 0.85              |
| 11:L:8:GLN:N      | 11:L:8:GLN:HE21   | 1.75                     | 0.85              |
| 5:E:18:ARG:HD2    | 5:E:22:ILE:HD11   | 1.60                     | 0.84              |
| 15:U:72:TYR:HB3   | 15:U:73:PRO:HD3   | 1.57                     | 0.84              |
| 2:B:250:PHE:CD1   | 28:B:528:DGD:HB92 | 2.12                     | 0.84              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:J:11:TRP:CH2    | 17:y:36:ILE:HD11  | 2.12                     | 0.84              |
| 3:C:305:THR:HG23  | 3:C:307:PRO:HD2   | 1.60                     | 0.83              |
| 1:A:39:PRO:HG3    | 25:A:369:BCR:HC8  | 1.58                     | 0.83              |
| 28:B:533:DGD:HG31 | 12:M:6:LEU:HD12   | 1.59                     | 0.83              |
| 1:A:317:TRP:HZ3   | 4:D:180:ARG:HD3   | 1.39                     | 0.83              |
| 2:B:124:ARG:HE    | 2:B:131:PRO:HD3   | 1.43                     | 0.83              |
| 27:D:360:LMG:H221 | 14:T:13:ILE:HG21  | 1.60                     | 0.83              |
| 3:C:166:ILE:HG23  | 3:C:245:ILE:HG23  | 1.61                     | 0.83              |
| 21:C:478:CLA:H12  | 21:C:479:CLA:H42  | 1.61                     | 0.82              |
| 28:B:528:DGD:O2D  | 4:D:87:HIS:CB     | 2.27                     | 0.82              |
| 7:H:31:MET:HE3    | 7:H:35:MET:HE1    | 1.62                     | 0.82              |
| 1:A:214:MET:HB3   | 23:A:367:MES:H61  | 1.59                     | 0.82              |
| 4:D:135:LEU:HD23  | 30:D:361:SQD:O2   | 1.78                     | 0.82              |
| 21:B:518:CLA:CBB  | 4:D:123:ILE:HG12  | 2.10                     | 0.81              |
| 1:A:192:ILE:HA    | 1:A:293:MET:HE1   | 1.61                     | 0.81              |
| 3:C:407:VAL:HG22  | 28:C:493:DGD:O2E  | 1.81                     | 0.81              |
| 3:C:28:GLN:OE1    | 3:C:28:GLN:HA     | 1.78                     | 0.81              |
| 27:D:360:LMG:H341 | 14:T:21:ILE:HD11  | 1.62                     | 0.81              |
| 2:B:247:PHE:HE1   | 21:B:512:CLA:H8   | 1.46                     | 0.81              |
| 3:C:254:THR:HG22  | 3:C:255:THR:N     | 1.96                     | 0.81              |
| 4:D:23:LYS:NZ     | 30:D:361:SQD:H462 | 1.97                     | 0.80              |
| 4:D:148:ALA:HB3   | 4:D:149:PRO:HD3   | 1.63                     | 0.80              |
| 17:y:39:LEU:HB3   | 17:y:46:LEU:HD21  | 1.64                     | 0.80              |
| 4:D:323:GLU:HG2   | 13:O:194:TYR:OH   | 1.81                     | 0.80              |
| 5:E:84:LYS:HB2    | 5:E:84:LYS:NZ     | 1.97                     | 0.80              |
| 3:C:135:ARG:HE    | 19:Z:33:TRP:NE1   | 1.80                     | 0.80              |
| 27:A:373:LMG:C20  | 32:D:357:PL9:H212 | 2.13                     | 0.79              |
| 25:C:489:BCR:HC22 | 10:K:18:PHE:HD1   | 1.46                     | 0.79              |
| 1:A:214:MET:HE1   | 4:D:142:ASN:HD21  | 1.45                     | 0.79              |
| 3:C:473:ASP:HB2   | 14:T:26:PRO:CB    | 2.11                     | 0.79              |
| 30:C:475:SQD:C3   | 30:C:475:SQD:C5   | 2.60                     | 0.79              |
| 28:B:533:DGD:HAH1 | 12:M:17:VAL:CG2   | 2.08                     | 0.79              |
| 10:K:10:LYS:O     | 10:K:10:LYS:CG    | 2.30                     | 0.78              |
| 13:O:230:VAL:HG12 | 13:O:231:ASP:N    | 1.98                     | 0.78              |
| 2:B:434:THR:CG2   | 13:O:204:LYS:HE3  | 2.12                     | 0.78              |
| 21:C:484:CLA:H141 | 21:K:483:CLA:H162 | 1.64                     | 0.78              |
| 19:Z:32:ASP:CG    | 19:Z:33:TRP:H     | 1.90                     | 0.78              |
| 2:B:483:ASP:CG    | 2:B:484:PRO:HD2   | 2.07                     | 0.78              |
| 3:C:437:PHE:HA    | 21:C:484:CLA:HMC2 | 1.66                     | 0.78              |
| 1:A:190:HIS:HB3   | 1:A:293:MET:HE2   | 1.64                     | 0.78              |
| 19:Z:36:SER:HA    | 19:Z:39:LEU:HG    | 1.64                     | 0.78              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:215:HIS:HA    | 23:A:367:MES:H51  | 1.63                     | 0.78              |
| 2:B:383:PHE:O     | 13:O:192:SER:HA   | 1.84                     | 0.78              |
| 3:C:110:PRO:HG3   | 27:C:494:LMG:H141 | 1.65                     | 0.78              |
| 21:C:480:CLA:H143 | 21:C:484:CLA:H152 | 1.66                     | 0.77              |
| 2:B:348:ASN:HB3   | 2:B:354:LEU:HD21  | 1.65                     | 0.77              |
| 1:A:218:LEU:HD22  | 23:A:367:MES:H52  | 1.66                     | 0.77              |
| 3:C:233:VAL:HA    | 25:C:490:BCR:H281 | 1.65                     | 0.77              |
| 4:D:152:VAL:HG11  | 21:D:354:CLA:H11  | 1.67                     | 0.77              |
| 13:O:31:LEU:HB2   | 13:O:36:ILE:HD11  | 1.67                     | 0.77              |
| 1:A:271:LEU:HD21  | 23:A:367:MES:HN4  | 1.50                     | 0.77              |
| 27:D:360:LMG:H201 | 11:L:22:LEU:HD11  | 1.66                     | 0.77              |
| 17:y:34:MET:HE1   | 17:y:38:LEU:HD21  | 1.65                     | 0.77              |
| 27:A:373:LMG:H332 | 12:M:22:LEU:CD2   | 2.12                     | 0.77              |
| 3:C:284:PHE:HB3   | 28:C:491:DGD:HA52 | 1.66                     | 0.77              |
| 3:C:135:ARG:HE    | 19:Z:33:TRP:HE1   | 1.30                     | 0.76              |
| 3:C:315:MET:HE1   | 3:C:369:LEU:HD12  | 1.66                     | 0.76              |
| 2:B:134:ASP:OD2   | 2:B:137:LYS:HE3   | 1.86                     | 0.76              |
| 1:A:131:TRP:CH2   | 21:C:481:CLA:HBA2 | 2.20                     | 0.76              |
| 4:D:192:THR:HG23  | 21:D:354:CLA:HBC2 | 1.68                     | 0.76              |
| 1:A:214:MET:HE3   | 22:D:355:PHO:HMD2 | 1.68                     | 0.76              |
| 5:E:35:TRP:CD2    | 6:F:39:ALA:HB2    | 2.20                     | 0.76              |
| 2:B:271:THR:HG22  | 2:B:273:TYR:N     | 1.98                     | 0.76              |
| 3:C:209:ILE:HG23  | 25:C:490:BCR:H382 | 1.65                     | 0.76              |
| 19:Z:49:ALA:O     | 19:Z:53:VAL:HG23  | 1.86                     | 0.76              |
| 11:L:5:PRO:HA     | 11:L:7:ARG:NH2    | 2.00                     | 0.75              |
| 1:A:46:ILE:HD13   | 28:A:375:DGD:HBE2 | 1.68                     | 0.75              |
| 1:A:93:PHE:CZ     | 21:A:366:CLA:HBA1 | 2.20                     | 0.75              |
| 3:C:473:ASP:CB    | 14:T:26:PRO:HB3   | 2.14                     | 0.75              |
| 30:C:475:SQD:H251 | 26:C:476:LHG:H102 | 1.66                     | 0.75              |
| 1:A:258:LEU:HD12  | 4:D:128:ARG:HD3   | 1.66                     | 0.75              |
| 3:C:391:ARG:NH1   | 3:C:391:ARG:HB2   | 2.02                     | 0.75              |
| 21:C:477:CLA:HMB2 | 25:C:490:BCR:H403 | 1.67                     | 0.75              |
| 1:A:57:PRO:HG3    | 1:A:68:SER:HB3    | 1.67                     | 0.75              |
| 8:I:4:LEU:HD22    | 29:I:274:LMT:H52  | 1.69                     | 0.75              |
| 4:D:279:LEU:HG    | 22:D:355:PHO:HBC3 | 1.67                     | 0.75              |
| 6:F:28:VAL:HB     | 6:F:29:PRO:HD3    | 1.68                     | 0.75              |
| 13:O:35:ASP:C     | 13:O:36:ILE:HD12  | 2.12                     | 0.74              |
| 21:B:523:CLA:HED3 | 21:B:523:CLA:H2   | 1.68                     | 0.74              |
| 16:V:63:CYS:SG    | 33:V:164:HEM:CAB  | 2.61                     | 0.74              |
| 21:B:518:CLA:H42  | 4:D:127:LEU:CD1   | 2.03                     | 0.74              |
| 18:X:12:ILE:O     | 18:X:12:ILE:HG23  | 1.85                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:214:MET:CB    | 23:A:367:MES:H61  | 2.16                     | 0.74              |
| 27:A:373:LMG:H192 | 32:D:357:PL9:H221 | 1.69                     | 0.74              |
| 3:C:135:ARG:NE    | 19:Z:33:TRP:HE1   | 1.85                     | 0.74              |
| 3:C:223:TRP:CZ2   | 28:C:474:DGD:HA62 | 2.23                     | 0.74              |
| 2:B:483:ASP:CB    | 2:B:484:PRO:HD2   | 2.17                     | 0.74              |
| 19:Z:32:ASP:HB2   | 19:Z:35:ARG:HG2   | 1.67                     | 0.74              |
| 4:D:244:TYR:OH    | 4:D:264:LYS:HE3   | 1.88                     | 0.74              |
| 5:E:18:ARG:HB3    | 5:E:18:ARG:HH11   | 1.52                     | 0.74              |
| 27:A:373:LMG:C33  | 12:M:22:LEU:HD21  | 2.14                     | 0.74              |
| 16:V:31:PRO:HA    | 16:V:34:LEU:HD12  | 1.68                     | 0.74              |
| 3:C:418:ASN:HB2   | 28:C:493:DGD:O4E  | 1.88                     | 0.73              |
| 2:B:234:ILE:HD11  | 21:B:520:CLA:H191 | 1.70                     | 0.73              |
| 3:C:29:GLU:HB3    | 10:K:46:ARG:NH1   | 2.03                     | 0.73              |
| 3:C:135:ARG:HB2   | 19:Z:27:TYR:HB3   | 1.69                     | 0.73              |
| 3:C:155:ASN:HA    | 3:C:158:THR:HG22  | 1.69                     | 0.73              |
| 4:D:41:ALA:HB2    | 22:D:355:PHO:H43  | 1.70                     | 0.73              |
| 21:B:518:CLA:H102 | 21:B:518:CLA:H142 | 1.69                     | 0.73              |
| 5:E:81:GLU:C      | 5:E:83:LEU:H      | 1.96                     | 0.73              |
| 10:K:21:LEU:HD13  | 17:y:24:MET:HE2   | 1.70                     | 0.73              |
| 1:A:214:MET:HA    | 1:A:214:MET:CE    | 2.17                     | 0.73              |
| 1:A:41:LEU:O      | 1:A:45:THR:HG22   | 1.89                     | 0.73              |
| 5:E:15:THR:HG22   | 9:J:7:ARG:HG3     | 1.71                     | 0.73              |
| 30:C:475:SQD:C4   | 30:C:475:SQD:C2   | 2.66                     | 0.73              |
| 18:X:34:PHE:O     | 18:X:38:ILE:HG12  | 1.88                     | 0.73              |
| 1:A:42:LEU:HD12   | 25:A:369:BCR:C11  | 2.18                     | 0.73              |
| 3:C:85:GLY:O      | 21:C:480:CLA:HED1 | 1.89                     | 0.73              |
| 3:C:241:GLY:O     | 3:C:245:ILE:HG13  | 1.88                     | 0.73              |
| 4:D:60:THR:HG23   | 4:D:61:HIS:CD2    | 2.23                     | 0.73              |
| 5:E:17:VAL:O      | 5:E:21:VAL:HG23   | 1.88                     | 0.73              |
| 4:D:85:MET:HE1    | 5:E:69:ARG:HA     | 1.71                     | 0.72              |
| 27:A:373:LMG:H202 | 32:D:357:PL9:H212 | 1.70                     | 0.72              |
| 3:C:225:VAL:CG2   | 28:C:491:DGD:HG11 | 2.20                     | 0.72              |
| 1:A:35:VAL:HA     | 25:A:369:BCR:H333 | 1.70                     | 0.72              |
| 3:C:407:VAL:HA    | 28:C:493:DGD:HO2E | 1.52                     | 0.72              |
| 3:C:168:LEU:HD13  | 21:C:483:CLA:H43  | 1.71                     | 0.72              |
| 4:D:148:ALA:HB2   | 4:D:276:VAL:HG13  | 1.70                     | 0.72              |
| 2:B:27:THR:HG22   | 2:B:107:LEU:HD13  | 1.72                     | 0.72              |
| 2:B:124:ARG:HH11  | 2:B:124:ARG:HG3   | 1.55                     | 0.72              |
| 3:C:305:THR:CG2   | 3:C:308:GLU:H     | 2.02                     | 0.72              |
| 7:H:63:LYS:C      | 7:H:65:LEU:H      | 1.98                     | 0.72              |
| 3:C:240:ILE:O     | 3:C:244:CYS:HB2   | 1.88                     | 0.72              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:254:THR:CG2   | 3:C:255:THR:H     | 2.00                     | 0.72              |
| 3:C:415:ASN:O     | 3:C:416:SER:HB3   | 1.89                     | 0.72              |
| 25:C:489:BCR:H11C | 25:J:112:BCR:H322 | 1.69                     | 0.71              |
| 3:C:91:HIS:CD2    | 21:C:478:CLA:HBA1 | 2.25                     | 0.71              |
| 21:B:511:CLA:H152 | 21:B:511:CLA:HMD2 | 1.72                     | 0.71              |
| 3:C:404:LEU:HG    | 28:C:493:DGD:O1A  | 1.90                     | 0.71              |
| 27:D:360:LMG:H192 | 11:L:22:LEU:HD21  | 1.71                     | 0.71              |
| 2:B:68:ARG:NH1    | 2:B:262:THR:HG23  | 2.04                     | 0.71              |
| 2:B:135:LEU:HD23  | 2:B:138:MET:HE3   | 1.71                     | 0.71              |
| 2:B:327:THR:CA    | 21:B:517:CLA:O1A  | 2.36                     | 0.71              |
| 13:O:206:GLU:CD   | 13:O:206:GLU:H    | 1.97                     | 0.71              |
| 1:A:40:THR:HG21   | 1:A:121:LEU:HD23  | 1.73                     | 0.71              |
| 21:A:366:CLA:HMC2 | 25:A:369:BCR:H12C | 1.72                     | 0.71              |
| 21:B:513:CLA:H161 | 7:H:38:PHE:HE2    | 1.54                     | 0.71              |
| 13:O:92:VAL:CG1   | 13:O:93:PRO:HD2   | 2.19                     | 0.71              |
| 3:C:391:ARG:HB2   | 3:C:391:ARG:HH11  | 1.56                     | 0.71              |
| 1:A:93:PHE:HZ     | 21:A:366:CLA:HBA1 | 1.54                     | 0.71              |
| 2:B:250:PHE:CD1   | 28:B:528:DGD:C9B  | 2.72                     | 0.71              |
| 4:D:44:ALA:HB3    | 22:D:355:PHO:H92  | 1.72                     | 0.71              |
| 4:D:129:GLN:HE22  | 4:D:143:ALA:HA    | 1.55                     | 0.71              |
| 1:A:22:THR:HG21   | 8:I:30:ARG:HD3    | 1.72                     | 0.71              |
| 3:C:348:GLU:OE2   | 13:O:37:VAL:HA    | 1.91                     | 0.70              |
| 3:C:187:ASP:HB2   | 3:C:230:LEU:HD12  | 1.74                     | 0.70              |
| 1:A:129:ARG:NH2   | 4:D:256:ILE:HD12  | 2.02                     | 0.70              |
| 3:C:116:VAL:HG12  | 25:C:489:BCR:H332 | 1.72                     | 0.70              |
| 2:B:224:ARG:HG2   | 7:H:24:GLY:O      | 1.91                     | 0.70              |
| 13:O:33:TYR:O     | 13:O:37:VAL:HG23  | 1.92                     | 0.70              |
| 13:O:77:LEU:HD23  | 13:O:93:PRO:HA    | 1.74                     | 0.70              |
| 13:O:69:LEU:HD12  | 13:O:70:CYS:N     | 2.05                     | 0.70              |
| 1:A:93:PHE:CD2    | 1:A:95:PRO:HD3    | 2.26                     | 0.70              |
| 1:A:328:MET:HE1   | 4:D:183:LEU:HD22  | 1.73                     | 0.70              |
| 2:B:222:PRO:HG3   | 7:H:27:THR:H      | 1.57                     | 0.70              |
| 1:A:332:HIS:CD2   | 1:A:333:GLU:HG3   | 2.27                     | 0.70              |
| 2:B:135:LEU:HA    | 2:B:138:MET:HE3   | 1.74                     | 0.70              |
| 3:C:52:ALA:HA     | 21:C:486:CLA:HMB3 | 1.73                     | 0.70              |
| 16:V:115:ALA:CB   | 16:V:122:ARG:HD2  | 2.22                     | 0.70              |
| 3:C:219:GLY:HA2   | 28:C:491:DGD:O3D  | 1.92                     | 0.70              |
| 4:D:55:VAL:HG21   | 4:D:110:LEU:HD12  | 1.74                     | 0.70              |
| 28:B:533:DGD:CDA  | 12:M:17:VAL:HG21  | 2.12                     | 0.69              |
| 4:D:88:SER:HB2    | 5:E:69:ARG:NH2    | 2.06                     | 0.69              |
| 3:C:54:VAL:HG13   | 21:C:487:CLA:HED1 | 1.74                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:259:ILE:HG12  | 27:D:360:LMG:C30  | 2.21                     | 0.69              |
| 15:U:38:GLU:HG2   | 15:U:39:LEU:N     | 2.05                     | 0.69              |
| 2:B:65:PHE:O      | 21:B:515:CLA:HBA1 | 1.92                     | 0.69              |
| 21:B:521:CLA:H193 | 21:B:523:CLA:H92  | 1.74                     | 0.69              |
| 2:B:137:LYS:HD2   | 7:H:14:LEU:O      | 1.93                     | 0.69              |
| 2:B:284:ILE:HG12  | 2:B:309:LEU:CD1   | 2.22                     | 0.69              |
| 4:D:39:PRO:O      | 4:D:43:LEU:HD22   | 1.93                     | 0.69              |
| 21:B:513:CLA:H161 | 7:H:38:PHE:CE2    | 2.28                     | 0.69              |
| 3:C:404:LEU:HD21  | 28:C:493:DGD:HA31 | 1.73                     | 0.69              |
| 7:H:6:TRP:CE2     | 7:H:10:ILE:HD11   | 2.27                     | 0.69              |
| 1:A:119:PHE:HZ    | 21:A:362:CLA:H101 | 1.58                     | 0.69              |
| 2:B:4:PRO:HD2     | 2:B:7:ARG:HD2     | 1.74                     | 0.69              |
| 3:C:284:PHE:CB    | 28:C:491:DGD:HA52 | 2.23                     | 0.69              |
| 21:C:478:CLA:O1A  | 21:C:479:CLA:H11  | 1.92                     | 0.69              |
| 4:D:41:ALA:CB     | 22:D:355:PHO:H43  | 2.23                     | 0.69              |
| 9:J:22:ILE:HG21   | 27:J:492:LMG:H202 | 1.75                     | 0.69              |
| 19:Z:30:PRO:HG3   | 19:Z:33:TRP:HZ3   | 1.58                     | 0.69              |
| 2:B:222:PRO:HG3   | 7:H:26:GLY:HA3    | 1.74                     | 0.69              |
| 3:C:60:ILE:HG21   | 21:C:479:CLA:H191 | 1.75                     | 0.69              |
| 3:C:158:THR:O     | 3:C:251:HIS:HB3   | 1.92                     | 0.69              |
| 27:J:492:LMG:O8   | 27:J:492:LMG:O9   | 2.11                     | 0.69              |
| 19:Z:28:ALA:O     | 19:Z:30:PRO:HD3   | 1.93                     | 0.69              |
| 3:C:68:THR:OG1    | 21:C:479:CLA:HED1 | 1.92                     | 0.69              |
| 1:A:77:ILE:HD11   | 14:T:6:TYR:HB3    | 1.76                     | 0.68              |
| 2:B:264:PRO:HG2   | 2:B:267:LEU:HD12  | 1.75                     | 0.68              |
| 21:B:524:CLA:OBD  | 11:L:10:VAL:HG21  | 1.93                     | 0.68              |
| 5:E:81:GLU:O      | 5:E:83:LEU:N      | 2.24                     | 0.68              |
| 3:C:130:VAL:HG13  | 21:C:486:CLA:H92  | 1.74                     | 0.68              |
| 4:D:152:VAL:HG21  | 4:D:279:LEU:HD12  | 1.72                     | 0.68              |
| 19:Z:32:ASP:HB3   | 19:Z:35:ARG:NH1   | 2.07                     | 0.68              |
| 1:A:121:LEU:HD21  | 21:A:366:CLA:HMB3 | 1.75                     | 0.68              |
| 21:B:521:CLA:H52  | 21:B:524:CLA:HBC3 | 1.74                     | 0.68              |
| 27:A:373:LMG:HC92 | 2:B:5:TRP:HE1     | 1.59                     | 0.68              |
| 28:C:493:DGD:HD3  | 9:J:32:ALA:O      | 1.93                     | 0.68              |
| 25:D:358:BCR:H403 | 9:J:25:VAL:HG21   | 1.75                     | 0.68              |
| 2:B:188:ASP:HA    | 7:H:58:VAL:HG23   | 1.76                     | 0.68              |
| 16:V:29:LEU:HD13  | 16:V:151:ILE:HD11 | 1.75                     | 0.68              |
| 3:C:166:ILE:O     | 3:C:170:ILE:HG13  | 1.94                     | 0.68              |
| 10:K:19:ASP:N     | 10:K:20:PRO:HD2   | 2.09                     | 0.68              |
| 1:A:192:ILE:CA    | 1:A:293:MET:HE1   | 2.23                     | 0.68              |
| 2:B:270:PRO:HG3   | 2:B:312:TYR:HD2   | 1.59                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:405:ASN:HA    | 28:C:493:DGD:HG12 | 1.75                     | 0.68              |
| 2:B:471:ALA:HB2   | 4:D:130:PHE:CZ    | 2.29                     | 0.68              |
| 10:K:21:LEU:CD1   | 17:y:24:MET:HE2   | 2.24                     | 0.68              |
| 1:A:271:LEU:HD11  | 23:A:367:MES:H82  | 0.83                     | 0.68              |
| 1:A:307:ILE:HG13  | 6:F:45:ARG:HD2    | 1.76                     | 0.68              |
| 2:B:133:LEU:HB3   | 2:B:138:MET:CE    | 2.24                     | 0.68              |
| 2:B:328:GLY:O     | 21:B:517:CLA:HBA1 | 1.94                     | 0.67              |
| 2:B:332:LYS:HE3   | 28:B:533:DGD:C4D  | 2.24                     | 0.67              |
| 2:B:464:PHE:HD2   | 21:B:521:CLA:HAC2 | 1.58                     | 0.67              |
| 4:D:152:VAL:CG1   | 21:D:354:CLA:H11  | 2.24                     | 0.67              |
| 6:F:18:VAL:HG13   | 6:F:19:ARG:H      | 1.59                     | 0.67              |
| 3:C:30:SER:HB2    | 10:K:46:ARG:O     | 1.94                     | 0.67              |
| 3:C:472:LEU:HD12  | 3:C:473:ASP:H     | 1.59                     | 0.67              |
| 3:C:113:VAL:HG12  | 27:C:494:LMG:H192 | 1.76                     | 0.67              |
| 4:D:27:PHE:CD2    | 6:F:19:ARG:HD3    | 2.29                     | 0.67              |
| 5:E:78:THR:O      | 5:E:81:GLU:HB2    | 1.94                     | 0.67              |
| 1:A:39:PRO:HB2    | 21:A:366:CLA:HBB1 | 1.75                     | 0.67              |
| 1:A:183:MET:HG2   | 21:A:363:CLA:HBC1 | 1.77                     | 0.67              |
| 3:C:75:PHE:HD1    | 3:C:86:LEU:HD21   | 1.59                     | 0.67              |
| 28:B:533:DGD:HA81 | 12:M:14:PHE:HA    | 1.75                     | 0.67              |
| 3:C:215:LYS:HB3   | 3:C:223:TRP:HA    | 1.77                     | 0.67              |
| 4:D:87:HIS:HD2    | 4:D:162:LEU:HD23  | 1.58                     | 0.67              |
| 4:D:180:ARG:HH11  | 4:D:180:ARG:CG    | 2.08                     | 0.67              |
| 2:B:135:LEU:HD23  | 2:B:138:MET:CE    | 2.25                     | 0.67              |
| 2:B:462:PHE:HA    | 21:B:521:CLA:HMC2 | 1.75                     | 0.67              |
| 21:C:479:CLA:H171 | 21:K:483:CLA:HBB2 | 1.77                     | 0.67              |
| 28:C:492:DGD:O3D  | 25:J:115:BCR:H382 | 1.94                     | 0.67              |
| 1:A:45:THR:HB     | 22:A:365:PHO:H8   | 1.77                     | 0.67              |
| 1:A:278:TRP:HA    | 28:C:493:DGD:HAG1 | 1.76                     | 0.67              |
| 3:C:161:LEU:HG    | 3:C:165:LEU:HD12  | 1.78                     | 0.67              |
| 1:A:129:ARG:NH2   | 4:D:256:ILE:HA    | 2.08                     | 0.66              |
| 2:B:356:VAL:HG22  | 2:B:370:LEU:CD2   | 2.26                     | 0.66              |
| 25:C:489:BCR:HC22 | 10:K:18:PHE:CD1   | 2.31                     | 0.66              |
| 5:E:84:LYS:HB2    | 5:E:84:LYS:HZ2    | 1.60                     | 0.66              |
| 2:B:483:ASP:OD2   | 2:B:484:PRO:HD2   | 1.94                     | 0.66              |
| 3:C:150:ASP:HB3   | 3:C:153:ASP:HB2   | 1.77                     | 0.66              |
| 3:C:155:ASN:HD21  | 3:C:255:THR:CB    | 2.07                     | 0.66              |
| 3:C:377:LEU:O     | 3:C:381:LYS:HB2   | 1.95                     | 0.66              |
| 28:C:493:DGD:HBF1 | 27:D:359:LMG:H211 | 1.77                     | 0.66              |
| 2:B:62:VAL:CG1    | 21:B:515:CLA:HED3 | 2.26                     | 0.66              |
| 3:C:305:THR:HG22  | 3:C:308:GLU:CB    | 2.26                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:Z:33:TRP:O     | 19:Z:33:TRP:CD1   | 2.48                     | 0.66              |
| 1:A:161:TYR:HB3   | 1:A:162:PRO:HD3   | 1.77                     | 0.66              |
| 4:D:267:LEU:HD23  | 4:D:267:LEU:C     | 2.20                     | 0.66              |
| 9:J:11:TRP:CZ3    | 17:y:36:ILE:HD11  | 2.31                     | 0.66              |
| 27:A:373:LMG:C11  | 4:D:266:TRP:CH2   | 2.66                     | 0.66              |
| 2:B:271:THR:CG2   | 2:B:273:TYR:H     | 2.08                     | 0.66              |
| 3:C:44:ASN:C      | 3:C:45:LEU:HD12   | 2.20                     | 0.66              |
| 5:E:15:THR:HG22   | 9:J:7:ARG:CB      | 2.25                     | 0.66              |
| 19:Z:33:TRP:O     | 19:Z:37:LYS:HB2   | 1.95                     | 0.66              |
| 1:A:119:PHE:CZ    | 21:A:362:CLA:H101 | 2.30                     | 0.66              |
| 28:C:492:DGD:HB52 | 25:J:115:BCR:H352 | 1.78                     | 0.66              |
| 4:D:209:LEU:HD23  | 4:D:209:LEU:C     | 2.22                     | 0.65              |
| 2:B:385:ARG:HD3   | 13:O:191:ALA:O    | 1.96                     | 0.65              |
| 3:C:437:PHE:HZ    | 21:K:483:CLA:HMB3 | 1.62                     | 0.65              |
| 4:D:192:THR:CG2   | 21:D:354:CLA:HBC2 | 2.26                     | 0.65              |
| 4:D:250:ASN:HD22  | 4:D:262:SER:HB3   | 1.62                     | 0.65              |
| 2:B:271:THR:HB    | 2:B:274:GLN:HG3   | 1.78                     | 0.65              |
| 27:D:360:LMG:O9   | 27:D:360:LMG:C7   | 2.43                     | 0.65              |
| 3:C:437:PHE:HA    | 21:C:484:CLA:CMC  | 2.26                     | 0.65              |
| 21:C:486:CLA:H151 | 19:Z:24:PRO:HG3   | 1.79                     | 0.65              |
| 21:B:517:CLA:H141 | 21:B:517:CLA:H172 | 1.79                     | 0.65              |
| 3:C:453:ALA:O     | 8:I:34:ARG:HB2    | 1.97                     | 0.65              |
| 3:C:165:LEU:HD21  | 21:C:482:CLA:HHC  | 1.78                     | 0.65              |
| 3:C:220:GLY:N     | 28:C:491:DGD:O3D  | 2.29                     | 0.65              |
| 13:O:92:VAL:HG12  | 13:O:93:PRO:HD2   | 1.78                     | 0.65              |
| 15:U:83:ALA:CB    | 15:U:84:PRO:HD2   | 2.14                     | 0.65              |
| 2:B:86:ILE:HD12   | 2:B:86:ILE:O      | 1.97                     | 0.65              |
| 1:A:64:ARG:NH1    | 13:O:98:THR:HG21  | 2.12                     | 0.65              |
| 3:C:89:ILE:N      | 3:C:90:PRO:HD2    | 2.11                     | 0.65              |
| 21:B:513:CLA:H3A  | 21:B:513:CLA:O2A  | 1.97                     | 0.64              |
| 16:V:143:GLY:O    | 16:V:147:VAL:HG23 | 1.97                     | 0.64              |
| 2:B:135:LEU:HB2   | 2:B:136:PRO:HD3   | 1.79                     | 0.64              |
| 2:B:442:ILE:HD11  | 13:O:200:LEU:HD23 | 1.76                     | 0.64              |
| 32:D:357:PL9:H262 | 32:D:357:PL9:C30  | 2.27                     | 0.64              |
| 3:C:141:GLU:CD    | 3:C:141:GLU:H     | 2.05                     | 0.64              |
| 3:C:437:PHE:CZ    | 21:K:483:CLA:HMB3 | 2.33                     | 0.64              |
| 21:D:356:CLA:H42  | 18:X:26:GLY:HA3   | 1.79                     | 0.64              |
| 2:B:7:ARG:HA      | 21:B:521:CLA:HBA1 | 1.78                     | 0.64              |
| 2:B:139:PHE:CZ    | 2:B:143:LEU:HD22  | 2.32                     | 0.64              |
| 1:A:81:ALA:HB2    | 1:A:175:GLY:HA3   | 1.78                     | 0.64              |
| 2:B:250:PHE:HB3   | 28:B:528:DGD:HB82 | 1.78                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:L:7:ARG:O      | 11:L:7:ARG:HD2    | 1.97                     | 0.64              |
| 2:B:331:ASN:HB3   | 2:B:437:LEU:HD12  | 1.79                     | 0.64              |
| 21:C:483:CLA:OBD  | 21:C:485:CLA:H152 | 1.96                     | 0.64              |
| 2:B:286:ARG:HG2   | 2:B:286:ARG:HH11  | 1.63                     | 0.64              |
| 13:O:120:THR:HG22 | 13:O:154:SER:OG   | 1.96                     | 0.64              |
| 13:O:144:LEU:HD13 | 13:O:259:VAL:HG11 | 1.78                     | 0.64              |
| 3:C:186:TYR:HE2   | 3:C:188:THR:HG22  | 1.62                     | 0.64              |
| 5:E:36:LEU:O      | 5:E:40:THR:HG23   | 1.98                     | 0.64              |
| 2:B:284:ILE:HG23  | 2:B:305:ILE:HD12  | 1.80                     | 0.63              |
| 19:Z:55:GLY:HA2   | 25:Z:116:BCR:H312 | 1.80                     | 0.63              |
| 1:A:32:TRP:HA     | 1:A:32:TRP:CE3    | 2.32                     | 0.63              |
| 1:A:57:PRO:HG3    | 1:A:68:SER:CB     | 2.28                     | 0.63              |
| 3:C:318:LEU:HD23  | 3:C:318:LEU:C     | 2.24                     | 0.63              |
| 14:T:29:ILE:H     | 14:T:29:ILE:CD1   | 1.95                     | 0.63              |
| 5:E:27:ILE:HB     | 5:E:28:PRO:HD3    | 1.80                     | 0.63              |
| 2:B:297:THR:OG1   | 2:B:300:GLU:HG3   | 1.98                     | 0.63              |
| 2:B:486:LEU:O     | 2:B:486:LEU:HD13  | 1.98                     | 0.63              |
| 3:C:37:ALA:C      | 21:C:484:CLA:HBA1 | 2.23                     | 0.63              |
| 3:C:310:SER:OG    | 3:C:355:THR:HG23  | 1.98                     | 0.63              |
| 32:D:357:PL9:H262 | 32:D:357:PL9:H302 | 1.80                     | 0.63              |
| 6:F:19:ARG:NH2    | 33:F:85:HEM:O2D   | 2.32                     | 0.63              |
| 17:y:41:VAL:C     | 17:y:43:ARG:H     | 2.06                     | 0.63              |
| 5:E:26:THR:O      | 5:E:29:ALA:HB3    | 1.98                     | 0.63              |
| 2:B:247:PHE:HB2   | 21:B:518:CLA:HBC1 | 1.80                     | 0.63              |
| 1:A:300:PHE:CZ    | 3:C:404:LEU:HD23  | 2.33                     | 0.62              |
| 21:B:513:CLA:H3A  | 21:B:513:CLA:CGA  | 2.29                     | 0.62              |
| 21:B:517:CLA:H11  | 28:B:533:DGD:HB32 | 1.79                     | 0.62              |
| 3:C:407:VAL:CA    | 28:C:493:DGD:O2E  | 2.45                     | 0.62              |
| 1:A:136:ARG:NH2   | 8:I:27:ASP:OD1    | 2.32                     | 0.62              |
| 4:D:246:MET:HE3   | 4:D:262:SER:HA    | 1.82                     | 0.62              |
| 1:A:22:THR:HG21   | 8:I:30:ARG:CD     | 2.29                     | 0.62              |
| 27:A:373:LMG:H201 | 32:D:357:PL9:H212 | 1.80                     | 0.62              |
| 3:C:135:ARG:NE    | 19:Z:33:TRP:NE1   | 2.47                     | 0.62              |
| 3:C:293:ASN:CA    | 28:C:491:DGD:O2E  | 2.40                     | 0.62              |
| 3:C:305:THR:HG22  | 3:C:308:GLU:HB2   | 1.82                     | 0.62              |
| 11:L:7:ARG:C      | 11:L:8:GLN:HE21   | 2.06                     | 0.62              |
| 1:A:18:CYS:O      | 1:A:22:THR:HG22   | 2.00                     | 0.62              |
| 13:O:117:GLY:O    | 13:O:159:VAL:HG12 | 1.98                     | 0.62              |
| 5:E:23:HIS:HA     | 5:E:26:THR:OG1    | 2.00                     | 0.62              |
| 1:A:29:TYR:CG     | 1:A:133:LEU:HD13  | 2.34                     | 0.62              |
| 13:O:36:ILE:HG23  | 13:O:41:LEU:HB3   | 1.80                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:107:ASP:OD2   | 3:C:110:PRO:HD3   | 1.99                     | 0.62              |
| 21:C:486:CLA:H141 | 19:Z:20:VAL:O     | 2.00                     | 0.62              |
| 13:O:234:THR:OG1  | 13:O:236:GLU:HG2  | 2.00                     | 0.62              |
| 15:U:54:LYS:HB2   | 15:U:113:THR:HG23 | 1.82                     | 0.62              |
| 1:A:228:THR:HG22  | 1:A:229:GLU:H     | 1.65                     | 0.62              |
| 2:B:379:ALA:HA    | 2:B:390:TYR:HB3   | 1.80                     | 0.62              |
| 28:B:528:DGD:HE5  | 28:B:528:DGD:HD61 | 1.82                     | 0.62              |
| 3:C:418:ASN:HA    | 28:C:493:DGD:HE2  | 1.81                     | 0.62              |
| 10:K:18:PHE:HD2   | 10:K:18:PHE:N     | 1.97                     | 0.62              |
| 1:A:42:LEU:HD12   | 25:A:369:BCR:H11C | 1.81                     | 0.62              |
| 2:B:371:THR:HG22  | 2:B:377:VAL:HA    | 1.81                     | 0.62              |
| 5:E:10:PHE:CE2    | 6:F:19:ARG:NH1    | 2.67                     | 0.62              |
| 2:B:356:VAL:HG22  | 2:B:370:LEU:HD21  | 1.81                     | 0.61              |
| 3:C:44:ASN:O      | 3:C:45:LEU:HD12   | 1.99                     | 0.61              |
| 3:C:119:LEU:HG    | 25:C:489:BCR:H10C | 1.82                     | 0.61              |
| 5:E:18:ARG:O      | 5:E:22:ILE:HG13   | 2.00                     | 0.61              |
| 2:B:69:LEU:HD11   | 21:B:513:CLA:OBD  | 2.00                     | 0.61              |
| 3:C:80:PRO:HD2    | 16:V:129:LYS:HZ1  | 1.65                     | 0.61              |
| 26:C:476:LHG:H171 | 28:C:492:DGD:HBG2 | 1.82                     | 0.61              |
| 4:D:160:TYR:HB3   | 4:D:161:PRO:CD    | 2.30                     | 0.61              |
| 5:E:64:PRO:HB3    | 5:E:84:LYS:HE2    | 1.82                     | 0.61              |
| 17:y:42:ARG:HG2   | 17:y:42:ARG:HH11  | 1.66                     | 0.61              |
| 19:Z:32:ASP:CB    | 19:Z:35:ARG:HG2   | 2.30                     | 0.61              |
| 1:A:218:LEU:CD2   | 23:A:367:MES:H52  | 2.30                     | 0.61              |
| 2:B:69:LEU:HD12   | 21:B:515:CLA:HBA2 | 1.82                     | 0.61              |
| 3:C:41:ARG:NH1    | 21:C:486:CLA:OBD  | 2.33                     | 0.61              |
| 28:C:492:DGD:HB42 | 28:C:493:DGD:HA21 | 1.81                     | 0.61              |
| 15:U:66:ILE:O     | 15:U:66:ILE:HG22  | 1.98                     | 0.61              |
| 18:X:11:THR:HG23  | 18:X:12:ILE:HG22  | 1.81                     | 0.61              |
| 3:C:113:VAL:HG11  | 27:C:494:LMG:H172 | 1.81                     | 0.61              |
| 3:C:461:ARG:HH11  | 3:C:461:ARG:HG3   | 1.65                     | 0.61              |
| 4:D:342:PRO:O     | 4:D:345:VAL:HG12  | 2.01                     | 0.61              |
| 2:B:264:PRO:CG    | 2:B:267:LEU:HD12  | 2.31                     | 0.61              |
| 27:B:531:LMG:HC2  | 4:D:141:TYR:OH    | 2.00                     | 0.61              |
| 3:C:224:ILE:HD11  | 21:C:477:CLA:H93  | 1.81                     | 0.61              |
| 3:C:248:GLY:O     | 3:C:252:ILE:HG12  | 2.00                     | 0.61              |
| 3:C:374:GLY:O     | 3:C:375:LEU:C     | 2.44                     | 0.61              |
| 6:F:31:ILE:HD12   | 6:F:31:ILE:N      | 2.16                     | 0.61              |
| 14:T:29:ILE:HD12  | 14:T:29:ILE:N     | 2.10                     | 0.61              |
| 15:U:58:ASN:ND2   | 15:U:114:VAL:HG13 | 2.15                     | 0.61              |
| 15:U:94:ILE:O     | 15:U:97:LEU:HG    | 2.00                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:B:517:CLA:HBC3 | 25:B:529:BCR:H10C | 1.83                     | 0.61              |
| 3:C:52:ALA:HA     | 21:C:486:CLA:CMB  | 2.31                     | 0.61              |
| 3:C:318:LEU:HG    | 3:C:328:VAL:HG11  | 1.82                     | 0.61              |
| 3:C:405:ASN:HB2   | 28:C:493:DGD:HG32 | 1.82                     | 0.61              |
| 7:H:12:ARG:HD3    | 7:H:12:ARG:C      | 2.24                     | 0.61              |
| 1:A:53:ILE:HD11   | 32:D:357:PL9:H501 | 1.82                     | 0.61              |
| 3:C:114:VAL:HG22  | 27:C:494:LMG:H211 | 1.83                     | 0.61              |
| 4:D:49:LEU:O      | 4:D:53:THR:HG23   | 2.01                     | 0.61              |
| 5:E:15:THR:CG2    | 9:J:8:ILE:H       | 2.13                     | 0.61              |
| 5:E:79:PHE:O      | 5:E:84:LYS:HB3    | 2.01                     | 0.61              |
| 7:H:19:GLY:O      | 7:H:21:VAL:HG13   | 1.99                     | 0.61              |
| 13:O:39:THR:OG1   | 13:O:41:LEU:HB2   | 2.01                     | 0.61              |
| 1:A:214:MET:HE3   | 22:D:355:PHO:CMD  | 2.31                     | 0.61              |
| 27:A:373:LMG:H331 | 11:L:24:ILE:HD11  | 1.81                     | 0.61              |
| 10:K:18:PHE:N     | 10:K:18:PHE:CD2   | 2.68                     | 0.61              |
| 1:A:89:ILE:HD11   | 1:A:108:ASN:HB3   | 1.81                     | 0.61              |
| 3:C:88:LEU:HB3    | 21:C:479:CLA:HED3 | 1.83                     | 0.61              |
| 9:J:18:GLY:HA3    | 25:J:112:BCR:H371 | 1.82                     | 0.61              |
| 21:B:518:CLA:HBB2 | 4:D:123:ILE:HG12  | 1.82                     | 0.60              |
| 3:C:143:TYR:O     | 3:C:144:SER:HB2   | 2.00                     | 0.60              |
| 3:C:180:MET:HE3   | 3:C:202:PRO:HD3   | 1.82                     | 0.60              |
| 21:C:480:CLA:H93  | 28:C:492:DGD:HAT2 | 1.83                     | 0.60              |
| 16:V:90:PRO:O     | 16:V:92:ARG:HD3   | 2.01                     | 0.60              |
| 1:A:322:ASN:OD1   | 3:C:412:THR:HA    | 2.01                     | 0.60              |
| 21:A:362:CLA:H111 | 22:A:365:PHO:H3A  | 1.83                     | 0.60              |
| 27:A:373:LMG:H192 | 32:D:357:PL9:C22  | 2.31                     | 0.60              |
| 3:C:223:TRP:CD2   | 3:C:224:ILE:HG13  | 2.36                     | 0.60              |
| 6:F:38:ALA:O      | 6:F:41:GLN:HG2    | 2.01                     | 0.60              |
| 10:K:10:LYS:O     | 10:K:11:LEU:C     | 2.43                     | 0.60              |
| 13:O:86:ARG:HG3   | 13:O:86:ARG:HH11  | 1.66                     | 0.60              |
| 15:U:97:LEU:O     | 15:U:102:LYS:HE2  | 2.01                     | 0.60              |
| 2:B:315:ILE:HG22  | 2:B:426:PHE:HB3   | 1.82                     | 0.60              |
| 10:K:17:ILE:HD12  | 10:K:17:ILE:N     | 2.17                     | 0.60              |
| 2:B:124:ARG:NE    | 2:B:131:PRO:HD3   | 2.13                     | 0.60              |
| 3:C:204:LEU:HD21  | 3:C:238:ILE:HG21  | 1.84                     | 0.60              |
| 3:C:391:ARG:HD2   | 3:C:395:TYR:CE2   | 2.36                     | 0.60              |
| 13:O:230:VAL:CG1  | 13:O:231:ASP:H    | 2.10                     | 0.60              |
| 15:U:89:GLU:CD    | 15:U:89:GLU:H     | 2.09                     | 0.60              |
| 1:A:153:SER:HB2   | 21:A:362:CLA:H43  | 1.83                     | 0.60              |
| 7:H:58:VAL:HG13   | 7:H:58:VAL:O      | 2.00                     | 0.60              |
| 1:A:343:LEU:O     | 1:A:344:ALA:HB2   | 2.00                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:47:GLY:HA2    | 25:D:358:BCR:H332 | 1.83                     | 0.60              |
| 10:K:40:GLN:HA    | 10:K:43:VAL:HG12  | 1.83                     | 0.60              |
| 18:X:12:ILE:HG12  | 18:X:16:LEU:CD1   | 2.30                     | 0.60              |
| 19:Z:33:TRP:O     | 19:Z:33:TRP:HD1   | 1.84                     | 0.60              |
| 1:A:107:TYR:CD1   | 13:O:141:ARG:NH1  | 2.69                     | 0.60              |
| 1:A:136:ARG:HH22  | 8:I:27:ASP:CG     | 2.08                     | 0.60              |
| 2:B:41:GLU:OE1    | 2:B:63:LEU:HB2    | 2.02                     | 0.60              |
| 3:C:264:PHE:HE2   | 21:C:482:CLA:O1A  | 1.85                     | 0.60              |
| 10:K:24:VAL:HG21  | 17:y:25:ILE:HG12  | 1.84                     | 0.60              |
| 27:A:373:LMG:H311 | 11:L:20:GLY:HA2   | 1.82                     | 0.60              |
| 3:C:178:LYS:HB2   | 21:C:478:CLA:H162 | 1.83                     | 0.60              |
| 1:A:60:ILE:HD12   | 1:A:84:PRO:HD2    | 1.83                     | 0.60              |
| 1:A:306:VAL:HG13  | 1:A:314:ILE:O     | 2.01                     | 0.60              |
| 2:B:143:LEU:HA    | 21:B:520:CLA:HED1 | 1.83                     | 0.60              |
| 2:B:238:LEU:HD13  | 21:B:522:CLA:C1D  | 2.32                     | 0.60              |
| 5:E:18:ARG:HB3    | 5:E:18:ARG:NH1    | 2.17                     | 0.60              |
| 2:B:213:GLY:O     | 2:B:217:ILE:HG13  | 2.02                     | 0.60              |
| 3:C:39:ASN:OD1    | 21:C:485:CLA:HBB2 | 2.02                     | 0.59              |
| 4:D:56:THR:HG21   | 5:E:50:PRO:HD3    | 1.82                     | 0.59              |
| 13:O:87:GLN:O     | 13:O:88:GLU:HB3   | 2.02                     | 0.59              |
| 15:U:113:THR:O    | 15:U:114:VAL:HG23 | 2.02                     | 0.59              |
| 1:A:22:THR:HG21   | 8:I:30:ARG:NE     | 2.16                     | 0.59              |
| 21:B:517:CLA:H142 | 27:B:531:LMG:H382 | 1.84                     | 0.59              |
| 5:E:15:THR:HG23   | 9:J:8:ILE:O       | 2.01                     | 0.59              |
| 1:A:257:ARG:HG3   | 1:A:257:ARG:HH11  | 1.66                     | 0.59              |
| 27:B:531:LMG:H201 | 27:B:531:LMG:H291 | 1.83                     | 0.59              |
| 3:C:292:PHE:O     | 28:C:491:DGD:O2E  | 2.20                     | 0.59              |
| 13:O:31:LEU:HD12  | 13:O:31:LEU:N     | 2.17                     | 0.59              |
| 1:A:309:ALA:HB3   | 16:V:27:ALA:O     | 2.03                     | 0.59              |
| 21:B:520:CLA:HHC  | 21:B:520:CLA:HBB1 | 1.83                     | 0.59              |
| 3:C:233:VAL:HA    | 25:C:490:BCR:C28  | 2.32                     | 0.59              |
| 17:y:19:ILE:HG23  | 17:y:20:ALA:H     | 1.68                     | 0.59              |
| 2:B:172:TYR:O     | 2:B:174:LEU:HG    | 2.02                     | 0.59              |
| 4:D:87:HIS:CD2    | 4:D:162:LEU:HD23  | 2.37                     | 0.59              |
| 6:F:16:PHE:HE2    | 33:F:85:HEM:HMA2  | 1.66                     | 0.59              |
| 2:B:149:LEU:CG    | 21:B:513:CLA:HBC1 | 2.26                     | 0.59              |
| 4:D:261:PHE:HB2   | 32:D:357:PL9:H521 | 1.83                     | 0.59              |
| 10:K:33:LEU:HD23  | 21:K:483:CLA:OBD  | 2.03                     | 0.59              |
| 1:A:22:THR:HG21   | 8:I:30:ARG:HE     | 1.67                     | 0.59              |
| 21:B:512:CLA:C4   | 7:H:45:ILE:HD11   | 2.33                     | 0.59              |
| 6:F:27:ALA:HB1    | 33:F:85:HEM:HBC2  | 1.82                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:99:ALA:O      | 8:I:1:MET:HE3     | 2.02                     | 0.59              |
| 5:E:56:TYR:O      | 16:V:27:ALA:HB2   | 2.02                     | 0.59              |
| 2:B:133:LEU:HB3   | 2:B:138:MET:HE2   | 1.85                     | 0.59              |
| 21:B:511:CLA:HHC  | 21:B:511:CLA:HBB1 | 1.84                     | 0.59              |
| 3:C:418:ASN:CB    | 28:C:493:DGD:HE2  | 2.32                     | 0.59              |
| 21:C:480:CLA:H42  | 28:C:493:DGD:HA32 | 1.84                     | 0.59              |
| 6:F:41:GLN:OE1    | 9:J:31:GLY:HA3    | 2.01                     | 0.59              |
| 2:B:458:PHE:HB3   | 21:B:514:CLA:HBC2 | 1.84                     | 0.59              |
| 3:C:281:MET:HE1   | 21:C:481:CLA:HAC2 | 1.84                     | 0.59              |
| 21:C:480:CLA:H43  | 28:C:492:DGD:HA91 | 1.85                     | 0.59              |
| 6:F:23:VAL:O      | 6:F:27:ALA:HB2    | 2.03                     | 0.59              |
| 3:C:112:PHE:O     | 3:C:116:VAL:HG13  | 2.03                     | 0.58              |
| 3:C:186:TYR:CE2   | 3:C:188:THR:HG22  | 2.37                     | 0.58              |
| 2:B:68:ARG:HH11   | 2:B:262:THR:HG23  | 1.68                     | 0.58              |
| 3:C:369:LEU:HD21  | 3:C:384:ILE:HD13  | 1.85                     | 0.58              |
| 21:C:481:CLA:H12  | 8:I:23:PHE:CD2    | 2.38                     | 0.58              |
| 4:D:55:VAL:HG21   | 4:D:110:LEU:CD1   | 2.33                     | 0.58              |
| 9:J:22:ILE:HG13   | 25:J:115:BCR:H10C | 1.85                     | 0.58              |
| 13:O:80:GLU:O     | 13:O:89:ALA:HB1   | 2.03                     | 0.58              |
| 1:A:238:LYS:O     | 1:A:241:GLN:HG3   | 2.03                     | 0.58              |
| 3:C:95:LEU:HD11   | 21:C:479:CLA:HBA2 | 1.83                     | 0.58              |
| 3:C:380:ILE:HA    | 3:C:384:ILE:HD11  | 1.85                     | 0.58              |
| 3:C:418:ASN:CA    | 28:C:493:DGD:HE2  | 2.34                     | 0.58              |
| 27:D:360:LMG:O9   | 27:D:360:LMG:HC72 | 2.03                     | 0.58              |
| 5:E:8:ARG:N       | 6:F:13:TYR:CE1    | 2.71                     | 0.58              |
| 1:A:240:GLY:HA3   | 14:T:29:ILE:HG22  | 1.86                     | 0.58              |
| 3:C:28:GLN:HB2    | 21:C:486:CLA:HED2 | 1.86                     | 0.58              |
| 4:D:32:TRP:CG     | 30:D:361:SQD:H251 | 2.38                     | 0.58              |
| 10:K:17:ILE:HD12  | 10:K:17:ILE:H     | 1.69                     | 0.58              |
| 2:B:188:ASP:OD1   | 7:H:58:VAL:HA     | 2.04                     | 0.58              |
| 21:C:477:CLA:H71  | 21:C:477:CLA:HMB3 | 1.86                     | 0.58              |
| 5:E:15:THR:HG23   | 9:J:8:ILE:H       | 1.68                     | 0.58              |
| 5:E:76:VAL:O      | 5:E:80:LEU:HD22   | 2.03                     | 0.58              |
| 2:B:262:THR:HG21  | 21:B:513:CLA:HBA2 | 1.86                     | 0.58              |
| 21:B:516:CLA:H161 | 21:B:526:CLA:H161 | 1.84                     | 0.58              |
| 3:C:131:TYR:HE1   | 3:C:135:ARG:HD2   | 1.67                     | 0.58              |
| 2:B:150:CYS:HA    | 21:B:513:CLA:HBC2 | 1.85                     | 0.58              |
| 2:B:238:LEU:HB2   | 21:B:522:CLA:HMD3 | 1.84                     | 0.58              |
| 3:C:156:LYS:O     | 3:C:160:ILE:HG13  | 2.03                     | 0.58              |
| 4:D:279:LEU:HD13  | 21:D:354:CLA:HBA2 | 1.86                     | 0.58              |
| 1:A:142:TRP:HB2   | 4:D:220:ASN:OD1   | 2.03                     | 0.58              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:C:130:VAL:O    | 3:C:134:ILE:HG12  | 2.04                     | 0.58              |
| 13:O:123:GLU:HG2 | 13:O:124:GLU:N    | 2.18                     | 0.58              |
| 15:U:38:GLU:HG2  | 15:U:39:LEU:H     | 1.68                     | 0.58              |
| 16:V:81:ARG:CZ   | 16:V:157:GLY:HA3  | 2.34                     | 0.58              |
| 19:Z:14:ILE:O    | 19:Z:18:VAL:HG23  | 2.04                     | 0.58              |
| 2:B:462:PHE:HA   | 21:B:521:CLA:CMC  | 2.33                     | 0.58              |
| 3:C:122:SER:OG   | 25:C:489:BCR:H14C | 2.04                     | 0.58              |
| 3:C:305:THR:HG23 | 3:C:307:PRO:CD    | 2.32                     | 0.58              |
| 4:D:239:GLN:O    | 4:D:240:ALA:HB3   | 2.03                     | 0.58              |
| 1:A:203:ALA:HB1  | 28:C:493:DGD:HBV2 | 1.86                     | 0.57              |
| 1:A:272:HIS:CD2  | 4:D:218:VAL:HG21  | 2.39                     | 0.57              |
| 3:C:60:ILE:HG21  | 21:C:479:CLA:C19  | 2.34                     | 0.57              |
| 32:D:357:PL9:H43 | 27:D:360:LMG:C25  | 2.34                     | 0.57              |
| 9:J:14:ALA:HB1   | 25:J:112:BCR:C38  | 2.34                     | 0.57              |
| 2:B:12:LEU:HD22  | 2:B:18:ARG:HB2    | 1.87                     | 0.57              |
| 3:C:289:PHE:CD1  | 21:C:477:CLA:H12  | 2.38                     | 0.57              |
| 3:C:447:ARG:HH11 | 3:C:447:ARG:CG    | 2.14                     | 0.57              |
| 32:D:357:PL9:H23 | 32:D:357:PL9:H303 | 1.87                     | 0.57              |
| 5:E:15:THR:O     | 9:J:8:ILE:HD12    | 2.03                     | 0.57              |
| 19:Z:30:PRO:C    | 19:Z:32:ASP:H     | 2.12                     | 0.57              |
| 2:B:55:MET:HE2   | 2:B:80:ILE:HD12   | 1.85                     | 0.57              |
| 2:B:393:GLU:HG2  | 15:U:44:ASP:O     | 2.03                     | 0.57              |
| 3:C:362:ARG:HG2  | 28:C:491:DGD:HE61 | 1.86                     | 0.57              |
| 28:C:493:DGD:O3D | 9:J:37:GLY:O      | 2.22                     | 0.57              |
| 19:Z:32:ASP:C    | 19:Z:34:ASP:N     | 2.60                     | 0.57              |
| 19:Z:55:GLY:CA   | 25:Z:116:BCR:H312 | 2.34                     | 0.57              |
| 2:B:150:CYS:CA   | 21:B:513:CLA:HBC2 | 2.35                     | 0.57              |
| 2:B:224:ARG:NE   | 7:H:25:TRP:NE1    | 2.52                     | 0.57              |
| 3:C:281:MET:HE2  | 28:C:474:DGD:HAE1 | 1.85                     | 0.57              |
| 4:D:252:PHE:O    | 4:D:256:ILE:HG22  | 2.05                     | 0.57              |
| 4:D:279:LEU:CD1  | 21:D:354:CLA:HBA2 | 2.35                     | 0.57              |
| 6:F:20:TRP:O     | 6:F:24:HIS:HB2    | 2.04                     | 0.57              |
| 1:A:234:ASN:HB2  | 27:A:373:LMG:HC3  | 1.87                     | 0.57              |
| 3:C:39:ASN:HB2   | 21:C:484:CLA:HBA2 | 1.85                     | 0.57              |
| 4:D:122:LEU:HD21 | 22:D:355:PHO:H62  | 1.86                     | 0.57              |
| 4:D:188:PHE:HE2  | 4:D:329:MET:CE    | 2.17                     | 0.57              |
| 7:H:63:LYS:O     | 7:H:65:LEU:N      | 2.37                     | 0.57              |
| 16:V:74:THR:O    | 16:V:75:ASN:HB2   | 2.04                     | 0.57              |
| 17:y:19:ILE:HG23 | 17:y:20:ALA:N     | 2.19                     | 0.57              |
| 2:B:10:THR:C     | 2:B:12:LEU:H      | 2.12                     | 0.57              |
| 21:B:521:CLA:OBD | 27:B:531:LMG:HC8  | 2.05                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:y:39:LEU:CB    | 17:y:46:LEU:HD21  | 2.32                     | 0.57              |
| 1:A:214:MET:HB3   | 23:A:367:MES:C6   | 2.33                     | 0.57              |
| 1:A:233:ALA:HB3   | 27:B:531:LMG:HC4  | 1.86                     | 0.57              |
| 3:C:286:ALA:HB2   | 21:C:478:CLA:CMD  | 2.30                     | 0.57              |
| 27:D:360:LMG:C20  | 11:L:22:LEU:HD11  | 2.34                     | 0.57              |
| 12:M:29:THR:O     | 12:M:32:GLN:HG3   | 2.05                     | 0.57              |
| 1:A:38:ILE:O      | 1:A:42:LEU:HG     | 2.05                     | 0.57              |
| 1:A:244:GLU:HG3   | 1:A:246:TYR:H     | 1.70                     | 0.57              |
| 2:B:230:ARG:O     | 2:B:233:ASN:HB3   | 2.05                     | 0.57              |
| 2:B:262:THR:HG21  | 21:B:513:CLA:CBA  | 2.35                     | 0.57              |
| 3:C:343:ARG:NH1   | 3:C:347:GLY:O     | 2.38                     | 0.57              |
| 10:K:31:LEU:O     | 10:K:34:ALA:HB3   | 2.04                     | 0.57              |
| 15:U:72:TYR:HB3   | 15:U:73:PRO:CD    | 2.34                     | 0.57              |
| 18:X:45:LYS:HD3   | 18:X:45:LYS:N     | 2.20                     | 0.57              |
| 1:A:160:ILE:HD11  | 28:C:491:DGD:HA91 | 1.86                     | 0.56              |
| 2:B:256:MET:HA    | 2:B:263:THR:HG21  | 1.87                     | 0.56              |
| 28:B:528:DGD:HO2D | 4:D:87:HIS:CB     | 2.09                     | 0.56              |
| 3:C:193:GLY:O     | 3:C:194:GLY:C     | 2.48                     | 0.56              |
| 3:C:350:ILE:HG21  | 3:C:359:TRP:HB2   | 1.88                     | 0.56              |
| 4:D:113:PHE:CE2   | 25:D:358:BCR:HC41 | 2.40                     | 0.56              |
| 4:D:152:VAL:HG21  | 4:D:279:LEU:CD1   | 2.35                     | 0.56              |
| 10:K:26:PRO:O     | 10:K:29:PRO:HD2   | 2.05                     | 0.56              |
| 1:A:13:LEU:H      | 1:A:13:LEU:HD12   | 1.69                     | 0.56              |
| 1:A:183:MET:HE1   | 21:A:363:CLA:HMD2 | 1.87                     | 0.56              |
| 27:A:373:LMG:H202 | 32:D:357:PL9:H201 | 1.86                     | 0.56              |
| 2:B:174:LEU:HD23  | 2:B:308:LYS:HG2   | 1.87                     | 0.56              |
| 2:B:191:ASN:HB2   | 7:H:58:VAL:CG2    | 2.35                     | 0.56              |
| 2:B:192:PRO:HD2   | 7:H:60:VAL:HG12   | 1.88                     | 0.56              |
| 3:C:305:THR:HG22  | 3:C:308:GLU:N     | 2.16                     | 0.56              |
| 4:D:36:LEU:O      | 4:D:39:PRO:HD2    | 2.05                     | 0.56              |
| 16:V:125:ASP:HA   | 16:V:131:ARG:HH21 | 1.70                     | 0.56              |
| 18:X:12:ILE:CG1   | 18:X:16:LEU:HD12  | 2.33                     | 0.56              |
| 1:A:77:ILE:HG12   | 14:T:6:TYR:CD1    | 2.40                     | 0.56              |
| 1:A:84:PRO:HA     | 1:A:112:TYR:CG    | 2.40                     | 0.56              |
| 1:A:193:LEU:HD21  | 21:A:362:CLA:C2C  | 2.36                     | 0.56              |
| 1:A:265:PHE:CD1   | 1:A:271:LEU:HA    | 2.41                     | 0.56              |
| 27:A:373:LMG:C25  | 27:D:360:LMG:C22  | 2.83                     | 0.56              |
| 17:y:33:PRO:O     | 17:y:36:ILE:HG13  | 2.05                     | 0.56              |
| 19:Z:16:SER:O     | 19:Z:20:VAL:HG23  | 2.04                     | 0.56              |
| 4:D:18:LEU:O      | 4:D:22:LEU:HG     | 2.05                     | 0.56              |
| 13:O:178:ARG:CG   | 13:O:178:ARG:NH1  | 2.55                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:149:TYR:HA    | 3:C:156:LYS:HD3   | 1.88                     | 0.56              |
| 4:D:18:LEU:HD22   | 18:X:38:ILE:HD13  | 1.86                     | 0.56              |
| 7:H:58:VAL:O      | 7:H:58:VAL:CG1    | 2.53                     | 0.56              |
| 1:A:334:ARG:NH1   | 13:O:184:ASP:C    | 2.64                     | 0.56              |
| 3:C:113:VAL:CG1   | 27:C:494:LMG:H192 | 2.36                     | 0.56              |
| 2:B:224:ARG:HG3   | 7:H:25:TRP:CD1    | 2.41                     | 0.56              |
| 4:D:157:PHE:CE1   | 4:D:171:PRO:HG2   | 2.41                     | 0.56              |
| 13:O:31:LEU:HD12  | 13:O:31:LEU:H     | 1.71                     | 0.56              |
| 4:D:267:LEU:HD23  | 4:D:267:LEU:O     | 2.06                     | 0.56              |
| 13:O:88:GLU:OE2   | 13:O:90:GLU:HG2   | 2.06                     | 0.56              |
| 1:A:292:THR:OG1   | 28:C:492:DGD:CEA  | 2.54                     | 0.56              |
| 4:D:113:PHE:CZ    | 25:D:358:BCR:HC41 | 2.41                     | 0.56              |
| 6:F:18:VAL:HG13   | 6:F:19:ARG:N      | 2.21                     | 0.56              |
| 16:V:87:LEU:HD12  | 16:V:87:LEU:N     | 2.20                     | 0.56              |
| 1:A:187:GLN:HB2   | 21:A:362:CLA:HAC2 | 1.88                     | 0.55              |
| 18:X:16:LEU:HD13  | 18:X:16:LEU:C     | 2.31                     | 0.55              |
| 19:Z:26:ALA:CB    | 19:Z:40:ILE:HD11  | 2.36                     | 0.55              |
| 21:A:362:CLA:H202 | 21:A:363:CLA:H112 | 1.88                     | 0.55              |
| 2:B:293:ALA:C     | 2:B:295:GLY:H     | 2.14                     | 0.55              |
| 3:C:135:ARG:HG2   | 19:Z:33:TRP:CE2   | 2.41                     | 0.55              |
| 3:C:167:VAL:CG1   | 21:C:487:CLA:H11  | 2.36                     | 0.55              |
| 13:O:59:ASP:C     | 13:O:61:SER:H     | 2.14                     | 0.55              |
| 19:Z:21:ILE:O     | 19:Z:25:VAL:HG22  | 2.07                     | 0.55              |
| 2:B:133:LEU:HB3   | 2:B:138:MET:HE1   | 1.88                     | 0.55              |
| 3:C:107:ASP:OD2   | 3:C:109:PHE:HB3   | 2.06                     | 0.55              |
| 4:D:189:HIS:HA    | 4:D:294:ARG:HD2   | 1.88                     | 0.55              |
| 15:U:72:TYR:O     | 15:U:73:PRO:C     | 2.48                     | 0.55              |
| 1:A:37:MET:HG2    | 1:A:41:LEU:HD12   | 1.89                     | 0.55              |
| 21:B:512:CLA:H203 | 28:B:528:DGD:HB91 | 1.88                     | 0.55              |
| 25:J:112:BCR:HC31 | 10:K:21:LEU:HD21  | 1.89                     | 0.55              |
| 1:A:217:SER:HA    | 1:A:220:THR:HG22  | 1.88                     | 0.55              |
| 3:C:199:ILE:N     | 3:C:199:ILE:HD12  | 2.22                     | 0.55              |
| 3:C:250:TRP:CD1   | 3:C:250:TRP:C     | 2.84                     | 0.55              |
| 4:D:48:TRP:CE2    | 22:D:355:PHO:H161 | 2.42                     | 0.55              |
| 5:E:30:LEU:HD12   | 33:F:85:HEM:HMC1  | 1.88                     | 0.55              |
| 11:L:11:GLU:HG2   | 11:L:12:LEU:N     | 2.19                     | 0.55              |
| 13:O:66:ILE:HD12  | 13:O:121:PHE:CD1  | 2.42                     | 0.55              |
| 15:U:57:LEU:HD22  | 15:U:79:ILE:HG21  | 1.87                     | 0.55              |
| 4:D:68:LEU:HD13   | 6:F:40:MET:HE2    | 1.88                     | 0.55              |
| 1:A:20:TRP:O      | 1:A:21:VAL:C      | 2.50                     | 0.55              |
| 1:A:29:TYR:CD2    | 1:A:133:LEU:HD13  | 2.41                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:191:ASN:HD21  | 7:H:60:VAL:HA     | 1.72                     | 0.55              |
| 2:B:386:ALA:HB3   | 15:U:132:LEU:HD11 | 1.88                     | 0.55              |
| 3:C:239:TRP:CE3   | 3:C:243:ILE:HD11  | 2.42                     | 0.55              |
| 3:C:337:LEU:HD12  | 13:O:131:PRO:HG3  | 1.88                     | 0.55              |
| 4:D:54:PHE:HB3    | 5:E:47:PHE:CD2    | 2.42                     | 0.55              |
| 4:D:85:MET:CE     | 5:E:69:ARG:HA     | 2.36                     | 0.55              |
| 7:H:63:LYS:C      | 7:H:65:LEU:N      | 2.65                     | 0.55              |
| 16:V:59:PHE:HA    | 16:V:63:CYS:SG    | 2.47                     | 0.55              |
| 3:C:64:ALA:HB2    | 21:C:479:CLA:HMD2 | 1.89                     | 0.55              |
| 3:C:135:ARG:HG2   | 19:Z:33:TRP:CZ2   | 2.42                     | 0.55              |
| 8:I:11:VAL:O      | 8:I:15:PHE:HD2    | 1.89                     | 0.55              |
| 13:O:227:VAL:HG12 | 13:O:228:ALA:N    | 2.22                     | 0.55              |
| 18:X:32:LEU:HD23  | 18:X:32:LEU:N     | 2.22                     | 0.55              |
| 19:Z:29:SER:HB2   | 19:Z:31:GLN:HG3   | 1.88                     | 0.55              |
| 2:B:100:HIS:CE1   | 21:B:516:CLA:H11  | 2.42                     | 0.55              |
| 5:E:8:ARG:NE      | 5:E:13:ILE:HG12   | 2.22                     | 0.55              |
| 13:O:180:ALA:HB1  | 13:O:191:ALA:HB2  | 1.89                     | 0.55              |
| 19:Z:23:VAL:O     | 19:Z:26:ALA:HB3   | 2.06                     | 0.55              |
| 26:A:371:LHG:HC2  | 4:D:229:ALA:HB1   | 1.87                     | 0.55              |
| 3:C:29:GLU:HB3    | 10:K:46:ARG:HH11  | 1.70                     | 0.55              |
| 3:C:223:TRP:CG    | 3:C:224:ILE:H     | 2.25                     | 0.55              |
| 21:C:488:CLA:HMB2 | 25:Z:116:BCR:H402 | 1.89                     | 0.55              |
| 19:Z:36:SER:OG    | 19:Z:39:LEU:HD12  | 2.07                     | 0.55              |
| 2:B:25:MET:HE1    | 2:B:108:PHE:CE1   | 2.42                     | 0.54              |
| 2:B:170:ASP:HB2   | 2:B:171:PRO:CD    | 2.36                     | 0.54              |
| 4:D:250:ASN:ND2   | 4:D:262:SER:HB3   | 2.22                     | 0.54              |
| 1:A:76:ASN:OD1    | 1:A:79:THR:HG23   | 2.07                     | 0.54              |
| 1:A:82:VAL:HB     | 1:A:174:LEU:HB2   | 1.88                     | 0.54              |
| 1:A:131:TRP:CE3   | 1:A:132:GLU:N     | 2.75                     | 0.54              |
| 21:B:520:CLA:H111 | 21:B:525:CLA:HAA1 | 1.88                     | 0.54              |
| 3:C:55:ALA:HB1    | 25:C:489:BCR:H373 | 1.89                     | 0.54              |
| 3:C:127:PHE:HE1   | 19:Z:23:VAL:HG21  | 1.72                     | 0.54              |
| 3:C:178:LYS:HA    | 3:C:182:PHE:HB2   | 1.90                     | 0.54              |
| 5:E:55:TYR:O      | 5:E:84:LYS:HE3    | 2.07                     | 0.54              |
| 13:O:141:ARG:HG2  | 13:O:141:ARG:HH11 | 1.71                     | 0.54              |
| 13:O:154:SER:O    | 13:O:168:PHE:HA   | 2.07                     | 0.54              |
| 27:A:373:LMG:C25  | 27:D:360:LMG:H222 | 2.37                     | 0.54              |
| 2:B:23:HIS:C      | 21:B:525:CLA:HED1 | 2.33                     | 0.54              |
| 2:B:169:SER:O     | 7:H:65:LEU:HD13   | 2.06                     | 0.54              |
| 3:C:45:LEU:HD23   | 3:C:48:LYS:HD2    | 1.89                     | 0.54              |
| 3:C:155:ASN:O     | 3:C:158:THR:HG22  | 2.07                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:C:487:CLA:H172 | 21:C:487:CLA:CMA  | 2.37                     | 0.54              |
| 4:D:152:VAL:HG11  | 21:D:354:CLA:C1   | 2.34                     | 0.54              |
| 4:D:152:VAL:HG11  | 21:D:354:CLA:HBA1 | 1.88                     | 0.54              |
| 30:L:213:SQD:H261 | 27:M:217:LMG:H191 | 1.90                     | 0.54              |
| 15:U:66:ILE:O     | 15:U:66:ILE:CG2   | 2.56                     | 0.54              |
| 1:A:197:PHE:CE2   | 28:C:492:DGD:CEA  | 2.90                     | 0.54              |
| 21:C:477:CLA:H3A  | 21:C:477:CLA:O2A  | 2.08                     | 0.54              |
| 15:U:58:ASN:OD1   | 15:U:84:PRO:HA    | 2.07                     | 0.54              |
| 19:Z:36:SER:HA    | 19:Z:39:LEU:CG    | 2.35                     | 0.54              |
| 2:B:247:PHE:CE1   | 21:B:512:CLA:H8   | 2.33                     | 0.54              |
| 21:B:518:CLA:H111 | 4:D:120:PHE:CE1   | 2.42                     | 0.54              |
| 4:D:180:ARG:HG3   | 4:D:180:ARG:NH1   | 2.23                     | 0.54              |
| 17:y:20:ALA:C     | 17:y:22:LEU:H     | 2.15                     | 0.54              |
| 1:A:45:THR:OG1    | 21:A:363:CLA:H141 | 2.08                     | 0.54              |
| 3:C:386:PRO:HB3   | 16:V:116:GLU:HG2  | 1.89                     | 0.54              |
| 21:C:477:CLA:C3D  | 21:C:479:CLA:H2   | 2.38                     | 0.54              |
| 15:U:100:ARG:O    | 15:U:103:GLN:HB3  | 2.07                     | 0.54              |
| 21:B:519:CLA:HAC2 | 7:H:34:PHE:CE2    | 2.43                     | 0.54              |
| 3:C:259:TRP:H     | 3:C:259:TRP:CD1   | 2.26                     | 0.54              |
| 13:O:92:VAL:HG13  | 13:O:93:PRO:HD2   | 1.90                     | 0.54              |
| 16:V:135:GLU:O    | 16:V:139:VAL:HG23 | 2.08                     | 0.54              |
| 4:D:303:ILE:HD13  | 12:M:2:GLU:HG2    | 1.88                     | 0.54              |
| 6:F:43:ILE:HG22   | 9:J:36:LEU:HD21   | 1.90                     | 0.54              |
| 13:O:218:LEU:HD22 | 15:U:119:THR:CG2  | 2.35                     | 0.54              |
| 21:A:364:CLA:H203 | 27:D:359:LMG:H402 | 1.89                     | 0.54              |
| 2:B:474:LEU:O     | 4:D:134:ARG:NH1   | 2.41                     | 0.54              |
| 21:B:511:CLA:HBB2 | 7:H:44:ILE:HG21   | 1.90                     | 0.54              |
| 19:Z:35:ARG:O     | 19:Z:38:GLN:HB3   | 2.07                     | 0.54              |
| 1:A:235:TYR:C     | 1:A:237:TYR:H     | 2.16                     | 0.53              |
| 3:C:125:LEU:HD22  | 21:C:487:CLA:CED  | 2.37                     | 0.53              |
| 7:H:12:ARG:N      | 7:H:13:PRO:HD2    | 2.23                     | 0.53              |
| 3:C:80:PRO:HB2    | 3:C:83:GLU:HG3    | 1.90                     | 0.53              |
| 4:D:86:GLY:O      | 4:D:166:SER:HB2   | 2.08                     | 0.53              |
| 4:D:239:GLN:O     | 4:D:240:ALA:CB    | 2.55                     | 0.53              |
| 5:E:15:THR:O      | 9:J:8:ILE:CD1     | 2.56                     | 0.53              |
| 6:F:9:GLU:C       | 6:F:11:VAL:H      | 2.15                     | 0.53              |
| 3:C:165:LEU:HD21  | 21:C:482:CLA:HBB1 | 1.89                     | 0.53              |
| 3:C:418:ASN:HB2   | 28:C:493:DGD:HE2  | 1.89                     | 0.53              |
| 28:C:492:DGD:HG11 | 27:J:492:LMG:H301 | 1.91                     | 0.53              |
| 4:D:103:ARG:HG3   | 5:E:73:LYS:HG3    | 1.90                     | 0.53              |
| 32:D:357:PL9:H352 | 11:L:26:VAL:HB    | 1.90                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:235:GLU:HG2   | 2:B:235:GLU:O     | 2.08                     | 0.53              |
| 21:B:521:CLA:H52  | 21:B:524:CLA:CBC  | 2.38                     | 0.53              |
| 25:B:530:BCR:HC31 | 29:B:535:LMT:H72  | 1.90                     | 0.53              |
| 3:C:174:LEU:HD12  | 21:C:487:CLA:H51  | 1.89                     | 0.53              |
| 3:C:223:TRP:CH2   | 28:C:474:DGD:HA62 | 2.44                     | 0.53              |
| 4:D:330:ALA:HB3   | 4:D:331:PRO:HD3   | 1.91                     | 0.53              |
| 10:K:43:VAL:O     | 10:K:43:VAL:HG13  | 2.09                     | 0.53              |
| 2:B:150:CYS:N     | 21:B:513:CLA:HBC2 | 2.23                     | 0.53              |
| 2:B:471:ALA:HB2   | 4:D:130:PHE:CE2   | 2.44                     | 0.53              |
| 9:J:15:THR:O      | 9:J:19:MET:HG3    | 2.08                     | 0.53              |
| 1:A:160:ILE:HD11  | 28:C:491:DGD:HA81 | 1.90                     | 0.53              |
| 21:B:512:CLA:H201 | 4:D:159:ILE:HG12  | 1.89                     | 0.53              |
| 3:C:243:ILE:O     | 21:C:482:CLA:HMC1 | 2.09                     | 0.53              |
| 3:C:407:VAL:CG2   | 28:C:493:DGD:O2E  | 2.55                     | 0.53              |
| 3:C:416:SER:H     | 28:C:493:DGD:C3E  | 2.22                     | 0.53              |
| 3:C:425:TRP:CZ2   | 21:C:480:CLA:HBA2 | 2.44                     | 0.53              |
| 12:M:25:LEU:O     | 12:M:28:GLN:HG3   | 2.08                     | 0.53              |
| 13:O:82:PRO:HB3   | 13:O:87:GLN:HG3   | 1.89                     | 0.53              |
| 16:V:116:GLU:HG3  | 16:V:116:GLU:O    | 2.08                     | 0.53              |
| 1:A:81:ALA:CB     | 1:A:175:GLY:HA3   | 2.37                     | 0.53              |
| 2:B:106:LEU:HD22  | 21:B:516:CLA:H193 | 1.90                     | 0.53              |
| 3:C:54:VAL:HA     | 21:C:487:CLA:CED  | 2.39                     | 0.53              |
| 3:C:404:LEU:CD2   | 28:C:493:DGD:HA31 | 2.37                     | 0.53              |
| 19:Z:32:ASP:C     | 19:Z:34:ASP:H     | 2.17                     | 0.53              |
| 21:A:363:CLA:H101 | 27:D:360:LMG:C25  | 2.39                     | 0.53              |
| 4:D:77:ALA:HB2    | 4:D:174:GLY:HA3   | 1.91                     | 0.53              |
| 7:H:55:LEU:O      | 7:H:58:VAL:HG12   | 2.09                     | 0.53              |
| 1:A:196:PRO:HA    | 1:A:199:GLN:OE1   | 2.09                     | 0.53              |
| 3:C:53:HIS:HB3    | 21:C:487:CLA:OBD  | 2.09                     | 0.53              |
| 25:C:489:BCR:C11  | 25:J:112:BCR:H322 | 2.38                     | 0.53              |
| 4:D:18:LEU:HD22   | 18:X:38:ILE:CD1   | 2.38                     | 0.53              |
| 32:D:357:PL9:C35  | 11:L:26:VAL:HB    | 2.38                     | 0.53              |
| 13:O:190:LEU:HB2  | 13:O:214:LYS:HB2  | 1.90                     | 0.53              |
| 33:V:164:HEM:HMA2 | 33:V:164:HEM:HBA1 | 1.90                     | 0.53              |
| 1:A:107:TYR:HD1   | 13:O:141:ARG:NH1  | 2.05                     | 0.53              |
| 21:B:515:CLA:H92  | 21:B:522:CLA:H18  | 1.91                     | 0.53              |
| 4:D:238:THR:O     | 4:D:239:GLN:O     | 2.27                     | 0.53              |
| 21:B:520:CLA:H121 | 21:B:520:CLA:O1D  | 2.09                     | 0.52              |
| 3:C:449:ARG:HG2   | 21:C:481:CLA:HED3 | 1.91                     | 0.52              |
| 28:C:493:DGD:O2D  | 9:J:32:ALA:HB1    | 2.10                     | 0.52              |
| 25:D:358:BCR:H391 | 9:J:21:VAL:HG11   | 1.91                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:K:24:VAL:O     | 10:K:27:VAL:HG12  | 2.10                     | 0.52              |
| 1:A:10:SER:C      | 1:A:12:ASN:H      | 2.16                     | 0.52              |
| 1:A:140:ARG:NH2   | 1:A:142:TRP:HZ3   | 2.07                     | 0.52              |
| 1:A:278:TRP:HA    | 28:C:493:DGD:CIA  | 2.38                     | 0.52              |
| 2:B:328:GLY:C     | 21:B:517:CLA:HBA1 | 2.34                     | 0.52              |
| 3:C:216:SER:HB3   | 3:C:221:GLU:HB2   | 1.90                     | 0.52              |
| 3:C:239:TRP:HE3   | 3:C:243:ILE:HD11  | 1.74                     | 0.52              |
| 3:C:391:ARG:HH11  | 3:C:391:ARG:CB    | 2.19                     | 0.52              |
| 21:C:484:CLA:H43  | 21:C:486:CLA:HAC1 | 1.90                     | 0.52              |
| 4:D:44:ALA:CB     | 22:D:355:PHO:H92  | 2.39                     | 0.52              |
| 13:O:190:LEU:HD12 | 15:U:41:ASN:ND2   | 2.24                     | 0.52              |
| 15:U:100:ARG:HH11 | 15:U:103:GLN:HG2  | 1.73                     | 0.52              |
| 19:Z:3:ILE:O      | 19:Z:7:LEU:HG     | 2.09                     | 0.52              |
| 3:C:216:SER:HB2   | 28:C:474:DGD:HG31 | 1.91                     | 0.52              |
| 26:C:476:LHG:H142 | 25:J:115:BCR:HC21 | 1.89                     | 0.52              |
| 4:D:71:CYS:HB2    | 4:D:76:VAL:HG12   | 1.91                     | 0.52              |
| 4:D:337:GLU:O     | 4:D:338:ASN:C     | 2.51                     | 0.52              |
| 1:A:114:LEU:HD23  | 1:A:114:LEU:C     | 2.34                     | 0.52              |
| 1:A:279:PRO:CG    | 4:D:212:ALA:HB2   | 2.40                     | 0.52              |
| 2:B:7:ARG:HE      | 21:B:521:CLA:HED1 | 1.74                     | 0.52              |
| 2:B:143:LEU:CA    | 21:B:520:CLA:HED1 | 2.39                     | 0.52              |
| 2:B:464:PHE:CD2   | 21:B:521:CLA:HAC2 | 2.44                     | 0.52              |
| 28:B:528:DGD:HE5  | 28:B:528:DGD:C6D  | 2.39                     | 0.52              |
| 3:C:276:LEU:HD11  | 3:C:444:HIS:HD2   | 1.73                     | 0.52              |
| 4:D:76:VAL:O      | 4:D:77:ALA:HB2    | 2.10                     | 0.52              |
| 13:O:31:LEU:HB2   | 13:O:36:ILE:CD1   | 2.38                     | 0.52              |
| 13:O:223:ILE:HG13 | 13:O:243:SER:HB3  | 1.92                     | 0.52              |
| 19:Z:55:GLY:N     | 25:Z:116:BCR:H312 | 2.23                     | 0.52              |
| 1:A:218:LEU:HD23  | 23:A:367:MES:H72  | 1.90                     | 0.52              |
| 21:C:480:CLA:H193 | 28:C:492:DGD:HBV1 | 1.91                     | 0.52              |
| 17:y:36:ILE:C     | 17:y:36:ILE:HD12  | 2.35                     | 0.52              |
| 1:A:232:SER:HB3   | 1:A:235:TYR:CD1   | 2.45                     | 0.52              |
| 1:A:334:ARG:NH1   | 13:O:183:LEU:O    | 2.42                     | 0.52              |
| 1:A:334:ARG:HD2   | 13:O:183:LEU:HB2  | 1.92                     | 0.52              |
| 2:B:191:ASN:ND2   | 7:H:60:VAL:HA     | 2.24                     | 0.52              |
| 28:B:533:DGD:HAE1 | 12:M:17:VAL:HG21  | 1.92                     | 0.52              |
| 3:C:405:ASN:CB    | 28:C:493:DGD:HG32 | 2.40                     | 0.52              |
| 3:C:452:ALA:O     | 3:C:454:GLY:N     | 2.42                     | 0.52              |
| 27:D:360:LMG:H212 | 14:T:17:PHE:CZ    | 2.28                     | 0.52              |
| 13:O:240:THR:HA   | 13:O:264:VAL:HA   | 1.92                     | 0.52              |
| 15:U:72:TYR:CB    | 15:U:73:PRO:HD3   | 2.34                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:y:21:GLN:HA    | 17:y:23:THR:HG22  | 1.90                     | 0.52              |
| 9:J:11:TRP:CG     | 10:K:42:ALA:HA    | 2.45                     | 0.52              |
| 15:U:83:ALA:CB    | 15:U:84:PRO:CD    | 2.77                     | 0.52              |
| 1:A:232:SER:HB3   | 1:A:235:TYR:HD1   | 1.75                     | 0.52              |
| 2:B:341:LYS:HD2   | 2:B:429:ILE:HG22  | 1.90                     | 0.52              |
| 3:C:47:GLY:O      | 3:C:50:LEU:HB3    | 2.10                     | 0.52              |
| 3:C:393:ALA:HB1   | 33:V:164:HEM:HBC1 | 1.91                     | 0.52              |
| 3:C:447:ARG:HG2   | 3:C:447:ARG:NH1   | 2.16                     | 0.52              |
| 4:D:221:THR:O     | 4:D:221:THR:HG23  | 2.10                     | 0.52              |
| 5:E:61:ARG:HH22   | 16:V:153:GLY:HA3  | 1.74                     | 0.52              |
| 13:O:141:ARG:NH1  | 13:O:141:ARG:HG2  | 2.24                     | 0.52              |
| 15:U:66:ILE:HG13  | 15:U:72:TYR:CD1   | 2.44                     | 0.52              |
| 19:Z:31:GLN:O     | 19:Z:32:ASP:HB3   | 2.10                     | 0.52              |
| 1:A:49:VAL:O      | 1:A:53:ILE:HG13   | 2.10                     | 0.52              |
| 3:C:271:TYR:CE1   | 21:C:483:CLA:HAC1 | 2.44                     | 0.52              |
| 3:C:281:MET:CE    | 21:C:481:CLA:HAC2 | 2.40                     | 0.52              |
| 4:D:161:PRO:HG3   | 4:D:170:ALA:HB2   | 1.91                     | 0.52              |
| 7:H:25:TRP:O      | 7:H:26:GLY:C      | 2.53                     | 0.52              |
| 11:L:1:MET:O      | 11:L:1:MET:CG     | 2.48                     | 0.52              |
| 13:O:225:LEU:C    | 13:O:226:ASN:HD22 | 2.17                     | 0.52              |
| 19:Z:29:SER:C     | 19:Z:31:GLN:H     | 2.17                     | 0.52              |
| 19:Z:32:ASP:CG    | 19:Z:33:TRP:N     | 2.60                     | 0.52              |
| 2:B:12:LEU:CD2    | 2:B:18:ARG:HB2    | 2.40                     | 0.52              |
| 3:C:425:TRP:HB3   | 21:C:480:CLA:HMB3 | 1.91                     | 0.52              |
| 13:O:178:ARG:HD2  | 13:O:182:PHE:CD1  | 2.45                     | 0.52              |
| 1:A:228:THR:HG22  | 1:A:229:GLU:N     | 2.25                     | 0.51              |
| 4:D:334:GLN:N     | 4:D:335:PRO:HD3   | 2.25                     | 0.51              |
| 5:E:61:ARG:NH2    | 16:V:153:GLY:HA3  | 2.25                     | 0.51              |
| 2:B:222:PRO:CG    | 7:H:27:THR:H      | 2.21                     | 0.51              |
| 4:D:42:TYR:HE1    | 6:F:26:LEU:HD23   | 1.75                     | 0.51              |
| 4:D:87:HIS:CD2    | 4:D:162:LEU:HA    | 2.45                     | 0.51              |
| 4:D:136:VAL:O     | 4:D:136:VAL:HG12  | 2.10                     | 0.51              |
| 4:D:346:LEU:O     | 4:D:348:ARG:HG3   | 2.10                     | 0.51              |
| 25:D:358:BCR:H391 | 25:J:115:BCR:H332 | 1.91                     | 0.51              |
| 10:K:30:VAL:HA    | 21:K:483:CLA:H191 | 1.93                     | 0.51              |
| 19:Z:32:ASP:OD1   | 19:Z:36:SER:HB2   | 2.11                     | 0.51              |
| 1:A:202:VAL:HG11  | 21:A:364:CLA:OBD  | 2.09                     | 0.51              |
| 3:C:346:THR:O     | 13:O:40:GLY:HA2   | 2.10                     | 0.51              |
| 7:H:38:PHE:HB2    | 25:X:107:BCR:H10C | 1.92                     | 0.51              |
| 16:V:147:VAL:O    | 16:V:150:LYS:HB2  | 2.10                     | 0.51              |
| 18:X:12:ILE:O     | 18:X:12:ILE:CG2   | 2.58                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:334:ASP:HB3   | 13:O:202:GLN:HG3  | 1.92                     | 0.51              |
| 2:B:383:PHE:CZ    | 13:O:193:GLY:HA2  | 2.45                     | 0.51              |
| 3:C:95:LEU:CD1    | 21:C:479:CLA:HBA2 | 2.40                     | 0.51              |
| 3:C:227:VAL:HG11  | 25:C:490:BCR:H282 | 1.93                     | 0.51              |
| 5:E:36:LEU:HA     | 5:E:39:SER:OG     | 2.11                     | 0.51              |
| 1:A:10:SER:C      | 1:A:12:ASN:N      | 2.69                     | 0.51              |
| 2:B:149:LEU:HD22  | 21:B:514:CLA:H161 | 1.92                     | 0.51              |
| 21:C:477:CLA:H151 | 21:C:483:CLA:HMB3 | 1.93                     | 0.51              |
| 5:E:9:PRO:O       | 5:E:10:PHE:C      | 2.53                     | 0.51              |
| 1:A:78:ILE:O      | 1:A:176:ILE:HB    | 2.10                     | 0.51              |
| 1:A:150:PRO:O     | 21:A:362:CLA:H43  | 2.11                     | 0.51              |
| 1:A:183:MET:HB3   | 21:A:362:CLA:HBC2 | 1.92                     | 0.51              |
| 21:A:363:CLA:HED2 | 4:D:198:MET:SD    | 2.50                     | 0.51              |
| 3:C:128:GLY:HA3   | 21:C:488:CLA:C3C  | 2.40                     | 0.51              |
| 3:C:269:GLU:OE1   | 3:C:447:ARG:HG2   | 2.10                     | 0.51              |
| 5:E:15:THR:CG2    | 9:J:7:ARG:CB      | 2.85                     | 0.51              |
| 25:J:112:BCR:C15  | 10:K:31:LEU:HB3   | 2.41                     | 0.51              |
| 14:T:25:GLU:O     | 14:T:26:PRO:C     | 2.54                     | 0.51              |
| 2:B:327:THR:HG22  | 21:B:517:CLA:H12  | 1.92                     | 0.51              |
| 2:B:414:PRO:HB2   | 2:B:415:PRO:CD    | 2.35                     | 0.51              |
| 3:C:415:ASN:O     | 3:C:416:SER:CB    | 2.57                     | 0.51              |
| 13:O:118:SER:HB3  | 13:O:157:PRO:HA   | 1.93                     | 0.51              |
| 19:Z:47:TRP:O     | 19:Z:50:LEU:HB2   | 2.11                     | 0.51              |
| 1:A:188:ALA:HB2   | 1:A:328:MET:HB2   | 1.92                     | 0.51              |
| 2:B:246:PHE:CD1   | 2:B:246:PHE:C     | 2.88                     | 0.51              |
| 3:C:266:TRP:HB3   | 3:C:271:TYR:OH    | 2.11                     | 0.51              |
| 10:K:17:ILE:H     | 10:K:17:ILE:CD1   | 2.24                     | 0.51              |
| 1:A:149:ALA:HB3   | 1:A:150:PRO:CD    | 2.41                     | 0.51              |
| 2:B:172:TYR:O     | 2:B:173:GLY:C     | 2.52                     | 0.51              |
| 2:B:229:LEU:O     | 2:B:231:MET:N     | 2.43                     | 0.51              |
| 3:C:158:THR:HG21  | 3:C:254:THR:O     | 2.10                     | 0.51              |
| 4:D:221:THR:HG23  | 4:D:244:TYR:HB2   | 1.91                     | 0.51              |
| 18:X:17:LYS:O     | 18:X:21:ILE:HG13  | 2.10                     | 0.51              |
| 27:A:373:LMG:O4   | 11:L:13:ASN:ND2   | 2.44                     | 0.51              |
| 2:B:91:TRP:HE1    | 29:B:535:LMT:H41  | 1.75                     | 0.51              |
| 10:K:25:LEU:HB2   | 10:K:26:PRO:HD3   | 1.93                     | 0.51              |
| 16:V:30:THR:HB    | 16:V:31:PRO:CD    | 2.35                     | 0.51              |
| 19:Z:36:SER:C     | 19:Z:38:GLN:N     | 2.69                     | 0.51              |
| 4:D:53:THR:HG22   | 4:D:67:TYR:CD2    | 2.46                     | 0.50              |
| 19:Z:17:PHE:CE2   | 19:Z:21:ILE:HD11  | 2.45                     | 0.50              |
| 1:A:227:THR:HA    | 1:A:231:GLU:OE2   | 2.10                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:A:364:CLA:HBB1 | 4:D:157:PHE:CE2   | 2.45                     | 0.50              |
| 21:B:518:CLA:HBA1 | 30:D:361:SQD:H101 | 1.93                     | 0.50              |
| 4:D:86:GLY:HA2    | 4:D:166:SER:HB3   | 1.93                     | 0.50              |
| 19:Z:5:PHE:HA     | 19:Z:57:LEU:CD2   | 2.40                     | 0.50              |
| 21:A:364:CLA:HED1 | 28:C:493:DGD:HBW2 | 1.93                     | 0.50              |
| 2:B:125:ASP:OD2   | 2:B:127:ARG:HB3   | 2.11                     | 0.50              |
| 3:C:81:MET:CE     | 3:C:89:ILE:HG22   | 2.41                     | 0.50              |
| 3:C:137:PRO:HB2   | 3:C:139:THR:O     | 2.12                     | 0.50              |
| 21:C:481:CLA:O1A  | 8:I:23:PHE:CZ     | 2.64                     | 0.50              |
| 4:D:88:SER:HB2    | 5:E:69:ARG:CZ     | 2.40                     | 0.50              |
| 4:D:99:GLY:HA3    | 29:D:363:LMT:H2'  | 1.94                     | 0.50              |
| 8:I:27:ASP:N      | 8:I:28:PRO:CD     | 2.74                     | 0.50              |
| 13:O:271:PRO:HG2  | 13:O:272:ALA:H    | 1.76                     | 0.50              |
| 1:A:190:HIS:CB    | 1:A:293:MET:HE2   | 2.38                     | 0.50              |
| 1:A:214:MET:O     | 1:A:215:HIS:C     | 2.54                     | 0.50              |
| 27:A:373:LMG:C25  | 27:D:360:LMG:H231 | 2.41                     | 0.50              |
| 2:B:137:LYS:O     | 2:B:141:ILE:HG13  | 2.11                     | 0.50              |
| 2:B:229:LEU:O     | 2:B:230:ARG:C     | 2.54                     | 0.50              |
| 28:C:493:DGD:HG31 | 9:J:33:TYR:CZ     | 2.47                     | 0.50              |
| 28:C:493:DGD:HB51 | 27:D:359:LMG:H121 | 1.94                     | 0.50              |
| 1:A:215:HIS:O     | 1:A:216:GLY:C     | 2.53                     | 0.50              |
| 1:A:283:VAL:O     | 1:A:286:THR:HG22  | 2.11                     | 0.50              |
| 27:A:373:LMG:HC61 | 11:L:11:GLU:OE2   | 2.11                     | 0.50              |
| 2:B:250:PHE:O     | 28:B:528:DGD:HB82 | 2.11                     | 0.50              |
| 3:C:56:HIS:C      | 3:C:58:GLY:N      | 2.68                     | 0.50              |
| 3:C:125:LEU:HA    | 21:C:488:CLA:HMC1 | 1.94                     | 0.50              |
| 4:D:53:THR:HG22   | 4:D:67:TYR:CE2    | 2.47                     | 0.50              |
| 7:H:55:LEU:HB2    | 7:H:58:VAL:HG12   | 1.92                     | 0.50              |
| 7:H:62:TRP:O      | 7:H:63:LYS:O      | 2.30                     | 0.50              |
| 2:B:220:ARG:HB3   | 2:B:221:PRO:HD2   | 1.93                     | 0.50              |
| 3:C:155:ASN:CA    | 3:C:158:THR:HG22  | 2.39                     | 0.50              |
| 3:C:159:THR:HG23  | 3:C:252:ILE:HD13  | 1.93                     | 0.50              |
| 4:D:262:SER:OG    | 27:D:360:LMG:O3   | 2.28                     | 0.50              |
| 32:D:357:PL9:H33  | 32:D:357:PL9:H301 | 1.93                     | 0.50              |
| 29:D:363:LMT:O2'  | 18:X:21:ILE:HD12  | 2.11                     | 0.50              |
| 13:O:94:THR:HB    | 13:O:135:GLN:O    | 2.12                     | 0.50              |
| 2:B:55:MET:CE     | 2:B:80:ILE:HD12   | 2.42                     | 0.50              |
| 2:B:173:GLY:HA3   | 2:B:265:ILE:HD11  | 1.93                     | 0.50              |
| 2:B:377:VAL:HG11  | 4:D:342:PRO:HG2   | 1.93                     | 0.50              |
| 21:B:512:CLA:HBD  | 21:B:512:CLA:H43  | 1.92                     | 0.50              |
| 3:C:452:ALA:C     | 3:C:454:GLY:N     | 2.68                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:C:481:CLA:HAA2 | 21:C:481:CLA:HBD  | 1.92                     | 0.50              |
| 21:C:486:CLA:H13  | 19:Z:20:VAL:HG13  | 1.93                     | 0.50              |
| 4:D:135:LEU:HD23  | 30:D:361:SQD:HO2  | 1.77                     | 0.50              |
| 4:D:180:ARG:CG    | 4:D:180:ARG:NH1   | 2.70                     | 0.50              |
| 1:A:126:TYR:OH    | 22:A:365:PHO:O1D  | 2.23                     | 0.50              |
| 1:A:243:GLU:H     | 1:A:243:GLU:CD    | 2.16                     | 0.50              |
| 3:C:72:LEU:HD11   | 3:C:108:THR:HB    | 1.93                     | 0.50              |
| 3:C:116:VAL:CG1   | 25:C:489:BCR:H332 | 2.40                     | 0.50              |
| 3:C:405:ASN:HA    | 28:C:493:DGD:C1G  | 2.40                     | 0.50              |
| 4:D:36:LEU:C      | 4:D:39:PRO:HD2    | 2.37                     | 0.50              |
| 4:D:302:GLU:OE1   | 13:O:186:LYS:NZ   | 2.34                     | 0.50              |
| 13:O:43:ASN:OD1   | 13:O:103:SER:HB2  | 2.12                     | 0.50              |
| 1:A:249:VAL:HG11  | 2:B:486:LEU:HD23  | 1.92                     | 0.50              |
| 2:B:26:HIS:CE1    | 21:B:522:CLA:HMA2 | 2.47                     | 0.50              |
| 2:B:27:THR:HG22   | 2:B:107:LEU:CD1   | 2.40                     | 0.50              |
| 3:C:224:ILE:CD1   | 21:C:477:CLA:H93  | 2.42                     | 0.50              |
| 19:Z:5:PHE:CE1    | 19:Z:54:VAL:HG13  | 2.46                     | 0.50              |
| 1:A:106:LEU:HD11  | 25:A:369:BCR:H402 | 1.94                     | 0.49              |
| 1:A:239:PHE:O     | 14:T:29:ILE:HA    | 2.12                     | 0.49              |
| 28:B:533:DGD:HAW2 | 12:M:13:LEU:HD13  | 1.93                     | 0.49              |
| 3:C:155:ASN:HA    | 3:C:158:THR:CG2   | 2.38                     | 0.49              |
| 3:C:460:ASP:O     | 3:C:461:ARG:C     | 2.55                     | 0.49              |
| 1:A:96:ILE:HG12   | 1:A:105:TRP:CE2   | 2.47                     | 0.49              |
| 3:C:90:PRO:O      | 3:C:94:THR:HG23   | 2.12                     | 0.49              |
| 3:C:126:GLY:O     | 3:C:130:VAL:HG23  | 2.12                     | 0.49              |
| 3:C:391:ARG:HD2   | 3:C:395:TYR:CZ    | 2.47                     | 0.49              |
| 18:X:43:ILE:HG22  | 18:X:43:ILE:O     | 2.12                     | 0.49              |
| 1:A:192:ILE:CB    | 1:A:293:MET:HE1   | 2.42                     | 0.49              |
| 1:A:215:HIS:N     | 23:A:367:MES:H61  | 2.27                     | 0.49              |
| 27:A:373:LMG:H202 | 32:D:357:PL9:C21  | 2.40                     | 0.49              |
| 3:C:33:PHE:CE1    | 4:D:229:ALA:CB    | 2.96                     | 0.49              |
| 3:C:264:PHE:CE1   | 21:C:483:CLA:HBB1 | 2.48                     | 0.49              |
| 3:C:405:ASN:CA    | 28:C:493:DGD:HG12 | 2.42                     | 0.49              |
| 3:C:449:ARG:HG2   | 21:C:481:CLA:CED  | 2.42                     | 0.49              |
| 21:C:484:CLA:C4   | 21:C:486:CLA:HAC1 | 2.42                     | 0.49              |
| 27:D:360:LMG:H192 | 11:L:22:LEU:CD2   | 2.42                     | 0.49              |
| 2:B:256:MET:O     | 2:B:448:ARG:NH1   | 2.42                     | 0.49              |
| 13:O:178:ARG:HG3  | 13:O:178:ARG:NH1  | 2.01                     | 0.49              |
| 17:y:24:MET:O     | 17:y:25:ILE:C     | 2.55                     | 0.49              |
| 19:Z:12:LEU:HB2   | 19:Z:50:LEU:HD22  | 1.93                     | 0.49              |
| 21:A:363:CLA:H11  | 22:A:365:PHO:HMB2 | 1.94                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:165:LEU:HD21  | 21:C:482:CLA:CHC  | 2.43                     | 0.49              |
| 4:D:192:THR:HG23  | 21:D:354:CLA:CBC  | 2.39                     | 0.49              |
| 1:A:143:ILE:HD11  | 4:D:217:THR:HA    | 1.93                     | 0.49              |
| 2:B:134:ASP:OD2   | 2:B:137:LYS:HB2   | 2.12                     | 0.49              |
| 2:B:183:PRO:HB2   | 2:B:185:TRP:CH2   | 2.46                     | 0.49              |
| 2:B:286:ARG:HG2   | 2:B:286:ARG:NH1   | 2.26                     | 0.49              |
| 4:D:210:LEU:HA    | 4:D:213:ILE:HG22  | 1.95                     | 0.49              |
| 5:E:30:LEU:CD1    | 6:F:28:VAL:HG13   | 2.41                     | 0.49              |
| 7:H:53:LEU:HD12   | 18:X:19:PHE:CD1   | 2.47                     | 0.49              |
| 13:O:59:ASP:HB3   | 13:O:62:GLN:HB3   | 1.93                     | 0.49              |
| 13:O:159:VAL:HG13 | 13:O:159:VAL:O    | 2.13                     | 0.49              |
| 19:Z:5:PHE:HA     | 19:Z:57:LEU:HD21  | 1.95                     | 0.49              |
| 2:B:349:LYS:HG3   | 2:B:350:GLU:OE1   | 2.12                     | 0.49              |
| 6:F:45:ARG:NH1    | 9:J:40:LEU:OXT    | 2.46                     | 0.49              |
| 21:B:518:CLA:H161 | 21:B:519:CLA:H203 | 1.95                     | 0.49              |
| 3:C:452:ALA:O     | 3:C:453:ALA:C     | 2.55                     | 0.49              |
| 4:D:283:ALA:HA    | 21:D:354:CLA:CED  | 2.43                     | 0.49              |
| 9:J:34:ALA:O      | 9:J:35:GLY:O      | 2.31                     | 0.49              |
| 10:K:17:ILE:C     | 10:K:18:PHE:HD2   | 2.21                     | 0.49              |
| 1:A:183:MET:HE1   | 21:A:363:CLA:CMD  | 2.43                     | 0.49              |
| 1:A:190:HIS:O     | 1:A:298:ASN:HB3   | 2.13                     | 0.49              |
| 3:C:89:ILE:N      | 3:C:90:PRO:CD     | 2.75                     | 0.49              |
| 4:D:19:ASP:O      | 4:D:20:ASP:C      | 2.55                     | 0.49              |
| 27:A:373:LMG:H192 | 32:D:357:PL9:C23  | 2.43                     | 0.49              |
| 2:B:86:ILE:HD12   | 2:B:86:ILE:C      | 2.38                     | 0.49              |
| 2:B:471:ALA:HB2   | 4:D:130:PHE:HZ    | 1.73                     | 0.49              |
| 28:B:533:DGD:C3G  | 12:M:6:LEU:HD12   | 2.38                     | 0.49              |
| 3:C:109:PHE:HB3   | 3:C:110:PRO:HD3   | 1.94                     | 0.49              |
| 3:C:367:GLU:HB2   | 3:C:368:PRO:HD3   | 1.95                     | 0.49              |
| 21:C:478:CLA:CGA  | 21:C:479:CLA:H11  | 2.43                     | 0.49              |
| 21:C:481:CLA:HAA2 | 21:C:481:CLA:CBD  | 2.41                     | 0.49              |
| 4:D:126:MET:CE    | 4:D:150:ILE:HG13  | 2.43                     | 0.49              |
| 10:K:11:LEU:HD11  | 10:K:22:VAL:HG21  | 1.93                     | 0.49              |
| 11:L:12:LEU:HD22  | 12:M:25:LEU:HD12  | 1.93                     | 0.49              |
| 13:O:126:GLY:O    | 13:O:128:ASP:N    | 2.45                     | 0.49              |
| 1:A:159:LEU:C     | 1:A:162:PRO:HD2   | 2.38                     | 0.48              |
| 21:C:486:CLA:H111 | 10:K:32:PHE:HE1   | 1.77                     | 0.48              |
| 10:K:30:VAL:HA    | 21:K:483:CLA:H201 | 1.94                     | 0.48              |
| 16:V:95:ILE:O     | 16:V:99:VAL:HG23  | 2.12                     | 0.48              |
| 1:A:13:LEU:H      | 1:A:13:LEU:CD1    | 2.27                     | 0.48              |
| 2:B:435:GLU:O     | 2:B:436:THR:C     | 2.56                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:B:520:CLA:H11  | 21:B:522:CLA:H201 | 1.95                     | 0.48              |
| 3:C:48:LYS:HD2    | 3:C:138:GLU:HG3   | 1.94                     | 0.48              |
| 4:D:261:PHE:HB2   | 32:D:357:PL9:C52  | 2.43                     | 0.48              |
| 5:E:28:PRO:O      | 5:E:32:ILE:HG13   | 2.13                     | 0.48              |
| 9:J:14:ALA:HB1    | 25:J:112:BCR:H382 | 1.94                     | 0.48              |
| 13:O:226:ASN:HD22 | 13:O:226:ASN:N    | 2.11                     | 0.48              |
| 18:X:42:GLN:O     | 18:X:43:ILE:HG13  | 2.12                     | 0.48              |
| 1:A:224:ILE:O     | 1:A:226:GLU:OE2   | 2.30                     | 0.48              |
| 3:C:167:VAL:HG13  | 21:C:487:CLA:H11  | 1.96                     | 0.48              |
| 3:C:315:MET:O     | 3:C:319:ILE:HG13  | 2.12                     | 0.48              |
| 3:C:390:ARG:NH2   | 16:V:126:ILE:HD13 | 2.29                     | 0.48              |
| 21:C:486:CLA:H161 | 19:Z:20:VAL:HG13  | 1.94                     | 0.48              |
| 4:D:210:LEU:HD21  | 32:D:357:PL9:H13  | 1.95                     | 0.48              |
| 6:F:31:ILE:N      | 6:F:31:ILE:CD1    | 2.76                     | 0.48              |
| 13:O:223:ILE:HG12 | 13:O:224:SER:N    | 2.27                     | 0.48              |
| 33:V:164:HEM:HBA1 | 33:V:164:HEM:CMA  | 2.42                     | 0.48              |
| 17:y:21:GLN:O     | 17:y:21:GLN:HG2   | 2.13                     | 0.48              |
| 18:X:32:LEU:O     | 18:X:36:VAL:HG23  | 2.13                     | 0.48              |
| 2:B:35:GLY:O      | 2:B:38:ALA:HB3    | 2.13                     | 0.48              |
| 2:B:118:TRP:CH2   | 11:L:5:PRO:HD2    | 2.48                     | 0.48              |
| 4:D:60:THR:HG23   | 4:D:61:HIS:HD2    | 1.75                     | 0.48              |
| 13:O:86:ARG:HG3   | 13:O:86:ARG:NH1   | 2.26                     | 0.48              |
| 1:A:193:LEU:HD21  | 21:A:362:CLA:HMC2 | 1.96                     | 0.48              |
| 21:A:364:CLA:HMA1 | 22:D:355:PHO:H203 | 1.96                     | 0.48              |
| 2:B:154:GLY:O     | 2:B:159:THR:HG23  | 2.13                     | 0.48              |
| 3:C:296:VAL:HG23  | 3:C:297:TYR:CD2   | 2.49                     | 0.48              |
| 4:D:193:LEU:O     | 4:D:193:LEU:HG    | 2.14                     | 0.48              |
| 27:D:360:LMG:C22  | 14:T:13:ILE:HG21  | 2.36                     | 0.48              |
| 16:V:63:CYS:O     | 16:V:64:ALA:C     | 2.55                     | 0.48              |
| 1:A:13:LEU:HD12   | 1:A:13:LEU:N      | 2.28                     | 0.48              |
| 1:A:172:MET:HE1   | 21:A:363:CLA:CHC  | 2.43                     | 0.48              |
| 1:A:199:GLN:NE2   | 21:A:364:CLA:HED2 | 2.29                     | 0.48              |
| 21:A:366:CLA:C1   | 28:C:474:DGD:HB22 | 2.44                     | 0.48              |
| 2:B:10:THR:C      | 2:B:12:LEU:N      | 2.71                     | 0.48              |
| 28:B:528:DGD:HD3  | 4:D:87:HIS:ND1    | 2.29                     | 0.48              |
| 3:C:91:HIS:NE2    | 21:C:478:CLA:HBA1 | 2.28                     | 0.48              |
| 3:C:315:MET:CE    | 3:C:366:LEU:HD13  | 2.44                     | 0.48              |
| 4:D:274:VAL:HA    | 32:D:357:PL9:H253 | 1.95                     | 0.48              |
| 4:D:303:ILE:CD1   | 12:M:2:GLU:HG2    | 2.44                     | 0.48              |
| 8:I:6:ILE:O       | 8:I:10:ILE:HG12   | 2.13                     | 0.48              |
| 27:A:373:LMG:H312 | 12:M:22:LEU:HD11  | 1.95                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:B:516:CLA:H62  | 25:B:530:BCR:H342 | 1.95                     | 0.48              |
| 1:A:184:ILE:HD11  | 4:D:186:GLN:CD    | 2.38                     | 0.48              |
| 2:B:25:MET:HE3    | 25:B:527:BCR:H23C | 1.95                     | 0.48              |
| 3:C:71:GLU:OE1    | 3:C:89:ILE:HG13   | 2.13                     | 0.48              |
| 3:C:135:ARG:HB2   | 19:Z:27:TYR:CB    | 2.42                     | 0.48              |
| 3:C:442:LEU:HD21  | 21:C:481:CLA:HMB2 | 1.96                     | 0.48              |
| 21:C:480:CLA:C4   | 28:C:493:DGD:HA32 | 2.43                     | 0.48              |
| 21:C:486:CLA:C4D  | 10:K:39:TRP:HH2   | 2.26                     | 0.48              |
| 4:D:180:ARG:HH11  | 4:D:180:ARG:HG3   | 1.79                     | 0.48              |
| 16:V:64:ALA:O     | 16:V:65:SER:C     | 2.56                     | 0.48              |
| 21:B:523:CLA:H161 | 25:B:529:BCR:H312 | 1.96                     | 0.48              |
| 3:C:154:LYS:HE2   | 3:C:261:ARG:HD2   | 1.94                     | 0.48              |
| 3:C:413:GLU:HG3   | 3:C:414:ILE:H     | 1.78                     | 0.48              |
| 4:D:26:ARG:HD3    | 6:F:18:VAL:HG21   | 1.95                     | 0.48              |
| 4:D:201:VAL:O     | 4:D:205:LEU:HB2   | 2.13                     | 0.48              |
| 10:K:11:LEU:HD12  | 10:K:19:ASP:HA    | 1.96                     | 0.48              |
| 1:A:205:VAL:HG21  | 21:A:362:CLA:HMA2 | 1.96                     | 0.48              |
| 2:B:9:HIS:HB2     | 21:B:521:CLA:O1A  | 2.13                     | 0.48              |
| 21:B:512:CLA:H42  | 7:H:45:ILE:CD1    | 2.44                     | 0.48              |
| 21:B:523:CLA:H61  | 21:B:523:CLA:H41  | 1.59                     | 0.48              |
| 3:C:413:GLU:HG3   | 3:C:414:ILE:N     | 2.28                     | 0.48              |
| 4:D:146:PHE:O     | 4:D:150:ILE:HG12  | 2.14                     | 0.48              |
| 10:K:20:PRO:O     | 10:K:23:ASP:HB2   | 2.13                     | 0.48              |
| 13:O:36:ILE:HD12  | 13:O:36:ILE:N     | 2.29                     | 0.48              |
| 2:B:175:THR:O     | 2:B:176:GLY:O     | 2.31                     | 0.47              |
| 2:B:221:PRO:HA    | 21:B:519:CLA:HED3 | 1.95                     | 0.47              |
| 2:B:364:GLU:HG3   | 4:D:296:TYR:CE2   | 2.48                     | 0.47              |
| 3:C:67:MET:HE1    | 21:C:480:CLA:C1D  | 2.43                     | 0.47              |
| 3:C:457:LYS:HE3   | 4:D:228:GLY:O     | 2.13                     | 0.47              |
| 30:C:475:SQD:O8   | 4:D:233:ARG:HG3   | 2.14                     | 0.47              |
| 21:C:487:CLA:H172 | 21:C:487:CLA:HMA1 | 1.95                     | 0.47              |
| 7:H:30:LEU:HD11   | 7:H:34:PHE:HE1    | 1.78                     | 0.47              |
| 8:I:24:LEU:O      | 8:I:26:GLY:N      | 2.41                     | 0.47              |
| 12:M:8:LEU:HD21   | 29:T:226:LMT:H81  | 1.95                     | 0.47              |
| 1:A:111:PRO:O     | 1:A:115:ILE:HG13  | 2.14                     | 0.47              |
| 1:A:287:ALA:HA    | 21:A:362:CLA:HED2 | 1.96                     | 0.47              |
| 1:A:330:VAL:HG11  | 4:D:348:ARG:HG2   | 1.96                     | 0.47              |
| 2:B:106:LEU:CD2   | 21:B:516:CLA:H193 | 2.44                     | 0.47              |
| 3:C:30:SER:OG     | 4:D:233:ARG:NH2   | 2.47                     | 0.47              |
| 3:C:55:ALA:C      | 25:C:489:BCR:H373 | 2.39                     | 0.47              |
| 3:C:466:VAL:HG13  | 4:D:251:ARG:HD2   | 1.95                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:C:487:CLA:H121 | 21:C:488:CLA:H202 | 1.96                     | 0.47              |
| 4:D:93:TRP:HA     | 4:D:99:GLY:H      | 1.80                     | 0.47              |
| 5:E:22:ILE:O      | 5:E:26:THR:HG23   | 2.14                     | 0.47              |
| 6:F:33:PHE:C      | 6:F:35:GLY:H      | 2.22                     | 0.47              |
| 7:H:39:LEU:C      | 7:H:39:LEU:HD23   | 2.39                     | 0.47              |
| 13:O:79:LYS:HE2   | 13:O:89:ALA:HB3   | 1.95                     | 0.47              |
| 1:A:281:VAL:HB    | 28:C:493:DGD:HAG3 | 1.96                     | 0.47              |
| 21:B:517:CLA:H61  | 21:B:517:CLA:H41  | 1.67                     | 0.47              |
| 3:C:94:THR:HG22   | 3:C:298:PRO:HD2   | 1.96                     | 0.47              |
| 2:B:124:ARG:HG3   | 2:B:124:ARG:NH1   | 2.26                     | 0.47              |
| 2:B:124:ARG:HD3   | 2:B:131:PRO:N     | 2.30                     | 0.47              |
| 2:B:235:GLU:OE1   | 2:B:472:ARG:NH1   | 2.47                     | 0.47              |
| 32:D:357:PL9:H301 | 32:D:357:PL9:C33  | 2.45                     | 0.47              |
| 5:E:77:GLU:HA     | 5:E:80:LEU:HD23   | 1.95                     | 0.47              |
| 16:V:45:ILE:HG12  | 16:V:46:THR:N     | 2.28                     | 0.47              |
| 1:A:287:ALA:HA    | 21:A:362:CLA:CED  | 2.44                     | 0.47              |
| 26:A:371:LHG:H341 | 21:C:480:CLA:H203 | 1.96                     | 0.47              |
| 2:B:215:PHE:CD2   | 2:B:215:PHE:C     | 2.93                     | 0.47              |
| 2:B:250:PHE:CB    | 28:B:528:DGD:HB82 | 2.45                     | 0.47              |
| 2:B:265:ILE:HG13  | 2:B:266:GLU:N     | 2.30                     | 0.47              |
| 2:B:373:LYS:HA    | 2:B:373:LYS:HD2   | 1.55                     | 0.47              |
| 3:C:116:VAL:HG23  | 3:C:117:VAL:N     | 2.28                     | 0.47              |
| 4:D:176:ALA:HA    | 4:D:179:PHE:CD2   | 2.49                     | 0.47              |
| 4:D:350:ASN:O     | 4:D:352:LEU:N     | 2.42                     | 0.47              |
| 5:E:35:TRP:C      | 5:E:35:TRP:CD1    | 2.93                     | 0.47              |
| 15:U:89:GLU:CD    | 15:U:89:GLU:N     | 2.73                     | 0.47              |
| 19:Z:30:PRO:C     | 19:Z:32:ASP:N     | 2.72                     | 0.47              |
| 1:A:124:SER:O     | 1:A:127:MET:HB3   | 2.15                     | 0.47              |
| 1:A:212:CYS:HB2   | 4:D:211:CYS:HB2   | 1.96                     | 0.47              |
| 1:A:243:GLU:HA    | 4:D:241:GLU:HA    | 1.97                     | 0.47              |
| 2:B:258:TYR:CE2   | 28:B:528:DGD:O1B  | 2.67                     | 0.47              |
| 2:B:274:GLN:NE2   | 7:H:62:TRP:NE1    | 2.63                     | 0.47              |
| 2:B:348:ASN:O     | 2:B:349:LYS:C     | 2.57                     | 0.47              |
| 21:B:515:CLA:HMA2 | 21:B:516:CLA:HMA2 | 1.97                     | 0.47              |
| 3:C:29:GLU:HA     | 10:K:46:ARG:HH12  | 1.79                     | 0.47              |
| 3:C:363:GLY:O     | 3:C:364:PRO:C     | 2.56                     | 0.47              |
| 4:D:23:LYS:HZ1    | 30:D:361:SQD:C46  | 2.18                     | 0.47              |
| 4:D:32:TRP:CZ3    | 30:D:361:SQD:H282 | 2.49                     | 0.47              |
| 27:D:360:LMG:H361 | 14:T:21:ILE:HD11  | 1.97                     | 0.47              |
| 6:F:20:TRP:NE1    | 6:F:24:HIS:CE1    | 2.83                     | 0.47              |
| 9:J:14:ALA:C      | 25:J:112:BCR:H382 | 2.40                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:K:35:LEU:HA    | 10:K:38:VAL:HG23  | 1.96                     | 0.47              |
| 13:O:77:LEU:HB3   | 13:O:91:PHE:HB3   | 1.96                     | 0.47              |
| 1:A:22:THR:CG2    | 8:I:30:ARG:HD3    | 2.42                     | 0.47              |
| 2:B:24:LEU:HD21   | 21:B:526:CLA:CAB  | 2.44                     | 0.47              |
| 2:B:68:ARG:HH22   | 21:B:514:CLA:HED3 | 1.80                     | 0.47              |
| 2:B:248:ALA:HA    | 21:B:513:CLA:H42  | 1.97                     | 0.47              |
| 3:C:67:MET:HE1    | 21:C:480:CLA:CHD  | 2.45                     | 0.47              |
| 3:C:288:CYS:SG    | 28:C:491:DGD:HA21 | 2.55                     | 0.47              |
| 3:C:447:ARG:CG    | 3:C:447:ARG:NH1   | 2.74                     | 0.47              |
| 4:D:122:LEU:CD2   | 22:D:355:PHO:H62  | 2.44                     | 0.47              |
| 4:D:259:ILE:HG12  | 27:D:360:LMG:C29  | 2.44                     | 0.47              |
| 5:E:81:GLU:C      | 5:E:83:LEU:N      | 2.64                     | 0.47              |
| 8:I:30:ARG:O      | 8:I:31:ASN:HB3    | 2.14                     | 0.47              |
| 11:L:24:ILE:HD12  | 11:L:24:ILE:N     | 2.29                     | 0.47              |
| 13:O:194:TYR:CE1  | 13:O:198:ILE:HD13 | 2.49                     | 0.47              |
| 2:B:201:HIS:CE1   | 21:B:513:CLA:HMB2 | 2.49                     | 0.47              |
| 3:C:135:ARG:HB2   | 19:Z:27:TYR:CG    | 2.50                     | 0.47              |
| 4:D:134:ARG:HA    | 4:D:134:ARG:HE    | 1.78                     | 0.47              |
| 10:K:44:GLY:O     | 10:K:45:PHE:C     | 2.57                     | 0.47              |
| 1:A:176:ILE:HG23  | 21:A:363:CLA:O1D  | 2.14                     | 0.47              |
| 21:B:517:CLA:HBC3 | 25:B:529:BCR:HC8  | 1.97                     | 0.47              |
| 3:C:407:VAL:CA    | 28:C:493:DGD:HO2E | 2.26                     | 0.47              |
| 16:V:83:GLU:CD    | 16:V:83:GLU:H     | 2.23                     | 0.47              |
| 21:B:522:CLA:H12  | 21:B:525:CLA:HAA2 | 1.96                     | 0.47              |
| 3:C:365:TRP:CB    | 3:C:391:ARG:HG2   | 2.45                     | 0.47              |
| 4:D:202:ALA:HB3   | 32:D:357:PL9:C30  | 2.44                     | 0.47              |
| 13:O:135:GLN:HG2  | 13:O:141:ARG:HG3  | 1.97                     | 0.47              |
| 14:T:22:PHE:C     | 14:T:23:PHE:CD2   | 2.93                     | 0.47              |
| 1:A:129:ARG:C     | 1:A:131:TRP:H     | 2.23                     | 0.46              |
| 26:A:371:LHG:O4   | 4:D:230:SER:HA    | 2.14                     | 0.46              |
| 5:E:8:ARG:HA      | 6:F:13:TYR:CE2    | 2.50                     | 0.46              |
| 13:O:184:ASP:OD2  | 13:O:188:ARG:HB2  | 2.15                     | 0.46              |
| 2:B:270:PRO:HG3   | 2:B:312:TYR:CD2   | 2.43                     | 0.46              |
| 21:B:519:CLA:OBD  | 7:H:27:THR:HB     | 2.15                     | 0.46              |
| 3:C:127:PHE:HA    | 21:C:486:CLA:H192 | 1.96                     | 0.46              |
| 3:C:436:PHE:O     | 21:C:484:CLA:HAC1 | 2.14                     | 0.46              |
| 29:D:536:LMT:H5'  | 30:D:361:SQD:H5   | 1.97                     | 0.46              |
| 13:O:113:VAL:HA   | 13:O:119:LEU:HD23 | 1.97                     | 0.46              |
| 16:V:68:VAL:O     | 16:V:68:VAL:HG13  | 2.15                     | 0.46              |
| 18:X:12:ILE:HD13  | 18:X:12:ILE:C     | 2.40                     | 0.46              |
| 19:Z:23:VAL:HB    | 19:Z:24:PRO:HD3   | 1.97                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:105:TRP:CZ3   | 25:A:369:BCR:H371 | 2.49                     | 0.46              |
| 28:B:528:DGD:O2D  | 4:D:87:HIS:CG     | 2.54                     | 0.46              |
| 3:C:193:GLY:O     | 3:C:194:GLY:O     | 2.33                     | 0.46              |
| 4:D:261:PHE:O     | 4:D:262:SER:HB3   | 2.14                     | 0.46              |
| 16:V:148:GLU:OE1  | 16:V:148:GLU:HA   | 2.14                     | 0.46              |
| 28:B:533:DGD:HA81 | 12:M:14:PHE:CA    | 2.42                     | 0.46              |
| 3:C:208:VAL:O     | 3:C:209:ILE:C     | 2.57                     | 0.46              |
| 4:D:27:PHE:CD2    | 6:F:19:ARG:CD     | 2.97                     | 0.46              |
| 10:K:11:LEU:O     | 10:K:12:PRO:C     | 2.57                     | 0.46              |
| 1:A:12:ASN:O      | 1:A:16:ARG:HG3    | 2.15                     | 0.46              |
| 2:B:63:LEU:N      | 2:B:64:PRO:HD2    | 2.30                     | 0.46              |
| 2:B:138:MET:SD    | 21:B:525:CLA:HAC1 | 2.55                     | 0.46              |
| 2:B:234:ILE:C     | 2:B:236:THR:H     | 2.23                     | 0.46              |
| 2:B:252:VAL:HG13  | 21:B:513:CLA:H12  | 1.97                     | 0.46              |
| 3:C:265:ILE:HG13  | 21:C:481:CLA:HED1 | 1.97                     | 0.46              |
| 4:D:128:ARG:O     | 4:D:129:GLN:C     | 2.59                     | 0.46              |
| 4:D:274:VAL:HG13  | 32:D:357:PL9:H253 | 1.97                     | 0.46              |
| 13:O:82:PRO:O     | 13:O:83:LYS:CB    | 2.64                     | 0.46              |
| 16:V:102:MET:HE1  | 16:V:141:ILE:CD1  | 2.45                     | 0.46              |
| 1:A:157:VAL:HG21  | 21:A:363:CLA:CMC  | 2.45                     | 0.46              |
| 1:A:216:GLY:O     | 1:A:220:THR:HG22  | 2.16                     | 0.46              |
| 1:A:278:TRP:HB3   | 1:A:279:PRO:CD    | 2.46                     | 0.46              |
| 3:C:213:LEU:HD21  | 25:C:490:BCR:C20  | 2.46                     | 0.46              |
| 4:D:122:LEU:HB3   | 4:D:150:ILE:CD1   | 2.45                     | 0.46              |
| 11:L:31:PHE:HB3   | 11:L:35:PHE:CE1   | 2.51                     | 0.46              |
| 16:V:98:LEU:O     | 16:V:102:MET:HG3  | 2.15                     | 0.46              |
| 1:A:221:SER:HB2   | 4:D:139:ARG:O     | 2.16                     | 0.46              |
| 3:C:390:ARG:CZ    | 16:V:126:ILE:HD13 | 2.46                     | 0.46              |
| 9:J:15:THR:HA     | 25:J:112:BCR:C37  | 2.46                     | 0.46              |
| 9:J:36:LEU:C      | 9:J:38:SER:H      | 2.23                     | 0.46              |
| 17:y:42:ARG:HG2   | 17:y:42:ARG:NH1   | 2.30                     | 0.46              |
| 19:Z:5:PHE:HE1    | 19:Z:54:VAL:HG13  | 1.80                     | 0.46              |
| 1:A:45:THR:HG23   | 1:A:46:ILE:N      | 2.31                     | 0.46              |
| 1:A:330:VAL:HG12  | 4:D:348:ARG:HA    | 1.97                     | 0.46              |
| 2:B:24:LEU:HB3    | 2:B:111:ALA:HB2   | 1.96                     | 0.46              |
| 2:B:413:ASP:O     | 2:B:414:PRO:C     | 2.57                     | 0.46              |
| 3:C:42:LEU:CD2    | 21:C:486:CLA:HED3 | 2.44                     | 0.46              |
| 3:C:45:LEU:O      | 3:C:46:SER:C      | 2.58                     | 0.46              |
| 3:C:189:TRP:O     | 3:C:190:ALA:C     | 2.58                     | 0.46              |
| 3:C:229:ASN:ND2   | 3:C:232:ASP:OD1   | 2.44                     | 0.46              |
| 3:C:276:LEU:HD21  | 21:C:484:CLA:CBB  | 2.46                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:342:MET:HE1   | 3:C:356:MET:HE2   | 1.98                     | 0.46              |
| 3:C:370:ARG:HD3   | 13:O:33:TYR:CE2   | 2.51                     | 0.46              |
| 3:C:472:LEU:HD12  | 3:C:473:ASP:N     | 2.28                     | 0.46              |
| 4:D:217:THR:O     | 4:D:221:THR:HB    | 2.15                     | 0.46              |
| 7:H:35:MET:HG3    | 25:X:107:BCR:H323 | 1.98                     | 0.46              |
| 12:M:18:PRO:O     | 12:M:21:PHE:HB3   | 2.16                     | 0.46              |
| 16:V:54:GLU:OE1   | 16:V:54:GLU:HA    | 2.16                     | 0.46              |
| 17:y:39:LEU:CD2   | 19:Z:25:VAL:HG12  | 2.46                     | 0.46              |
| 1:A:96:ILE:C      | 1:A:98:GLU:H      | 2.23                     | 0.46              |
| 1:A:121:LEU:HD11  | 21:C:481:CLA:H171 | 1.98                     | 0.46              |
| 2:B:222:PRO:O     | 2:B:223:GLN:C     | 2.59                     | 0.46              |
| 2:B:298:LEU:HD12  | 2:B:298:LEU:HA    | 1.75                     | 0.46              |
| 3:C:308:GLU:HB2   | 3:C:361:PHE:CE1   | 2.51                     | 0.46              |
| 28:C:492:DGD:HBE2 | 28:C:493:DGD:HA92 | 1.97                     | 0.46              |
| 5:E:36:LEU:HA     | 5:E:39:SER:HG     | 1.79                     | 0.46              |
| 1:A:64:ARG:O      | 13:O:178:ARG:NH2  | 2.49                     | 0.46              |
| 1:A:306:VAL:HG11  | 1:A:316:THR:HG23  | 1.97                     | 0.46              |
| 3:C:39:ASN:HD21   | 21:C:486:CLA:C1C  | 2.29                     | 0.46              |
| 3:C:49:LEU:O      | 3:C:53:HIS:ND1    | 2.43                     | 0.46              |
| 3:C:142:GLU:C     | 3:C:144:SER:H     | 2.24                     | 0.46              |
| 3:C:143:TYR:O     | 3:C:144:SER:CB    | 2.64                     | 0.46              |
| 21:D:354:CLA:H101 | 22:D:355:PHO:H2   | 1.98                     | 0.46              |
| 5:E:51:ARG:O      | 5:E:53:ASP:N      | 2.49                     | 0.46              |
| 19:Z:36:SER:C     | 19:Z:38:GLN:H     | 2.24                     | 0.46              |
| 1:A:32:TRP:HA     | 1:A:32:TRP:HE3    | 1.76                     | 0.45              |
| 1:A:72:LEU:CD2    | 14:T:3:THR:HG21   | 2.46                     | 0.45              |
| 1:A:317:TRP:CD1   | 4:D:177:ALA:HB2   | 2.51                     | 0.45              |
| 1:A:326:LEU:HD21  | 3:C:412:THR:HB    | 1.98                     | 0.45              |
| 2:B:341:LYS:HA    | 2:B:405:GLU:HB2   | 1.98                     | 0.45              |
| 3:C:342:MET:HE3   | 3:C:352:GLY:HA2   | 1.98                     | 0.45              |
| 3:C:435:PHE:O     | 3:C:438:LEU:N     | 2.49                     | 0.45              |
| 3:C:451:ALA:HA    | 3:C:456:GLU:CD    | 2.41                     | 0.45              |
| 21:C:486:CLA:H8   | 25:C:489:BCR:H402 | 1.97                     | 0.45              |
| 4:D:41:ALA:HB2    | 22:D:355:PHO:C4   | 2.44                     | 0.45              |
| 27:D:359:LMG:O3   | 9:J:32:ALA:HA     | 2.16                     | 0.45              |
| 7:H:11:LEU:C      | 7:H:13:PRO:HD2    | 2.41                     | 0.45              |
| 1:A:131:TRP:CZ3   | 21:C:481:CLA:HBA2 | 2.51                     | 0.45              |
| 21:A:366:CLA:H12  | 28:C:474:DGD:HB22 | 1.98                     | 0.45              |
| 2:B:27:THR:CG2    | 2:B:107:LEU:HD13  | 2.45                     | 0.45              |
| 2:B:110:ALA:CB    | 21:B:526:CLA:HMB2 | 2.47                     | 0.45              |
| 21:B:519:CLA:C3D  | 7:H:31:MET:HB2    | 2.45                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:328:VAL:HG23  | 3:C:329:GLY:N     | 2.31                     | 0.45              |
| 5:E:64:PRO:HD3    | 5:E:84:LYS:HE2    | 1.98                     | 0.45              |
| 10:K:18:PHE:O     | 10:K:22:VAL:HG23  | 2.16                     | 0.45              |
| 1:A:39:PRO:HB2    | 21:A:366:CLA:CBB  | 2.44                     | 0.45              |
| 1:A:202:VAL:O     | 1:A:206:PHE:HB2   | 2.17                     | 0.45              |
| 2:B:15:ASP:O      | 2:B:17:GLY:N      | 2.50                     | 0.45              |
| 2:B:68:ARG:HH12   | 21:B:514:CLA:CED  | 2.30                     | 0.45              |
| 2:B:380:ASP:C     | 2:B:380:ASP:OD1   | 2.60                     | 0.45              |
| 3:C:54:VAL:HG22   | 21:C:487:CLA:HED1 | 1.99                     | 0.45              |
| 3:C:176:VAL:HG11  | 3:C:238:ILE:HG12  | 1.99                     | 0.45              |
| 3:C:210:PHE:HZ    | 3:C:243:ILE:HD11  | 1.81                     | 0.45              |
| 3:C:223:TRP:CH2   | 28:C:474:DGD:HA82 | 2.51                     | 0.45              |
| 6:F:12:SER:O      | 6:F:13:TYR:HB2    | 2.16                     | 0.45              |
| 13:O:144:LEU:CD1  | 13:O:259:VAL:HG11 | 2.45                     | 0.45              |
| 15:U:56:ASP:HB3   | 15:U:60:THR:H     | 1.80                     | 0.45              |
| 1:A:255:PHE:HD2   | 1:A:264:SER:HG    | 1.63                     | 0.45              |
| 2:B:68:ARG:HH12   | 21:B:514:CLA:HED1 | 1.81                     | 0.45              |
| 21:B:518:CLA:H102 | 21:B:518:CLA:C14  | 2.41                     | 0.45              |
| 28:B:528:DGD:C6D  | 28:B:528:DGD:C5E  | 2.94                     | 0.45              |
| 3:C:276:LEU:CD1   | 3:C:444:HIS:HD2   | 2.30                     | 0.45              |
| 4:D:14:TRP:CE3    | 18:X:38:ILE:HD12  | 2.52                     | 0.45              |
| 6:F:23:VAL:O      | 6:F:23:VAL:HG22   | 2.17                     | 0.45              |
| 6:F:33:PHE:C      | 6:F:35:GLY:N      | 2.74                     | 0.45              |
| 13:O:190:LEU:HD12 | 15:U:41:ASN:CG    | 2.41                     | 0.45              |
| 19:Z:35:ARG:HG3   | 19:Z:36:SER:N     | 2.30                     | 0.45              |
| 1:A:309:ALA:HB2   | 5:E:52:PRO:C      | 2.42                     | 0.45              |
| 2:B:306:PRO:HG2   | 2:B:309:LEU:HB2   | 1.97                     | 0.45              |
| 21:B:515:CLA:H41  | 21:B:515:CLA:H61  | 1.51                     | 0.45              |
| 3:C:35:TRP:CG     | 3:C:36:TRP:N      | 2.84                     | 0.45              |
| 3:C:245:ILE:O     | 3:C:249:ILE:HG12  | 2.16                     | 0.45              |
| 3:C:258:GLY:CA    | 3:C:262:ARG:HH12  | 2.28                     | 0.45              |
| 4:D:126:MET:HE3   | 4:D:150:ILE:HG13  | 1.99                     | 0.45              |
| 5:E:10:PHE:CZ     | 6:F:19:ARG:HD2    | 2.51                     | 0.45              |
| 9:J:14:ALA:HB1    | 25:J:112:BCR:C26  | 2.46                     | 0.45              |
| 13:O:56:TYR:O     | 13:O:161:SER:HA   | 2.17                     | 0.45              |
| 13:O:88:GLU:HG2   | 13:O:89:ALA:N     | 2.31                     | 0.45              |
| 15:U:99:GLU:HA    | 15:U:102:LYS:HE3  | 1.99                     | 0.45              |
| 16:V:30:THR:O     | 16:V:34:LEU:HG    | 2.17                     | 0.45              |
| 26:A:371:LHG:HC11 | 3:C:447:ARG:CZ    | 2.46                     | 0.45              |
| 21:B:516:CLA:HBB1 | 21:B:516:CLA:HHC  | 1.99                     | 0.45              |
| 21:B:517:CLA:C1   | 28:B:533:DGD:HB32 | 2.46                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:168:LEU:HD13  | 21:C:483:CLA:C4   | 2.45                     | 0.45              |
| 3:C:318:LEU:HD23  | 3:C:318:LEU:O     | 2.16                     | 0.45              |
| 10:K:18:PHE:O     | 10:K:19:ASP:C     | 2.60                     | 0.45              |
| 15:U:80:VAL:HG22  | 15:U:127:ARG:HH21 | 1.82                     | 0.45              |
| 15:U:80:VAL:HG22  | 15:U:127:ARG:NH2  | 2.31                     | 0.45              |
| 1:A:38:ILE:HB     | 25:A:369:BCR:H331 | 1.99                     | 0.45              |
| 2:B:364:GLU:HG3   | 4:D:296:TYR:CD2   | 2.52                     | 0.45              |
| 7:H:21:VAL:HG23   | 7:H:22:ALA:O      | 2.16                     | 0.45              |
| 1:A:221:SER:HB3   | 4:D:141:TYR:HB2   | 1.98                     | 0.45              |
| 21:A:363:CLA:H2   | 27:A:373:LMG:H242 | 1.99                     | 0.45              |
| 2:B:62:VAL:HG11   | 21:B:515:CLA:HED3 | 1.99                     | 0.45              |
| 2:B:463:PHE:C     | 2:B:463:PHE:CD2   | 2.94                     | 0.45              |
| 3:C:258:GLY:C     | 3:C:262:ARG:NH1   | 2.74                     | 0.45              |
| 4:D:56:THR:HB     | 5:E:49:THR:HG23   | 1.97                     | 0.45              |
| 4:D:213:ILE:HG23  | 4:D:214:HIS:N     | 2.30                     | 0.45              |
| 13:O:92:VAL:HG12  | 13:O:93:PRO:CD    | 2.43                     | 0.45              |
| 1:A:11:ALA:HB1    | 1:A:15:GLU:OE1    | 2.17                     | 0.45              |
| 27:A:373:LMG:O10  | 27:A:373:LMG:O9   | 2.34                     | 0.45              |
| 2:B:10:THR:O      | 2:B:13:ILE:HG13   | 2.16                     | 0.45              |
| 2:B:422:ARG:HG2   | 2:B:422:ARG:HH11  | 1.82                     | 0.45              |
| 3:C:33:PHE:HE1    | 4:D:229:ALA:CB    | 2.29                     | 0.45              |
| 3:C:258:GLY:HA3   | 3:C:262:ARG:HH12  | 1.81                     | 0.45              |
| 13:O:69:LEU:HB3   | 13:O:107:ILE:CB   | 2.35                     | 0.45              |
| 13:O:132:VAL:O    | 13:O:144:LEU:HD23 | 2.17                     | 0.45              |
| 14:T:22:PHE:C     | 14:T:23:PHE:HD2   | 2.24                     | 0.45              |
| 2:B:71:VAL:HG21   | 2:B:96:VAL:CG2    | 2.47                     | 0.45              |
| 2:B:247:PHE:CD2   | 21:B:513:CLA:H111 | 2.52                     | 0.45              |
| 3:C:163:PHE:CD1   | 3:C:252:ILE:HD11  | 2.52                     | 0.45              |
| 3:C:225:VAL:HG13  | 3:C:289:PHE:HA    | 1.99                     | 0.45              |
| 21:C:479:CLA:H61  | 21:C:479:CLA:H41  | 1.58                     | 0.45              |
| 4:D:67:TYR:CE1    | 4:D:76:VAL:HG11   | 2.51                     | 0.45              |
| 15:U:100:ARG:NH1  | 15:U:103:GLN:HG2  | 2.31                     | 0.45              |
| 16:V:119:PRO:HG3  | 16:V:127:PHE:CD1  | 2.52                     | 0.45              |
| 27:A:373:LMG:H171 | 11:L:23:LEU:HD13  | 1.99                     | 0.44              |
| 2:B:141:ILE:O     | 2:B:144:PHE:HB3   | 2.17                     | 0.44              |
| 2:B:225:LEU:O     | 2:B:226:TYR:C     | 2.60                     | 0.44              |
| 2:B:385:ARG:O     | 2:B:386:ALA:C     | 2.60                     | 0.44              |
| 2:B:450:TRP:HB3   | 21:B:517:CLA:CMB  | 2.47                     | 0.44              |
| 25:B:529:BCR:H361 | 25:B:529:BCR:H20C | 1.80                     | 0.44              |
| 3:C:68:THR:OG1    | 21:C:479:CLA:CED  | 2.63                     | 0.44              |
| 3:C:110:PRO:O     | 3:C:114:VAL:HG23  | 2.17                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:337:LEU:CD1   | 13:O:131:PRO:HG3  | 2.47                     | 0.44              |
| 5:E:14:ILE:CG2    | 9:J:13:VAL:HG11   | 2.47                     | 0.44              |
| 13:O:173:ASN:ND2  | 13:O:220:LYS:HD3  | 2.32                     | 0.44              |
| 2:B:18:ARG:HD2    | 2:B:115:TRP:CE3   | 2.52                     | 0.44              |
| 4:D:122:LEU:CG    | 22:D:355:PHO:H62  | 2.47                     | 0.44              |
| 5:E:34:GLY:HA2    | 6:F:32:PHE:CE2    | 2.53                     | 0.44              |
| 7:H:9:ASP:O       | 7:H:12:ARG:HB3    | 2.17                     | 0.44              |
| 7:H:28:THR:O      | 7:H:31:MET:HB3    | 2.18                     | 0.44              |
| 8:I:4:LEU:O       | 8:I:8:VAL:HG23    | 2.17                     | 0.44              |
| 2:B:148:LEU:HG    | 21:B:514:CLA:H193 | 1.99                     | 0.44              |
| 3:C:334:PRO:HA    | 13:O:179:THR:OG1  | 2.17                     | 0.44              |
| 3:C:436:PHE:HB3   | 21:K:483:CLA:H93  | 1.99                     | 0.44              |
| 25:D:358:BCR:H331 | 25:D:358:BCR:C8   | 2.47                     | 0.44              |
| 27:D:360:LMG:H221 | 14:T:13:ILE:CG2   | 2.38                     | 0.44              |
| 6:F:36:ALA:O      | 6:F:38:ALA:N      | 2.50                     | 0.44              |
| 7:H:16:SER:C      | 7:H:18:TYR:H      | 2.25                     | 0.44              |
| 18:X:16:LEU:HD11  | 18:X:20:PHE:CE2   | 2.53                     | 0.44              |
| 1:A:185:VAL:O     | 1:A:186:PHE:C     | 2.61                     | 0.44              |
| 3:C:264:PHE:CE2   | 21:C:482:CLA:O1A  | 2.66                     | 0.44              |
| 3:C:269:GLU:O     | 3:C:272:LEU:HB3   | 2.18                     | 0.44              |
| 9:J:22:ILE:HG21   | 27:J:492:LMG:C20  | 2.45                     | 0.44              |
| 10:K:17:ILE:N     | 10:K:17:ILE:CD1   | 2.81                     | 0.44              |
| 13:O:116:ASP:OD2  | 13:O:116:ASP:C    | 2.58                     | 0.44              |
| 15:U:89:GLU:C     | 15:U:91:VAL:N     | 2.76                     | 0.44              |
| 1:A:182:PHE:O     | 1:A:186:PHE:HB2   | 2.18                     | 0.44              |
| 2:B:71:VAL:HG21   | 2:B:96:VAL:HG21   | 1.99                     | 0.44              |
| 21:B:512:CLA:C20  | 28:B:528:DGD:HB91 | 2.48                     | 0.44              |
| 3:C:28:GLN:CB     | 21:C:486:CLA:HED2 | 2.47                     | 0.44              |
| 3:C:276:LEU:HD21  | 21:C:484:CLA:HBB1 | 1.99                     | 0.44              |
| 4:D:190:ASN:HB2   | 4:D:296:TYR:CD1   | 2.52                     | 0.44              |
| 4:D:253:TRP:HB2   | 4:D:260:ALA:HB2   | 2.00                     | 0.44              |
| 15:U:72:TYR:CB    | 15:U:73:PRO:CD    | 2.92                     | 0.44              |
| 16:V:59:PHE:CD1   | 16:V:63:CYS:SG    | 3.08                     | 0.44              |
| 16:V:81:ARG:HG2   | 16:V:81:ARG:HH11  | 1.83                     | 0.44              |
| 1:A:60:ILE:HG23   | 1:A:61:ASP:N      | 2.32                     | 0.44              |
| 2:B:201:HIS:HD2   | 2:B:202:HIS:ND1   | 2.16                     | 0.44              |
| 4:D:333:ASP:C     | 4:D:335:PRO:HD3   | 2.43                     | 0.44              |
| 5:E:15:THR:CG2    | 9:J:7:ARG:HB3     | 2.47                     | 0.44              |
| 6:F:36:ALA:O      | 6:F:39:ALA:N      | 2.51                     | 0.44              |
| 17:y:32:GLY:N     | 17:y:33:PRO:HD2   | 2.32                     | 0.44              |
| 1:A:333:GLU:HB2   | 1:A:337:HIS:HE1   | 1.83                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:15:ASP:O      | 2:B:16:PRO:C      | 2.60                     | 0.44              |
| 4:D:185:PHE:CE2   | 4:D:289:LEU:HD12  | 2.52                     | 0.44              |
| 4:D:209:LEU:O     | 4:D:213:ILE:HG22  | 2.18                     | 0.44              |
| 7:H:41:PHE:O      | 7:H:45:ILE:HG23   | 2.18                     | 0.44              |
| 1:A:110:GLY:O     | 1:A:111:PRO:C     | 2.60                     | 0.44              |
| 2:B:444:ARG:HH11  | 2:B:444:ARG:HG3   | 1.82                     | 0.44              |
| 3:C:394:GLU:OE2   | 3:C:398:HIS:CD2   | 2.71                     | 0.44              |
| 4:D:202:ALA:HB3   | 32:D:357:PL9:H302 | 2.00                     | 0.44              |
| 32:D:357:PL9:C43  | 27:D:360:LMG:C25  | 2.95                     | 0.44              |
| 13:O:120:THR:HG22 | 13:O:154:SER:CB   | 2.47                     | 0.44              |
| 18:X:44:ASP:O     | 18:X:45:LYS:HB3   | 2.17                     | 0.44              |
| 1:A:129:ARG:C     | 1:A:131:TRP:N     | 2.76                     | 0.44              |
| 1:A:220:THR:O     | 1:A:223:LEU:HG    | 2.18                     | 0.44              |
| 2:B:187:PRO:C     | 2:B:189:GLY:H     | 2.26                     | 0.44              |
| 2:B:366:PHE:CD1   | 2:B:367:PRO:HD2   | 2.53                     | 0.44              |
| 21:B:517:CLA:CBC  | 25:B:529:BCR:H10C | 2.48                     | 0.44              |
| 3:C:54:VAL:HA     | 21:C:487:CLA:HED1 | 2.00                     | 0.44              |
| 3:C:82:TYR:HA     | 3:C:422:PRO:HG2   | 2.00                     | 0.44              |
| 3:C:92:ILE:HD11   | 21:C:479:CLA:HED2 | 1.99                     | 0.44              |
| 4:D:154:VAL:O     | 4:D:158:LEU:HB2   | 2.18                     | 0.44              |
| 4:D:221:THR:CG2   | 4:D:244:TYR:HB2   | 2.48                     | 0.44              |
| 25:D:358:BCR:C39  | 9:J:21:VAL:HG11   | 2.48                     | 0.44              |
| 27:D:360:LMG:H111 | 27:D:360:LMG:H292 | 1.98                     | 0.44              |
| 5:E:63:ILE:HG23   | 5:E:64:PRO:HD2    | 1.99                     | 0.44              |
| 7:H:44:ILE:HG12   | 18:X:19:PHE:CZ    | 2.52                     | 0.44              |
| 1:A:217:SER:O     | 1:A:220:THR:HG22  | 2.18                     | 0.43              |
| 2:B:283:GLU:OE1   | 2:B:283:GLU:HA    | 2.17                     | 0.43              |
| 2:B:447:PRO:O     | 2:B:448:ARG:C     | 2.60                     | 0.43              |
| 21:C:487:CLA:HBB1 | 21:C:487:CLA:HHC  | 2.00                     | 0.43              |
| 21:C:488:CLA:C1   | 21:C:488:CLA:HAA1 | 2.47                     | 0.43              |
| 4:D:67:TYR:OH     | 27:D:359:LMG:H291 | 2.18                     | 0.43              |
| 5:E:74:GLN:HG3    | 5:E:75:GLN:N      | 2.31                     | 0.43              |
| 6:F:45:ARG:NH2    | 6:F:45:ARG:HB3    | 2.33                     | 0.43              |
| 8:I:27:ASP:O      | 8:I:28:PRO:C      | 2.59                     | 0.43              |
| 10:K:17:ILE:O     | 10:K:17:ILE:HG22  | 2.17                     | 0.43              |
| 10:K:20:PRO:HB2   | 17:y:21:GLN:CB    | 2.48                     | 0.43              |
| 13:O:59:ASP:C     | 13:O:61:SER:N     | 2.76                     | 0.43              |
| 26:A:371:LHG:HC32 | 4:D:229:ALA:O     | 2.18                     | 0.43              |
| 2:B:206:GLY:O     | 2:B:210:ILE:HG13  | 2.18                     | 0.43              |
| 2:B:271:THR:CG2   | 2:B:273:TYR:HB2   | 2.48                     | 0.43              |
| 2:B:484:PRO:O     | 2:B:485:GLU:HG2   | 2.18                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:B:518:CLA:C1   | 4:D:127:LEU:HD21  | 2.48                     | 0.43              |
| 28:B:533:DGD:HA32 | 12:M:10:ALA:HB1   | 2.00                     | 0.43              |
| 3:C:235:GLY:O     | 3:C:238:ILE:HB    | 2.18                     | 0.43              |
| 4:D:101:PHE:O     | 4:D:104:TRP:HB3   | 2.18                     | 0.43              |
| 21:D:356:CLA:C4   | 18:X:26:GLY:HA3   | 2.47                     | 0.43              |
| 13:O:116:ASP:OD1  | 13:O:157:PRO:HB3  | 2.18                     | 0.43              |
| 13:O:225:LEU:N    | 13:O:225:LEU:HD12 | 2.33                     | 0.43              |
| 16:V:39:ASN:HD21  | 16:V:43:LYS:HB3   | 1.82                     | 0.43              |
| 1:A:29:TYR:OH     | 1:A:132:GLU:OE2   | 2.26                     | 0.43              |
| 1:A:198:HIS:O     | 1:A:202:VAL:HG12  | 2.18                     | 0.43              |
| 2:B:164:PRO:HG2   | 2:B:165:GLY:H     | 1.82                     | 0.43              |
| 2:B:434:THR:HG21  | 13:O:204:LYS:HE3  | 1.97                     | 0.43              |
| 2:B:463:PHE:CE1   | 28:B:528:DGD:CFA  | 3.01                     | 0.43              |
| 3:C:242:LEU:O     | 3:C:243:ILE:C     | 2.61                     | 0.43              |
| 3:C:338:GLY:O     | 3:C:339:LYS:C     | 2.60                     | 0.43              |
| 3:C:390:ARG:NE    | 16:V:126:ILE:CG2  | 2.82                     | 0.43              |
| 3:C:416:SER:OG    | 16:V:68:VAL:HG23  | 2.17                     | 0.43              |
| 4:D:238:THR:O     | 4:D:239:GLN:C     | 2.60                     | 0.43              |
| 4:D:329:MET:O     | 4:D:330:ALA:C     | 2.61                     | 0.43              |
| 5:E:72:ALA:O      | 5:E:76:VAL:HG23   | 2.18                     | 0.43              |
| 10:K:20:PRO:O     | 17:y:21:GLN:HG3   | 2.18                     | 0.43              |
| 19:Z:5:PHE:CG     | 19:Z:61:VAL:HG21  | 2.53                     | 0.43              |
| 19:Z:17:PHE:HE2   | 19:Z:21:ILE:HD11  | 1.84                     | 0.43              |
| 1:A:210:LEU:C     | 1:A:210:LEU:CD2   | 2.92                     | 0.43              |
| 2:B:327:THR:HG22  | 21:B:517:CLA:C1   | 2.49                     | 0.43              |
| 2:B:348:ASN:OD1   | 2:B:352:GLU:HB2   | 2.18                     | 0.43              |
| 21:B:514:CLA:H142 | 21:B:525:CLA:H52  | 2.01                     | 0.43              |
| 28:B:533:DGD:HA32 | 12:M:10:ALA:CB    | 2.49                     | 0.43              |
| 3:C:33:PHE:CD1    | 4:D:229:ALA:HB3   | 2.54                     | 0.43              |
| 3:C:362:ARG:CG    | 28:C:491:DGD:HE61 | 2.48                     | 0.43              |
| 3:C:370:ARG:HD3   | 13:O:33:TYR:CD2   | 2.54                     | 0.43              |
| 4:D:176:ALA:C     | 4:D:178:ILE:H     | 2.26                     | 0.43              |
| 10:K:18:PHE:CE1   | 19:Z:9:LEU:HG     | 2.53                     | 0.43              |
| 10:K:30:VAL:N     | 21:K:483:CLA:H191 | 2.34                     | 0.43              |
| 13:O:72:GLN:O     | 13:O:263:GLY:HA3  | 2.17                     | 0.43              |
| 15:U:54:LYS:HD2   | 15:U:113:THR:CG2  | 2.49                     | 0.43              |
| 1:A:309:ALA:HB3   | 5:E:53:ASP:HA     | 2.00                     | 0.43              |
| 2:B:238:LEU:N     | 21:B:522:CLA:HMD1 | 2.33                     | 0.43              |
| 2:B:247:PHE:HD2   | 21:B:513:CLA:H111 | 1.83                     | 0.43              |
| 21:B:512:CLA:CAA  | 7:H:45:ILE:HD12   | 2.48                     | 0.43              |
| 3:C:60:ILE:CG2    | 21:C:479:CLA:HMD1 | 2.48                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:72:LEU:HG     | 10:K:10:LYS:N     | 2.33                     | 0.43              |
| 21:C:486:CLA:H122 | 10:K:32:PHE:CE1   | 2.53                     | 0.43              |
| 5:E:38:VAL:CG2    | 6:F:36:ALA:HB1    | 2.47                     | 0.43              |
| 13:O:70:CYS:O     | 13:O:265:PHE:HB2  | 2.18                     | 0.43              |
| 19:Z:36:SER:HA    | 19:Z:39:LEU:CD1   | 2.48                     | 0.43              |
| 1:A:12:ASN:O      | 1:A:13:LEU:C      | 2.60                     | 0.43              |
| 1:A:63:ILE:HB     | 3:C:335:THR:HG21  | 1.99                     | 0.43              |
| 3:C:160:ILE:HA    | 3:C:163:PHE:CD2   | 2.53                     | 0.43              |
| 5:E:8:ARG:HA      | 6:F:13:TYR:CZ     | 2.52                     | 0.43              |
| 19:Z:22:GLY:O     | 19:Z:23:VAL:C     | 2.61                     | 0.43              |
| 1:A:42:LEU:HA     | 1:A:45:THR:HG22   | 2.00                     | 0.43              |
| 1:A:187:GLN:HB2   | 21:A:362:CLA:CAC  | 2.48                     | 0.43              |
| 27:A:373:LMG:H301 | 12:M:22:LEU:HD22  | 1.99                     | 0.43              |
| 2:B:252:VAL:HG11  | 21:B:514:CLA:OBD  | 2.18                     | 0.43              |
| 2:B:284:ILE:HG23  | 2:B:305:ILE:CD1   | 2.48                     | 0.43              |
| 3:C:128:GLY:N     | 21:C:488:CLA:HAC2 | 2.33                     | 0.43              |
| 4:D:62:GLY:HA3    | 5:E:63:ILE:HD13   | 2.00                     | 0.43              |
| 4:D:253:TRP:HA    | 4:D:256:ILE:HG23  | 2.01                     | 0.43              |
| 29:I:274:LMT:H6D  | 13:O:95:LYS:NZ    | 2.34                     | 0.43              |
| 10:K:46:ARG:NH1   | 10:K:46:ARG:HB2   | 2.34                     | 0.43              |
| 2:B:263:THR:HB    | 2:B:448:ARG:HH12  | 1.82                     | 0.43              |
| 2:B:289:GLN:OE1   | 2:B:292:LEU:HD12  | 2.19                     | 0.43              |
| 3:C:50:LEU:O      | 3:C:54:VAL:HG23   | 2.17                     | 0.43              |
| 3:C:433:LEU:HD13  | 21:C:478:CLA:CHC  | 2.49                     | 0.43              |
| 3:C:455:PHE:C     | 3:C:457:LYS:H     | 2.26                     | 0.43              |
| 3:C:473:ASP:HA    | 14:T:27:PRO:HD2   | 2.01                     | 0.43              |
| 4:D:263:ASN:O     | 4:D:265:ARG:N     | 2.52                     | 0.43              |
| 4:D:291:LEU:O     | 4:D:292:ASN:HB2   | 2.18                     | 0.43              |
| 13:O:109:GLY:HA3  | 13:O:122:VAL:O    | 2.18                     | 0.43              |
| 13:O:171:GLU:HA   | 13:O:221:GLY:O    | 2.19                     | 0.43              |
| 17:y:31:ALA:O     | 17:y:35:ILE:HG23  | 2.19                     | 0.43              |
| 18:X:44:ASP:C     | 18:X:45:LYS:CD    | 2.92                     | 0.43              |
| 2:B:33:TRP:NE1    | 21:B:517:CLA:HMC2 | 2.34                     | 0.43              |
| 2:B:327:THR:O     | 2:B:444:ARG:NE    | 2.46                     | 0.43              |
| 4:D:161:PRO:HB3   | 4:D:170:ALA:HB2   | 2.01                     | 0.43              |
| 7:H:55:LEU:HB2    | 7:H:58:VAL:CG1    | 2.49                     | 0.43              |
| 12:M:33:GLN:HG2   | 12:M:34:LYS:N     | 2.33                     | 0.43              |
| 17:y:41:VAL:C     | 17:y:43:ARG:N     | 2.71                     | 0.43              |
| 18:X:32:LEU:HD23  | 18:X:32:LEU:H     | 1.83                     | 0.43              |
| 1:A:157:VAL:HG21  | 21:A:363:CLA:HMC1 | 2.00                     | 0.43              |
| 3:C:33:PHE:CE1    | 4:D:229:ALA:HB3   | 2.54                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:48:LYS:CD     | 3:C:138:GLU:HG3   | 2.49                     | 0.43              |
| 3:C:55:ALA:HB1    | 25:C:489:BCR:C37  | 2.49                     | 0.43              |
| 3:C:56:HIS:C      | 3:C:58:GLY:H      | 2.27                     | 0.43              |
| 3:C:310:SER:HG    | 3:C:355:THR:HG23  | 1.84                     | 0.43              |
| 3:C:453:ALA:C     | 8:I:34:ARG:HB2    | 2.44                     | 0.43              |
| 28:C:492:DGD:HB41 | 9:J:29:PHE:CZ     | 2.54                     | 0.43              |
| 4:D:199:MET:O     | 4:D:200:GLY:C     | 2.60                     | 0.43              |
| 8:I:20:VAL:C      | 8:I:22:GLY:H      | 2.26                     | 0.43              |
| 10:K:43:VAL:O     | 10:K:46:ARG:HG3   | 2.19                     | 0.43              |
| 12:M:1:MET:HG2    | 12:M:2:GLU:H      | 1.84                     | 0.43              |
| 16:V:103:LYS:O    | 16:V:122:ARG:HG2  | 2.19                     | 0.43              |
| 17:y:20:ALA:HA    | 17:y:22:LEU:HD12  | 2.01                     | 0.43              |
| 1:A:45:THR:CB     | 22:A:365:PHO:H8   | 2.48                     | 0.42              |
| 1:A:247:ASN:HB3   | 1:A:250:ALA:HB3   | 2.00                     | 0.42              |
| 1:A:286:THR:CG2   | 21:A:362:CLA:HED3 | 2.35                     | 0.42              |
| 2:B:222:PRO:HG3   | 7:H:27:THR:N      | 2.28                     | 0.42              |
| 2:B:275:TRP:CH2   | 2:B:358:ARG:HD3   | 2.54                     | 0.42              |
| 2:B:413:ASP:OD1   | 2:B:416:THR:HB    | 2.19                     | 0.42              |
| 3:C:63:TRP:O      | 3:C:64:ALA:C      | 2.62                     | 0.42              |
| 21:C:484:CLA:H41  | 21:C:484:CLA:H62  | 1.64                     | 0.42              |
| 21:C:487:CLA:H172 | 21:C:487:CLA:HMA3 | 2.00                     | 0.42              |
| 4:D:125:PHE:O     | 4:D:128:ARG:HB3   | 2.19                     | 0.42              |
| 5:E:34:GLY:O      | 5:E:37:PHE:HB3    | 2.19                     | 0.42              |
| 9:J:12:ILE:O      | 9:J:16:VAL:HG23   | 2.19                     | 0.42              |
| 15:U:91:VAL:HG13  | 15:U:92:LEU:N     | 2.33                     | 0.42              |
| 1:A:55:ALA:HA     | 25:A:369:BCR:C27  | 2.50                     | 0.42              |
| 1:A:340:PRO:HG3   | 15:U:133:TYR:CG   | 2.55                     | 0.42              |
| 28:B:528:DGD:HD61 | 28:B:528:DGD:C5E  | 2.48                     | 0.42              |
| 3:C:164:HIS:CB    | 21:C:483:CLA:HED3 | 2.49                     | 0.42              |
| 3:C:164:HIS:HB2   | 21:C:483:CLA:HED3 | 2.00                     | 0.42              |
| 3:C:318:LEU:HG    | 3:C:328:VAL:CG1   | 2.48                     | 0.42              |
| 4:D:279:LEU:HD22  | 21:D:354:CLA:HMA2 | 2.01                     | 0.42              |
| 12:M:33:GLN:CG    | 12:M:34:LYS:N     | 2.82                     | 0.42              |
| 18:X:44:ASP:C     | 18:X:45:LYS:HD3   | 2.44                     | 0.42              |
| 1:A:239:PHE:HB3   | 14:T:28:ARG:O     | 2.19                     | 0.42              |
| 1:A:291:SER:HB3   | 3:C:431:PHE:CE2   | 2.54                     | 0.42              |
| 2:B:105:GLY:O     | 2:B:108:PHE:HB3   | 2.19                     | 0.42              |
| 2:B:349:LYS:HG2   | 2:B:395:GLN:O     | 2.19                     | 0.42              |
| 3:C:29:GLU:CB     | 10:K:46:ARG:NH1   | 2.80                     | 0.42              |
| 3:C:101:PRO:O     | 3:C:104:GLU:HB2   | 2.19                     | 0.42              |
| 3:C:155:ASN:C     | 3:C:158:THR:HG22  | 2.45                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:203:THR:O     | 3:C:235:GLY:HA3   | 2.20                     | 0.42              |
| 3:C:259:TRP:C     | 3:C:261:ARG:N     | 2.74                     | 0.42              |
| 3:C:406:SER:HA    | 3:C:420:VAL:CG2   | 2.49                     | 0.42              |
| 10:K:20:PRO:HB2   | 17:y:21:GLN:HB3   | 2.01                     | 0.42              |
| 26:A:371:LHG:H351 | 21:K:483:CLA:H71  | 2.01                     | 0.42              |
| 27:A:373:LMG:HC92 | 2:B:5:TRP:NE1     | 2.32                     | 0.42              |
| 2:B:251:VAL:HB    | 21:B:513:CLA:C4   | 2.50                     | 0.42              |
| 3:C:37:ALA:O      | 21:C:484:CLA:HBA1 | 2.19                     | 0.42              |
| 3:C:202:PRO:HB2   | 3:C:235:GLY:HA2   | 2.01                     | 0.42              |
| 21:C:483:CLA:H61  | 21:C:483:CLA:H41  | 1.92                     | 0.42              |
| 5:E:60:GLN:HG2    | 5:E:62:SER:H      | 1.84                     | 0.42              |
| 12:M:19:SER:O     | 12:M:23:ILE:HG13  | 2.18                     | 0.42              |
| 13:O:59:ASP:O     | 13:O:61:SER:N     | 2.53                     | 0.42              |
| 13:O:230:VAL:CG1  | 13:O:231:ASP:N    | 2.70                     | 0.42              |
| 16:V:130:MET:SD   | 16:V:133:LEU:HD12 | 2.60                     | 0.42              |
| 1:A:207:GLY:O     | 1:A:210:LEU:HB3   | 2.20                     | 0.42              |
| 2:B:433:ASP:OD1   | 2:B:433:ASP:C     | 2.61                     | 0.42              |
| 3:C:162:GLY:O     | 3:C:166:ILE:HG13  | 2.18                     | 0.42              |
| 3:C:223:TRP:CE3   | 3:C:224:ILE:HG13  | 2.53                     | 0.42              |
| 6:F:21:VAL:O      | 6:F:22:ALA:C      | 2.62                     | 0.42              |
| 10:K:16:ALA:O     | 10:K:19:ASP:HB2   | 2.20                     | 0.42              |
| 17:y:42:ARG:O     | 17:y:43:ARG:C     | 2.61                     | 0.42              |
| 1:A:33:PHE:CE2    | 21:C:481:CLA:O1A  | 2.73                     | 0.42              |
| 1:A:160:ILE:HD11  | 28:C:491:DGD:C9A  | 2.50                     | 0.42              |
| 1:A:222:SER:O     | 1:A:246:TYR:HB2   | 2.19                     | 0.42              |
| 2:B:330:MET:SD    | 2:B:446:SER:HB3   | 2.59                     | 0.42              |
| 21:B:524:CLA:H41  | 21:B:524:CLA:H61  | 1.85                     | 0.42              |
| 21:B:526:CLA:C1D  | 7:H:7:LEU:HD23    | 2.50                     | 0.42              |
| 3:C:205:ASP:OD1   | 3:C:207:ARG:HB3   | 2.19                     | 0.42              |
| 3:C:396:MET:HE1   | 16:V:73:LYS:O     | 2.19                     | 0.42              |
| 3:C:464:GLU:HA    | 3:C:465:PRO:HD2   | 1.72                     | 0.42              |
| 21:C:477:CLA:C2D  | 21:C:479:CLA:H2   | 2.50                     | 0.42              |
| 5:E:69:ARG:HG3    | 5:E:70:PHE:N      | 2.34                     | 0.42              |
| 13:O:168:PHE:O    | 13:O:224:SER:HA   | 2.19                     | 0.42              |
| 3:C:414:ILE:HG22  | 3:C:415:ASN:N     | 2.35                     | 0.42              |
| 28:C:493:DGD:HBW1 | 27:D:359:LMG:H181 | 2.02                     | 0.42              |
| 5:E:35:TRP:CG     | 6:F:39:ALA:HB2    | 2.55                     | 0.42              |
| 11:L:36:PHE:O     | 11:L:37:ASN:C     | 2.61                     | 0.42              |
| 1:A:21:VAL:HG11   | 1:A:32:TRP:CE3    | 2.55                     | 0.42              |
| 1:A:39:PRO:CB     | 21:A:366:CLA:HBB1 | 2.45                     | 0.42              |
| 1:A:273:PHE:CD1   | 26:A:371:LHG:H242 | 2.55                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:16:PRO:HB3    | 2:B:133:LEU:HD21  | 2.02                     | 0.42              |
| 2:B:179:GLN:HA    | 2:B:180:PRO:HD3   | 1.92                     | 0.42              |
| 2:B:222:PRO:HB3   | 7:H:26:GLY:N      | 2.34                     | 0.42              |
| 2:B:413:ASP:O     | 2:B:413:ASP:CG    | 2.63                     | 0.42              |
| 3:C:365:TRP:HB3   | 3:C:391:ARG:HG2   | 2.02                     | 0.42              |
| 26:C:476:LHG:H171 | 28:C:492:DGD:HBN1 | 2.00                     | 0.42              |
| 4:D:52:THR:HG22   | 4:D:67:TYR:CE2    | 2.54                     | 0.42              |
| 5:E:78:THR:HA     | 5:E:81:GLU:HG2    | 2.02                     | 0.42              |
| 10:K:43:VAL:CG2   | 10:K:46:ARG:HE    | 2.33                     | 0.42              |
| 30:L:213:SQD:H82  | 27:M:217:LMG:H152 | 2.01                     | 0.42              |
| 1:A:42:LEU:HA     | 1:A:45:THR:CG2    | 2.49                     | 0.42              |
| 1:A:210:LEU:C     | 1:A:210:LEU:HD23  | 2.45                     | 0.42              |
| 1:A:234:ASN:CB    | 27:A:373:LMG:HC3  | 2.48                     | 0.42              |
| 1:A:317:TRP:O     | 1:A:321:ILE:HG13  | 2.20                     | 0.42              |
| 2:B:191:ASN:HB2   | 7:H:58:VAL:HG22   | 2.00                     | 0.42              |
| 2:B:448:ARG:HH11  | 2:B:448:ARG:HG3   | 1.84                     | 0.42              |
| 3:C:84:GLN:C      | 3:C:86:LEU:HD13   | 2.45                     | 0.42              |
| 3:C:125:LEU:HG    | 25:Z:116:BCR:C36  | 2.49                     | 0.42              |
| 3:C:148:GLY:O     | 3:C:156:LYS:NZ    | 2.51                     | 0.42              |
| 28:C:492:DGD:HB52 | 25:J:115:BCR:C35  | 2.47                     | 0.42              |
| 5:E:15:THR:HG23   | 9:J:8:ILE:N       | 2.34                     | 0.42              |
| 7:H:35:MET:HA     | 25:X:107:BCR:C32  | 2.50                     | 0.42              |
| 8:I:7:THR:O       | 8:I:8:VAL:C       | 2.63                     | 0.42              |
| 8:I:17:LEU:O      | 8:I:18:LEU:C      | 2.61                     | 0.42              |
| 8:I:20:VAL:C      | 8:I:22:GLY:N      | 2.77                     | 0.42              |
| 13:O:248:ASP:CG   | 13:O:250:ASP:H    | 2.27                     | 0.42              |
| 29:O:274:LMT:H5'  | 29:O:274:LMT:H1B  | 1.92                     | 0.42              |
| 15:U:41:ASN:O     | 15:U:42:VAL:C     | 2.62                     | 0.42              |
| 22:A:365:PHO:HAC2 | 4:D:212:ALA:HB3   | 2.01                     | 0.42              |
| 27:A:373:LMG:C31  | 12:M:22:LEU:HD21  | 2.50                     | 0.42              |
| 2:B:243:ALA:HB2   | 2:B:466:HIS:CE1   | 2.54                     | 0.42              |
| 2:B:338:GLN:HB2   | 2:B:431:GLU:O     | 2.20                     | 0.42              |
| 2:B:472:ARG:HG2   | 2:B:472:ARG:HH11  | 1.84                     | 0.42              |
| 3:C:140:LEU:HB2   | 3:C:148:GLY:HA2   | 2.02                     | 0.42              |
| 3:C:279:LEU:HD23  | 3:C:282:MET:HE3   | 2.01                     | 0.42              |
| 3:C:461:ARG:HG3   | 3:C:461:ARG:NH1   | 2.32                     | 0.42              |
| 4:D:261:PHE:N     | 32:D:357:PL9:O1   | 2.51                     | 0.42              |
| 7:H:18:TYR:CG     | 7:H:19:GLY:N      | 2.85                     | 0.42              |
| 10:K:30:VAL:CA    | 21:K:483:CLA:H191 | 2.50                     | 0.42              |
| 16:V:153:GLY:O    | 16:V:154:ASP:C    | 2.62                     | 0.42              |
| 27:A:373:LMG:C25  | 27:D:360:LMG:C21  | 2.97                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:A:373:LMG:C31  | 11:L:20:GLY:HA2   | 2.49                     | 0.41              |
| 27:A:373:LMG:H131 | 4:D:273:PHE:CE2   | 2.55                     | 0.41              |
| 2:B:18:ARG:HD3    | 2:B:118:TRP:HB3   | 2.01                     | 0.41              |
| 2:B:280:PHE:O     | 2:B:284:ILE:HG13  | 2.20                     | 0.41              |
| 28:B:533:DGD:HG11 | 12:M:6:LEU:HD12   | 2.02                     | 0.41              |
| 21:C:486:CLA:H122 | 10:K:32:PHE:HE1   | 1.85                     | 0.41              |
| 4:D:204:VAL:HG22  | 4:D:279:LEU:HD21  | 2.01                     | 0.41              |
| 6:F:9:GLU:C       | 6:F:11:VAL:N      | 2.78                     | 0.41              |
| 6:F:45:ARG:CZ     | 9:J:40:LEU:OXT    | 2.68                     | 0.41              |
| 9:J:15:THR:O      | 25:J:112:BCR:H372 | 2.19                     | 0.41              |
| 13:O:227:VAL:CG1  | 13:O:228:ALA:N    | 2.82                     | 0.41              |
| 16:V:119:PRO:HA   | 16:V:127:PHE:CD2  | 2.55                     | 0.41              |
| 1:A:104:GLU:OE2   | 13:O:99:ARG:HD3   | 2.20                     | 0.41              |
| 1:A:131:TRP:CH2   | 21:C:481:CLA:CBA  | 2.99                     | 0.41              |
| 1:A:228:THR:HB    | 1:A:231:GLU:HB3   | 2.01                     | 0.41              |
| 3:C:405:ASN:HB2   | 28:C:493:DGD:O6D  | 2.20                     | 0.41              |
| 3:C:417:VAL:C     | 28:C:493:DGD:O3E  | 2.62                     | 0.41              |
| 21:C:478:CLA:O1A  | 21:C:479:CLA:HBD  | 2.19                     | 0.41              |
| 4:D:122:LEU:HG    | 22:D:355:PHO:H62  | 2.02                     | 0.41              |
| 7:H:27:THR:O      | 7:H:28:THR:C      | 2.63                     | 0.41              |
| 17:y:36:ILE:O     | 17:y:39:LEU:HB2   | 2.20                     | 0.41              |
| 1:A:236:GLY:HA3   | 4:D:265:ARG:NH1   | 2.35                     | 0.41              |
| 1:A:332:HIS:HB3   | 4:D:321:LEU:HD21  | 2.01                     | 0.41              |
| 2:B:260:SER:C     | 2:B:262:THR:H     | 2.28                     | 0.41              |
| 2:B:260:SER:C     | 2:B:262:THR:N     | 2.76                     | 0.41              |
| 2:B:326:ARG:HH21  | 4:D:297:ASP:CG    | 2.28                     | 0.41              |
| 3:C:125:LEU:HD22  | 21:C:487:CLA:HED3 | 2.00                     | 0.41              |
| 3:C:315:MET:HE1   | 3:C:369:LEU:CD1   | 2.45                     | 0.41              |
| 4:D:302:GLU:OE1   | 4:D:302:GLU:HA    | 2.20                     | 0.41              |
| 14:T:16:LEU:O     | 14:T:17:PHE:C     | 2.63                     | 0.41              |
| 15:U:50:ALA:HB1   | 15:U:113:THR:HG21 | 2.01                     | 0.41              |
| 15:U:75:LEU:O     | 15:U:79:ILE:HG13  | 2.20                     | 0.41              |
| 15:U:82:ASN:ND2   | 15:U:94:ILE:HG23  | 2.34                     | 0.41              |
| 1:A:10:SER:OG     | 1:A:13:LEU:HD12   | 2.20                     | 0.41              |
| 1:A:193:LEU:HD21  | 21:A:362:CLA:CMC  | 2.50                     | 0.41              |
| 2:B:170:ASP:HB2   | 2:B:171:PRO:HD2   | 2.02                     | 0.41              |
| 21:B:513:CLA:H203 | 21:B:519:CLA:H92  | 2.02                     | 0.41              |
| 3:C:72:LEU:O      | 10:K:10:LYS:N     | 2.52                     | 0.41              |
| 3:C:109:PHE:CD2   | 27:C:494:LMG:H112 | 2.55                     | 0.41              |
| 3:C:264:PHE:HE2   | 21:C:482:CLA:CGA  | 2.33                     | 0.41              |
| 3:C:292:PHE:CD2   | 28:C:491:DGD:HG31 | 2.55                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:456:GLU:N     | 3:C:456:GLU:OE1   | 2.53                     | 0.41              |
| 4:D:176:ALA:C     | 4:D:178:ILE:N     | 2.78                     | 0.41              |
| 4:D:189:HIS:O     | 4:D:190:ASN:C     | 2.63                     | 0.41              |
| 4:D:274:VAL:HG13  | 32:D:357:PL9:H222 | 2.02                     | 0.41              |
| 15:U:55:ILE:HG21  | 15:U:65:PHE:CE1   | 2.56                     | 0.41              |
| 19:Z:5:PHE:CD2    | 19:Z:61:VAL:HG21  | 2.54                     | 0.41              |
| 1:A:205:VAL:HG21  | 21:A:362:CLA:CMA  | 2.51                     | 0.41              |
| 1:A:260:PHE:CD1   | 1:A:260:PHE:C     | 2.98                     | 0.41              |
| 1:A:292:THR:C     | 1:A:294:ALA:H     | 2.28                     | 0.41              |
| 21:B:521:CLA:HBB2 | 21:B:523:CLA:HMB3 | 2.01                     | 0.41              |
| 27:B:531:LMG:C2   | 4:D:141:TYR:OH    | 2.67                     | 0.41              |
| 3:C:55:ALA:CB     | 25:C:489:BCR:H373 | 2.51                     | 0.41              |
| 26:C:476:LHG:H242 | 26:C:476:LHG:H121 | 2.02                     | 0.41              |
| 4:D:205:LEU:HD12  | 4:D:205:LEU:HA    | 1.71                     | 0.41              |
| 4:D:259:ILE:HG21  | 27:D:360:LMG:H292 | 2.01                     | 0.41              |
| 6:F:28:VAL:CB     | 6:F:29:PRO:HD3    | 2.46                     | 0.41              |
| 7:H:31:MET:HE3    | 7:H:35:MET:CE     | 2.40                     | 0.41              |
| 9:J:11:TRP:CE2    | 9:J:12:ILE:HG12   | 2.55                     | 0.41              |
| 11:L:22:LEU:O     | 11:L:26:VAL:HG13  | 2.21                     | 0.41              |
| 13:O:215:ARG:NE   | 15:U:39:LEU:HD22  | 2.34                     | 0.41              |
| 1:A:190:HIS:HB3   | 1:A:293:MET:CE    | 2.43                     | 0.41              |
| 1:A:296:ASN:HB2   | 3:C:400:PRO:O     | 2.20                     | 0.41              |
| 1:A:307:ILE:HG13  | 6:F:45:ARG:CD     | 2.49                     | 0.41              |
| 2:B:328:GLY:N     | 21:B:517:CLA:O1A  | 2.54                     | 0.41              |
| 3:C:75:PHE:CD1    | 3:C:86:LEU:HD21   | 2.48                     | 0.41              |
| 3:C:272:LEU:O     | 3:C:273:SER:C     | 2.63                     | 0.41              |
| 3:C:464:GLU:O     | 3:C:467:LEU:HB2   | 2.19                     | 0.41              |
| 4:D:161:PRO:CB    | 4:D:170:ALA:HB2   | 2.51                     | 0.41              |
| 7:H:55:LEU:O      | 7:H:56:ASP:C      | 2.62                     | 0.41              |
| 10:K:28:ILE:O     | 10:K:31:LEU:HB2   | 2.21                     | 0.41              |
| 13:O:36:ILE:O     | 13:O:37:VAL:C     | 2.63                     | 0.41              |
| 15:U:59:ASN:O     | 15:U:60:THR:C     | 2.64                     | 0.41              |
| 16:V:121:LEU:C    | 16:V:123:SER:H    | 2.28                     | 0.41              |
| 19:Z:24:PRO:C     | 19:Z:26:ALA:N     | 2.76                     | 0.41              |
| 1:A:12:ASN:O      | 1:A:15:GLU:HB3    | 2.20                     | 0.41              |
| 1:A:105:TRP:CZ3   | 1:A:111:PRO:HG3   | 2.55                     | 0.41              |
| 1:A:155:PHE:CD1   | 28:C:491:DGD:HAE2 | 2.56                     | 0.41              |
| 2:B:12:LEU:O      | 2:B:14:ASN:N      | 2.54                     | 0.41              |
| 2:B:127:ARG:C     | 2:B:127:ARG:HD2   | 2.45                     | 0.41              |
| 2:B:289:GLN:OE1   | 2:B:289:GLN:HA    | 2.21                     | 0.41              |
| 2:B:479:PHE:O     | 2:B:480:SER:CB    | 2.68                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:187:ASP:HB2   | 3:C:230:LEU:CD1   | 2.48                     | 0.41              |
| 3:C:321:ASP:HA    | 3:C:324:LEU:HD23  | 2.01                     | 0.41              |
| 4:D:263:ASN:O     | 4:D:266:TRP:N     | 2.50                     | 0.41              |
| 13:O:136:MET:O    | 13:O:137:ALA:C    | 2.63                     | 0.41              |
| 13:O:184:ASP:C    | 13:O:184:ASP:OD1  | 2.63                     | 0.41              |
| 15:U:58:ASN:HD22  | 15:U:114:VAL:HG13 | 1.84                     | 0.41              |
| 1:A:83:VAL:HA     | 1:A:84:PRO:HD3    | 1.85                     | 0.41              |
| 1:A:277:ALA:O     | 1:A:281:VAL:HG23  | 2.21                     | 0.41              |
| 2:B:49:ASP:HA     | 2:B:50:PRO:HD2    | 1.88                     | 0.41              |
| 2:B:160:GLY:O     | 2:B:161:LEU:C     | 2.63                     | 0.41              |
| 2:B:220:ARG:NH1   | 7:H:20:LYS:O      | 2.51                     | 0.41              |
| 3:C:259:TRP:O     | 3:C:260:ALA:C     | 2.62                     | 0.41              |
| 21:C:480:CLA:HHC  | 21:C:480:CLA:HBB1 | 2.03                     | 0.41              |
| 5:E:44:TYR:OH     | 6:F:43:ILE:HD13   | 2.21                     | 0.41              |
| 6:F:24:HIS:HE1    | 33:F:85:HEM:ND    | 2.19                     | 0.41              |
| 6:F:38:ALA:HB1    | 9:J:27:LEU:CD2    | 2.50                     | 0.41              |
| 7:H:13:PRO:HG2    | 7:H:14:LEU:H      | 1.85                     | 0.41              |
| 9:J:9:PRO:HB2     | 9:J:12:ILE:HG13   | 2.03                     | 0.41              |
| 13:O:120:THR:HA   | 13:O:153:ALA:O    | 2.21                     | 0.41              |
| 15:U:75:LEU:HD21  | 15:U:101:GLN:HB3  | 2.03                     | 0.41              |
| 16:V:124:ALA:HB1  | 16:V:131:ARG:CG   | 2.51                     | 0.41              |
| 1:A:114:LEU:HD23  | 1:A:114:LEU:O     | 2.21                     | 0.41              |
| 1:A:279:PRO:HG2   | 4:D:212:ALA:HB2   | 2.01                     | 0.41              |
| 2:B:76:SER:HG     | 2:B:78:TRP:CD1    | 2.39                     | 0.41              |
| 2:B:305:ILE:HA    | 2:B:306:PRO:HD2   | 1.88                     | 0.41              |
| 2:B:354:LEU:HD12  | 2:B:378:LYS:HB2   | 2.02                     | 0.41              |
| 2:B:475:PHE:HB3   | 2:B:478:VAL:CG2   | 2.51                     | 0.41              |
| 3:C:67:MET:HE1    | 21:C:480:CLA:C4C  | 2.51                     | 0.41              |
| 3:C:175:LEU:HA    | 21:C:478:CLA:H141 | 2.02                     | 0.41              |
| 3:C:199:ILE:N     | 3:C:199:ILE:CD1   | 2.83                     | 0.41              |
| 25:C:489:BCR:H20C | 25:C:489:BCR:H361 | 1.87                     | 0.41              |
| 16:V:58:LEU:HD13  | 16:V:137:ASP:HB3  | 2.02                     | 0.41              |
| 1:A:18:CYS:O      | 1:A:22:THR:CG2    | 2.69                     | 0.41              |
| 1:A:131:TRP:CE3   | 1:A:132:GLU:CA    | 3.03                     | 0.41              |
| 1:A:278:TRP:CH2   | 28:C:493:DGD:HBV1 | 2.56                     | 0.41              |
| 21:A:364:CLA:H91  | 21:D:354:CLA:H203 | 2.02                     | 0.41              |
| 2:B:191:ASN:OD1   | 2:B:193:TYR:N     | 2.52                     | 0.41              |
| 3:C:62:PHE:HE2    | 10:K:29:PRO:HD3   | 1.86                     | 0.41              |
| 3:C:267:SER:O     | 3:C:271:TYR:CD2   | 2.74                     | 0.41              |
| 3:C:318:LEU:C     | 3:C:318:LEU:CD2   | 2.94                     | 0.41              |
| 4:D:84:SER:HB2    | 4:D:85:MET:HE2    | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:64:PRO:HB3    | 5:E:84:LYS:CD     | 2.51                     | 0.41              |
| 6:F:31:ILE:HG12   | 33:F:85:HEM:HMC2  | 2.03                     | 0.41              |
| 6:F:37:ILE:O      | 6:F:37:ILE:HG22   | 2.20                     | 0.41              |
| 7:H:10:ILE:H      | 7:H:10:ILE:HG13   | 1.70                     | 0.41              |
| 13:O:73:PRO:HG2   | 13:O:102:THR:HB   | 2.03                     | 0.41              |
| 13:O:147:THR:OG1  | 13:O:148:VAL:N    | 2.54                     | 0.41              |
| 16:V:160:LYS:HA   | 16:V:163:TYR:CD2  | 2.57                     | 0.41              |
| 1:A:234:ASN:HD22  | 1:A:234:ASN:HA    | 1.66                     | 0.40              |
| 21:A:363:CLA:H92  | 32:D:357:PL9:H422 | 2.02                     | 0.40              |
| 2:B:238:LEU:HD13  | 21:B:522:CLA:C2D  | 2.51                     | 0.40              |
| 2:B:414:PRO:CB    | 2:B:415:PRO:HD3   | 2.40                     | 0.40              |
| 2:B:457:VAL:O     | 2:B:458:PHE:C     | 2.62                     | 0.40              |
| 3:C:64:ALA:HB2    | 21:C:479:CLA:C2D  | 2.51                     | 0.40              |
| 3:C:216:SER:HA    | 28:C:474:DGD:HG12 | 2.03                     | 0.40              |
| 3:C:271:TYR:CE1   | 21:C:483:CLA:CAC  | 3.04                     | 0.40              |
| 3:C:307:PRO:HG3   | 3:C:358:PHE:CD1   | 2.56                     | 0.40              |
| 3:C:308:GLU:HG3   | 3:C:361:PHE:CZ    | 2.56                     | 0.40              |
| 3:C:327:ASN:HB3   | 13:O:125:ASP:OD1  | 2.21                     | 0.40              |
| 3:C:369:LEU:CD2   | 3:C:384:ILE:HD13  | 2.51                     | 0.40              |
| 4:D:190:ASN:HB2   | 4:D:296:TYR:CE1   | 2.55                     | 0.40              |
| 4:D:274:VAL:HG22  | 32:D:357:PL9:H253 | 2.03                     | 0.40              |
| 10:K:28:ILE:O     | 10:K:29:PRO:C     | 2.61                     | 0.40              |
| 12:M:10:ALA:O     | 12:M:14:PHE:HB2   | 2.21                     | 0.40              |
| 12:M:31:SER:HA    | 27:M:217:LMG:HC72 | 2.03                     | 0.40              |
| 15:U:91:VAL:C     | 15:U:93:ASN:N     | 2.78                     | 0.40              |
| 17:y:20:ALA:O     | 17:y:23:THR:HG22  | 2.21                     | 0.40              |
| 17:y:46:LEU:N     | 17:y:46:LEU:HD23  | 2.36                     | 0.40              |
| 1:A:141:PRO:O     | 1:A:143:ILE:N     | 2.53                     | 0.40              |
| 1:A:288:LEU:O     | 1:A:292:THR:HB    | 2.21                     | 0.40              |
| 2:B:224:ARG:NE    | 7:H:25:TRP:HE1    | 2.19                     | 0.40              |
| 2:B:472:ARG:HE    | 21:B:521:CLA:HED2 | 1.86                     | 0.40              |
| 21:B:518:CLA:H11  | 4:D:127:LEU:HD21  | 2.04                     | 0.40              |
| 21:B:525:CLA:H62  | 21:B:525:CLA:H41  | 1.72                     | 0.40              |
| 3:C:116:VAL:CG2   | 3:C:117:VAL:N     | 2.84                     | 0.40              |
| 3:C:188:THR:CG2   | 3:C:298:PRO:HB3   | 2.50                     | 0.40              |
| 4:D:90:LEU:O      | 21:D:356:CLA:HED1 | 2.21                     | 0.40              |
| 5:E:15:THR:HG22   | 9:J:8:ILE:H       | 1.83                     | 0.40              |
| 5:E:84:LYS:HB2    | 5:E:84:LYS:HZ3    | 1.79                     | 0.40              |
| 6:F:45:ARG:CB     | 6:F:45:ARG:HH21   | 2.35                     | 0.40              |
| 25:J:115:BCR:H20C | 25:J:115:BCR:H361 | 1.96                     | 0.40              |
| 13:O:226:ASN:N    | 13:O:226:ASN:ND2  | 2.68                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:217:SER:HA    | 1:A:220:THR:CG2   | 2.51                     | 0.40              |
| 27:A:373:LMG:C20  | 32:D:357:PL9:C21  | 2.92                     | 0.40              |
| 21:B:513:CLA:CBB  | 21:B:515:CLA:H171 | 2.42                     | 0.40              |
| 21:B:517:CLA:C2   | 28:B:533:DGD:HB52 | 2.52                     | 0.40              |
| 3:C:59:LEU:HD11   | 25:C:489:BCR:H372 | 2.03                     | 0.40              |
| 3:C:350:ILE:CG2   | 3:C:359:TRP:HB2   | 2.51                     | 0.40              |
| 7:H:53:LEU:HD21   | 7:H:55:LEU:HD21   | 2.03                     | 0.40              |
| 9:J:24:ILE:HG23   | 9:J:25:VAL:N      | 2.37                     | 0.40              |
| 10:K:34:ALA:O     | 10:K:37:PHE:HB2   | 2.20                     | 0.40              |
| 13:O:157:PRO:O    | 13:O:158:ASN:O    | 2.38                     | 0.40              |
| 13:O:208:LEU:O    | 13:O:209:ALA:C    | 2.63                     | 0.40              |
| 18:X:11:THR:OG1   | 25:X:107:BCR:H282 | 2.21                     | 0.40              |
| 1:A:258:LEU:O     | 4:D:128:ARG:NH1   | 2.55                     | 0.40              |
| 2:B:150:CYS:HA    | 21:B:513:CLA:CBC  | 2.52                     | 0.40              |
| 2:B:272:ARG:HG3   | 2:B:273:TYR:N     | 2.36                     | 0.40              |
| 21:B:522:CLA:H102 | 21:B:522:CLA:H13  | 1.86                     | 0.40              |
| 3:C:127:PHE:CE1   | 19:Z:23:VAL:HG21  | 2.54                     | 0.40              |
| 21:C:483:CLA:H121 | 25:C:490:BCR:H362 | 2.04                     | 0.40              |
| 21:C:486:CLA:C14  | 19:Z:24:PRO:HG2   | 2.51                     | 0.40              |
| 4:D:84:SER:HB3    | 5:E:68:ASP:HA     | 2.04                     | 0.40              |
| 4:D:185:PHE:HE2   | 4:D:289:LEU:HD12  | 1.87                     | 0.40              |
| 4:D:239:GLN:HB3   | 4:D:240:ALA:H     | 1.33                     | 0.40              |
| 27:D:360:LMG:H361 | 14:T:21:ILE:CD1   | 2.51                     | 0.40              |
| 5:E:30:LEU:CD2    | 6:F:28:VAL:HG13   | 2.51                     | 0.40              |
| 21:K:483:CLA:HHC  | 21:K:483:CLA:HBB1 | 2.03                     | 0.40              |
| 13:O:49:ASP:CG    | 13:O:50:ASP:N     | 2.79                     | 0.40              |
| 1:A:72:LEU:HD23   | 14:T:3:THR:HG21   | 2.03                     | 0.40              |
| 1:A:113:GLN:O     | 1:A:114:LEU:C     | 2.65                     | 0.40              |
| 1:A:116:ILE:HG13  | 1:A:117:PHE:N     | 2.37                     | 0.40              |
| 1:A:214:MET:HB2   | 23:A:367:MES:H61  | 1.99                     | 0.40              |
| 1:A:238:LYS:HA    | 1:A:238:LYS:HD3   | 1.86                     | 0.40              |
| 1:A:244:GLU:CD    | 1:A:245:THR:H     | 2.27                     | 0.40              |
| 2:B:153:PHE:O     | 2:B:157:HIS:HB3   | 2.22                     | 0.40              |
| 2:B:262:THR:HG21  | 21:B:513:CLA:HBA1 | 2.03                     | 0.40              |
| 2:B:483:ASP:CB    | 2:B:484:PRO:CD    | 2.97                     | 0.40              |
| 3:C:141:GLU:HA    | 3:C:148:GLY:HA3   | 2.04                     | 0.40              |
| 21:C:481:CLA:O1A  | 8:I:23:PHE:CE1    | 2.74                     | 0.40              |
| 4:D:17:ILE:HG21   | 18:X:42:GLN:HG3   | 2.03                     | 0.40              |
| 4:D:279:LEU:CD1   | 21:D:354:CLA:CBA  | 3.00                     | 0.40              |
| 6:F:42:PHE:N      | 6:F:42:PHE:CD1    | 2.90                     | 0.40              |
| 7:H:7:LEU:HG      | 7:H:11:LEU:CD1    | 2.52                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 13:O:215:ARG:HD2 | 15:U:39:LEU:HD22 | 2.04                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 1   | A     | 333/344 (97%) | 285 (86%) | 41 (12%) | 7 (2%)   | 5           | 31  |
| 2   | B     | 483/510 (95%) | 416 (86%) | 54 (11%) | 13 (3%)  | 4           | 27  |
| 3   | C     | 446/461 (97%) | 370 (83%) | 60 (14%) | 16 (4%)  | 2           | 22  |
| 4   | D     | 338/352 (96%) | 286 (85%) | 43 (13%) | 9 (3%)   | 4           | 27  |
| 5   | E     | 75/83 (90%)   | 66 (88%)  | 5 (7%)   | 4 (5%)   | 1           | 14  |
| 6   | F     | 36/44 (82%)   | 22 (61%)  | 9 (25%)  | 5 (14%)  | 0           | 3   |
| 7   | H     | 63/65 (97%)   | 45 (71%)  | 9 (14%)  | 9 (14%)  | 0           | 3   |
| 8   | I     | 33/38 (87%)   | 20 (61%)  | 11 (33%) | 2 (6%)   | 1           | 13  |
| 9   | J     | 32/40 (80%)   | 26 (81%)  | 4 (12%)  | 2 (6%)   | 1           | 12  |
| 10  | K     | 35/37 (95%)   | 26 (74%)  | 7 (20%)  | 2 (6%)   | 1           | 13  |
| 11  | L     | 35/37 (95%)   | 33 (94%)  | 2 (6%)   | 0        | 100         | 100 |
| 12  | M     | 32/36 (89%)   | 23 (72%)  | 9 (28%)  | 0        | 100         | 100 |
| 13  | O     | 241/246 (98%) | 201 (83%) | 29 (12%) | 11 (5%)  | 2           | 17  |
| 14  | T     | 28/32 (88%)   | 25 (89%)  | 3 (11%)  | 0        | 100         | 100 |
| 15  | U     | 95/104 (91%)  | 79 (83%)  | 12 (13%) | 4 (4%)   | 2           | 19  |
| 16  | V     | 135/137 (98%) | 111 (82%) | 23 (17%) | 1 (1%)   | 18          | 51  |
| 17  | y     | 26/46 (56%)   | 14 (54%)  | 8 (31%)  | 4 (15%)  | 0           | 2   |
| 18  | X     | 33/40 (82%)   | 25 (76%)  | 5 (15%)  | 3 (9%)   | 0           | 6   |
| 19  | Z     | 60/62 (97%)   | 48 (80%)  | 9 (15%)  | 3 (5%)   | 1           | 16  |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| All | All   | 2559/2714 (94%) | 2121 (83%) | 343 (13%) | 95 (4%)  | 2           | 21 |

All (95) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 12  | ASN  |
| 1   | A     | 141 | PRO  |
| 1   | A     | 142 | TRP  |
| 2   | B     | 176 | GLY  |
| 2   | B     | 230 | ARG  |
| 2   | B     | 484 | PRO  |
| 3   | C     | 144 | SER  |
| 3   | C     | 257 | PHE  |
| 3   | C     | 416 | SER  |
| 3   | C     | 452 | ALA  |
| 4   | D     | 239 | GLN  |
| 4   | D     | 240 | ALA  |
| 4   | D     | 262 | SER  |
| 5   | E     | 82  | GLN  |
| 7   | H     | 18  | TYR  |
| 7   | H     | 63  | LYS  |
| 8   | I     | 25  | SER  |
| 9   | J     | 35  | GLY  |
| 13  | O     | 52  | ALA  |
| 15  | U     | 72  | TYR  |
| 15  | U     | 83  | ALA  |
| 16  | V     | 75  | ASN  |
| 17  | y     | 43  | ARG  |
| 19  | Z     | 32  | ASP  |
| 2   | B     | 349 | LYS  |
| 3   | C     | 46  | SER  |
| 3   | C     | 136 | GLY  |
| 3   | C     | 194 | GLY  |
| 3   | C     | 209 | ILE  |
| 3   | C     | 456 | GLU  |
| 4   | D     | 234 | ALA  |
| 4   | D     | 264 | LYS  |
| 6   | F     | 37  | ILE  |
| 7   | H     | 26  | GLY  |
| 9   | J     | 38  | SER  |
| 13  | O     | 83  | LYS  |
| 13  | O     | 231 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | U     | 73  | PRO  |
| 17  | y     | 25  | ILE  |
| 18  | X     | 43  | ILE  |
| 2   | B     | 13  | ILE  |
| 2   | B     | 127 | ARG  |
| 2   | B     | 183 | PRO  |
| 2   | B     | 414 | PRO  |
| 2   | B     | 436 | THR  |
| 3   | C     | 32  | GLY  |
| 3   | C     | 141 | GLU  |
| 3   | C     | 375 | LEU  |
| 3   | C     | 453 | ALA  |
| 4   | D     | 263 | ASN  |
| 5   | E     | 9   | PRO  |
| 6   | F     | 17  | THR  |
| 7   | H     | 16  | SER  |
| 7   | H     | 64  | ALA  |
| 10  | K     | 13  | GLU  |
| 10  | K     | 45  | PHE  |
| 13  | O     | 60  | SER  |
| 13  | O     | 158 | ASN  |
| 13  | O     | 165 | SER  |
| 19  | Z     | 24  | PRO  |
| 19  | Z     | 28  | ALA  |
| 2   | B     | 173 | GLY  |
| 2   | B     | 231 | MET  |
| 2   | B     | 235 | GLU  |
| 3   | C     | 154 | LYS  |
| 4   | D     | 73  | PHE  |
| 5   | E     | 10  | PHE  |
| 13  | O     | 51  | THR  |
| 17  | y     | 24  | MET  |
| 18  | X     | 44  | ASP  |
| 1   | A     | 97  | TRP  |
| 3   | C     | 462 | GLU  |
| 6   | F     | 13  | TYR  |
| 7   | H     | 6   | TRP  |
| 7   | H     | 65  | LEU  |
| 15  | U     | 42  | VAL  |
| 18  | X     | 12  | ILE  |
| 1   | A     | 334 | ARG  |
| 4   | D     | 351 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | H     | 14  | LEU  |
| 1   | A     | 21  | VAL  |
| 2   | B     | 16  | PRO  |
| 13  | O     | 159 | VAL  |
| 3   | C     | 201 | ASN  |
| 6   | F     | 9   | GLU  |
| 6   | F     | 11  | VAL  |
| 17  | y     | 35  | ILE  |
| 5   | E     | 52  | PRO  |
| 7   | H     | 60  | VAL  |
| 8   | I     | 32  | PRO  |
| 13  | O     | 232 | GLY  |
| 1   | A     | 176 | ILE  |
| 4   | D     | 160 | TYR  |
| 13  | O     | 127 | ILE  |
| 13  | O     | 152 | VAL  |

### 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%) | 255 (94%) | 16 (6%)  | 18          | 45 |
| 2   | B     | 385/407 (95%) | 368 (96%) | 17 (4%)  | 25          | 52 |
| 3   | C     | 348/362 (96%) | 332 (95%) | 16 (5%)  | 24          | 51 |
| 4   | D     | 275/283 (97%) | 257 (94%) | 18 (6%)  | 15          | 43 |
| 5   | E     | 69/72 (96%)   | 63 (91%)  | 6 (9%)   | 9           | 34 |
| 6   | F     | 32/38 (84%)   | 31 (97%)  | 1 (3%)   | 35          | 59 |
| 7   | H     | 53/54 (98%)   | 49 (92%)  | 4 (8%)   | 12          | 39 |
| 8   | I     | 32/35 (91%)   | 30 (94%)  | 2 (6%)   | 16          | 44 |
| 9   | J     | 24/28 (86%)   | 23 (96%)  | 1 (4%)   | 26          | 53 |
| 10  | K     | 30/30 (100%)  | 27 (90%)  | 3 (10%)  | 7           | 30 |
| 11  | L     | 35/35 (100%)  | 31 (89%)  | 4 (11%)  | 5           | 26 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 12  | M     | 31/33 (94%)     | 30 (97%)   | 1 (3%)   | 34          | 58 |
| 13  | O     | 202/208 (97%)   | 194 (96%)  | 8 (4%)   | 28          | 54 |
| 14  | T     | 27/29 (93%)     | 26 (96%)   | 1 (4%)   | 30          | 56 |
| 15  | U     | 84/89 (94%)     | 80 (95%)   | 4 (5%)   | 23          | 50 |
| 16  | V     | 116/117 (99%)   | 112 (97%)  | 4 (3%)   | 32          | 57 |
| 17  | y     | 20/37 (54%)     | 17 (85%)   | 3 (15%)  | 3           | 17 |
| 18  | X     | 28/33 (85%)     | 23 (82%)   | 5 (18%)  | 2           | 11 |
| 19  | Z     | 52/52 (100%)    | 47 (90%)   | 5 (10%)  | 8           | 32 |
| All | All   | 2114/2222 (95%) | 1995 (94%) | 119 (6%) | 19          | 47 |

All (119) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 12  | ASN  |
| 1   | A     | 30  | VAL  |
| 1   | A     | 32  | TRP  |
| 1   | A     | 157 | VAL  |
| 1   | A     | 202 | VAL  |
| 1   | A     | 206 | PHE  |
| 1   | A     | 210 | LEU  |
| 1   | A     | 214 | MET  |
| 1   | A     | 218 | LEU  |
| 1   | A     | 243 | GLU  |
| 1   | A     | 271 | LEU  |
| 1   | A     | 275 | LEU  |
| 1   | A     | 286 | THR  |
| 1   | A     | 292 | THR  |
| 1   | A     | 306 | VAL  |
| 1   | A     | 308 | ASP  |
| 2   | B     | 11  | VAL  |
| 2   | B     | 18  | ARG  |
| 2   | B     | 84  | THR  |
| 2   | B     | 116 | VAL  |
| 2   | B     | 223 | GLN  |
| 2   | B     | 262 | THR  |
| 2   | B     | 271 | THR  |
| 2   | B     | 308 | LYS  |
| 2   | B     | 309 | LEU  |
| 2   | B     | 362 | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 373 | LYS  |
| 2   | B     | 374 | ASN  |
| 2   | B     | 414 | PRO  |
| 2   | B     | 422 | ARG  |
| 2   | B     | 433 | ASP  |
| 2   | B     | 436 | THR  |
| 2   | B     | 486 | LEU  |
| 3   | C     | 26  | ARG  |
| 3   | C     | 27  | ASP  |
| 3   | C     | 28  | GLN  |
| 3   | C     | 29  | GLU  |
| 3   | C     | 86  | LEU  |
| 3   | C     | 165 | LEU  |
| 3   | C     | 174 | LEU  |
| 3   | C     | 244 | CYS  |
| 3   | C     | 289 | PHE  |
| 3   | C     | 305 | THR  |
| 3   | C     | 355 | THR  |
| 3   | C     | 391 | ARG  |
| 3   | C     | 401 | LEU  |
| 3   | C     | 417 | VAL  |
| 3   | C     | 447 | ARG  |
| 3   | C     | 472 | LEU  |
| 4   | D     | 20  | ASP  |
| 4   | D     | 43  | LEU  |
| 4   | D     | 53  | THR  |
| 4   | D     | 60  | THR  |
| 4   | D     | 84  | SER  |
| 4   | D     | 91  | LEU  |
| 4   | D     | 130 | PHE  |
| 4   | D     | 180 | ARG  |
| 4   | D     | 201 | VAL  |
| 4   | D     | 221 | THR  |
| 4   | D     | 236 | ASN  |
| 4   | D     | 241 | GLU  |
| 4   | D     | 256 | ILE  |
| 4   | D     | 259 | ILE  |
| 4   | D     | 279 | LEU  |
| 4   | D     | 291 | LEU  |
| 4   | D     | 323 | GLU  |
| 4   | D     | 346 | LEU  |
| 5   | E     | 9   | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | E     | 18  | ARG  |
| 5   | E     | 52  | PRO  |
| 5   | E     | 77  | GLU  |
| 5   | E     | 82  | GLN  |
| 5   | E     | 84  | LYS  |
| 6   | F     | 24  | HIS  |
| 7   | H     | 21  | VAL  |
| 7   | H     | 27  | THR  |
| 7   | H     | 56  | ASP  |
| 7   | H     | 60  | VAL  |
| 8   | I     | 32  | PRO  |
| 8   | I     | 33  | LYS  |
| 9   | J     | 7   | ARG  |
| 10  | K     | 10  | LYS  |
| 10  | K     | 18  | PHE  |
| 10  | K     | 19  | ASP  |
| 11  | L     | 1   | MET  |
| 11  | L     | 8   | GLN  |
| 11  | L     | 11  | GLU  |
| 11  | L     | 15  | THR  |
| 12  | M     | 20  | VAL  |
| 13  | O     | 31  | LEU  |
| 13  | O     | 87  | GLN  |
| 13  | O     | 88  | GLU  |
| 13  | O     | 97  | VAL  |
| 13  | O     | 106 | GLN  |
| 13  | O     | 114 | ASN  |
| 13  | O     | 178 | ARG  |
| 13  | O     | 219 | THR  |
| 14  | T     | 29  | ILE  |
| 15  | U     | 61  | ASN  |
| 15  | U     | 88  | VAL  |
| 15  | U     | 114 | VAL  |
| 15  | U     | 132 | LEU  |
| 16  | V     | 32  | GLU  |
| 16  | V     | 45  | ILE  |
| 16  | V     | 63  | CYS  |
| 16  | V     | 116 | GLU  |
| 17  | y     | 25  | ILE  |
| 17  | y     | 28  | ILE  |
| 17  | y     | 46  | LEU  |
| 18  | X     | 11  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18  | X     | 12  | ILE  |
| 18  | X     | 32  | LEU  |
| 18  | X     | 42  | GLN  |
| 18  | X     | 45  | LYS  |
| 19  | Z     | 14  | ILE  |
| 19  | Z     | 25  | VAL  |
| 19  | Z     | 33  | TRP  |
| 19  | Z     | 58  | ASN  |
| 19  | Z     | 62  | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 19  | ASN  |
| 1   | A     | 165 | GLN  |
| 1   | A     | 241 | GLN  |
| 1   | A     | 247 | ASN  |
| 1   | A     | 261 | GLN  |
| 1   | A     | 337 | HIS  |
| 2   | B     | 26  | HIS  |
| 2   | B     | 201 | HIS  |
| 2   | B     | 216 | HIS  |
| 2   | B     | 282 | GLN  |
| 2   | B     | 374 | ASN  |
| 3   | C     | 44  | ASN  |
| 3   | C     | 118 | HIS  |
| 3   | C     | 155 | ASN  |
| 3   | C     | 251 | HIS  |
| 3   | C     | 398 | HIS  |
| 3   | C     | 418 | ASN  |
| 3   | C     | 441 | HIS  |
| 3   | C     | 444 | HIS  |
| 4   | D     | 98  | GLN  |
| 4   | D     | 129 | GLN  |
| 4   | D     | 142 | ASN  |
| 4   | D     | 224 | GLN  |
| 4   | D     | 239 | GLN  |
| 4   | D     | 250 | ASN  |
| 4   | D     | 301 | GLN  |
| 6   | F     | 44  | GLN  |
| 7   | H     | 59  | ASN  |
| 11  | L     | 8   | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | M     | 33  | GLN  |
| 13  | O     | 87  | GLN  |
| 13  | O     | 106 | GLN  |
| 13  | O     | 135 | GLN  |
| 13  | O     | 150 | ASN  |
| 13  | O     | 173 | ASN  |
| 13  | O     | 222 | GLN  |
| 13  | O     | 226 | ASN  |
| 15  | U     | 82  | ASN  |
| 16  | V     | 104 | ASN  |
| 18  | X     | 42  | GLN  |
| 19  | Z     | 6   | GLN  |
| 19  | Z     | 31  | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 87 ligands modelled in this entry, 4 are monoatomic - leaving 83 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 | $\# Z  > 2$ |
| 26  | LHG  | A     | 371 | -    | 38,38,48     | 2.27 | 6 (15%)     | 41,44,54    | 1.41 | 4 (9%)      |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 21  | CLA  | B     | 522 | 2    | 69,73,73     | 2.23 | 17 (24%) | 82,113,113  | 1.70 | 11 (13%) |
| 21  | CLA  | K     | 483 | 3    | 69,73,73     | 2.24 | 17 (24%) | 82,113,113  | 1.78 | 13 (15%) |
| 28  | DGD  | C     | 491 | -    | 54,54,67     | 1.67 | 9 (16%)  | 68,68,81    | 2.94 | 24 (35%) |
| 21  | CLA  | C     | 479 | 3    | 69,73,73     | 2.47 | 19 (27%) | 82,113,113  | 1.91 | 13 (15%) |
| 29  | LMT  | I     | 274 | -    | 36,36,36     | 1.88 | 12 (33%) | 47,47,47    | 1.34 | 7 (14%)  |
| 21  | CLA  | C     | 488 | 3    | 69,73,73     | 2.55 | 21 (30%) | 82,113,113  | 1.85 | 15 (18%) |
| 29  | LMT  | D     | 536 | -    | 36,36,36     | 1.71 | 10 (27%) | 47,47,47    | 1.61 | 8 (17%)  |
| 27  | LMG  | A     | 373 | -    | 51,51,55     | 0.56 | 1 (1%)   | 59,59,63    | 1.10 | 5 (8%)   |
| 25  | BCR  | A     | 369 | -    | 41,41,41     | 1.97 | 6 (14%)  | 56,56,56    | 2.13 | 23 (41%) |
| 27  | LMG  | D     | 359 | -    | 46,46,55     | 1.80 | 6 (13%)  | 54,54,63    | 2.54 | 17 (31%) |
| 28  | DGD  | B     | 533 | -    | 67,67,67     | 1.55 | 15 (22%) | 81,81,81    | 1.83 | 19 (23%) |
| 25  | BCR  | J     | 115 | -    | 41,41,41     | 2.22 | 8 (19%)  | 56,56,56    | 3.32 | 17 (30%) |
| 21  | CLA  | C     | 480 | -    | 69,73,73     | 2.42 | 19 (27%) | 82,113,113  | 1.97 | 13 (15%) |
| 25  | BCR  | B     | 527 | -    | 41,41,41     | 1.83 | 7 (17%)  | 56,56,56    | 2.40 | 21 (37%) |
| 21  | CLA  | B     | 518 | 2    | 69,73,73     | 2.55 | 19 (27%) | 82,113,113  | 2.11 | 16 (19%) |
| 21  | CLA  | B     | 520 | -    | 69,73,73     | 2.29 | 19 (27%) | 82,113,113  | 1.71 | 11 (13%) |
| 21  | CLA  | C     | 483 | -    | 69,73,73     | 2.59 | 23 (33%) | 82,113,113  | 1.79 | 13 (15%) |
| 27  | LMG  | B     | 531 | -    | 49,49,55     | 1.74 | 6 (12%)  | 57,57,63    | 2.81 | 18 (31%) |
| 21  | CLA  | B     | 519 | 2    | 69,73,73     | 2.34 | 17 (24%) | 82,113,113  | 1.83 | 15 (18%) |
| 21  | CLA  | B     | 524 | 2    | 69,73,73     | 2.56 | 22 (31%) | 82,113,113  | 1.85 | 15 (18%) |
| 28  | DGD  | C     | 474 | -    | 57,57,67     | 2.11 | 15 (26%) | 71,71,81    | 3.51 | 25 (35%) |
| 21  | CLA  | A     | 362 | 1    | 69,73,73     | 2.15 | 19 (27%) | 82,113,113  | 1.76 | 11 (13%) |
| 21  | CLA  | B     | 514 | 2    | 69,73,73     | 2.33 | 16 (23%) | 82,113,113  | 1.60 | 12 (14%) |
| 25  | BCR  | B     | 530 | -    | 41,41,41     | 2.56 | 9 (21%)  | 56,56,56    | 2.27 | 23 (41%) |
| 25  | BCR  | Z     | 116 | -    | 41,41,41     | 2.02 | 8 (19%)  | 56,56,56    | 2.14 | 21 (37%) |
| 21  | CLA  | B     | 523 | 2    | 69,73,73     | 2.28 | 19 (27%) | 82,113,113  | 1.67 | 13 (15%) |
| 30  | SQD  | D     | 361 | -    | 41,43,54     | 2.64 | 19 (46%) | 51,54,65    | 2.81 | 16 (31%) |
| 21  | CLA  | C     | 487 | 3    | 69,73,73     | 2.79 | 25 (36%) | 82,113,113  | 1.85 | 11 (13%) |
| 21  | CLA  | B     | 525 | 2    | 69,73,73     | 2.46 | 19 (27%) | 82,113,113  | 1.83 | 12 (14%) |
| 27  | LMG  | J     | 492 | -    | 48,48,55     | 2.03 | 10 (20%) | 56,56,63    | 1.88 | 17 (30%) |
| 27  | LMG  | C     | 494 | -    | 45,45,55     | 1.98 | 8 (17%)  | 53,53,63    | 2.20 | 16 (30%) |
| 21  | CLA  | C     | 478 | 3    | 69,73,73     | 2.28 | 17 (24%) | 82,113,113  | 1.75 | 15 (18%) |
| 25  | BCR  | X     | 107 | -    | 41,41,41     | 1.55 | 5 (12%)  | 56,56,56    | 2.46 | 21 (37%) |
| 25  | BCR  | C     | 489 | -    | 41,41,41     | 1.92 | 7 (17%)  | 56,56,56    | 2.13 | 19 (33%) |
| 29  | LMT  | A     | 376 | -    | 36,36,36     | 2.00 | 10 (27%) | 47,47,47    | 1.47 | 8 (17%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 21  | CLA  | C     | 486 | 3    | 69,73,73     | 2.95 | 25 (36%) | 82,113,113  | 1.79 | 15 (18%) |
| 33  | HEM  | F     | 85  | 5    | 50,50,50     | 2.91 | 21 (42%) | 67,82,82    | 2.49 | 20 (29%) |
| 23  | MES  | A     | 367 | -    | 12,12,12     | 1.51 | 1 (8%)   | 15,16,16    | 1.06 | 0        |
| 28  | DGD  | D     | 362 | -    | 64,64,67     | 2.15 | 22 (34%) | 78,78,81    | 2.47 | 21 (26%) |
| 21  | CLA  | B     | 515 | 2    | 69,73,73     | 2.40 | 19 (27%) | 82,113,113  | 1.78 | 14 (17%) |
| 32  | PL9  | D     | 357 | -    | 55,55,55     | 3.24 | 22 (40%) | 68,69,69    | 2.85 | 27 (39%) |
| 21  | CLA  | C     | 484 | 3    | 69,73,73     | 2.43 | 19 (27%) | 82,113,113  | 1.82 | 14 (17%) |
| 21  | CLA  | C     | 485 | 3    | 69,73,73     | 2.47 | 20 (28%) | 82,113,113  | 1.76 | 13 (15%) |
| 21  | CLA  | D     | 354 | 4    | 69,73,73     | 2.56 | 18 (26%) | 82,113,113  | 1.68 | 14 (17%) |
| 28  | DGD  | B     | 528 | -    | 59,59,67     | 0.61 | 2 (3%)   | 73,73,81    | 1.07 | 8 (10%)  |
| 21  | CLA  | B     | 513 | 2    | 69,73,73     | 2.24 | 18 (26%) | 82,113,113  | 1.88 | 14 (17%) |
| 29  | LMT  | B     | 535 | -    | 36,36,36     | 1.88 | 9 (25%)  | 47,47,47    | 1.15 | 2 (4%)   |
| 21  | CLA  | B     | 516 | 2    | 69,73,73     | 2.55 | 19 (27%) | 82,113,113  | 1.96 | 17 (20%) |
| 21  | CLA  | B     | 517 | -    | 69,73,73     | 2.69 | 22 (31%) | 82,113,113  | 2.04 | 20 (24%) |
| 25  | BCR  | B     | 529 | -    | 41,41,41     | 2.18 | 7 (17%)  | 56,56,56    | 2.21 | 19 (33%) |
| 27  | LMG  | I     | 220 | -    | 43,43,55     | 2.09 | 12 (27%) | 51,51,63    | 2.18 | 13 (25%) |
| 28  | DGD  | C     | 492 | -    | 63,63,67     | 1.43 | 11 (17%) | 77,77,81    | 2.73 | 20 (25%) |
| 28  | DGD  | A     | 375 | -    | 53,53,67     | 2.09 | 13 (24%) | 67,67,81    | 2.47 | 22 (32%) |
| 25  | BCR  | J     | 112 | -    | 41,41,41     | 1.93 | 7 (17%)  | 56,56,56    | 2.47 | 24 (42%) |
| 30  | SQD  | C     | 475 | -    | 49,51,54     | 2.71 | 27 (55%) | 59,62,65    | 2.65 | 17 (28%) |
| 21  | CLA  | A     | 363 | -    | 69,73,73     | 2.22 | 19 (27%) | 82,113,113  | 1.90 | 14 (17%) |
| 28  | DGD  | C     | 493 | -    | 67,67,67     | 1.51 | 16 (23%) | 81,81,81    | 2.95 | 28 (34%) |
| 21  | CLA  | B     | 526 | 2    | 69,73,73     | 2.65 | 22 (31%) | 82,113,113  | 1.78 | 12 (14%) |
| 21  | CLA  | B     | 512 | 2    | 69,73,73     | 2.15 | 17 (24%) | 82,113,113  | 1.62 | 11 (13%) |
| 21  | CLA  | C     | 481 | 3    | 69,73,73     | 2.73 | 22 (31%) | 82,113,113  | 2.02 | 16 (19%) |
| 30  | SQD  | L     | 213 | -    | 45,47,54     | 2.70 | 25 (55%) | 55,58,65    | 2.76 | 19 (34%) |
| 26  | LHG  | C     | 476 | -    | 36,36,48     | 2.44 | 6 (16%)  | 39,42,54    | 1.50 | 4 (10%)  |
| 27  | LMG  | M     | 217 | -    | 42,42,55     | 2.02 | 8 (19%)  | 50,50,63    | 1.47 | 7 (14%)  |
| 21  | CLA  | D     | 356 | 4    | 69,73,73     | 2.38 | 20 (28%) | 82,113,113  | 1.87 | 14 (17%) |
| 33  | HEM  | V     | 164 | 16   | 50,50,50     | 2.72 | 25 (50%) | 67,82,82    | 2.41 | 19 (28%) |
| 21  | CLA  | B     | 511 | -    | 69,73,73     | 2.82 | 28 (40%) | 82,113,113  | 1.79 | 14 (17%) |
| 21  | CLA  | C     | 482 | 3    | 69,73,73     | 2.86 | 23 (33%) | 82,113,113  | 1.85 | 15 (18%) |
| 21  | CLA  | C     | 477 | 3    | 69,73,73     | 2.35 | 16 (23%) | 82,113,113  | 1.91 | 16 (19%) |
| 29  | LMT  | T     | 226 | -    | 36,36,36     | 1.80 | 9 (25%)  | 47,47,47    | 0.98 | 2 (4%)   |
| 31  | BCT  | D     | 353 | 20   | 3,3,3        | 0.53 | 0        | 2,3,3       | 0.36 | 0        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 22  | PHO  | D     | 355 | -    | 58,69,69     | 3.74 | 16 (27%) | 55,99,99    | 1.96 | 11 (20%) |
| 21  | CLA  | B     | 521 | 2    | 69,73,73     | 2.45 | 17 (24%) | 82,113,113  | 1.92 | 20 (24%) |
| 29  | LMT  | D     | 363 | -    | 32,32,36     | 1.83 | 7 (21%)  | 43,43,47    | 1.50 | 6 (13%)  |
| 21  | CLA  | A     | 364 | -    | 69,73,73     | 2.33 | 20 (28%) | 82,113,113  | 1.90 | 16 (19%) |
| 25  | BCR  | D     | 358 | -    | 41,41,41     | 1.76 | 7 (17%)  | 56,56,56    | 2.34 | 21 (37%) |
| 21  | CLA  | A     | 366 | 1    | 69,73,73     | 2.34 | 20 (28%) | 82,113,113  | 1.77 | 11 (13%) |
| 25  | BCR  | C     | 490 | -    | 41,41,41     | 1.99 | 6 (14%)  | 56,56,56    | 2.26 | 24 (42%) |
| 29  | LMT  | O     | 274 | -    | 36,36,36     | 2.01 | 12 (33%) | 47,47,47    | 1.41 | 8 (17%)  |
| 30  | SQD  | F     | 224 | -    | 43,45,54     | 2.74 | 22 (51%) | 53,56,65    | 2.73 | 20 (37%) |
| 22  | PHO  | A     | 365 | -    | 58,69,69     | 4.00 | 16 (27%) | 55,99,99    | 2.06 | 11 (20%) |
| 27  | LMG  | D     | 360 | -    | 48,48,55     | 0.57 | 1 (2%)   | 56,56,63    | 1.12 | 6 (10%)  |

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   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 26  | LHG  | A     | 371 | -    | -         | 16/43/43/53   | -       |
| 21  | CLA  | B     | 522 | 2    | 1/1/15/20 | 14/39/115/115 | -       |
| 21  | CLA  | K     | 483 | 3    | 1/1/15/20 | 6/39/115/115  | -       |
| 28  | DGD  | C     | 491 | -    | -         | 5/42/82/95    | 0/2/2/2 |
| 21  | CLA  | C     | 479 | 3    | 1/1/15/20 | 12/39/115/115 | -       |
| 29  | LMT  | I     | 274 | -    | -         | 2/21/61/61    | 0/2/2/2 |
| 21  | CLA  | C     | 488 | 3    | 1/1/15/20 | 7/39/115/115  | -       |
| 29  | LMT  | D     | 536 | -    | -         | 1/21/61/61    | 0/2/2/2 |
| 27  | LMG  | A     | 373 | -    | -         | 20/46/66/70   | 0/1/1/1 |
| 25  | BCR  | A     | 369 | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 27  | LMG  | D     | 359 | -    | -         | 5/41/61/70    | 0/1/1/1 |
| 28  | DGD  | B     | 533 | -    | -         | 9/55/95/95    | 0/2/2/2 |
| 25  | BCR  | J     | 115 | -    | -         | 3/29/63/63    | 0/2/2/2 |
| 21  | CLA  | C     | 480 | -    | 1/1/15/20 | 14/39/115/115 | -       |
| 25  | BCR  | B     | 527 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 21  | CLA  | B     | 518 | 2    | 1/1/15/20 | 8/39/115/115  | -       |
| 21  | CLA  | B     | 520 | -    | 1/1/15/20 | 14/39/115/115 | -       |
| 21  | CLA  | C     | 483 | -    | 1/1/15/20 | 10/39/115/115 | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 27  | LMG  | B     | 531 | -    | -         | 4/44/64/70    | 0/1/1/1 |
| 21  | CLA  | B     | 519 | 2    | 1/1/15/20 | 7/39/115/115  | -       |
| 21  | CLA  | B     | 524 | 2    | 1/1/15/20 | 12/39/115/115 | -       |
| 28  | DGD  | C     | 474 | -    | -         | 7/45/85/95    | 0/2/2/2 |
| 21  | CLA  | A     | 362 | 1    | 1/1/15/20 | 9/39/115/115  | -       |
| 21  | CLA  | B     | 514 | 2    | 1/1/15/20 | 10/39/115/115 | -       |
| 25  | BCR  | B     | 530 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 25  | BCR  | Z     | 116 | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 21  | CLA  | B     | 523 | 2    | 1/1/15/20 | 11/39/115/115 | -       |
| 30  | SQD  | D     | 361 | -    | -         | 16/38/58/69   | 0/1/1/1 |
| 21  | CLA  | C     | 487 | 3    | 1/1/15/20 | 8/39/115/115  | -       |
| 21  | CLA  | B     | 525 | 2    | 1/1/15/20 | 9/39/115/115  | -       |
| 27  | LMG  | J     | 492 | -    | -         | 5/43/63/70    | 0/1/1/1 |
| 27  | LMG  | C     | 494 | -    | -         | 3/40/60/70    | 0/1/1/1 |
| 21  | CLA  | C     | 478 | 3    | 1/1/15/20 | 7/39/115/115  | -       |
| 25  | BCR  | X     | 107 | -    | -         | 3/29/63/63    | 0/2/2/2 |
| 25  | BCR  | C     | 489 | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 29  | LMT  | A     | 376 | -    | -         | 3/21/61/61    | 0/2/2/2 |
| 21  | CLA  | C     | 486 | 3    | 1/1/15/20 | 6/39/115/115  | -       |
| 33  | HEM  | F     | 85  | 5    | -         | 8/14/54/54    | -       |
| 23  | MES  | A     | 367 | -    | -         | 3/6/14/14     | 0/1/1/1 |
| 28  | DGD  | D     | 362 | -    | -         | 10/52/92/95   | 0/2/2/2 |
| 21  | CLA  | B     | 515 | 2    | 1/1/15/20 | 8/39/115/115  | -       |
| 32  | PL9  | D     | 357 | -    | -         | 17/53/73/73   | 0/1/1/1 |
| 21  | CLA  | C     | 484 | 3    | 1/1/15/20 | 12/39/115/115 | -       |
| 21  | CLA  | C     | 485 | 3    | 1/1/15/20 | 10/39/115/115 | -       |
| 21  | CLA  | D     | 354 | 4    | 1/1/15/20 | 10/39/115/115 | -       |
| 28  | DGD  | B     | 528 | -    | -         | 18/47/87/95   | 0/2/2/2 |
| 21  | CLA  | B     | 513 | 2    | 1/1/15/20 | 10/39/115/115 | -       |
| 29  | LMT  | B     | 535 | -    | -         | 3/21/61/61    | 0/2/2/2 |
| 21  | CLA  | B     | 516 | 2    | 1/1/15/20 | 10/39/115/115 | -       |
| 21  | CLA  | B     | 517 | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 25  | BCR  | B     | 529 | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 27  | LMG  | I     | 220 | -    | -         | 4/38/58/70    | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 28  | DGD  | C     | 492 | -    | 1/1/13/13 | 8/51/91/95    | 0/2/2/2 |
| 28  | DGD  | A     | 375 | -    | -         | 6/41/81/95    | 0/2/2/2 |
| 25  | BCR  | J     | 112 | -    | -         | 1/29/63/63    | 0/2/2/2 |
| 30  | SQD  | C     | 475 | -    | -         | 22/46/66/69   | 0/1/1/1 |
| 21  | CLA  | A     | 363 | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 28  | DGD  | C     | 493 | -    | 1/1/13/13 | 9/55/95/95    | 0/2/2/2 |
| 21  | CLA  | B     | 526 | 2    | 1/1/15/20 | 9/39/115/115  | -       |
| 21  | CLA  | B     | 512 | 2    | 1/1/15/20 | 7/39/115/115  | -       |
| 21  | CLA  | C     | 481 | 3    | 1/1/15/20 | 11/39/115/115 | -       |
| 30  | SQD  | L     | 213 | -    | -         | 16/42/62/69   | 0/1/1/1 |
| 26  | LHG  | C     | 476 | -    | -         | 16/41/41/53   | -       |
| 27  | LMG  | M     | 217 | -    | -         | 3/37/57/70    | 0/1/1/1 |
| 21  | CLA  | D     | 356 | 4    | 1/1/15/20 | 8/39/115/115  | -       |
| 33  | HEM  | V     | 164 | 16   | -         | 10/14/54/54   | -       |
| 21  | CLA  | B     | 511 | -    | 1/1/15/20 | 16/39/115/115 | -       |
| 21  | CLA  | C     | 482 | 3    | 1/1/15/20 | 10/39/115/115 | -       |
| 21  | CLA  | C     | 477 | 3    | 1/1/15/20 | 10/39/115/115 | -       |
| 29  | LMT  | T     | 226 | -    | -         | 1/21/61/61    | 0/2/2/2 |
| 22  | PHO  | D     | 355 | -    | 1/1/17/22 | 16/37/103/103 | 0/5/6/6 |
| 21  | CLA  | B     | 521 | 2    | 1/1/15/20 | 9/39/115/115  | -       |
| 29  | LMT  | D     | 363 | -    | -         | 1/17/57/61    | 0/2/2/2 |
| 21  | CLA  | A     | 364 | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 25  | BCR  | D     | 358 | -    | -         | 3/29/63/63    | 0/2/2/2 |
| 21  | CLA  | A     | 366 | 1    | 1/1/15/20 | 6/39/115/115  | -       |
| 25  | BCR  | C     | 490 | -    | -         | 3/29/63/63    | 0/2/2/2 |
| 29  | LMT  | O     | 274 | -    | -         | 3/21/61/61    | 0/2/2/2 |
| 30  | SQD  | F     | 224 | -    | -         | 18/40/60/69   | 0/1/1/1 |
| 22  | PHO  | A     | 365 | -    | 1/1/17/22 | 6/37/103/103  | 0/5/6/6 |
| 27  | LMG  | D     | 360 | -    | -         | 20/43/63/70   | 0/1/1/1 |

All (1199) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 22  | A     | 365 | PHO  | C3A-C2A | -17.56 | 1.39        | 1.54     |
| 22  | D     | 355 | PHO  | C3A-C2A | -17.49 | 1.39        | 1.54     |
| 32  | D     | 357 | PL9  | C28-C29 | 11.74  | 1.60        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 22  | A     | 365 | PHO  | C1D-C2D | 11.48  | 1.52        | 1.39     |
| 21  | C     | 486 | CLA  | MG-NA   | 11.31  | 2.33        | 2.06     |
| 21  | B     | 524 | CLA  | C2-C3   | 11.25  | 1.58        | 1.33     |
| 22  | A     | 365 | PHO  | C3B-C4B | 11.03  | 1.52        | 1.41     |
| 21  | C     | 482 | CLA  | C2-C3   | 10.97  | 1.58        | 1.33     |
| 21  | B     | 521 | CLA  | C2-C3   | 10.89  | 1.58        | 1.33     |
| 21  | B     | 517 | CLA  | C2-C3   | 10.77  | 1.57        | 1.33     |
| 22  | D     | 355 | PHO  | C1D-C2D | 10.70  | 1.51        | 1.39     |
| 21  | B     | 518 | CLA  | C2-C3   | 10.63  | 1.57        | 1.33     |
| 21  | C     | 487 | CLA  | C2-C3   | 10.59  | 1.57        | 1.33     |
| 21  | B     | 514 | CLA  | C2-C3   | 10.13  | 1.56        | 1.33     |
| 21  | C     | 477 | CLA  | C2-C3   | 10.09  | 1.56        | 1.33     |
| 32  | D     | 357 | PL9  | C13-C14 | 10.06  | 1.56        | 1.33     |
| 21  | B     | 526 | CLA  | C2-C3   | 10.04  | 1.56        | 1.33     |
| 21  | B     | 515 | CLA  | C2-C3   | 10.03  | 1.56        | 1.33     |
| 27  | B     | 531 | LMG  | O1-C1   | -10.01 | 1.23        | 1.40     |
| 21  | B     | 516 | CLA  | C2-C3   | 10.00  | 1.56        | 1.33     |
| 21  | C     | 486 | CLA  | C2-C3   | 9.99   | 1.56        | 1.33     |
| 27  | M     | 217 | LMG  | O1-C1   | -9.98  | 1.23        | 1.40     |
| 27  | I     | 220 | LMG  | O1-C1   | -9.93  | 1.23        | 1.40     |
| 27  | C     | 494 | LMG  | O1-C1   | -9.90  | 1.23        | 1.40     |
| 27  | J     | 492 | LMG  | O1-C1   | -9.89  | 1.23        | 1.40     |
| 21  | B     | 519 | CLA  | C2-C3   | 9.89   | 1.55        | 1.33     |
| 27  | D     | 359 | LMG  | O1-C1   | -9.88  | 1.23        | 1.40     |
| 21  | C     | 479 | CLA  | C2-C3   | 9.88   | 1.55        | 1.33     |
| 21  | C     | 481 | CLA  | C2-C3   | 9.80   | 1.55        | 1.33     |
| 21  | B     | 525 | CLA  | C2-C3   | 9.76   | 1.55        | 1.33     |
| 21  | D     | 354 | CLA  | MG-NA   | 9.67   | 2.29        | 2.06     |
| 21  | C     | 480 | CLA  | C2-C3   | 9.55   | 1.55        | 1.33     |
| 21  | B     | 511 | CLA  | C2-C3   | 9.52   | 1.55        | 1.33     |
| 21  | B     | 520 | CLA  | C2-C3   | 9.49   | 1.54        | 1.33     |
| 21  | C     | 483 | CLA  | C2-C3   | 9.41   | 1.54        | 1.33     |
| 22  | D     | 355 | PHO  | C3B-C4B | 9.38   | 1.51        | 1.41     |
| 21  | C     | 481 | CLA  | MG-NA   | 9.27   | 2.28        | 2.06     |
| 21  | A     | 364 | CLA  | C2-C3   | 9.27   | 1.54        | 1.33     |
| 21  | D     | 356 | CLA  | C2-C3   | 9.22   | 1.54        | 1.33     |
| 21  | B     | 522 | CLA  | C2-C3   | 9.11   | 1.54        | 1.33     |
| 21  | C     | 485 | CLA  | C2-C3   | 9.10   | 1.54        | 1.33     |
| 21  | B     | 523 | CLA  | C2-C3   | 9.08   | 1.54        | 1.33     |
| 26  | C     | 476 | LHG  | P-O5    | 9.08   | 1.82        | 1.50     |
| 21  | C     | 478 | CLA  | C2-C3   | 9.06   | 1.53        | 1.33     |
| 25  | B     | 530 | BCR  | C30-C25 | 8.98   | 1.65        | 1.53     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | D     | 354 | CLA  | C2-C3   | 8.95  | 1.53        | 1.33     |
| 22  | A     | 365 | PHO  | C2-C3   | 8.89  | 1.53        | 1.33     |
| 21  | K     | 483 | CLA  | C2-C3   | 8.86  | 1.53        | 1.33     |
| 32  | D     | 357 | PL9  | C2-C3   | 8.86  | 1.56        | 1.34     |
| 26  | A     | 371 | LHG  | P-O5    | 8.78  | 1.81        | 1.50     |
| 21  | C     | 488 | CLA  | C2-C3   | 8.78  | 1.53        | 1.33     |
| 21  | C     | 484 | CLA  | C2-C3   | 8.76  | 1.53        | 1.33     |
| 21  | A     | 366 | CLA  | C2-C3   | 8.68  | 1.53        | 1.33     |
| 22  | A     | 365 | PHO  | CHA-CBD | 8.63  | 1.61        | 1.51     |
| 30  | C     | 475 | SQD  | C4-C3   | 8.59  | 1.74        | 1.52     |
| 21  | B     | 513 | CLA  | C2-C3   | 8.53  | 1.52        | 1.33     |
| 21  | A     | 363 | CLA  | C2-C3   | 8.49  | 1.52        | 1.33     |
| 22  | D     | 355 | PHO  | C3B-C2B | 8.45  | 1.51        | 1.40     |
| 21  | B     | 512 | CLA  | C2-C3   | 8.36  | 1.52        | 1.33     |
| 30  | F     | 224 | SQD  | C4-C3   | 8.01  | 1.73        | 1.52     |
| 21  | B     | 518 | CLA  | O2A-CGA | 7.81  | 1.56        | 1.33     |
| 21  | C     | 488 | CLA  | MG-NA   | 7.80  | 2.24        | 2.06     |
| 22  | A     | 365 | PHO  | C3B-C2B | 7.80  | 1.50        | 1.40     |
| 30  | D     | 361 | SQD  | C4-C3   | 7.79  | 1.72        | 1.52     |
| 33  | F     | 85  | HEM  | O1D-CGD | 7.53  | 1.46        | 1.22     |
| 25  | B     | 529 | BCR  | C30-C25 | 7.49  | 1.63        | 1.53     |
| 33  | V     | 164 | HEM  | O1D-CGD | 7.45  | 1.46        | 1.22     |
| 22  | D     | 355 | PHO  | C2-C3   | 7.32  | 1.49        | 1.33     |
| 25  | C     | 489 | BCR  | C1-C6   | 7.31  | 1.63        | 1.53     |
| 25  | B     | 530 | BCR  | C1-C6   | 7.28  | 1.63        | 1.53     |
| 30  | L     | 213 | SQD  | C4-C3   | 7.22  | 1.71        | 1.52     |
| 33  | F     | 85  | HEM  | C3B-C2B | 7.21  | 1.51        | 1.37     |
| 28  | A     | 375 | DGD  | O3G-C1D | 7.17  | 1.52        | 1.40     |
| 21  | A     | 362 | CLA  | C2-C3   | 7.15  | 1.49        | 1.33     |
| 25  | J     | 112 | BCR  | C30-C25 | 7.06  | 1.62        | 1.53     |
| 25  | J     | 115 | BCR  | C30-C25 | 6.95  | 1.62        | 1.53     |
| 21  | B     | 511 | CLA  | C4C-C3C | 6.80  | 1.56        | 1.45     |
| 26  | C     | 476 | LHG  | P-O3    | 6.73  | 1.85        | 1.59     |
| 25  | A     | 369 | BCR  | C30-C25 | 6.66  | 1.62        | 1.53     |
| 21  | B     | 517 | CLA  | O2A-CGA | 6.64  | 1.52        | 1.33     |
| 21  | B     | 524 | CLA  | O2A-CGA | 6.53  | 1.52        | 1.33     |
| 28  | C     | 474 | DGD  | O5D-C1E | 6.52  | 1.51        | 1.40     |
| 28  | D     | 362 | DGD  | O5D-C1E | 6.52  | 1.51        | 1.40     |
| 25  | Z     | 116 | BCR  | C30-C25 | 6.46  | 1.62        | 1.53     |
| 21  | B     | 511 | CLA  | O2D-CGD | 6.38  | 1.48        | 1.33     |
| 21  | C     | 487 | CLA  | O2A-CGA | 6.37  | 1.51        | 1.33     |
| 32  | D     | 357 | PL9  | C3-C4   | -6.30 | 1.39        | 1.49     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | C     | 484 | CLA  | O2D-CGD | 6.26  | 1.48        | 1.33     |
| 21  | B     | 517 | CLA  | MG-NA   | 6.25  | 2.21        | 2.06     |
| 21  | B     | 526 | CLA  | MG-NA   | 6.25  | 2.21        | 2.06     |
| 25  | C     | 490 | BCR  | C1-C6   | 6.24  | 1.61        | 1.53     |
| 28  | D     | 362 | DGD  | O3G-C1D | 6.17  | 1.50        | 1.40     |
| 21  | B     | 515 | CLA  | O2A-CGA | 6.14  | 1.51        | 1.33     |
| 25  | Z     | 116 | BCR  | C1-C6   | 6.13  | 1.61        | 1.53     |
| 21  | C     | 482 | CLA  | O2D-CGD | 6.08  | 1.48        | 1.33     |
| 21  | C     | 487 | CLA  | MG-NA   | 6.01  | 2.20        | 2.06     |
| 25  | J     | 115 | BCR  | C5-C6   | 5.99  | 1.44        | 1.34     |
| 25  | C     | 490 | BCR  | C30-C25 | 5.97  | 1.61        | 1.53     |
| 21  | B     | 511 | CLA  | O2A-CGA | 5.91  | 1.50        | 1.33     |
| 26  | A     | 371 | LHG  | P-O3    | 5.85  | 1.82        | 1.59     |
| 21  | B     | 526 | CLA  | O2A-CGA | 5.82  | 1.50        | 1.33     |
| 21  | B     | 516 | CLA  | O2A-CGA | 5.82  | 1.50        | 1.33     |
| 21  | C     | 482 | CLA  | C1C-C2C | 5.78  | 1.56        | 1.44     |
| 21  | C     | 486 | CLA  | O2A-CGA | 5.78  | 1.50        | 1.33     |
| 21  | C     | 477 | CLA  | O2D-CGD | 5.73  | 1.47        | 1.33     |
| 21  | B     | 511 | CLA  | MG-NA   | 5.72  | 2.19        | 2.06     |
| 21  | B     | 513 | CLA  | O2A-CGA | 5.69  | 1.49        | 1.33     |
| 21  | A     | 364 | CLA  | O2A-CGA | 5.68  | 1.49        | 1.33     |
| 21  | C     | 482 | CLA  | C4C-C3C | 5.63  | 1.54        | 1.45     |
| 28  | C     | 491 | DGD  | O5D-C1E | 5.61  | 1.49        | 1.40     |
| 21  | C     | 482 | CLA  | O2A-CGA | 5.61  | 1.49        | 1.33     |
| 25  | A     | 369 | BCR  | C1-C6   | 5.61  | 1.61        | 1.53     |
| 21  | B     | 516 | CLA  | C3A-C2A | -5.60 | 1.39        | 1.54     |
| 21  | C     | 477 | CLA  | O2A-CGA | 5.58  | 1.49        | 1.33     |
| 21  | B     | 517 | CLA  | C3A-C2A | -5.58 | 1.39        | 1.54     |
| 21  | C     | 477 | CLA  | C3A-C2A | -5.58 | 1.39        | 1.54     |
| 21  | B     | 513 | CLA  | C3A-C2A | -5.57 | 1.39        | 1.54     |
| 21  | B     | 523 | CLA  | C3A-C2A | -5.57 | 1.39        | 1.54     |
| 21  | D     | 356 | CLA  | C3A-C2A | -5.57 | 1.39        | 1.54     |
| 21  | B     | 521 | CLA  | C3A-C2A | -5.57 | 1.39        | 1.54     |
| 21  | B     | 512 | CLA  | C3A-C2A | -5.56 | 1.39        | 1.54     |
| 21  | A     | 366 | CLA  | C3A-C2A | -5.56 | 1.39        | 1.54     |
| 21  | C     | 478 | CLA  | C3A-C2A | -5.56 | 1.39        | 1.54     |
| 21  | C     | 481 | CLA  | O2A-CGA | 5.56  | 1.49        | 1.33     |
| 21  | C     | 485 | CLA  | C3A-C2A | -5.56 | 1.39        | 1.54     |
| 21  | C     | 484 | CLA  | C3A-C2A | -5.56 | 1.39        | 1.54     |
| 21  | B     | 514 | CLA  | C3A-C2A | -5.56 | 1.39        | 1.54     |
| 21  | A     | 362 | CLA  | C3A-C2A | -5.56 | 1.39        | 1.54     |
| 21  | A     | 364 | CLA  | C3A-C2A | -5.55 | 1.39        | 1.54     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | C     | 488 | CLA  | C3A-C2A | -5.55 | 1.39        | 1.54     |
| 21  | B     | 518 | CLA  | C3A-C2A | -5.55 | 1.39        | 1.54     |
| 21  | B     | 522 | CLA  | C3A-C2A | -5.54 | 1.39        | 1.54     |
| 21  | B     | 520 | CLA  | C3A-C2A | -5.53 | 1.39        | 1.54     |
| 21  | C     | 482 | CLA  | C3A-C2A | -5.53 | 1.39        | 1.54     |
| 21  | B     | 519 | CLA  | C3A-C2A | -5.53 | 1.39        | 1.54     |
| 21  | C     | 480 | CLA  | C3A-C2A | -5.53 | 1.39        | 1.54     |
| 21  | C     | 479 | CLA  | C3A-C2A | -5.53 | 1.39        | 1.54     |
| 21  | B     | 515 | CLA  | C3A-C2A | -5.52 | 1.39        | 1.54     |
| 21  | C     | 481 | CLA  | C3A-C2A | -5.52 | 1.39        | 1.54     |
| 21  | B     | 524 | CLA  | C3A-C2A | -5.52 | 1.39        | 1.54     |
| 21  | C     | 487 | CLA  | C3A-C2A | -5.52 | 1.39        | 1.54     |
| 21  | K     | 483 | CLA  | C3A-C2A | -5.51 | 1.39        | 1.54     |
| 33  | V     | 164 | HEM  | C3B-C2B | 5.51  | 1.48        | 1.37     |
| 21  | A     | 363 | CLA  | C3A-C2A | -5.51 | 1.39        | 1.54     |
| 21  | B     | 525 | CLA  | C3A-C2A | -5.50 | 1.39        | 1.54     |
| 21  | B     | 511 | CLA  | C3A-C2A | -5.50 | 1.39        | 1.54     |
| 21  | C     | 486 | CLA  | C3A-C2A | -5.49 | 1.39        | 1.54     |
| 21  | D     | 354 | CLA  | C3A-C2A | -5.49 | 1.39        | 1.54     |
| 21  | B     | 526 | CLA  | C3A-C2A | -5.48 | 1.39        | 1.54     |
| 21  | C     | 481 | CLA  | C1C-C2C | 5.46  | 1.55        | 1.44     |
| 21  | C     | 483 | CLA  | C3A-C2A | -5.46 | 1.39        | 1.54     |
| 21  | B     | 525 | CLA  | O2A-CGA | 5.46  | 1.49        | 1.33     |
| 21  | B     | 520 | CLA  | C4C-C3C | 5.46  | 1.54        | 1.45     |
| 32  | D     | 357 | PL9  | C6-C1   | -5.44 | 1.39        | 1.48     |
| 25  | B     | 527 | BCR  | C1-C6   | 5.42  | 1.60        | 1.53     |
| 21  | C     | 483 | CLA  | O2D-CGD | 5.36  | 1.46        | 1.33     |
| 21  | C     | 487 | CLA  | C4C-C3C | 5.35  | 1.54        | 1.45     |
| 21  | B     | 519 | CLA  | O2D-CGD | 5.34  | 1.46        | 1.33     |
| 21  | D     | 354 | CLA  | O2A-CGA | 5.30  | 1.48        | 1.33     |
| 21  | B     | 521 | CLA  | O2D-CGD | 5.30  | 1.46        | 1.33     |
| 26  | C     | 476 | LHG  | P-O6    | 5.29  | 1.80        | 1.59     |
| 33  | F     | 85  | HEM  | FE-NB   | 5.29  | 2.11        | 1.94     |
| 21  | C     | 479 | CLA  | O2A-CGA | 5.29  | 1.48        | 1.33     |
| 30  | D     | 361 | SQD  | O47-C7  | 5.26  | 1.49        | 1.34     |
| 25  | J     | 115 | BCR  | C26-C25 | 5.24  | 1.43        | 1.34     |
| 21  | B     | 526 | CLA  | O2D-CGD | 5.22  | 1.46        | 1.33     |
| 28  | C     | 474 | DGD  | O6D-C1D | 5.21  | 1.55        | 1.41     |
| 22  | D     | 355 | PHO  | CHA-CBD | 5.20  | 1.57        | 1.51     |
| 21  | C     | 485 | CLA  | C4C-C3C | 5.18  | 1.53        | 1.45     |
| 21  | C     | 486 | CLA  | C1C-C2C | 5.17  | 1.55        | 1.44     |
| 33  | F     | 85  | HEM  | C4D-ND  | -5.11 | 1.31        | 1.40     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | B     | 516 | CLA  | O2D-CGD | 5.11  | 1.45        | 1.33     |
| 21  | C     | 485 | CLA  | O2D-CGD | 5.10  | 1.45        | 1.33     |
| 21  | C     | 478 | CLA  | O2A-CGA | 5.10  | 1.48        | 1.33     |
| 21  | B     | 525 | CLA  | O2D-CGD | 5.09  | 1.45        | 1.33     |
| 21  | C     | 483 | CLA  | MG-NA   | 5.08  | 2.18        | 2.06     |
| 25  | B     | 527 | BCR  | C30-C25 | 5.05  | 1.60        | 1.53     |
| 21  | C     | 486 | CLA  | O2D-CGD | 5.04  | 1.45        | 1.33     |
| 30  | L     | 213 | SQD  | O5-C5   | 5.04  | 1.56        | 1.44     |
| 21  | D     | 356 | CLA  | O2A-CGA | 5.02  | 1.48        | 1.33     |
| 28  | D     | 362 | DGD  | O6D-C1D | 5.01  | 1.54        | 1.41     |
| 21  | B     | 516 | CLA  | C4C-C3C | 5.01  | 1.53        | 1.45     |
| 28  | C     | 491 | DGD  | O6D-C1D | 5.01  | 1.54        | 1.41     |
| 21  | C     | 483 | CLA  | C4C-C3C | 5.01  | 1.53        | 1.45     |
| 21  | B     | 522 | CLA  | O2D-CGD | 5.01  | 1.45        | 1.33     |
| 21  | C     | 486 | CLA  | C4C-C3C | 4.99  | 1.53        | 1.45     |
| 25  | B     | 529 | BCR  | C5-C6   | 4.98  | 1.42        | 1.34     |
| 21  | B     | 525 | CLA  | MG-NA   | 4.98  | 2.18        | 2.06     |
| 21  | C     | 488 | CLA  | O2A-CGA | 4.96  | 1.47        | 1.33     |
| 33  | F     | 85  | HEM  | C4A-C3A | 4.96  | 1.54        | 1.43     |
| 29  | T     | 226 | LMT  | C4B-C3B | -4.95 | 1.39        | 1.52     |
| 21  | C     | 483 | CLA  | O2A-CGA | 4.95  | 1.47        | 1.33     |
| 29  | O     | 274 | LMT  | C4B-C3B | -4.94 | 1.39        | 1.52     |
| 25  | B     | 529 | BCR  | C26-C25 | 4.93  | 1.42        | 1.34     |
| 28  | C     | 491 | DGD  | O3G-C1D | 4.91  | 1.48        | 1.40     |
| 29  | A     | 376 | LMT  | C4B-C3B | -4.91 | 1.39        | 1.52     |
| 21  | C     | 487 | CLA  | C1C-C2C | 4.91  | 1.54        | 1.44     |
| 29  | D     | 363 | LMT  | C4B-C3B | -4.91 | 1.39        | 1.52     |
| 21  | B     | 514 | CLA  | O2A-CGA | 4.90  | 1.47        | 1.33     |
| 29  | D     | 536 | LMT  | C4B-C3B | -4.89 | 1.39        | 1.52     |
| 29  | B     | 535 | LMT  | C4B-C3B | -4.89 | 1.39        | 1.52     |
| 30  | L     | 213 | SQD  | O7-S    | 4.88  | 1.58        | 1.45     |
| 30  | F     | 224 | SQD  | O47-C7  | 4.88  | 1.48        | 1.34     |
| 29  | I     | 274 | LMT  | C4B-C3B | -4.87 | 1.39        | 1.52     |
| 21  | C     | 488 | CLA  | O2D-CGD | 4.86  | 1.45        | 1.33     |
| 21  | B     | 521 | CLA  | C1D-C2D | 4.85  | 1.54        | 1.45     |
| 28  | B     | 533 | DGD  | O5D-C1E | 4.84  | 1.48        | 1.40     |
| 21  | D     | 356 | CLA  | C1C-C2C | 4.84  | 1.54        | 1.44     |
| 21  | B     | 515 | CLA  | C1C-C2C | 4.82  | 1.54        | 1.44     |
| 21  | C     | 487 | CLA  | O2D-CGD | 4.81  | 1.45        | 1.33     |
| 21  | B     | 524 | CLA  | C1C-C2C | 4.81  | 1.54        | 1.44     |
| 21  | B     | 512 | CLA  | O2A-CGA | 4.81  | 1.47        | 1.33     |
| 33  | F     | 85  | HEM  | C1C-C2C | 4.81  | 1.54        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | C     | 485 | CLA  | C1C-C2C | 4.80  | 1.54        | 1.44     |
| 21  | B     | 526 | CLA  | C4C-C3C | 4.80  | 1.53        | 1.45     |
| 25  | D     | 358 | BCR  | C26-C25 | 4.80  | 1.42        | 1.34     |
| 21  | B     | 521 | CLA  | C4C-C3C | 4.79  | 1.53        | 1.45     |
| 21  | C     | 488 | CLA  | C1C-C2C | 4.79  | 1.54        | 1.44     |
| 21  | C     | 484 | CLA  | O2A-CGA | 4.79  | 1.47        | 1.33     |
| 21  | K     | 483 | CLA  | O2A-CGA | 4.79  | 1.47        | 1.33     |
| 29  | A     | 376 | LMT  | O5B-C1B | 4.79  | 1.54        | 1.41     |
| 33  | F     | 85  | HEM  | CBC-CAC | 4.78  | 1.53        | 1.30     |
| 30  | F     | 224 | SQD  | O48-C23 | 4.77  | 1.47        | 1.33     |
| 21  | D     | 354 | CLA  | C4C-C3C | 4.77  | 1.53        | 1.45     |
| 33  | V     | 164 | HEM  | CBC-CAC | 4.76  | 1.53        | 1.30     |
| 26  | A     | 371 | LHG  | P-O6    | 4.76  | 1.78        | 1.59     |
| 25  | D     | 358 | BCR  | C30-C25 | 4.76  | 1.59        | 1.53     |
| 21  | C     | 480 | CLA  | O2A-CGA | 4.74  | 1.47        | 1.33     |
| 21  | A     | 362 | CLA  | O2D-CGD | 4.74  | 1.44        | 1.33     |
| 21  | C     | 483 | CLA  | C1C-C2C | 4.73  | 1.54        | 1.44     |
| 30  | L     | 213 | SQD  | O47-C7  | 4.72  | 1.47        | 1.34     |
| 21  | K     | 483 | CLA  | O2D-CGD | 4.72  | 1.44        | 1.33     |
| 21  | C     | 482 | CLA  | MG-NC   | 4.71  | 2.17        | 2.06     |
| 25  | B     | 530 | BCR  | C26-C25 | 4.70  | 1.42        | 1.34     |
| 33  | F     | 85  | HEM  | C3B-C4B | 4.70  | 1.54        | 1.44     |
| 22  | D     | 355 | PHO  | CMC-C2C | 4.69  | 1.57        | 1.50     |
| 21  | A     | 363 | CLA  | O2A-CGA | 4.69  | 1.47        | 1.33     |
| 21  | B     | 518 | CLA  | C4-C3   | -4.69 | 1.39        | 1.50     |
| 21  | C     | 479 | CLA  | C1D-C2D | 4.68  | 1.54        | 1.45     |
| 22  | A     | 365 | PHO  | O2D-CGD | 4.67  | 1.44        | 1.33     |
| 21  | B     | 520 | CLA  | C4-C3   | -4.67 | 1.39        | 1.50     |
| 30  | D     | 361 | SQD  | O7-S    | 4.66  | 1.58        | 1.45     |
| 21  | D     | 354 | CLA  | C4-C3   | -4.66 | 1.39        | 1.50     |
| 21  | A     | 362 | CLA  | C4-C3   | -4.66 | 1.39        | 1.50     |
| 21  | C     | 481 | CLA  | CAA-CBA | -4.65 | 1.39        | 1.52     |
| 21  | B     | 512 | CLA  | C4-C3   | -4.65 | 1.39        | 1.50     |
| 21  | B     | 517 | CLA  | C4-C3   | -4.65 | 1.39        | 1.50     |
| 21  | A     | 366 | CLA  | O2A-CGA | 4.65  | 1.46        | 1.33     |
| 22  | D     | 355 | PHO  | C4-C3   | -4.65 | 1.39        | 1.50     |
| 21  | B     | 516 | CLA  | C4-C3   | -4.65 | 1.39        | 1.50     |
| 21  | B     | 522 | CLA  | O2A-CGA | 4.64  | 1.46        | 1.33     |
| 21  | C     | 482 | CLA  | C4-C3   | -4.64 | 1.39        | 1.50     |
| 22  | A     | 365 | PHO  | C4-C3   | -4.63 | 1.39        | 1.50     |
| 21  | A     | 366 | CLA  | C4-C3   | -4.63 | 1.39        | 1.50     |
| 21  | B     | 519 | CLA  | C4-C3   | -4.63 | 1.39        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | B     | 514 | CLA  | C4-C3   | -4.62 | 1.39        | 1.50     |
| 21  | D     | 356 | CLA  | C4-C3   | -4.62 | 1.39        | 1.50     |
| 21  | D     | 356 | CLA  | C4C-C3C | 4.62  | 1.52        | 1.45     |
| 21  | B     | 511 | CLA  | C3B-C2B | 4.62  | 1.56        | 1.41     |
| 21  | C     | 481 | CLA  | C4-C3   | -4.62 | 1.39        | 1.50     |
| 21  | B     | 513 | CLA  | C4-C3   | -4.62 | 1.39        | 1.50     |
| 21  | C     | 483 | CLA  | C4-C3   | -4.61 | 1.39        | 1.50     |
| 21  | B     | 515 | CLA  | C4-C3   | -4.61 | 1.39        | 1.50     |
| 21  | C     | 479 | CLA  | C4-C3   | -4.61 | 1.39        | 1.50     |
| 21  | A     | 366 | CLA  | C1C-C2C | 4.61  | 1.53        | 1.44     |
| 21  | C     | 484 | CLA  | C4-C3   | -4.61 | 1.39        | 1.50     |
| 21  | B     | 523 | CLA  | C4-C3   | -4.61 | 1.39        | 1.50     |
| 21  | B     | 524 | CLA  | C4-C3   | -4.61 | 1.39        | 1.50     |
| 21  | A     | 363 | CLA  | C4-C3   | -4.60 | 1.39        | 1.50     |
| 21  | C     | 484 | CLA  | C3B-C4B | 4.60  | 1.56        | 1.42     |
| 21  | B     | 511 | CLA  | C4-C3   | -4.60 | 1.39        | 1.50     |
| 21  | A     | 364 | CLA  | C4-C3   | -4.60 | 1.39        | 1.50     |
| 21  | C     | 485 | CLA  | C3B-C4B | 4.60  | 1.56        | 1.42     |
| 21  | C     | 477 | CLA  | C4-C3   | -4.60 | 1.39        | 1.50     |
| 21  | C     | 480 | CLA  | C4-C3   | -4.60 | 1.39        | 1.50     |
| 21  | C     | 486 | CLA  | C4-C3   | -4.60 | 1.39        | 1.50     |
| 21  | C     | 485 | CLA  | C1D-C2D | 4.60  | 1.54        | 1.45     |
| 25  | B     | 530 | BCR  | C5-C6   | 4.59  | 1.42        | 1.34     |
| 21  | C     | 485 | CLA  | C4-C3   | -4.59 | 1.39        | 1.50     |
| 21  | K     | 483 | CLA  | C4-C3   | -4.59 | 1.39        | 1.50     |
| 21  | C     | 487 | CLA  | C4-C3   | -4.59 | 1.39        | 1.50     |
| 21  | B     | 522 | CLA  | C4-C3   | -4.59 | 1.39        | 1.50     |
| 21  | B     | 526 | CLA  | C4-C3   | -4.59 | 1.39        | 1.50     |
| 21  | C     | 488 | CLA  | C4-C3   | -4.58 | 1.39        | 1.50     |
| 21  | B     | 518 | CLA  | CAA-CBA | -4.58 | 1.39        | 1.52     |
| 21  | C     | 478 | CLA  | O2D-CGD | 4.58  | 1.44        | 1.33     |
| 21  | C     | 478 | CLA  | C4-C3   | -4.57 | 1.39        | 1.50     |
| 21  | B     | 525 | CLA  | C4-C3   | -4.57 | 1.39        | 1.50     |
| 21  | B     | 517 | CLA  | CAA-CBA | -4.57 | 1.39        | 1.52     |
| 21  | B     | 515 | CLA  | CAA-CBA | -4.56 | 1.39        | 1.52     |
| 21  | C     | 484 | CLA  | CAA-CBA | -4.56 | 1.39        | 1.52     |
| 21  | A     | 362 | CLA  | MG-NA   | 4.56  | 2.17        | 2.06     |
| 28  | A     | 375 | DGD  | O6D-C1D | 4.56  | 1.53        | 1.41     |
| 21  | B     | 521 | CLA  | C4-C3   | -4.56 | 1.39        | 1.50     |
| 21  | B     | 519 | CLA  | CAA-CBA | -4.55 | 1.39        | 1.52     |
| 21  | C     | 480 | CLA  | CAA-CBA | -4.54 | 1.39        | 1.52     |
| 25  | C     | 489 | BCR  | C30-C25 | 4.54  | 1.59        | 1.53     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | C     | 480 | CLA  | O2D-CGD | 4.54  | 1.44        | 1.33     |
| 21  | C     | 478 | CLA  | CAA-CBA | -4.54 | 1.39        | 1.52     |
| 30  | C     | 475 | SQD  | O47-C7  | 4.53  | 1.47        | 1.34     |
| 21  | B     | 522 | CLA  | CAA-CBA | -4.53 | 1.39        | 1.52     |
| 21  | B     | 520 | CLA  | CAA-CBA | -4.52 | 1.39        | 1.52     |
| 21  | C     | 479 | CLA  | CAA-CBA | -4.52 | 1.39        | 1.52     |
| 21  | C     | 488 | CLA  | CAA-CBA | -4.52 | 1.39        | 1.52     |
| 21  | C     | 477 | CLA  | CAA-CBA | -4.52 | 1.39        | 1.52     |
| 21  | B     | 514 | CLA  | C4C-C3C | 4.52  | 1.52        | 1.45     |
| 21  | C     | 480 | CLA  | C4C-C3C | 4.52  | 1.52        | 1.45     |
| 21  | C     | 479 | CLA  | C1C-C2C | 4.51  | 1.53        | 1.44     |
| 28  | A     | 375 | DGD  | O6D-C5D | 4.51  | 1.55        | 1.44     |
| 22  | A     | 365 | PHO  | CAA-CBA | -4.51 | 1.39        | 1.52     |
| 21  | A     | 366 | CLA  | O2D-CGD | 4.51  | 1.44        | 1.33     |
| 21  | C     | 484 | CLA  | C1C-C2C | 4.51  | 1.53        | 1.44     |
| 21  | B     | 521 | CLA  | CAA-CBA | -4.51 | 1.39        | 1.52     |
| 21  | B     | 512 | CLA  | CAA-CBA | -4.51 | 1.39        | 1.52     |
| 21  | A     | 362 | CLA  | CAA-CBA | -4.50 | 1.39        | 1.52     |
| 21  | K     | 483 | CLA  | CAA-CBA | -4.50 | 1.39        | 1.52     |
| 25  | B     | 530 | BCR  | C2-C1   | 4.50  | 1.64        | 1.54     |
| 21  | B     | 524 | CLA  | CAA-CBA | -4.50 | 1.39        | 1.52     |
| 25  | J     | 115 | BCR  | C29-C30 | 4.49  | 1.64        | 1.54     |
| 33  | V     | 164 | HEM  | C1C-C2C | 4.49  | 1.54        | 1.45     |
| 21  | D     | 356 | CLA  | CAA-CBA | -4.49 | 1.39        | 1.52     |
| 21  | B     | 514 | CLA  | CAA-CBA | -4.49 | 1.39        | 1.52     |
| 21  | B     | 523 | CLA  | CAA-CBA | -4.49 | 1.39        | 1.52     |
| 29  | O     | 274 | LMT  | O5B-C1B | 4.48  | 1.53        | 1.41     |
| 21  | D     | 354 | CLA  | CAA-CBA | -4.48 | 1.39        | 1.52     |
| 21  | C     | 486 | CLA  | CAA-CBA | -4.48 | 1.39        | 1.52     |
| 25  | B     | 529 | BCR  | C1-C6   | 4.48  | 1.59        | 1.53     |
| 21  | B     | 513 | CLA  | O2D-CGD | 4.47  | 1.44        | 1.33     |
| 21  | B     | 511 | CLA  | MG-NC   | 4.47  | 2.16        | 2.06     |
| 21  | A     | 364 | CLA  | CAA-CBA | -4.47 | 1.39        | 1.52     |
| 25  | J     | 112 | BCR  | C5-C6   | 4.47  | 1.42        | 1.34     |
| 21  | A     | 366 | CLA  | CAA-CBA | -4.46 | 1.39        | 1.52     |
| 21  | B     | 513 | CLA  | CAA-CBA | -4.46 | 1.39        | 1.52     |
| 21  | B     | 516 | CLA  | CAA-CBA | -4.46 | 1.39        | 1.52     |
| 21  | C     | 482 | CLA  | CAA-CBA | -4.46 | 1.39        | 1.52     |
| 30  | F     | 224 | SQD  | O7-S    | 4.45  | 1.57        | 1.45     |
| 21  | C     | 485 | CLA  | CAA-CBA | -4.45 | 1.39        | 1.52     |
| 22  | D     | 355 | PHO  | CAA-CBA | -4.45 | 1.39        | 1.52     |
| 21  | C     | 483 | CLA  | CAA-CBA | -4.44 | 1.39        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 29  | D     | 363 | LMT  | O1'-C1' | 4.44  | 1.47        | 1.40     |
| 21  | B     | 526 | CLA  | CAA-CBA | -4.44 | 1.39        | 1.52     |
| 21  | B     | 523 | CLA  | C1C-C2C | 4.44  | 1.53        | 1.44     |
| 21  | A     | 363 | CLA  | CAA-CBA | -4.44 | 1.39        | 1.52     |
| 21  | B     | 516 | CLA  | MG-NC   | 4.43  | 2.16        | 2.06     |
| 21  | B     | 520 | CLA  | O2D-CGD | 4.43  | 1.44        | 1.33     |
| 21  | B     | 521 | CLA  | O2A-CGA | 4.42  | 1.46        | 1.33     |
| 21  | B     | 525 | CLA  | CAA-CBA | -4.42 | 1.39        | 1.52     |
| 21  | B     | 523 | CLA  | C3B-C4B | 4.41  | 1.55        | 1.42     |
| 21  | K     | 483 | CLA  | C1C-C2C | 4.40  | 1.53        | 1.44     |
| 27  | J     | 492 | LMG  | O7-C8   | 4.40  | 1.57        | 1.46     |
| 21  | B     | 511 | CLA  | CAA-CBA | -4.40 | 1.39        | 1.52     |
| 21  | C     | 487 | CLA  | CAA-CBA | -4.39 | 1.39        | 1.52     |
| 30  | F     | 224 | SQD  | O5-C5   | 4.38  | 1.55        | 1.44     |
| 21  | C     | 478 | CLA  | C1C-C2C | 4.38  | 1.53        | 1.44     |
| 21  | B     | 515 | CLA  | O2D-CGD | 4.37  | 1.44        | 1.33     |
| 28  | C     | 492 | DGD  | O6D-C1D | 4.37  | 1.53        | 1.41     |
| 21  | C     | 485 | CLA  | O2A-CGA | 4.35  | 1.46        | 1.33     |
| 30  | D     | 361 | SQD  | O5-C5   | 4.35  | 1.55        | 1.44     |
| 21  | C     | 482 | CLA  | C1B-NB  | 4.35  | 1.43        | 1.37     |
| 21  | C     | 481 | CLA  | C4C-C3C | 4.34  | 1.52        | 1.45     |
| 21  | B     | 523 | CLA  | O2A-CGA | 4.34  | 1.46        | 1.33     |
| 21  | C     | 482 | CLA  | C3B-C4B | 4.33  | 1.55        | 1.42     |
| 21  | A     | 366 | CLA  | MG-NC   | 4.33  | 2.16        | 2.06     |
| 21  | B     | 517 | CLA  | C1C-C2C | 4.33  | 1.53        | 1.44     |
| 33  | F     | 85  | HEM  | FE-NC   | 4.33  | 2.09        | 1.95     |
| 21  | C     | 478 | CLA  | C4C-C3C | 4.33  | 1.52        | 1.45     |
| 21  | K     | 483 | CLA  | C4C-C3C | 4.33  | 1.52        | 1.45     |
| 21  | A     | 363 | CLA  | C3B-C4B | 4.33  | 1.55        | 1.42     |
| 21  | B     | 517 | CLA  | C4C-C3C | 4.33  | 1.52        | 1.45     |
| 21  | C     | 482 | CLA  | C1D-C2D | 4.32  | 1.53        | 1.45     |
| 25  | B     | 530 | BCR  | C29-C30 | 4.31  | 1.64        | 1.54     |
| 21  | D     | 354 | CLA  | C1C-C2C | 4.31  | 1.53        | 1.44     |
| 21  | B     | 525 | CLA  | C1C-C2C | 4.31  | 1.53        | 1.44     |
| 28  | C     | 474 | DGD  | O3G-C1D | 4.29  | 1.47        | 1.40     |
| 28  | C     | 493 | DGD  | O6D-C1D | 4.28  | 1.52        | 1.41     |
| 25  | C     | 490 | BCR  | C5-C6   | 4.28  | 1.41        | 1.34     |
| 33  | V     | 164 | HEM  | C3C-C4C | 4.25  | 1.53        | 1.46     |
| 21  | B     | 519 | CLA  | C4C-C3C | 4.25  | 1.52        | 1.45     |
| 30  | L     | 213 | SQD  | O48-C23 | 4.24  | 1.45        | 1.33     |
| 21  | B     | 519 | CLA  | O2A-CGA | 4.24  | 1.45        | 1.33     |
| 23  | A     | 367 | MES  | C8-S    | 4.23  | 1.83        | 1.77     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | A     | 364 | CLA  | C4C-C3C | 4.23  | 1.52        | 1.45     |
| 30  | C     | 475 | SQD  | O5-C5   | 4.23  | 1.54        | 1.44     |
| 21  | B     | 523 | CLA  | O2D-CGD | 4.23  | 1.43        | 1.33     |
| 21  | B     | 512 | CLA  | O2D-CGD | 4.22  | 1.43        | 1.33     |
| 21  | B     | 517 | CLA  | O2D-CGD | 4.22  | 1.43        | 1.33     |
| 21  | B     | 517 | CLA  | C1D-C2D | 4.22  | 1.53        | 1.45     |
| 21  | B     | 522 | CLA  | C1C-C2C | 4.21  | 1.53        | 1.44     |
| 21  | A     | 364 | CLA  | O2D-CGD | 4.21  | 1.43        | 1.33     |
| 21  | B     | 518 | CLA  | C1C-C2C | 4.19  | 1.53        | 1.44     |
| 21  | B     | 519 | CLA  | C1D-C2D | 4.18  | 1.53        | 1.45     |
| 22  | A     | 365 | PHO  | O2A-CGA | 4.18  | 1.45        | 1.33     |
| 21  | C     | 480 | CLA  | C1C-C2C | 4.18  | 1.53        | 1.44     |
| 21  | C     | 479 | CLA  | O2D-CGD | 4.17  | 1.43        | 1.33     |
| 21  | B     | 524 | CLA  | O2D-CGD | 4.17  | 1.43        | 1.33     |
| 21  | B     | 517 | CLA  | C3B-C4B | 4.15  | 1.54        | 1.42     |
| 26  | A     | 371 | LHG  | O7-C7   | 4.15  | 1.46        | 1.34     |
| 28  | A     | 375 | DGD  | O5D-C1E | 4.15  | 1.47        | 1.40     |
| 25  | D     | 358 | BCR  | C1-C6   | 4.15  | 1.59        | 1.53     |
| 28  | C     | 474 | DGD  | O1G-C1A | 4.15  | 1.45        | 1.33     |
| 21  | B     | 524 | CLA  | C4C-C3C | 4.14  | 1.52        | 1.45     |
| 21  | B     | 518 | CLA  | O2D-CGD | 4.14  | 1.43        | 1.33     |
| 21  | C     | 479 | CLA  | C4C-C3C | 4.13  | 1.52        | 1.45     |
| 21  | C     | 487 | CLA  | MG-NC   | 4.13  | 2.16        | 2.06     |
| 21  | A     | 363 | CLA  | C1C-C2C | 4.12  | 1.52        | 1.44     |
| 21  | B     | 524 | CLA  | C1D-C2D | 4.11  | 1.53        | 1.45     |
| 25  | X     | 107 | BCR  | C26-C25 | 4.10  | 1.41        | 1.34     |
| 33  | V     | 164 | HEM  | C4D-ND  | -4.10 | 1.33        | 1.40     |
| 21  | C     | 477 | CLA  | C4C-C3C | 4.09  | 1.52        | 1.45     |
| 25  | Z     | 116 | BCR  | C26-C25 | 4.09  | 1.41        | 1.34     |
| 33  | V     | 164 | HEM  | FE-NC   | 4.09  | 2.08        | 1.95     |
| 21  | D     | 354 | CLA  | O2D-CGD | 4.08  | 1.43        | 1.33     |
| 21  | C     | 486 | CLA  | CHC-C1C | 4.07  | 1.46        | 1.38     |
| 30  | L     | 213 | SQD  | O6-C1   | 4.07  | 1.47        | 1.40     |
| 21  | C     | 479 | CLA  | MG-NC   | 4.06  | 2.15        | 2.06     |
| 28  | C     | 474 | DGD  | O6D-C5D | 4.06  | 1.54        | 1.44     |
| 30  | D     | 361 | SQD  | C1-C2   | 4.06  | 1.64        | 1.52     |
| 25  | B     | 529 | BCR  | C29-C30 | 4.06  | 1.63        | 1.54     |
| 21  | C     | 481 | CLA  | O2D-CGD | 4.06  | 1.43        | 1.33     |
| 25  | D     | 358 | BCR  | C29-C30 | 4.05  | 1.63        | 1.54     |
| 21  | B     | 516 | CLA  | C1C-C2C | 4.05  | 1.52        | 1.44     |
| 21  | C     | 488 | CLA  | C4C-C3C | 4.04  | 1.51        | 1.45     |
| 21  | A     | 366 | CLA  | C3B-C4B | 4.04  | 1.54        | 1.42     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 21  | B     | 516 | CLA  | CBA-CGA | 4.02 | 1.62        | 1.50     |
| 22  | D     | 355 | PHO  | O2A-CGA | 4.02 | 1.45        | 1.33     |
| 21  | B     | 518 | CLA  | C1D-C2D | 4.01 | 1.53        | 1.45     |
| 22  | A     | 365 | PHO  | CMC-C2C | 4.00 | 1.56        | 1.50     |
| 21  | B     | 515 | CLA  | C3B-C4B | 4.00 | 1.54        | 1.42     |
| 21  | B     | 518 | CLA  | C4C-C3C | 4.00 | 1.51        | 1.45     |
| 21  | B     | 513 | CLA  | C3B-C4B | 4.00 | 1.54        | 1.42     |
| 21  | B     | 519 | CLA  | C1C-C2C | 3.99 | 1.52        | 1.44     |
| 30  | L     | 213 | SQD  | C1-C2   | 3.99 | 1.64        | 1.52     |
| 21  | C     | 480 | CLA  | MG-NB   | 3.98 | 2.13        | 2.05     |
| 21  | C     | 481 | CLA  | C1B-NB  | 3.98 | 1.43        | 1.37     |
| 21  | B     | 526 | CLA  | C3B-C4B | 3.97 | 1.54        | 1.42     |
| 21  | C     | 483 | CLA  | MG-NC   | 3.96 | 2.15        | 2.06     |
| 21  | C     | 483 | CLA  | C1D-C2D | 3.96 | 1.53        | 1.45     |
| 21  | A     | 362 | CLA  | C4C-C3C | 3.95 | 1.51        | 1.45     |
| 21  | C     | 481 | CLA  | C3B-C4B | 3.94 | 1.54        | 1.42     |
| 33  | V     | 164 | HEM  | O2D-CGD | 3.94 | 1.43        | 1.30     |
| 21  | A     | 366 | CLA  | C4C-C3C | 3.94 | 1.51        | 1.45     |
| 30  | C     | 475 | SQD  | C1-C2   | 3.94 | 1.64        | 1.52     |
| 21  | B     | 526 | CLA  | C1D-C2D | 3.94 | 1.53        | 1.45     |
| 21  | B     | 520 | CLA  | O2A-CGA | 3.94 | 1.44        | 1.33     |
| 21  | C     | 478 | CLA  | C3B-C4B | 3.94 | 1.54        | 1.42     |
| 21  | C     | 486 | CLA  | MG-NB   | 3.93 | 2.13        | 2.05     |
| 21  | B     | 514 | CLA  | C1C-C2C | 3.93 | 1.52        | 1.44     |
| 28  | C     | 474 | DGD  | O6E-C1E | 3.93 | 1.51        | 1.41     |
| 21  | B     | 520 | CLA  | C1C-C2C | 3.91 | 1.52        | 1.44     |
| 21  | C     | 485 | CLA  | MG-NA   | 3.91 | 2.15        | 2.06     |
| 21  | D     | 356 | CLA  | O2D-CGD | 3.89 | 1.42        | 1.33     |
| 29  | B     | 535 | LMT  | O5B-C1B | 3.89 | 1.51        | 1.41     |
| 21  | B     | 513 | CLA  | C1C-C2C | 3.89 | 1.52        | 1.44     |
| 21  | B     | 526 | CLA  | C1B-NB  | 3.88 | 1.43        | 1.37     |
| 28  | C     | 474 | DGD  | O2G-C1B | 3.88 | 1.45        | 1.34     |
| 25  | A     | 369 | BCR  | C26-C25 | 3.87 | 1.41        | 1.34     |
| 21  | C     | 483 | CLA  | C3B-C4B | 3.87 | 1.54        | 1.42     |
| 26  | C     | 476 | LHG  | O8-C23  | 3.87 | 1.44        | 1.33     |
| 28  | B     | 533 | DGD  | O6D-C1D | 3.86 | 1.51        | 1.41     |
| 21  | B     | 523 | CLA  | C4C-C3C | 3.86 | 1.51        | 1.45     |
| 25  | B     | 527 | BCR  | C26-C25 | 3.85 | 1.41        | 1.34     |
| 22  | D     | 355 | PHO  | O2D-CGD | 3.85 | 1.42        | 1.33     |
| 21  | B     | 514 | CLA  | O2D-CGD | 3.85 | 1.42        | 1.33     |
| 21  | B     | 513 | CLA  | C4C-C3C | 3.84 | 1.51        | 1.45     |
| 21  | C     | 487 | CLA  | C5-C3   | 3.84 | 1.59        | 1.51     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 21  | B     | 520 | CLA  | MG-NC   | 3.83 | 2.15        | 2.06     |
| 28  | C     | 474 | DGD  | C3G-C2G | 3.83 | 1.62        | 1.50     |
| 21  | A     | 364 | CLA  | C1C-C2C | 3.82 | 1.52        | 1.44     |
| 21  | B     | 522 | CLA  | C4C-C3C | 3.82 | 1.51        | 1.45     |
| 21  | B     | 512 | CLA  | C1C-C2C | 3.82 | 1.52        | 1.44     |
| 28  | A     | 375 | DGD  | C3G-C2G | 3.81 | 1.62        | 1.50     |
| 21  | K     | 483 | CLA  | MG-NC   | 3.81 | 2.15        | 2.06     |
| 21  | C     | 482 | CLA  | MG-NB   | 3.81 | 2.13        | 2.05     |
| 33  | V     | 164 | HEM  | C4A-C3A | 3.81 | 1.52        | 1.43     |
| 21  | B     | 512 | CLA  | C4C-C3C | 3.80 | 1.51        | 1.45     |
| 21  | A     | 364 | CLA  | C1D-C2D | 3.80 | 1.52        | 1.45     |
| 21  | B     | 511 | CLA  | CMC-C2C | 3.79 | 1.58        | 1.50     |
| 21  | B     | 524 | CLA  | C3B-C4B | 3.79 | 1.53        | 1.42     |
| 21  | B     | 525 | CLA  | MG-NC   | 3.79 | 2.15        | 2.06     |
| 21  | A     | 363 | CLA  | O2D-CGD | 3.79 | 1.42        | 1.33     |
| 21  | B     | 516 | CLA  | C5-C3   | 3.78 | 1.59        | 1.51     |
| 21  | B     | 511 | CLA  | C1D-C2D | 3.78 | 1.52        | 1.45     |
| 30  | C     | 475 | SQD  | O7-S    | 3.78 | 1.55        | 1.45     |
| 28  | B     | 533 | DGD  | O6E-C1E | 3.78 | 1.51        | 1.41     |
| 21  | C     | 484 | CLA  | C4C-C3C | 3.78 | 1.51        | 1.45     |
| 21  | C     | 486 | CLA  | C1D-C2D | 3.77 | 1.52        | 1.45     |
| 21  | B     | 524 | CLA  | C5-C3   | 3.77 | 1.59        | 1.51     |
| 25  | J     | 112 | BCR  | C1-C6   | 3.77 | 1.58        | 1.53     |
| 21  | C     | 488 | CLA  | C3B-C4B | 3.77 | 1.53        | 1.42     |
| 25  | A     | 369 | BCR  | C5-C6   | 3.76 | 1.40        | 1.34     |
| 21  | C     | 484 | CLA  | MG-NC   | 3.76 | 2.15        | 2.06     |
| 30  | C     | 475 | SQD  | O6-C1   | 3.75 | 1.46        | 1.40     |
| 25  | C     | 489 | BCR  | C2-C1   | 3.75 | 1.62        | 1.54     |
| 21  | C     | 485 | CLA  | MG-NC   | 3.74 | 2.15        | 2.06     |
| 21  | B     | 522 | CLA  | C3B-C4B | 3.74 | 1.53        | 1.42     |
| 21  | B     | 525 | CLA  | C4C-C3C | 3.72 | 1.51        | 1.45     |
| 21  | C     | 481 | CLA  | C1D-C2D | 3.72 | 1.52        | 1.45     |
| 21  | B     | 511 | CLA  | CHB-C4A | 3.72 | 1.47        | 1.37     |
| 25  | J     | 115 | BCR  | C1-C6   | 3.71 | 1.58        | 1.53     |
| 21  | C     | 480 | CLA  | C1B-NB  | 3.71 | 1.42        | 1.37     |
| 28  | A     | 375 | DGD  | O6E-C5E | 3.70 | 1.53        | 1.44     |
| 33  | F     | 85  | HEM  | C3C-C4C | 3.70 | 1.52        | 1.46     |
| 30  | C     | 475 | SQD  | O48-C23 | 3.69 | 1.44        | 1.33     |
| 33  | V     | 164 | HEM  | CAC-C3C | 3.69 | 1.57        | 1.47     |
| 21  | B     | 521 | CLA  | C1C-C2C | 3.69 | 1.52        | 1.44     |
| 21  | C     | 486 | CLA  | O1D-CGD | 3.69 | 1.30        | 1.21     |
| 21  | B     | 521 | CLA  | O1D-CGD | 3.68 | 1.30        | 1.21     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | C     | 484 | CLA  | C1D-C2D | 3.68  | 1.52        | 1.45     |
| 25  | X     | 107 | BCR  | C29-C30 | 3.68  | 1.62        | 1.54     |
| 21  | C     | 480 | CLA  | CMC-C2C | 3.68  | 1.58        | 1.50     |
| 21  | C     | 486 | CLA  | C3B-C4B | 3.67  | 1.53        | 1.42     |
| 21  | C     | 481 | CLA  | C3B-C2B | 3.67  | 1.53        | 1.41     |
| 28  | D     | 362 | DGD  | C2A-C1A | 3.67  | 1.61        | 1.50     |
| 21  | B     | 519 | CLA  | C3B-C4B | 3.66  | 1.53        | 1.42     |
| 21  | B     | 511 | CLA  | O1D-CGD | 3.66  | 1.30        | 1.21     |
| 21  | B     | 521 | CLA  | C5-C3   | 3.66  | 1.58        | 1.51     |
| 25  | B     | 529 | BCR  | C2-C1   | 3.65  | 1.62        | 1.54     |
| 21  | C     | 482 | CLA  | C3B-C2B | 3.65  | 1.53        | 1.41     |
| 32  | D     | 357 | PL9  | C12-C13 | -3.65 | 1.39        | 1.50     |
| 32  | D     | 357 | PL9  | C6-C5   | 3.64  | 1.53        | 1.35     |
| 21  | B     | 512 | CLA  | C3B-C4B | 3.64  | 1.53        | 1.42     |
| 21  | C     | 480 | CLA  | C3B-C4B | 3.64  | 1.53        | 1.42     |
| 21  | C     | 478 | CLA  | C1D-C2D | 3.63  | 1.52        | 1.45     |
| 25  | C     | 490 | BCR  | C2-C1   | 3.63  | 1.62        | 1.54     |
| 21  | B     | 521 | CLA  | MG-NC   | 3.62  | 2.14        | 2.06     |
| 21  | C     | 482 | CLA  | O1D-CGD | 3.62  | 1.30        | 1.21     |
| 21  | C     | 477 | CLA  | C1C-C2C | 3.62  | 1.51        | 1.44     |
| 21  | D     | 356 | CLA  | MG-NC   | 3.61  | 2.14        | 2.06     |
| 21  | B     | 525 | CLA  | C3B-C4B | 3.60  | 1.53        | 1.42     |
| 32  | D     | 357 | PL9  | C32-C33 | -3.60 | 1.39        | 1.50     |
| 21  | C     | 487 | CLA  | CMC-C2C | 3.60  | 1.58        | 1.50     |
| 21  | C     | 488 | CLA  | C1D-C2D | 3.60  | 1.52        | 1.45     |
| 21  | C     | 485 | CLA  | C1B-NB  | 3.59  | 1.42        | 1.37     |
| 21  | C     | 488 | CLA  | O1D-CGD | 3.59  | 1.30        | 1.21     |
| 28  | C     | 493 | DGD  | O5D-C6D | -3.59 | 1.37        | 1.43     |
| 30  | C     | 475 | SQD  | O3-C3   | 3.59  | 1.51        | 1.43     |
| 21  | B     | 526 | CLA  | MG-NC   | 3.58  | 2.14        | 2.06     |
| 32  | D     | 357 | PL9  | C37-C38 | -3.58 | 1.39        | 1.50     |
| 26  | A     | 371 | LHG  | O8-C23  | 3.57  | 1.43        | 1.33     |
| 21  | K     | 483 | CLA  | C3B-C4B | 3.56  | 1.53        | 1.42     |
| 25  | J     | 112 | BCR  | C2-C1   | 3.55  | 1.62        | 1.54     |
| 21  | D     | 356 | CLA  | C1D-C2D | 3.55  | 1.52        | 1.45     |
| 33  | F     | 85  | HEM  | CAC-C3C | 3.55  | 1.56        | 1.47     |
| 21  | A     | 362 | CLA  | C1C-C2C | 3.55  | 1.51        | 1.44     |
| 33  | F     | 85  | HEM  | O2D-CGD | 3.55  | 1.42        | 1.30     |
| 21  | B     | 514 | CLA  | C1D-C2D | 3.54  | 1.52        | 1.45     |
| 21  | C     | 487 | CLA  | CAA-C2A | 3.54  | 1.60        | 1.54     |
| 32  | D     | 357 | PL9  | C27-C28 | -3.53 | 1.39        | 1.50     |
| 21  | B     | 526 | CLA  | MG-NB   | 3.53  | 2.12        | 2.05     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | B     | 523 | CLA  | MG-NC   | 3.52  | 2.14        | 2.06     |
| 21  | B     | 517 | CLA  | C5-C3   | 3.52  | 1.58        | 1.51     |
| 29  | B     | 535 | LMT  | O5'-C1' | 3.51  | 1.50        | 1.41     |
| 21  | A     | 362 | CLA  | MG-NB   | 3.51  | 2.12        | 2.05     |
| 29  | O     | 274 | LMT  | O1B-C4' | 3.50  | 1.52        | 1.43     |
| 28  | D     | 362 | DGD  | O2G-C1B | 3.49  | 1.44        | 1.34     |
| 25  | A     | 369 | BCR  | C2-C1   | 3.49  | 1.62        | 1.54     |
| 21  | C     | 483 | CLA  | CMC-C2C | 3.49  | 1.57        | 1.50     |
| 21  | B     | 511 | CLA  | C1C-C2C | 3.49  | 1.51        | 1.44     |
| 21  | B     | 518 | CLA  | MG-NB   | 3.48  | 2.12        | 2.05     |
| 29  | D     | 536 | LMT  | O5B-C1B | 3.48  | 1.50        | 1.41     |
| 21  | C     | 481 | CLA  | CMC-C2C | 3.48  | 1.57        | 1.50     |
| 21  | B     | 521 | CLA  | C3B-C4B | 3.48  | 1.52        | 1.42     |
| 21  | C     | 482 | CLA  | CBA-CGA | 3.47  | 1.60        | 1.50     |
| 21  | C     | 480 | CLA  | C1D-C2D | 3.47  | 1.52        | 1.45     |
| 29  | D     | 363 | LMT  | O5'-C1' | 3.47  | 1.50        | 1.41     |
| 29  | I     | 274 | LMT  | O5B-C1B | 3.46  | 1.50        | 1.41     |
| 28  | C     | 493 | DGD  | C5B-C4B | -3.46 | 1.34        | 1.51     |
| 25  | J     | 112 | BCR  | C29-C30 | 3.46  | 1.62        | 1.54     |
| 21  | A     | 364 | CLA  | C3B-C4B | 3.46  | 1.52        | 1.42     |
| 21  | C     | 482 | CLA  | CMC-C2C | 3.45  | 1.57        | 1.50     |
| 25  | Z     | 116 | BCR  | C5-C6   | 3.45  | 1.40        | 1.34     |
| 21  | B     | 515 | CLA  | CMC-C2C | 3.43  | 1.57        | 1.50     |
| 25  | B     | 527 | BCR  | C5-C6   | 3.43  | 1.40        | 1.34     |
| 21  | C     | 481 | CLA  | CHC-C1C | 3.43  | 1.45        | 1.38     |
| 21  | A     | 362 | CLA  | C3B-C4B | 3.42  | 1.52        | 1.42     |
| 21  | B     | 518 | CLA  | MG-NC   | 3.42  | 2.14        | 2.06     |
| 21  | C     | 477 | CLA  | MG-NB   | 3.42  | 2.12        | 2.05     |
| 21  | B     | 514 | CLA  | MG-NC   | 3.42  | 2.14        | 2.06     |
| 29  | A     | 376 | LMT  | O1B-C1B | 3.42  | 1.51        | 1.41     |
| 28  | A     | 375 | DGD  | O6E-C1E | 3.42  | 1.50        | 1.41     |
| 21  | B     | 517 | CLA  | CHC-C1C | 3.41  | 1.45        | 1.38     |
| 21  | C     | 487 | CLA  | C3B-C2B | 3.41  | 1.52        | 1.41     |
| 21  | C     | 485 | CLA  | CMC-C2C | 3.41  | 1.57        | 1.50     |
| 21  | B     | 518 | CLA  | C3B-C4B | 3.41  | 1.52        | 1.42     |
| 21  | A     | 362 | CLA  | C1D-C2D | 3.41  | 1.52        | 1.45     |
| 25  | Z     | 116 | BCR  | C29-C30 | 3.40  | 1.61        | 1.54     |
| 29  | B     | 535 | LMT  | O1'-C1' | 3.40  | 1.45        | 1.40     |
| 33  | V     | 164 | HEM  | CMC-C2C | 3.40  | 1.57        | 1.50     |
| 33  | V     | 164 | HEM  | O2A-CGA | -3.39 | 1.19        | 1.30     |
| 21  | B     | 515 | CLA  | C1D-C2D | 3.39  | 1.52        | 1.45     |
| 21  | B     | 526 | CLA  | O1D-CGD | 3.39  | 1.29        | 1.21     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 26  | C     | 476 | LHG  | O7-C7   | 3.39  | 1.43        | 1.34     |
| 21  | C     | 479 | CLA  | MG-NB   | 3.38  | 2.12        | 2.05     |
| 21  | C     | 484 | CLA  | MG-NB   | 3.38  | 2.12        | 2.05     |
| 21  | D     | 356 | CLA  | C3B-C4B | 3.38  | 1.52        | 1.42     |
| 29  | T     | 226 | LMT  | O5'-C1' | 3.38  | 1.50        | 1.41     |
| 21  | B     | 519 | CLA  | CMC-C2C | 3.38  | 1.57        | 1.50     |
| 21  | D     | 356 | CLA  | CMC-C2C | 3.38  | 1.57        | 1.50     |
| 25  | X     | 107 | BCR  | C1-C6   | 3.38  | 1.58        | 1.53     |
| 29  | B     | 535 | LMT  | O1B-C1B | 3.38  | 1.51        | 1.41     |
| 21  | A     | 363 | CLA  | CMC-C2C | 3.37  | 1.57        | 1.50     |
| 21  | B     | 511 | CLA  | C1B-NB  | 3.37  | 1.42        | 1.37     |
| 21  | B     | 523 | CLA  | C1D-C2D | 3.37  | 1.52        | 1.45     |
| 30  | D     | 361 | SQD  | O8-S    | 3.37  | 1.59        | 1.47     |
| 25  | A     | 369 | BCR  | C29-C30 | 3.36  | 1.61        | 1.54     |
| 25  | Z     | 116 | BCR  | C2-C1   | 3.36  | 1.61        | 1.54     |
| 21  | B     | 516 | CLA  | C3B-C4B | 3.35  | 1.52        | 1.42     |
| 21  | A     | 366 | CLA  | O1D-CGD | 3.35  | 1.29        | 1.21     |
| 21  | D     | 354 | CLA  | MG-ND   | -3.34 | 1.99        | 2.05     |
| 21  | C     | 478 | CLA  | CMC-C2C | 3.34  | 1.57        | 1.50     |
| 28  | D     | 362 | DGD  | O1G-C1G | 3.34  | 1.52        | 1.45     |
| 21  | B     | 513 | CLA  | MG-NC   | 3.34  | 2.14        | 2.06     |
| 33  | V     | 164 | HEM  | C4A-NA  | -3.33 | 1.33        | 1.39     |
| 25  | B     | 527 | BCR  | C2-C1   | 3.33  | 1.61        | 1.54     |
| 21  | B     | 520 | CLA  | CMC-C2C | 3.33  | 1.57        | 1.50     |
| 32  | D     | 357 | PL9  | C2-C1   | 3.32  | 1.53        | 1.44     |
| 21  | C     | 479 | CLA  | C3B-C2B | 3.32  | 1.52        | 1.41     |
| 21  | C     | 485 | CLA  | MG-NB   | 3.31  | 2.12        | 2.05     |
| 21  | C     | 486 | CLA  | C1B-NB  | 3.30  | 1.42        | 1.37     |
| 21  | B     | 511 | CLA  | CHB-C1B | 3.30  | 1.46        | 1.39     |
| 30  | D     | 361 | SQD  | O48-C23 | 3.29  | 1.42        | 1.33     |
| 21  | C     | 487 | CLA  | O1D-CGD | 3.29  | 1.29        | 1.21     |
| 21  | C     | 482 | CLA  | CAC-C3C | 3.29  | 1.59        | 1.51     |
| 21  | B     | 511 | CLA  | CBA-CGA | 3.28  | 1.60        | 1.50     |
| 28  | C     | 493 | DGD  | O5D-C1E | 3.28  | 1.45        | 1.40     |
| 25  | B     | 527 | BCR  | C29-C30 | 3.28  | 1.61        | 1.54     |
| 21  | C     | 486 | CLA  | CHD-C4C | 3.28  | 1.46        | 1.39     |
| 21  | B     | 525 | CLA  | C5-C3   | 3.27  | 1.58        | 1.51     |
| 29  | A     | 376 | LMT  | O1B-C4' | 3.27  | 1.52        | 1.43     |
| 30  | C     | 475 | SQD  | C20-C19 | -3.26 | 1.35        | 1.51     |
| 33  | F     | 85  | HEM  | O2A-CGA | -3.26 | 1.20        | 1.30     |
| 29  | O     | 274 | LMT  | O5'-C1' | 3.26  | 1.50        | 1.41     |
| 25  | C     | 489 | BCR  | C29-C30 | 3.26  | 1.61        | 1.54     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25  | Z     | 116 | BCR  | C38-C26 | 3.25  | 1.56        | 1.50     |
| 21  | C     | 484 | CLA  | C3B-C2B | 3.25  | 1.52        | 1.41     |
| 21  | B     | 515 | CLA  | MG-NC   | 3.25  | 2.14        | 2.06     |
| 33  | V     | 164 | HEM  | FE-NB   | 3.25  | 2.04        | 1.94     |
| 21  | B     | 512 | CLA  | C1D-C2D | 3.25  | 1.51        | 1.45     |
| 21  | C     | 477 | CLA  | MG-NC   | 3.24  | 2.14        | 2.06     |
| 33  | F     | 85  | HEM  | FE-NA   | 3.24  | 2.05        | 1.95     |
| 21  | C     | 477 | CLA  | C3B-C4B | 3.24  | 1.52        | 1.42     |
| 28  | C     | 491 | DGD  | C5B-C4B | -3.23 | 1.35        | 1.51     |
| 30  | F     | 224 | SQD  | C8-C7   | 3.23  | 1.60        | 1.50     |
| 21  | B     | 516 | CLA  | CMC-C2C | 3.23  | 1.57        | 1.50     |
| 21  | B     | 515 | CLA  | C5-C3   | 3.23  | 1.57        | 1.51     |
| 28  | D     | 362 | DGD  | O6E-C1E | 3.22  | 1.50        | 1.41     |
| 25  | D     | 358 | BCR  | C2-C1   | 3.22  | 1.61        | 1.54     |
| 25  | X     | 107 | BCR  | C2-C1   | 3.22  | 1.61        | 1.54     |
| 21  | D     | 354 | CLA  | C3B-C4B | 3.21  | 1.52        | 1.42     |
| 21  | A     | 366 | CLA  | C3B-C2B | 3.21  | 1.52        | 1.41     |
| 21  | C     | 477 | CLA  | C1D-C2D | 3.21  | 1.51        | 1.45     |
| 21  | C     | 487 | CLA  | C3B-C4B | 3.21  | 1.52        | 1.42     |
| 25  | C     | 490 | BCR  | C29-C30 | 3.21  | 1.61        | 1.54     |
| 29  | O     | 274 | LMT  | O1B-C1B | 3.20  | 1.50        | 1.41     |
| 21  | C     | 488 | CLA  | C3B-C2B | 3.20  | 1.52        | 1.41     |
| 21  | B     | 526 | CLA  | C3B-C2B | 3.20  | 1.52        | 1.41     |
| 21  | B     | 519 | CLA  | MG-NC   | 3.20  | 2.13        | 2.06     |
| 21  | B     | 526 | CLA  | C1C-C2C | 3.19  | 1.51        | 1.44     |
| 21  | A     | 362 | CLA  | O1D-CGD | 3.18  | 1.29        | 1.21     |
| 30  | L     | 213 | SQD  | O5-C1   | 3.18  | 1.50        | 1.41     |
| 21  | C     | 479 | CLA  | C3B-C4B | 3.18  | 1.52        | 1.42     |
| 21  | A     | 364 | CLA  | MG-NA   | 3.18  | 2.13        | 2.06     |
| 29  | T     | 226 | LMT  | O1'-C1' | 3.17  | 1.45        | 1.40     |
| 25  | J     | 115 | BCR  | C2-C1   | 3.17  | 1.61        | 1.54     |
| 30  | F     | 224 | SQD  | C1-C2   | 3.17  | 1.61        | 1.52     |
| 21  | B     | 514 | CLA  | C3B-C4B | 3.17  | 1.51        | 1.42     |
| 21  | B     | 514 | CLA  | C3B-C2B | 3.17  | 1.51        | 1.41     |
| 30  | C     | 475 | SQD  | C19-C18 | -3.16 | 1.36        | 1.51     |
| 30  | C     | 475 | SQD  | C33-C32 | -3.16 | 1.36        | 1.51     |
| 21  | B     | 517 | CLA  | O1D-CGD | 3.14  | 1.29        | 1.21     |
| 21  | C     | 486 | CLA  | CHC-C4B | 3.14  | 1.46        | 1.39     |
| 21  | K     | 483 | CLA  | CMC-C2C | 3.14  | 1.57        | 1.50     |
| 21  | B     | 519 | CLA  | C3B-C2B | 3.14  | 1.51        | 1.41     |
| 21  | B     | 512 | CLA  | O1D-CGD | 3.13  | 1.29        | 1.21     |
| 21  | B     | 515 | CLA  | C4C-C3C | 3.12  | 1.50        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 29  | I     | 274 | LMT  | C3'-C4' | 3.12  | 1.60        | 1.52     |
| 21  | C     | 484 | CLA  | CHC-C1C | 3.11  | 1.44        | 1.38     |
| 21  | C     | 484 | CLA  | C1B-NB  | 3.11  | 1.41        | 1.37     |
| 30  | L     | 213 | SQD  | O8-S    | 3.11  | 1.58        | 1.47     |
| 30  | D     | 361 | SQD  | O6-C1   | 3.10  | 1.45        | 1.40     |
| 28  | A     | 375 | DGD  | O1G-C1G | 3.10  | 1.52        | 1.45     |
| 21  | C     | 479 | CLA  | CMC-C2C | 3.10  | 1.57        | 1.50     |
| 30  | F     | 224 | SQD  | O5-C1   | 3.10  | 1.49        | 1.41     |
| 28  | D     | 362 | DGD  | C1G-C2G | 3.09  | 1.60        | 1.50     |
| 21  | C     | 483 | CLA  | C5-C3   | 3.09  | 1.57        | 1.51     |
| 21  | C     | 483 | CLA  | C3B-C2B | 3.09  | 1.51        | 1.41     |
| 21  | B     | 513 | CLA  | C1D-C2D | 3.08  | 1.51        | 1.45     |
| 21  | B     | 520 | CLA  | C1D-C2D | 3.08  | 1.51        | 1.45     |
| 21  | A     | 366 | CLA  | CMC-C2C | 3.07  | 1.57        | 1.50     |
| 21  | C     | 477 | CLA  | CMC-C2C | 3.07  | 1.57        | 1.50     |
| 21  | A     | 366 | CLA  | C1D-C2D | 3.07  | 1.51        | 1.45     |
| 30  | F     | 224 | SQD  | C14-C13 | -3.07 | 1.36        | 1.51     |
| 21  | B     | 525 | CLA  | C3B-C2B | 3.06  | 1.51        | 1.41     |
| 30  | D     | 361 | SQD  | C15-C14 | -3.06 | 1.36        | 1.51     |
| 21  | A     | 363 | CLA  | C1D-C2D | 3.06  | 1.51        | 1.45     |
| 21  | C     | 478 | CLA  | O1D-CGD | 3.06  | 1.29        | 1.21     |
| 30  | L     | 213 | SQD  | C12-C11 | -3.05 | 1.36        | 1.51     |
| 30  | C     | 475 | SQD  | C17-C16 | -3.05 | 1.36        | 1.51     |
| 21  | A     | 363 | CLA  | CBA-CGA | 3.05  | 1.59        | 1.50     |
| 21  | B     | 525 | CLA  | O1D-CGD | 3.05  | 1.28        | 1.21     |
| 21  | D     | 354 | CLA  | CMC-C2C | 3.05  | 1.57        | 1.50     |
| 21  | C     | 483 | CLA  | C1B-NB  | 3.05  | 1.41        | 1.37     |
| 30  | D     | 361 | SQD  | C14-C13 | -3.04 | 1.36        | 1.51     |
| 21  | C     | 484 | CLA  | O1D-CGD | 3.04  | 1.28        | 1.21     |
| 30  | F     | 224 | SQD  | C24-C23 | 3.04  | 1.59        | 1.50     |
| 21  | A     | 364 | CLA  | CMC-C2C | 3.04  | 1.57        | 1.50     |
| 21  | B     | 513 | CLA  | CMC-C2C | 3.04  | 1.57        | 1.50     |
| 29  | A     | 376 | LMT  | C4'-C5' | 3.04  | 1.61        | 1.52     |
| 30  | F     | 224 | SQD  | C13-C12 | -3.04 | 1.36        | 1.51     |
| 21  | C     | 488 | CLA  | CHC-C1C | 3.04  | 1.44        | 1.38     |
| 21  | B     | 513 | CLA  | O1D-CGD | 3.03  | 1.28        | 1.21     |
| 30  | C     | 475 | SQD  | C12-C11 | -3.03 | 1.36        | 1.51     |
| 21  | D     | 356 | CLA  | MG-NA   | 3.03  | 2.13        | 2.06     |
| 30  | F     | 224 | SQD  | O3-C3   | 3.03  | 1.50        | 1.43     |
| 21  | B     | 514 | CLA  | MG-ND   | -3.03 | 1.99        | 2.05     |
| 30  | D     | 361 | SQD  | C16-C15 | -3.02 | 1.36        | 1.51     |
| 29  | O     | 274 | LMT  | O1'-C1' | 3.02  | 1.45        | 1.40     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | C     | 487 | CLA  | CBA-CGA | 3.02  | 1.59        | 1.50     |
| 33  | F     | 85  | HEM  | CMC-C2C | 3.02  | 1.57        | 1.50     |
| 21  | C     | 480 | CLA  | C3B-C2B | 3.02  | 1.51        | 1.41     |
| 30  | D     | 361 | SQD  | C12-C11 | -3.01 | 1.36        | 1.51     |
| 27  | C     | 494 | LMG  | O6-C1   | 3.01  | 1.49        | 1.41     |
| 21  | A     | 362 | CLA  | O2A-CGA | 3.01  | 1.42        | 1.33     |
| 29  | I     | 274 | LMT  | C4'-C5' | 3.01  | 1.61        | 1.52     |
| 28  | B     | 533 | DGD  | O2G-C1B | 3.01  | 1.42        | 1.34     |
| 30  | D     | 361 | SQD  | C13-C12 | -3.01 | 1.36        | 1.51     |
| 21  | B     | 517 | CLA  | CMC-C2C | 3.01  | 1.56        | 1.50     |
| 21  | C     | 481 | CLA  | CAA-C2A | -3.00 | 1.48        | 1.54     |
| 30  | F     | 224 | SQD  | C17-C16 | -3.00 | 1.36        | 1.51     |
| 30  | L     | 213 | SQD  | C16-C15 | -2.99 | 1.36        | 1.51     |
| 21  | C     | 486 | CLA  | C3B-C2B | 2.98  | 1.51        | 1.41     |
| 21  | C     | 479 | CLA  | O1D-CGD | 2.98  | 1.28        | 1.21     |
| 21  | C     | 477 | CLA  | O1D-CGD | 2.98  | 1.28        | 1.21     |
| 21  | B     | 518 | CLA  | O1D-CGD | 2.98  | 1.28        | 1.21     |
| 30  | F     | 224 | SQD  | C12-C11 | -2.98 | 1.36        | 1.51     |
| 21  | A     | 366 | CLA  | MG-NB   | 2.98  | 2.11        | 2.05     |
| 30  | L     | 213 | SQD  | C17-C16 | -2.98 | 1.37        | 1.51     |
| 21  | C     | 481 | CLA  | O1D-CGD | 2.97  | 1.28        | 1.21     |
| 21  | B     | 514 | CLA  | CBA-CGA | 2.97  | 1.59        | 1.50     |
| 21  | B     | 516 | CLA  | C3B-C2B | 2.97  | 1.51        | 1.41     |
| 28  | D     | 362 | DGD  | O1G-C1A | 2.97  | 1.42        | 1.33     |
| 30  | F     | 224 | SQD  | O8-S    | 2.97  | 1.58        | 1.47     |
| 21  | B     | 516 | CLA  | C1D-C2D | 2.97  | 1.51        | 1.45     |
| 21  | A     | 363 | CLA  | O1D-CGD | 2.97  | 1.28        | 1.21     |
| 30  | F     | 224 | SQD  | C15-C14 | -2.96 | 1.37        | 1.51     |
| 30  | C     | 475 | SQD  | C11-C10 | -2.96 | 1.37        | 1.51     |
| 30  | D     | 361 | SQD  | C11-C10 | -2.95 | 1.37        | 1.51     |
| 21  | C     | 488 | CLA  | C1B-NB  | 2.95  | 1.41        | 1.37     |
| 21  | C     | 486 | CLA  | CHD-C1D | 2.95  | 1.44        | 1.38     |
| 27  | M     | 217 | LMG  | O7-C8   | 2.95  | 1.53        | 1.46     |
| 27  | C     | 494 | LMG  | O7-C8   | 2.94  | 1.53        | 1.46     |
| 32  | D     | 357 | PL9  | C33-C34 | 2.94  | 1.39        | 1.33     |
| 21  | C     | 482 | CLA  | MG-NA   | 2.94  | 2.13        | 2.06     |
| 30  | C     | 475 | SQD  | C32-C31 | -2.94 | 1.37        | 1.51     |
| 21  | C     | 478 | CLA  | MG-NC   | 2.93  | 2.13        | 2.06     |
| 30  | D     | 361 | SQD  | O3-C3   | 2.92  | 1.50        | 1.43     |
| 21  | B     | 522 | CLA  | MG-NC   | 2.92  | 2.13        | 2.06     |
| 30  | C     | 475 | SQD  | C18-C17 | -2.91 | 1.37        | 1.51     |
| 27  | D     | 359 | LMG  | C16-C15 | -2.91 | 1.37        | 1.51     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 28  | C     | 474 | DGD  | C4E-C3E | 2.91  | 1.59        | 1.52     |
| 21  | C     | 479 | CLA  | MG-NA   | 2.91  | 2.13        | 2.06     |
| 21  | B     | 516 | CLA  | O1D-CGD | 2.91  | 1.28        | 1.21     |
| 21  | B     | 523 | CLA  | MG-ND   | -2.90 | 2.00        | 2.05     |
| 30  | L     | 213 | SQD  | C11-C10 | -2.90 | 1.37        | 1.51     |
| 28  | A     | 375 | DGD  | C5B-C4B | -2.90 | 1.37        | 1.51     |
| 21  | C     | 488 | CLA  | MG-NB   | 2.90  | 2.11        | 2.05     |
| 21  | B     | 520 | CLA  | O1D-CGD | 2.89  | 1.28        | 1.21     |
| 29  | A     | 376 | LMT  | O5'-C1' | 2.89  | 1.49        | 1.41     |
| 21  | A     | 363 | CLA  | CAA-C2A | 2.89  | 1.59        | 1.54     |
| 21  | B     | 512 | CLA  | MG-NC   | 2.89  | 2.13        | 2.06     |
| 21  | B     | 520 | CLA  | C3B-C2B | 2.88  | 1.50        | 1.41     |
| 21  | B     | 524 | CLA  | O1D-CGD | 2.88  | 1.28        | 1.21     |
| 30  | C     | 475 | SQD  | C16-C15 | -2.87 | 1.37        | 1.51     |
| 21  | B     | 524 | CLA  | CMC-C2C | 2.86  | 1.56        | 1.50     |
| 21  | D     | 354 | CLA  | C3B-C2B | 2.86  | 1.50        | 1.41     |
| 21  | B     | 515 | CLA  | C1B-NB  | 2.86  | 1.41        | 1.37     |
| 21  | B     | 514 | CLA  | CMC-C2C | 2.86  | 1.56        | 1.50     |
| 21  | K     | 483 | CLA  | C1B-NB  | 2.86  | 1.41        | 1.37     |
| 21  | C     | 483 | CLA  | O1D-CGD | 2.85  | 1.28        | 1.21     |
| 25  | C     | 489 | BCR  | C5-C6   | 2.85  | 1.39        | 1.34     |
| 21  | C     | 487 | CLA  | C1B-NB  | 2.85  | 1.41        | 1.37     |
| 21  | B     | 523 | CLA  | O1D-CGD | 2.85  | 1.28        | 1.21     |
| 29  | O     | 274 | LMT  | C4'-C5' | 2.84  | 1.60        | 1.52     |
| 21  | C     | 480 | CLA  | MG-NC   | 2.84  | 2.13        | 2.06     |
| 32  | D     | 357 | PL9  | C8-C9   | 2.83  | 1.39        | 1.33     |
| 30  | F     | 224 | SQD  | C16-C15 | -2.83 | 1.37        | 1.51     |
| 27  | I     | 220 | LMG  | O6-C1   | 2.83  | 1.49        | 1.41     |
| 21  | B     | 522 | CLA  | CAC-C3C | 2.83  | 1.58        | 1.51     |
| 21  | B     | 525 | CLA  | C1D-C2D | 2.82  | 1.50        | 1.45     |
| 21  | C     | 487 | CLA  | C1D-C2D | 2.82  | 1.50        | 1.45     |
| 33  | V     | 164 | HEM  | C3B-C4B | 2.81  | 1.50        | 1.44     |
| 28  | C     | 474 | DGD  | C5B-C4B | -2.81 | 1.37        | 1.51     |
| 21  | A     | 364 | CLA  | O1D-CGD | 2.81  | 1.28        | 1.21     |
| 29  | B     | 535 | LMT  | O1B-C4' | 2.81  | 1.51        | 1.43     |
| 21  | C     | 483 | CLA  | MG-NB   | 2.80  | 2.11        | 2.05     |
| 21  | B     | 516 | CLA  | MG-ND   | -2.80 | 2.00        | 2.05     |
| 30  | L     | 213 | SQD  | C13-C12 | -2.80 | 1.37        | 1.51     |
| 21  | B     | 522 | CLA  | CMC-C2C | 2.79  | 1.56        | 1.50     |
| 32  | D     | 357 | PL9  | C18-C19 | 2.79  | 1.39        | 1.33     |
| 28  | C     | 492 | DGD  | O5D-C6D | -2.79 | 1.38        | 1.43     |
| 21  | B     | 512 | CLA  | C3B-C2B | 2.79  | 1.50        | 1.41     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | L     | 213 | SQD  | C15-C14 | -2.79 | 1.37        | 1.51     |
| 21  | B     | 515 | CLA  | C3B-C2B | 2.79  | 1.50        | 1.41     |
| 25  | D     | 358 | BCR  | C5-C6   | 2.78  | 1.39        | 1.34     |
| 28  | C     | 491 | DGD  | O2E-C2E | -2.78 | 1.36        | 1.43     |
| 32  | D     | 357 | PL9  | C38-C39 | 2.78  | 1.39        | 1.33     |
| 32  | D     | 357 | PL9  | C43-C44 | 2.78  | 1.39        | 1.33     |
| 21  | A     | 364 | CLA  | MG-NC   | 2.77  | 2.12        | 2.06     |
| 21  | D     | 354 | CLA  | C1D-ND  | -2.77 | 1.34        | 1.37     |
| 21  | A     | 363 | CLA  | C3B-C2B | 2.77  | 1.50        | 1.41     |
| 29  | A     | 376 | LMT  | O1'-C1' | 2.77  | 1.44        | 1.40     |
| 30  | L     | 213 | SQD  | C20-C19 | -2.77 | 1.38        | 1.51     |
| 25  | C     | 489 | BCR  | C26-C25 | 2.77  | 1.39        | 1.34     |
| 30  | C     | 475 | SQD  | C8-C7   | 2.77  | 1.58        | 1.50     |
| 21  | B     | 523 | CLA  | C1B-NB  | 2.77  | 1.41        | 1.37     |
| 21  | K     | 483 | CLA  | C1D-C2D | 2.77  | 1.50        | 1.45     |
| 29  | T     | 226 | LMT  | C1B-C2B | 2.77  | 1.60        | 1.52     |
| 29  | D     | 363 | LMT  | O5B-C1B | 2.76  | 1.48        | 1.41     |
| 30  | F     | 224 | SQD  | O6-C1   | 2.76  | 1.44        | 1.40     |
| 21  | C     | 479 | CLA  | C5-C3   | 2.76  | 1.57        | 1.51     |
| 33  | V     | 164 | HEM  | FE-NA   | 2.75  | 2.04        | 1.95     |
| 30  | C     | 475 | SQD  | C13-C12 | -2.75 | 1.38        | 1.51     |
| 21  | B     | 518 | CLA  | C3B-C2B | 2.75  | 1.50        | 1.41     |
| 21  | B     | 515 | CLA  | MG-NB   | 2.75  | 2.11        | 2.05     |
| 30  | L     | 213 | SQD  | C14-C13 | -2.74 | 1.38        | 1.51     |
| 25  | J     | 112 | BCR  | C26-C25 | 2.74  | 1.39        | 1.34     |
| 21  | B     | 526 | CLA  | CHB-C4A | 2.74  | 1.44        | 1.37     |
| 21  | C     | 487 | CLA  | CHB-C4A | 2.74  | 1.44        | 1.37     |
| 21  | B     | 517 | CLA  | MG-NB   | 2.74  | 2.11        | 2.05     |
| 27  | C     | 494 | LMG  | C16-C15 | -2.74 | 1.38        | 1.51     |
| 28  | D     | 362 | DGD  | O2G-C2G | 2.74  | 1.53        | 1.46     |
| 21  | B     | 519 | CLA  | O1D-CGD | 2.74  | 1.28        | 1.21     |
| 30  | C     | 475 | SQD  | C15-C14 | -2.73 | 1.38        | 1.51     |
| 27  | M     | 217 | LMG  | O7-C10  | 2.73  | 1.42        | 1.34     |
| 21  | B     | 520 | CLA  | C3B-C4B | 2.72  | 1.50        | 1.42     |
| 33  | V     | 164 | HEM  | C1A-C2A | -2.72 | 1.39        | 1.44     |
| 21  | B     | 520 | CLA  | MG-NB   | 2.72  | 2.11        | 2.05     |
| 27  | M     | 217 | LMG  | O6-C1   | 2.72  | 1.48        | 1.41     |
| 21  | C     | 481 | CLA  | MG-NB   | 2.72  | 2.11        | 2.05     |
| 27  | J     | 492 | LMG  | O6-C1   | 2.72  | 1.48        | 1.41     |
| 21  | B     | 513 | CLA  | CBA-CGA | 2.72  | 1.58        | 1.50     |
| 28  | C     | 492 | DGD  | O2G-C1B | 2.71  | 1.41        | 1.34     |
| 29  | D     | 363 | LMT  | C4'-C5' | 2.71  | 1.60        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | A     | 362 | CLA  | MG-NC   | 2.71  | 2.12        | 2.06     |
| 21  | D     | 356 | CLA  | CBA-CGA | 2.71  | 1.58        | 1.50     |
| 30  | C     | 475 | SQD  | O8-S    | 2.70  | 1.57        | 1.47     |
| 33  | F     | 85  | HEM  | CHC-C1C | 2.70  | 1.43        | 1.38     |
| 21  | B     | 518 | CLA  | O2A-C1  | 2.69  | 1.53        | 1.46     |
| 25  | C     | 489 | BCR  | C19-C18 | -2.69 | 1.40        | 1.46     |
| 21  | C     | 485 | CLA  | C3B-C2B | 2.69  | 1.50        | 1.41     |
| 27  | C     | 494 | LMG  | O1-C7   | 2.69  | 1.48        | 1.43     |
| 21  | A     | 363 | CLA  | C1D-ND  | -2.69 | 1.34        | 1.37     |
| 21  | B     | 518 | CLA  | CBA-CGA | 2.69  | 1.58        | 1.50     |
| 29  | I     | 274 | LMT  | O1'-C1' | 2.69  | 1.44        | 1.40     |
| 33  | V     | 164 | HEM  | C1D-C2D | 2.68  | 1.50        | 1.44     |
| 30  | C     | 475 | SQD  | O5-C1   | 2.68  | 1.48        | 1.41     |
| 25  | X     | 107 | BCR  | C5-C6   | 2.68  | 1.39        | 1.34     |
| 33  | F     | 85  | HEM  | C4D-C3D | 2.68  | 1.49        | 1.45     |
| 21  | A     | 364 | CLA  | CBA-CGA | 2.68  | 1.58        | 1.50     |
| 21  | B     | 524 | CLA  | MG-NA   | 2.67  | 2.12        | 2.06     |
| 28  | A     | 375 | DGD  | C2A-C1A | 2.67  | 1.58        | 1.50     |
| 27  | I     | 220 | LMG  | C4-C5   | 2.67  | 1.58        | 1.53     |
| 28  | C     | 493 | DGD  | C3G-C2G | 2.67  | 1.59        | 1.50     |
| 25  | B     | 530 | BCR  | C38-C26 | 2.66  | 1.55        | 1.50     |
| 30  | L     | 213 | SQD  | C19-C18 | -2.66 | 1.38        | 1.51     |
| 28  | C     | 492 | DGD  | O5D-C1E | 2.66  | 1.44        | 1.40     |
| 27  | J     | 492 | LMG  | O7-C10  | 2.66  | 1.41        | 1.34     |
| 21  | B     | 517 | CLA  | C6-C7   | 2.65  | 1.63        | 1.52     |
| 27  | I     | 220 | LMG  | C16-C15 | -2.65 | 1.38        | 1.51     |
| 21  | A     | 363 | CLA  | MG-NB   | 2.65  | 2.11        | 2.05     |
| 33  | V     | 164 | HEM  | FE-ND   | 2.65  | 2.03        | 1.94     |
| 29  | T     | 226 | LMT  | O5B-C1B | 2.65  | 1.48        | 1.41     |
| 21  | C     | 480 | CLA  | O1D-CGD | 2.65  | 1.27        | 1.21     |
| 21  | B     | 524 | CLA  | CBA-CGA | 2.65  | 1.58        | 1.50     |
| 21  | D     | 356 | CLA  | O1D-CGD | 2.65  | 1.27        | 1.21     |
| 21  | C     | 478 | CLA  | C3B-C2B | 2.65  | 1.50        | 1.41     |
| 27  | I     | 220 | LMG  | O8-C28  | 2.65  | 1.41        | 1.33     |
| 21  | C     | 482 | CLA  | CAA-C2A | 2.64  | 1.58        | 1.54     |
| 30  | C     | 475 | SQD  | C14-C13 | -2.64 | 1.38        | 1.51     |
| 28  | D     | 362 | DGD  | C3D-C2D | 2.64  | 1.59        | 1.52     |
| 27  | B     | 531 | LMG  | C16-C15 | -2.64 | 1.38        | 1.51     |
| 21  | B     | 517 | CLA  | O2A-C1  | 2.64  | 1.53        | 1.46     |
| 21  | B     | 526 | CLA  | C5-C3   | 2.64  | 1.56        | 1.51     |
| 21  | A     | 364 | CLA  | C3B-C2B | 2.63  | 1.50        | 1.41     |
| 28  | B     | 533 | DGD  | C4E-C3E | 2.63  | 1.59        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | B     | 511 | CLA  | C3B-C4B | 2.63  | 1.50        | 1.42     |
| 21  | C     | 484 | CLA  | CAC-C3C | 2.63  | 1.57        | 1.51     |
| 21  | C     | 477 | CLA  | C3B-C2B | 2.62  | 1.50        | 1.41     |
| 22  | D     | 355 | PHO  | C4C-C3C | 2.62  | 1.53        | 1.45     |
| 21  | C     | 487 | CLA  | CAC-C3C | 2.62  | 1.57        | 1.51     |
| 21  | C     | 487 | CLA  | MG-NB   | 2.62  | 2.11        | 2.05     |
| 21  | A     | 362 | CLA  | C3B-C2B | 2.61  | 1.50        | 1.41     |
| 21  | C     | 488 | CLA  | CAC-C3C | 2.61  | 1.57        | 1.51     |
| 33  | F     | 85  | HEM  | FE-ND   | 2.61  | 2.02        | 1.94     |
| 21  | B     | 523 | CLA  | CMC-C2C | 2.60  | 1.56        | 1.50     |
| 21  | C     | 488 | CLA  | CMC-C2C | 2.59  | 1.56        | 1.50     |
| 21  | D     | 356 | CLA  | C5-C3   | 2.59  | 1.56        | 1.51     |
| 21  | B     | 516 | CLA  | MG-NB   | 2.59  | 2.10        | 2.05     |
| 28  | C     | 491 | DGD  | O6D-C5D | 2.59  | 1.50        | 1.44     |
| 27  | M     | 217 | LMG  | C16-C15 | -2.58 | 1.38        | 1.51     |
| 21  | B     | 525 | CLA  | CMC-C2C | 2.58  | 1.56        | 1.50     |
| 29  | D     | 536 | LMT  | O5'-C1' | 2.58  | 1.48        | 1.41     |
| 25  | B     | 529 | BCR  | C38-C26 | 2.58  | 1.55        | 1.50     |
| 21  | D     | 354 | CLA  | O1D-CGD | 2.58  | 1.27        | 1.21     |
| 21  | B     | 525 | CLA  | C1B-NB  | 2.58  | 1.41        | 1.37     |
| 21  | B     | 513 | CLA  | MG-NB   | 2.58  | 2.10        | 2.05     |
| 21  | B     | 522 | CLA  | O1D-CGD | 2.57  | 1.27        | 1.21     |
| 21  | C     | 488 | CLA  | CHD-C4C | 2.57  | 1.45        | 1.39     |
| 21  | C     | 485 | CLA  | O1D-CGD | 2.57  | 1.27        | 1.21     |
| 21  | D     | 356 | CLA  | C3B-C2B | 2.57  | 1.49        | 1.41     |
| 28  | D     | 362 | DGD  | C1E-C2E | 2.57  | 1.60        | 1.52     |
| 28  | C     | 493 | DGD  | O3G-C1D | 2.57  | 1.44        | 1.40     |
| 21  | B     | 515 | CLA  | CHC-C1C | 2.57  | 1.43        | 1.38     |
| 21  | D     | 356 | CLA  | MG-NB   | 2.57  | 2.10        | 2.05     |
| 22  | A     | 365 | PHO  | O1D-CGD | 2.56  | 1.27        | 1.21     |
| 21  | B     | 521 | CLA  | C3B-C2B | 2.56  | 1.49        | 1.41     |
| 21  | K     | 483 | CLA  | C3B-C2B | 2.56  | 1.49        | 1.41     |
| 21  | B     | 516 | CLA  | O2A-C1  | 2.56  | 1.53        | 1.46     |
| 30  | F     | 224 | SQD  | C11-C10 | -2.55 | 1.39        | 1.51     |
| 21  | B     | 518 | CLA  | CMC-C2C | 2.55  | 1.56        | 1.50     |
| 21  | B     | 515 | CLA  | CBA-CGA | 2.55  | 1.58        | 1.50     |
| 21  | B     | 517 | CLA  | CHD-C1D | 2.55  | 1.43        | 1.38     |
| 30  | L     | 213 | SQD  | C8-C7   | 2.55  | 1.58        | 1.50     |
| 21  | A     | 364 | CLA  | MG-ND   | -2.55 | 2.00        | 2.05     |
| 22  | A     | 365 | PHO  | C3D-CAD | -2.54 | 1.42        | 1.47     |
| 21  | C     | 482 | CLA  | CMD-C2D | 2.54  | 1.56        | 1.50     |
| 30  | D     | 361 | SQD  | C8-C7   | 2.54  | 1.58        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | A     | 362 | CLA  | CMC-C2C | 2.54  | 1.56        | 1.50     |
| 21  | B     | 524 | CLA  | MG-NC   | 2.53  | 2.12        | 2.06     |
| 21  | B     | 523 | CLA  | MG-NB   | 2.53  | 2.10        | 2.05     |
| 21  | C     | 486 | CLA  | CBA-CGA | 2.53  | 1.58        | 1.50     |
| 21  | C     | 483 | CLA  | CAC-C3C | 2.53  | 1.57        | 1.51     |
| 29  | A     | 376 | LMT  | C1B-C2B | 2.53  | 1.59        | 1.52     |
| 25  | C     | 490 | BCR  | C26-C25 | 2.53  | 1.38        | 1.34     |
| 28  | D     | 362 | DGD  | O6D-C5D | 2.53  | 1.50        | 1.44     |
| 21  | C     | 480 | CLA  | C5-C3   | 2.53  | 1.56        | 1.51     |
| 28  | C     | 474 | DGD  | C4A-C3A | -2.52 | 1.39        | 1.51     |
| 28  | C     | 492 | DGD  | C9A-C8A | -2.52 | 1.39        | 1.51     |
| 28  | C     | 492 | DGD  | C4A-C3A | -2.52 | 1.39        | 1.51     |
| 21  | B     | 523 | CLA  | CHC-C1C | 2.52  | 1.43        | 1.38     |
| 28  | B     | 533 | DGD  | C4A-C3A | -2.51 | 1.39        | 1.51     |
| 25  | D     | 358 | BCR  | C19-C18 | -2.51 | 1.40        | 1.46     |
| 33  | V     | 164 | HEM  | C4D-C3D | 2.51  | 1.49        | 1.45     |
| 27  | B     | 531 | LMG  | C39-C38 | -2.50 | 1.39        | 1.51     |
| 30  | L     | 213 | SQD  | O3-C3   | 2.50  | 1.49        | 1.43     |
| 21  | B     | 519 | CLA  | CMD-C2D | 2.50  | 1.55        | 1.50     |
| 29  | B     | 535 | LMT  | C10-C9  | -2.50 | 1.39        | 1.51     |
| 27  | C     | 494 | LMG  | C34-C33 | -2.50 | 1.39        | 1.51     |
| 28  | C     | 493 | DGD  | C4A-C3A | -2.50 | 1.39        | 1.51     |
| 21  | A     | 366 | CLA  | C1B-NB  | 2.50  | 1.41        | 1.37     |
| 28  | B     | 533 | DGD  | CEB-CDB | -2.50 | 1.39        | 1.51     |
| 33  | V     | 164 | HEM  | C1B-C2B | -2.49 | 1.39        | 1.44     |
| 21  | B     | 518 | CLA  | C5-C3   | 2.49  | 1.56        | 1.51     |
| 29  | D     | 536 | LMT  | C10-C9  | -2.49 | 1.39        | 1.51     |
| 28  | C     | 493 | DGD  | CFB-CEB | -2.49 | 1.39        | 1.51     |
| 27  | D     | 359 | LMG  | C34-C33 | -2.49 | 1.39        | 1.51     |
| 28  | C     | 493 | DGD  | CEB-CDB | -2.49 | 1.39        | 1.51     |
| 28  | C     | 492 | DGD  | CFB-CEB | -2.48 | 1.39        | 1.51     |
| 29  | T     | 226 | LMT  | C10-C9  | -2.48 | 1.39        | 1.51     |
| 21  | C     | 479 | CLA  | CMD-C2D | 2.48  | 1.55        | 1.50     |
| 29  | I     | 274 | LMT  | C10-C9  | -2.48 | 1.39        | 1.51     |
| 29  | D     | 536 | LMT  | C5-C4   | -2.48 | 1.39        | 1.51     |
| 28  | C     | 493 | DGD  | C9A-C8A | -2.48 | 1.39        | 1.51     |
| 21  | A     | 366 | CLA  | CHC-C1C | 2.48  | 1.43        | 1.38     |
| 21  | D     | 354 | CLA  | C1D-C2D | 2.48  | 1.50        | 1.45     |
| 28  | C     | 474 | DGD  | C3E-C2E | 2.48  | 1.58        | 1.52     |
| 27  | I     | 220 | LMG  | C34-C33 | -2.48 | 1.39        | 1.51     |
| 28  | C     | 491 | DGD  | C4A-C3A | -2.47 | 1.39        | 1.51     |
| 28  | C     | 493 | DGD  | C9B-C8B | -2.47 | 1.39        | 1.51     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 29  | O     | 274 | LMT  | C10-C9  | -2.47 | 1.39        | 1.51     |
| 21  | A     | 366 | CLA  | MG-ND   | -2.47 | 2.00        | 2.05     |
| 28  | C     | 493 | DGD  | CDA-CCA | -2.47 | 1.39        | 1.51     |
| 29  | B     | 535 | LMT  | C5-C4   | -2.47 | 1.39        | 1.51     |
| 27  | D     | 359 | LMG  | C39-C38 | -2.47 | 1.39        | 1.51     |
| 28  | B     | 533 | DGD  | C5B-C4B | -2.47 | 1.39        | 1.51     |
| 21  | C     | 486 | CLA  | CMC-C2C | 2.47  | 1.55        | 1.50     |
| 28  | B     | 533 | DGD  | CDA-CCA | -2.47 | 1.39        | 1.51     |
| 27  | B     | 531 | LMG  | C20-C19 | -2.47 | 1.39        | 1.51     |
| 28  | D     | 362 | DGD  | C3G-C2G | 2.47  | 1.58        | 1.50     |
| 30  | L     | 213 | SQD  | C18-C17 | -2.47 | 1.39        | 1.51     |
| 27  | J     | 492 | LMG  | C34-C33 | -2.47 | 1.39        | 1.51     |
| 28  | B     | 533 | DGD  | C9A-C8A | -2.47 | 1.39        | 1.51     |
| 30  | C     | 475 | SQD  | C21-C20 | -2.46 | 1.36        | 1.51     |
| 32  | D     | 357 | PL9  | C5-C4   | 2.46  | 1.55        | 1.47     |
| 29  | O     | 274 | LMT  | C5-C4   | -2.46 | 1.39        | 1.51     |
| 27  | B     | 531 | LMG  | C34-C33 | -2.46 | 1.39        | 1.51     |
| 28  | B     | 533 | DGD  | CFB-CEB | -2.46 | 1.39        | 1.51     |
| 21  | B     | 525 | CLA  | MG-NB   | 2.46  | 2.10        | 2.05     |
| 28  | D     | 362 | DGD  | CEB-CDB | -2.46 | 1.39        | 1.51     |
| 28  | A     | 375 | DGD  | C4A-C3A | -2.46 | 1.39        | 1.51     |
| 21  | B     | 511 | CLA  | CAA-C2A | 2.46  | 1.58        | 1.54     |
| 28  | C     | 492 | DGD  | CEB-CDB | -2.46 | 1.39        | 1.51     |
| 29  | O     | 274 | LMT  | O5B-C5B | 2.46  | 1.50        | 1.44     |
| 28  | D     | 362 | DGD  | CFB-CEB | -2.46 | 1.39        | 1.51     |
| 29  | A     | 376 | LMT  | C10-C9  | -2.46 | 1.39        | 1.51     |
| 29  | A     | 376 | LMT  | C5-C4   | -2.45 | 1.39        | 1.51     |
| 33  | F     | 85  | HEM  | C1B-C2B | -2.45 | 1.39        | 1.44     |
| 21  | C     | 487 | CLA  | C2A-C1A | 2.45  | 1.57        | 1.52     |
| 28  | D     | 362 | DGD  | CDA-CCA | -2.45 | 1.39        | 1.51     |
| 27  | M     | 217 | LMG  | C34-C33 | -2.45 | 1.39        | 1.51     |
| 27  | J     | 492 | LMG  | C39-C38 | -2.45 | 1.39        | 1.51     |
| 32  | D     | 357 | PL9  | C10-C9  | 2.45  | 1.56        | 1.50     |
| 28  | C     | 474 | DGD  | C9B-C8B | -2.45 | 1.39        | 1.51     |
| 29  | I     | 274 | LMT  | C5-C4   | -2.45 | 1.39        | 1.51     |
| 27  | C     | 494 | LMG  | C20-C19 | -2.45 | 1.39        | 1.51     |
| 28  | C     | 491 | DGD  | C9A-C8A | -2.45 | 1.39        | 1.51     |
| 21  | B     | 524 | CLA  | C3B-C2B | 2.44  | 1.49        | 1.41     |
| 28  | C     | 474 | DGD  | C9A-C8A | -2.44 | 1.39        | 1.51     |
| 27  | D     | 359 | LMG  | C20-C19 | -2.44 | 1.39        | 1.51     |
| 32  | D     | 357 | PL9  | C23-C24 | 2.44  | 1.38        | 1.33     |
| 29  | T     | 226 | LMT  | C5-C4   | -2.44 | 1.39        | 1.51     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | B     | 511 | CLA  | MG-NB   | 2.44  | 2.10        | 2.05     |
| 28  | A     | 375 | DGD  | C9B-C8B | -2.44 | 1.39        | 1.51     |
| 28  | C     | 492 | DGD  | C9B-C8B | -2.44 | 1.39        | 1.51     |
| 28  | B     | 533 | DGD  | C9B-C8B | -2.44 | 1.39        | 1.51     |
| 30  | D     | 361 | SQD  | C17-C16 | -2.43 | 1.36        | 1.51     |
| 27  | I     | 220 | LMG  | C20-C19 | -2.43 | 1.39        | 1.51     |
| 28  | D     | 362 | DGD  | C9A-C8A | -2.43 | 1.39        | 1.51     |
| 27  | J     | 492 | LMG  | C20-C19 | -2.43 | 1.39        | 1.51     |
| 21  | B     | 514 | CLA  | O1D-CGD | 2.43  | 1.27        | 1.21     |
| 28  | B     | 533 | DGD  | C2B-C1B | 2.42  | 1.57        | 1.50     |
| 27  | M     | 217 | LMG  | C20-C19 | -2.42 | 1.39        | 1.51     |
| 21  | B     | 512 | CLA  | MG-NA   | 2.42  | 2.12        | 2.06     |
| 29  | D     | 363 | LMT  | C5-C4   | -2.42 | 1.39        | 1.51     |
| 21  | A     | 362 | CLA  | CHC-C1C | 2.42  | 1.43        | 1.38     |
| 29  | D     | 363 | LMT  | O5'-C5' | 2.42  | 1.50        | 1.44     |
| 21  | B     | 524 | CLA  | MG-NB   | 2.41  | 2.10        | 2.05     |
| 28  | D     | 362 | DGD  | C5B-C4B | -2.41 | 1.39        | 1.51     |
| 28  | D     | 362 | DGD  | C4A-C3A | -2.41 | 1.39        | 1.51     |
| 28  | D     | 362 | DGD  | C9B-C8B | -2.41 | 1.39        | 1.51     |
| 21  | B     | 522 | CLA  | C1D-C2D | 2.41  | 1.50        | 1.45     |
| 27  | I     | 220 | LMG  | O6-C5   | 2.41  | 1.50        | 1.44     |
| 25  | B     | 530 | BCR  | C7-C6   | 2.40  | 1.53        | 1.45     |
| 21  | B     | 525 | CLA  | CBA-CGA | 2.40  | 1.57        | 1.50     |
| 30  | C     | 475 | SQD  | C34-C33 | -2.40 | 1.36        | 1.51     |
| 27  | D     | 359 | LMG  | O6-C1   | 2.39  | 1.48        | 1.41     |
| 29  | I     | 274 | LMT  | C1B-C2B | 2.39  | 1.59        | 1.52     |
| 21  | B     | 513 | CLA  | C1D-ND  | -2.39 | 1.34        | 1.37     |
| 29  | I     | 274 | LMT  | C3B-C2B | 2.39  | 1.58        | 1.52     |
| 21  | B     | 511 | CLA  | CHD-C1D | 2.38  | 1.43        | 1.38     |
| 21  | C     | 483 | CLA  | CHC-C1C | 2.38  | 1.43        | 1.38     |
| 21  | C     | 488 | CLA  | CHC-C4B | 2.37  | 1.44        | 1.39     |
| 25  | B     | 527 | BCR  | C38-C26 | 2.37  | 1.54        | 1.50     |
| 21  | K     | 483 | CLA  | MG-NB   | 2.37  | 2.10        | 2.05     |
| 32  | D     | 357 | PL9  | C48-C49 | 2.36  | 1.39        | 1.32     |
| 28  | C     | 491 | DGD  | C3G-C2G | 2.36  | 1.58        | 1.50     |
| 22  | D     | 355 | PHO  | C1C-C2C | 2.36  | 1.53        | 1.45     |
| 28  | C     | 492 | DGD  | C5B-C4B | -2.36 | 1.40        | 1.51     |
| 29  | D     | 536 | LMT  | C4'-C5' | 2.36  | 1.59        | 1.52     |
| 21  | B     | 523 | CLA  | C3B-C2B | 2.36  | 1.49        | 1.41     |
| 21  | B     | 522 | CLA  | MG-ND   | -2.36 | 2.01        | 2.05     |
| 21  | A     | 364 | CLA  | C1D-ND  | -2.36 | 1.34        | 1.37     |
| 21  | C     | 481 | CLA  | CHC-C4B | 2.35  | 1.44        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | B     | 517 | CLA  | CHD-C4C | 2.35  | 1.44        | 1.39     |
| 21  | B     | 513 | CLA  | C3B-C2B | 2.34  | 1.49        | 1.41     |
| 26  | C     | 476 | LHG  | C4-C5   | 2.34  | 1.58        | 1.50     |
| 25  | Z     | 116 | BCR  | C23-C22 | -2.34 | 1.40        | 1.46     |
| 27  | B     | 531 | LMG  | O6-C1   | 2.34  | 1.47        | 1.41     |
| 21  | B     | 511 | CLA  | CAC-C3C | 2.34  | 1.57        | 1.51     |
| 21  | B     | 524 | CLA  | CAC-C3C | 2.33  | 1.57        | 1.51     |
| 29  | I     | 274 | LMT  | O5'-C1' | 2.33  | 1.47        | 1.41     |
| 33  | F     | 85  | HEM  | C1D-C2D | 2.33  | 1.49        | 1.44     |
| 21  | B     | 521 | CLA  | CBA-CGA | 2.33  | 1.57        | 1.50     |
| 21  | B     | 511 | CLA  | C5-C3   | 2.33  | 1.56        | 1.51     |
| 32  | D     | 357 | PL9  | C36-C37 | -2.33 | 1.46        | 1.53     |
| 30  | F     | 224 | SQD  | C18-C17 | -2.33 | 1.37        | 1.51     |
| 29  | D     | 536 | LMT  | C4B-C5B | 2.32  | 1.58        | 1.53     |
| 21  | B     | 521 | CLA  | CMD-C2D | 2.32  | 1.55        | 1.50     |
| 21  | C     | 486 | CLA  | MG-NC   | 2.32  | 2.11        | 2.06     |
| 21  | B     | 524 | CLA  | CMD-C2D | 2.32  | 1.55        | 1.50     |
| 28  | C     | 493 | DGD  | C4E-C3E | 2.32  | 1.58        | 1.52     |
| 21  | A     | 362 | CLA  | CHD-C4C | 2.31  | 1.44        | 1.39     |
| 21  | D     | 354 | CLA  | CHD-C1D | 2.31  | 1.42        | 1.38     |
| 29  | O     | 274 | LMT  | O5'-C5' | 2.31  | 1.50        | 1.44     |
| 21  | B     | 522 | CLA  | C1D-ND  | -2.30 | 1.34        | 1.37     |
| 30  | D     | 361 | SQD  | O5-C1   | 2.30  | 1.47        | 1.41     |
| 30  | L     | 213 | SQD  | C21-C20 | -2.30 | 1.37        | 1.51     |
| 21  | C     | 488 | CLA  | CMD-C2D | 2.30  | 1.55        | 1.50     |
| 21  | C     | 485 | CLA  | CHC-C1C | 2.29  | 1.43        | 1.38     |
| 27  | J     | 492 | LMG  | C16-C15 | -2.29 | 1.40        | 1.51     |
| 28  | C     | 493 | DGD  | O2E-C2E | -2.29 | 1.37        | 1.43     |
| 21  | A     | 363 | CLA  | C4C-C3C | 2.28  | 1.48        | 1.45     |
| 22  | D     | 355 | PHO  | C1A-C2A | 2.28  | 1.54        | 1.51     |
| 22  | A     | 365 | PHO  | C1C-C2C | 2.28  | 1.52        | 1.45     |
| 21  | A     | 364 | CLA  | C3D-C2D | -2.28 | 1.32        | 1.39     |
| 28  | C     | 493 | DGD  | C4D-C3D | -2.28 | 1.46        | 1.52     |
| 21  | B     | 519 | CLA  | MG-ND   | -2.27 | 2.01        | 2.05     |
| 22  | A     | 365 | PHO  | CAC-C3C | 2.27  | 1.56        | 1.51     |
| 21  | B     | 511 | CLA  | MG-ND   | -2.27 | 2.01        | 2.05     |
| 27  | I     | 220 | LMG  | O1-C7   | 2.27  | 1.47        | 1.43     |
| 28  | B     | 528 | DGD  | O5D-C1E | 2.27  | 1.44        | 1.40     |
| 21  | D     | 356 | CLA  | C1D-ND  | -2.27 | 1.34        | 1.37     |
| 30  | L     | 213 | SQD  | C44-C45 | 2.27  | 1.57        | 1.50     |
| 28  | C     | 474 | DGD  | C2A-C1A | 2.26  | 1.57        | 1.50     |
| 21  | B     | 521 | CLA  | CMC-C2C | 2.26  | 1.55        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 33  | V     | 164 | HEM  | CAB-C3B | -2.26 | 1.41        | 1.47     |
| 21  | C     | 478 | CLA  | CAC-C3C | 2.25  | 1.56        | 1.51     |
| 21  | C     | 486 | CLA  | C5-C3   | 2.25  | 1.55        | 1.51     |
| 27  | I     | 220 | LMG  | O8-C9   | 2.25  | 1.50        | 1.45     |
| 21  | B     | 524 | CLA  | C1B-NB  | 2.25  | 1.40        | 1.37     |
| 27  | D     | 360 | LMG  | O1-C1   | 2.25  | 1.43        | 1.40     |
| 21  | B     | 511 | CLA  | CBD-CHA | 2.25  | 1.62        | 1.51     |
| 21  | C     | 484 | CLA  | OBD-CAD | 2.25  | 1.26        | 1.22     |
| 21  | C     | 481 | CLA  | CHD-C4C | 2.25  | 1.44        | 1.39     |
| 28  | B     | 528 | DGD  | O3G-C1D | 2.24  | 1.43        | 1.40     |
| 21  | C     | 478 | CLA  | C5-C3   | 2.24  | 1.55        | 1.51     |
| 21  | B     | 520 | CLA  | CAC-C3C | 2.23  | 1.56        | 1.51     |
| 29  | T     | 226 | LMT  | C4B-C5B | 2.23  | 1.57        | 1.53     |
| 21  | B     | 519 | CLA  | MG-NB   | 2.22  | 2.10        | 2.05     |
| 27  | A     | 373 | LMG  | O1-C1   | 2.22  | 1.43        | 1.40     |
| 27  | J     | 492 | LMG  | C11-C10 | 2.22  | 1.57        | 1.50     |
| 21  | D     | 354 | CLA  | CHC-C1C | 2.22  | 1.42        | 1.38     |
| 21  | C     | 483 | CLA  | MG-ND   | -2.21 | 2.01        | 2.05     |
| 21  | A     | 366 | CLA  | MG-NA   | 2.21  | 2.11        | 2.06     |
| 30  | L     | 213 | SQD  | C24-C23 | 2.21  | 1.57        | 1.50     |
| 25  | J     | 115 | BCR  | C24-C23 | 2.21  | 1.39        | 1.33     |
| 27  | J     | 492 | LMG  | C4-C5   | 2.21  | 1.57        | 1.53     |
| 21  | K     | 483 | CLA  | MG-ND   | -2.20 | 2.01        | 2.05     |
| 21  | C     | 479 | CLA  | CBA-CGA | 2.20  | 1.57        | 1.50     |
| 21  | B     | 513 | CLA  | CHC-C1C | 2.20  | 1.42        | 1.38     |
| 29  | I     | 274 | LMT  | O5'-C5' | 2.19  | 1.49        | 1.44     |
| 21  | B     | 520 | CLA  | MG-ND   | -2.19 | 2.01        | 2.05     |
| 25  | B     | 530 | BCR  | C24-C23 | 2.19  | 1.39        | 1.33     |
| 21  | C     | 483 | CLA  | CBA-CGA | 2.19  | 1.57        | 1.50     |
| 21  | C     | 478 | CLA  | C1B-NB  | 2.18  | 1.40        | 1.37     |
| 21  | B     | 515 | CLA  | O1D-CGD | 2.18  | 1.26        | 1.21     |
| 22  | D     | 355 | PHO  | O1D-CGD | 2.18  | 1.26        | 1.21     |
| 21  | B     | 526 | CLA  | CMC-C2C | 2.17  | 1.55        | 1.50     |
| 21  | B     | 523 | CLA  | C5-C3   | 2.17  | 1.55        | 1.51     |
| 28  | C     | 493 | DGD  | O6E-C5E | -2.17 | 1.39        | 1.44     |
| 21  | B     | 512 | CLA  | CMC-C2C | 2.17  | 1.55        | 1.50     |
| 21  | C     | 477 | CLA  | CBA-CGA | 2.17  | 1.57        | 1.50     |
| 21  | B     | 511 | CLA  | CHD-C4C | 2.16  | 1.44        | 1.39     |
| 29  | B     | 535 | LMT  | C1B-C2B | 2.16  | 1.58        | 1.52     |
| 21  | C     | 482 | CLA  | CHD-C4C | 2.16  | 1.44        | 1.39     |
| 21  | B     | 524 | CLA  | CHC-C1C | 2.14  | 1.42        | 1.38     |
| 21  | B     | 512 | CLA  | MG-NB   | 2.14  | 2.10        | 2.05     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 33  | V     | 164 | HEM  | CHB-C1B | -2.13 | 1.34        | 1.38     |
| 21  | C     | 485 | CLA  | MG-ND   | -2.13 | 2.01        | 2.05     |
| 21  | A     | 363 | CLA  | MG-NC   | 2.12  | 2.11        | 2.06     |
| 21  | C     | 487 | CLA  | CHB-C1B | 2.12  | 1.44        | 1.39     |
| 30  | F     | 224 | SQD  | C19-C18 | -2.12 | 1.35        | 1.50     |
| 27  | I     | 220 | LMG  | C7-C8   | 2.12  | 1.57        | 1.50     |
| 27  | M     | 217 | LMG  | C11-C10 | 2.12  | 1.56        | 1.50     |
| 21  | B     | 517 | CLA  | C3B-C2B | 2.12  | 1.48        | 1.41     |
| 29  | T     | 226 | LMT  | O5B-C5B | 2.11  | 1.49        | 1.44     |
| 21  | C     | 486 | CLA  | C4B-NB  | 2.11  | 1.40        | 1.37     |
| 21  | A     | 362 | CLA  | C1D-ND  | -2.10 | 1.35        | 1.37     |
| 21  | C     | 484 | CLA  | CMD-C2D | 2.10  | 1.55        | 1.50     |
| 21  | B     | 526 | CLA  | CHD-C4C | 2.10  | 1.44        | 1.39     |
| 29  | D     | 536 | LMT  | C3'-C4' | 2.10  | 1.58        | 1.52     |
| 28  | B     | 533 | DGD  | O2G-C2G | 2.10  | 1.51        | 1.46     |
| 30  | C     | 475 | SQD  | C22-C21 | -2.09 | 1.35        | 1.50     |
| 21  | C     | 487 | CLA  | O2A-C1  | 2.09  | 1.51        | 1.46     |
| 27  | C     | 494 | LMG  | C7-C8   | 2.09  | 1.57        | 1.50     |
| 21  | B     | 512 | CLA  | MG-ND   | -2.08 | 2.01        | 2.05     |
| 25  | J     | 112 | BCR  | C19-C18 | -2.08 | 1.41        | 1.46     |
| 21  | C     | 485 | CLA  | CMD-C2D | 2.08  | 1.55        | 1.50     |
| 32  | D     | 357 | PL9  | C11-C9  | 2.08  | 1.55        | 1.51     |
| 21  | B     | 522 | CLA  | C3B-C2B | 2.08  | 1.48        | 1.41     |
| 22  | A     | 365 | PHO  | C3D-C2D | -2.07 | 1.36        | 1.39     |
| 29  | D     | 536 | LMT  | C1B-C2B | 2.07  | 1.58        | 1.52     |
| 21  | B     | 526 | CLA  | CMD-C2D | 2.07  | 1.55        | 1.50     |
| 21  | C     | 482 | CLA  | C4B-NB  | 2.07  | 1.40        | 1.37     |
| 30  | C     | 475 | SQD  | C24-C23 | 2.07  | 1.56        | 1.50     |
| 28  | D     | 362 | DGD  | C2B-C1B | 2.07  | 1.56        | 1.50     |
| 33  | V     | 164 | HEM  | CHC-C1C | 2.07  | 1.42        | 1.38     |
| 21  | B     | 526 | CLA  | CHB-C1B | 2.07  | 1.44        | 1.39     |
| 30  | F     | 224 | SQD  | C44-C45 | 2.07  | 1.57        | 1.50     |
| 21  | B     | 520 | CLA  | C1D-ND  | -2.06 | 1.35        | 1.37     |
| 21  | K     | 483 | CLA  | O1D-CGD | 2.06  | 1.26        | 1.21     |
| 21  | C     | 481 | CLA  | CHD-C1D | 2.06  | 1.42        | 1.38     |
| 29  | D     | 536 | LMT  | O1B-C1B | 2.06  | 1.47        | 1.41     |
| 21  | C     | 481 | CLA  | CBD-CHA | 2.06  | 1.61        | 1.51     |
| 30  | L     | 213 | SQD  | C22-C21 | -2.06 | 1.35        | 1.50     |
| 21  | C     | 480 | CLA  | OBD-CAD | 2.06  | 1.26        | 1.22     |
| 33  | V     | 164 | HEM  | C1C-NC  | -2.05 | 1.35        | 1.39     |
| 25  | J     | 115 | BCR  | C4-C5   | 2.05  | 1.54        | 1.51     |
| 21  | C     | 483 | CLA  | CMD-C2D | 2.05  | 1.55        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | B     | 518 | CLA  | C1D-ND  | -2.04 | 1.35        | 1.37     |
| 33  | F     | 85  | HEM  | C4A-NA  | -2.04 | 1.35        | 1.39     |
| 21  | A     | 364 | CLA  | CBD-CHA | 2.04  | 1.61        | 1.51     |
| 21  | B     | 520 | CLA  | C1B-NB  | 2.03  | 1.40        | 1.37     |
| 21  | D     | 356 | CLA  | CHC-C1C | 2.03  | 1.42        | 1.38     |
| 21  | A     | 363 | CLA  | CHC-C1C | 2.03  | 1.42        | 1.38     |
| 21  | B     | 517 | CLA  | CHC-C4B | 2.03  | 1.44        | 1.39     |
| 29  | O     | 274 | LMT  | C1B-C2B | 2.03  | 1.58        | 1.52     |
| 21  | B     | 511 | CLA  | C4B-NB  | 2.03  | 1.40        | 1.37     |
| 21  | C     | 486 | CLA  | OBD-CAD | 2.02  | 1.26        | 1.22     |
| 28  | A     | 375 | DGD  | C1G-C2G | 2.02  | 1.57        | 1.50     |
| 30  | D     | 361 | SQD  | O6-C44  | -2.02 | 1.40        | 1.43     |
| 21  | C     | 480 | CLA  | CBA-CGA | 2.02  | 1.56        | 1.50     |
| 21  | A     | 366 | CLA  | C5-C3   | 2.02  | 1.55        | 1.51     |
| 26  | A     | 371 | LHG  | C3-C2   | 2.01  | 1.57        | 1.51     |
| 28  | C     | 492 | DGD  | CDA-CCA | -2.01 | 1.39        | 1.51     |
| 22  | D     | 355 | PHO  | C3D-CAD | -2.01 | 1.43        | 1.47     |
| 29  | I     | 274 | LMT  | O5B-C5B | 2.01  | 1.49        | 1.44     |
| 28  | B     | 533 | DGD  | C2A-C1A | 2.01  | 1.56        | 1.50     |
| 27  | I     | 220 | LMG  | C1-C2   | 2.00  | 1.58        | 1.52     |

All (1197) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 28  | C     | 474 | DGD  | O1G-C1G-C2G | 12.52  | 144.47      | 108.40   |
| 25  | J     | 115 | BCR  | C32-C1-C6   | -10.90 | 93.14       | 110.24   |
| 28  | C     | 492 | DGD  | O5D-C1E-C2E | 10.88  | 124.80      | 108.27   |
| 33  | F     | 85  | HEM  | CMA-C3A-C4A | 10.64  | 141.62      | 125.42   |
| 28  | C     | 491 | DGD  | O5D-C1E-C2E | 10.63  | 124.41      | 108.27   |
| 21  | B     | 518 | CLA  | C4A-NA-C1A  | 10.22  | 111.34      | 106.68   |
| 28  | D     | 362 | DGD  | O5D-C1E-C2E | 10.13  | 123.66      | 108.27   |
| 25  | J     | 115 | BCR  | C32-C1-C31  | -10.06 | 79.83       | 108.63   |
| 28  | C     | 493 | DGD  | O5D-C1E-C2E | 10.02  | 123.49      | 108.27   |
| 33  | V     | 164 | HEM  | CMA-C3A-C4A | 9.71   | 140.21      | 125.42   |
| 27  | D     | 359 | LMG  | C8-O7-C10   | 9.69   | 140.99      | 117.80   |
| 21  | C     | 487 | CLA  | C4A-NA-C1A  | 9.66   | 111.09      | 106.68   |
| 21  | B     | 525 | CLA  | C4A-NA-C1A  | 9.57   | 111.05      | 106.68   |
| 27  | C     | 494 | LMG  | C8-O7-C10   | 9.46   | 140.44      | 117.80   |
| 28  | C     | 474 | DGD  | O5D-C1E-C2E | 9.31   | 122.41      | 108.27   |
| 21  | C     | 477 | CLA  | C4A-NA-C1A  | 9.22   | 110.89      | 106.68   |
| 30  | L     | 213 | SQD  | O5-C1-O6    | 9.19   | 131.75      | 110.04   |
| 21  | B     | 516 | CLA  | C4A-NA-C1A  | 9.17   | 110.86      | 106.68   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | D     | 356 | CLA  | C4A-NA-C1A  | 9.15  | 110.86      | 106.68   |
| 21  | A     | 366 | CLA  | C4A-NA-C1A  | 9.07  | 110.82      | 106.68   |
| 27  | B     | 531 | LMG  | C8-O7-C10   | 8.94  | 139.20      | 117.80   |
| 28  | A     | 375 | DGD  | C2G-O2G-C1B | 8.92  | 139.15      | 117.80   |
| 21  | C     | 479 | CLA  | C4A-NA-C1A  | 8.91  | 110.74      | 106.68   |
| 30  | F     | 224 | SQD  | O5-C1-O6    | 8.86  | 130.97      | 110.04   |
| 21  | C     | 488 | CLA  | C4A-NA-C1A  | 8.82  | 110.70      | 106.68   |
| 21  | C     | 482 | CLA  | C4A-NA-C1A  | 8.82  | 110.70      | 106.68   |
| 32  | D     | 357 | PL9  | C7-C8-C9    | -8.78 | 111.71      | 126.83   |
| 33  | F     | 85  | HEM  | CMA-C3A-C2A | -8.74 | 107.09      | 125.62   |
| 28  | C     | 493 | DGD  | O5D-C6D-C5D | 8.74  | 129.11      | 109.42   |
| 28  | C     | 474 | DGD  | O6D-C5D-C6D | 8.70  | 123.95      | 106.69   |
| 28  | C     | 491 | DGD  | C2G-O2G-C1B | 8.70  | 138.62      | 117.80   |
| 21  | B     | 526 | CLA  | C4A-NA-C1A  | 8.67  | 110.64      | 106.68   |
| 21  | C     | 485 | CLA  | C4A-NA-C1A  | 8.59  | 110.60      | 106.68   |
| 21  | B     | 511 | CLA  | C4A-NA-C1A  | 8.55  | 110.58      | 106.68   |
| 28  | C     | 493 | DGD  | O6D-C5D-C6D | 8.54  | 123.63      | 106.69   |
| 21  | B     | 513 | CLA  | C4A-NA-C1A  | 8.54  | 110.58      | 106.68   |
| 21  | C     | 483 | CLA  | C4A-NA-C1A  | 8.38  | 110.50      | 106.68   |
| 32  | D     | 357 | PL9  | C7-C3-C4    | 8.37  | 123.80      | 116.91   |
| 21  | K     | 483 | CLA  | C4A-NA-C1A  | 8.35  | 110.49      | 106.68   |
| 27  | I     | 220 | LMG  | C8-O7-C10   | 8.28  | 137.60      | 117.80   |
| 30  | D     | 361 | SQD  | O5-C1-O6    | 8.25  | 129.54      | 110.04   |
| 21  | A     | 364 | CLA  | C4A-NA-C1A  | 8.23  | 110.44      | 106.68   |
| 30  | C     | 475 | SQD  | O5-C1-O6    | 8.20  | 129.41      | 110.04   |
| 21  | A     | 362 | CLA  | C4A-NA-C1A  | 8.19  | 110.42      | 106.68   |
| 21  | C     | 480 | CLA  | C4A-NA-C1A  | 8.15  | 110.39      | 106.68   |
| 28  | C     | 474 | DGD  | O5D-C6D-C5D | 8.12  | 127.71      | 109.42   |
| 21  | C     | 484 | CLA  | C4A-NA-C1A  | 8.08  | 110.37      | 106.68   |
| 21  | B     | 520 | CLA  | C4A-NA-C1A  | 8.08  | 110.36      | 106.68   |
| 21  | B     | 522 | CLA  | C4A-NA-C1A  | 7.99  | 110.32      | 106.68   |
| 33  | V     | 164 | HEM  | CMA-C3A-C2A | -7.91 | 108.84      | 125.62   |
| 28  | C     | 493 | DGD  | C2G-O2G-C1B | 7.88  | 136.66      | 117.80   |
| 21  | C     | 486 | CLA  | C4A-NA-C1A  | 7.77  | 110.22      | 106.68   |
| 21  | C     | 478 | CLA  | C4A-NA-C1A  | 7.75  | 110.21      | 106.68   |
| 21  | B     | 515 | CLA  | C4A-NA-C1A  | 7.72  | 110.20      | 106.68   |
| 21  | B     | 521 | CLA  | C4A-NA-C1A  | 7.71  | 110.20      | 106.68   |
| 21  | B     | 519 | CLA  | C4A-NA-C1A  | 7.53  | 110.12      | 106.68   |
| 28  | C     | 491 | DGD  | O6D-C5D-C6D | 7.49  | 121.54      | 106.69   |
| 21  | B     | 512 | CLA  | C4A-NA-C1A  | 7.35  | 110.03      | 106.68   |
| 30  | C     | 475 | SQD  | O6-C1-C2    | 7.34  | 119.43      | 108.27   |
| 21  | B     | 523 | CLA  | C4A-NA-C1A  | 7.34  | 110.03      | 106.68   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | A     | 363 | CLA  | C4A-NA-C1A  | 7.34  | 110.03      | 106.68   |
| 21  | B     | 517 | CLA  | C4A-NA-C1A  | 7.29  | 110.00      | 106.68   |
| 28  | C     | 492 | DGD  | O6D-C5D-C6D | 7.20  | 120.97      | 106.69   |
| 30  | D     | 361 | SQD  | O6-C1-C2    | 7.15  | 119.13      | 108.27   |
| 30  | D     | 361 | SQD  | O7-S-C6     | 7.14  | 117.42      | 106.76   |
| 25  | J     | 115 | BCR  | C2-C1-C6    | 7.13  | 120.79      | 110.44   |
| 28  | D     | 362 | DGD  | C3G-O3G-C1D | -7.11 | 98.55       | 113.80   |
| 22  | D     | 355 | PHO  | O2D-CGD-CBD | 7.03  | 118.67      | 110.95   |
| 21  | B     | 524 | CLA  | C4A-NA-C1A  | 7.03  | 109.88      | 106.68   |
| 28  | B     | 533 | DGD  | O2G-C1B-C2B | 7.00  | 126.63      | 111.48   |
| 30  | L     | 213 | SQD  | O6-C1-C2    | 6.99  | 118.89      | 108.27   |
| 25  | J     | 115 | BCR  | C32-C1-C2   | -6.93 | 82.33       | 108.95   |
| 25  | X     | 107 | BCR  | C38-C26-C25 | 6.93  | 132.04      | 124.48   |
| 28  | C     | 474 | DGD  | C6D-C5D-C4D | -6.92 | 97.53       | 112.07   |
| 22  | A     | 365 | PHO  | O2D-CGD-CBD | 6.90  | 118.53      | 110.95   |
| 27  | J     | 492 | LMG  | O7-C10-C11  | 6.89  | 126.39      | 111.48   |
| 21  | C     | 481 | CLA  | C4A-NA-C1A  | 6.88  | 109.82      | 106.68   |
| 28  | C     | 474 | DGD  | O1G-C1A-C2A | 6.77  | 132.49      | 111.83   |
| 30  | C     | 475 | SQD  | O7-S-C6     | 6.75  | 116.83      | 106.76   |
| 25  | D     | 358 | BCR  | C38-C26-C25 | 6.73  | 131.82      | 124.48   |
| 28  | C     | 474 | DGD  | O2G-C1B-C2B | 6.66  | 125.88      | 111.48   |
| 27  | B     | 531 | LMG  | C13-C12-C11 | -6.63 | 88.78       | 113.13   |
| 30  | L     | 213 | SQD  | O7-S-C6     | 6.62  | 116.64      | 106.76   |
| 21  | D     | 354 | CLA  | C4A-NA-C1A  | 6.57  | 109.68      | 106.68   |
| 30  | F     | 224 | SQD  | O7-S-C6     | 6.55  | 116.53      | 106.76   |
| 25  | J     | 112 | BCR  | C33-C5-C6   | 6.55  | 131.63      | 124.48   |
| 25  | A     | 369 | BCR  | C38-C26-C25 | 6.45  | 131.52      | 124.48   |
| 28  | C     | 491 | DGD  | O5D-C6D-C5D | 6.44  | 123.95      | 109.42   |
| 28  | D     | 362 | DGD  | O5D-C6D-C5D | 6.43  | 123.92      | 109.42   |
| 25  | B     | 529 | BCR  | C38-C26-C25 | 6.42  | 131.49      | 124.48   |
| 25  | J     | 115 | BCR  | C38-C26-C25 | 6.42  | 131.49      | 124.48   |
| 22  | A     | 365 | PHO  | C4D-CHA-CBD | -6.38 | 105.39      | 108.45   |
| 27  | B     | 531 | LMG  | C19-C18-C17 | -6.36 | 82.22       | 114.37   |
| 28  | C     | 493 | DGD  | C6D-O5D-C1E | -6.35 | 100.17      | 113.80   |
| 26  | C     | 476 | LHG  | C25-C24-C23 | 6.32  | 136.87      | 113.69   |
| 28  | C     | 492 | DGD  | C6D-O5D-C1E | -6.30 | 100.28      | 113.80   |
| 25  | J     | 115 | BCR  | C33-C5-C6   | 6.29  | 131.35      | 124.48   |
| 25  | B     | 529 | BCR  | C33-C5-C6   | 6.29  | 131.35      | 124.48   |
| 28  | C     | 474 | DGD  | O3G-C1D-C2D | -6.28 | 98.74       | 108.27   |
| 28  | C     | 493 | DGD  | C6D-C5D-C4D | -6.28 | 98.89       | 112.07   |
| 25  | B     | 527 | BCR  | C38-C26-C25 | 6.27  | 131.33      | 124.48   |
| 30  | F     | 224 | SQD  | O6-C1-C2    | 6.27  | 117.79      | 108.27   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 27  | M     | 217 | LMG  | O7-C10-C11  | 6.27  | 125.03      | 111.48   |
| 30  | F     | 224 | SQD  | C10-C9-C8   | 6.17  | 135.81      | 113.13   |
| 30  | D     | 361 | SQD  | C10-C9-C8   | 6.16  | 135.77      | 113.13   |
| 28  | C     | 474 | DGD  | O6D-C1D-O3G | 6.15  | 124.58      | 110.04   |
| 25  | B     | 527 | BCR  | C33-C5-C6   | 6.15  | 131.19      | 124.48   |
| 21  | C     | 481 | CLA  | CAA-C2A-C1A | -6.15 | 91.83       | 111.97   |
| 26  | A     | 371 | LHG  | C25-C24-C23 | 6.14  | 136.21      | 113.69   |
| 30  | C     | 475 | SQD  | C10-C9-C8   | 6.12  | 135.62      | 113.13   |
| 28  | C     | 493 | DGD  | C4B-C3B-C2B | -6.11 | 90.68       | 113.13   |
| 30  | D     | 361 | SQD  | C25-C24-C23 | 6.10  | 136.06      | 113.69   |
| 21  | A     | 364 | CLA  | C4D-C3D-CAD | 6.08  | 114.71      | 108.11   |
| 25  | Z     | 116 | BCR  | C38-C26-C25 | 6.06  | 131.10      | 124.48   |
| 27  | D     | 359 | LMG  | C13-C12-C11 | -6.06 | 90.85       | 113.13   |
| 21  | B     | 514 | CLA  | C4A-NA-C1A  | 6.06  | 109.44      | 106.68   |
| 25  | D     | 358 | BCR  | C33-C5-C6   | 6.06  | 131.09      | 124.48   |
| 28  | C     | 492 | DGD  | O5D-C6D-C5D | 6.05  | 123.05      | 109.42   |
| 32  | D     | 357 | PL9  | C32-C33-C34 | -6.03 | 113.82      | 127.62   |
| 30  | L     | 213 | SQD  | C10-C9-C8   | 6.01  | 135.21      | 113.13   |
| 30  | F     | 224 | SQD  | C25-C24-C23 | 6.00  | 135.67      | 113.69   |
| 28  | D     | 362 | DGD  | O3G-C3G-C2G | 5.94  | 125.28      | 110.82   |
| 30  | L     | 213 | SQD  | C25-C24-C23 | 5.90  | 135.31      | 113.69   |
| 28  | D     | 362 | DGD  | O6D-C5D-C6D | 5.86  | 118.32      | 106.69   |
| 21  | C     | 481 | CLA  | CBA-CAA-C2A | 5.86  | 131.24      | 113.79   |
| 27  | B     | 531 | LMG  | C17-C16-C15 | -5.80 | 85.05       | 114.37   |
| 25  | C     | 490 | BCR  | C33-C5-C6   | 5.76  | 130.77      | 124.48   |
| 25  | C     | 489 | BCR  | C38-C26-C25 | 5.73  | 130.74      | 124.48   |
| 21  | C     | 481 | CLA  | CAA-CBA-CGA | -5.71 | 96.99       | 113.21   |
| 21  | C     | 482 | CLA  | C4D-C3D-CAD | 5.67  | 114.27      | 108.11   |
| 25  | J     | 115 | BCR  | C31-C1-C6   | 5.66  | 119.12      | 110.24   |
| 28  | C     | 491 | DGD  | C1G-O1G-C1A | 5.64  | 137.74      | 117.12   |
| 28  | C     | 493 | DGD  | C3G-O3G-C1D | -5.64 | 101.70      | 113.80   |
| 21  | C     | 480 | CLA  | CBA-CAA-C2A | 5.64  | 130.57      | 113.79   |
| 21  | C     | 481 | CLA  | C4D-C3D-CAD | 5.61  | 114.20      | 108.11   |
| 25  | B     | 530 | BCR  | C38-C26-C25 | 5.57  | 130.56      | 124.48   |
| 30  | C     | 475 | SQD  | C25-C24-C23 | 5.56  | 134.07      | 113.69   |
| 28  | C     | 491 | DGD  | O1G-C1G-C2G | -5.54 | 92.41       | 108.40   |
| 28  | C     | 492 | DGD  | C6A-C5A-C4A | -5.54 | 86.37       | 114.37   |
| 28  | C     | 492 | DGD  | O2G-C1B-C2B | 5.51  | 123.39      | 111.48   |
| 28  | C     | 492 | DGD  | C4A-C3A-C2A | -5.48 | 92.99       | 113.13   |
| 21  | B     | 524 | CLA  | O2D-CGD-CBD | 5.48  | 120.81      | 111.23   |
| 27  | D     | 359 | LMG  | C7-O1-C1    | -5.46 | 102.08      | 113.80   |
| 25  | B     | 527 | BCR  | C8-C7-C6    | 5.44  | 141.54      | 127.00   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 28  | A     | 375 | DGD  | O3G-C1D-C2D | -5.44 | 100.01      | 108.27   |
| 28  | C     | 491 | DGD  | C4B-C3B-C2B | -5.43 | 93.17       | 113.13   |
| 29  | D     | 536 | LMT  | C1B-O1B-C4' | -5.41 | 105.14      | 117.98   |
| 28  | A     | 375 | DGD  | C6D-O5D-C1E | -5.37 | 102.29      | 113.80   |
| 32  | D     | 357 | PL9  | C12-C13-C14 | -5.37 | 115.34      | 127.62   |
| 25  | J     | 115 | BCR  | C23-C24-C25 | 5.33  | 141.25      | 127.00   |
| 25  | Z     | 116 | BCR  | C33-C5-C6   | 5.32  | 130.28      | 124.48   |
| 25  | X     | 107 | BCR  | C15-C14-C13 | 5.28  | 134.69      | 127.28   |
| 21  | B     | 517 | CLA  | C4D-C3D-CAD | 5.28  | 113.84      | 108.11   |
| 21  | C     | 483 | CLA  | C4D-C3D-CAD | 5.27  | 113.83      | 108.11   |
| 21  | B     | 511 | CLA  | O2D-CGD-CBD | 5.26  | 120.43      | 111.23   |
| 27  | I     | 220 | LMG  | C13-C12-C11 | -5.25 | 93.84       | 113.13   |
| 21  | A     | 362 | CLA  | C4D-C3D-CAD | 5.23  | 113.78      | 108.11   |
| 33  | F     | 85  | HEM  | CAD-C3D-C2D | 5.20  | 137.62      | 127.87   |
| 25  | A     | 369 | BCR  | C24-C23-C22 | 5.19  | 133.92      | 126.23   |
| 21  | C     | 480 | CLA  | CAA-C2A-C1A | -5.17 | 95.05       | 111.97   |
| 28  | C     | 474 | DGD  | C1G-O1G-C1A | -5.16 | 98.27       | 117.12   |
| 28  | C     | 491 | DGD  | C6D-C5D-C4D | -5.16 | 101.24      | 112.07   |
| 27  | B     | 531 | LMG  | C7-O1-C1    | -5.14 | 102.77      | 113.80   |
| 25  | A     | 369 | BCR  | C33-C5-C6   | 5.14  | 130.09      | 124.48   |
| 28  | C     | 474 | DGD  | C6D-O5D-C1E | -5.13 | 102.79      | 113.80   |
| 28  | A     | 375 | DGD  | O5D-C1E-C2E | 5.12  | 116.05      | 108.27   |
| 25  | C     | 490 | BCR  | C38-C26-C25 | 5.12  | 130.07      | 124.48   |
| 28  | C     | 492 | DGD  | C6D-C5D-C4D | -5.11 | 101.35      | 112.07   |
| 32  | D     | 357 | PL9  | C22-C23-C24 | -5.10 | 115.94      | 127.62   |
| 21  | D     | 354 | CLA  | C4D-C3D-CAD | 5.09  | 113.64      | 108.11   |
| 27  | D     | 359 | LMG  | O1-C7-C8    | 5.09  | 123.20      | 110.82   |
| 28  | A     | 375 | DGD  | C6D-C5D-C4D | -5.09 | 101.39      | 112.07   |
| 21  | B     | 513 | CLA  | C4D-C3D-CAD | 5.08  | 113.63      | 108.11   |
| 25  | B     | 530 | BCR  | C33-C5-C6   | 5.08  | 130.02      | 124.48   |
| 25  | J     | 112 | BCR  | C38-C26-C25 | 5.07  | 130.02      | 124.48   |
| 21  | B     | 511 | CLA  | C4D-C3D-CAD | 5.07  | 113.61      | 108.11   |
| 32  | D     | 357 | PL9  | C42-C43-C44 | -5.06 | 116.05      | 127.62   |
| 21  | B     | 518 | CLA  | CAA-C2A-C1A | -5.04 | 95.46       | 111.97   |
| 21  | C     | 479 | CLA  | O2D-CGD-CBD | 5.04  | 120.03      | 111.23   |
| 21  | C     | 486 | CLA  | C3B-C4B-NB  | -5.03 | 106.04      | 110.53   |
| 21  | D     | 356 | CLA  | C4D-C3D-CAD | 5.03  | 113.57      | 108.11   |
| 28  | A     | 375 | DGD  | C4B-C3B-C2B | -4.98 | 94.84       | 113.13   |
| 21  | B     | 525 | CLA  | C4D-C3D-CAD | 4.97  | 113.50      | 108.11   |
| 21  | A     | 366 | CLA  | C4D-C3D-CAD | 4.97  | 113.50      | 108.11   |
| 21  | B     | 520 | CLA  | C4D-C3D-CAD | 4.97  | 113.50      | 108.11   |
| 21  | C     | 484 | CLA  | C3B-C4B-NB  | -4.95 | 106.11      | 110.53   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 33  | V     | 164 | HEM  | C4A-C3A-C2A | -4.94 | 101.16      | 106.82   |
| 28  | C     | 493 | DGD  | C1D-O6D-C5D | -4.92 | 104.10      | 113.72   |
| 32  | D     | 357 | PL9  | C11-C9-C8   | -4.92 | 110.12      | 121.17   |
| 25  | X     | 107 | BCR  | C33-C5-C6   | 4.91  | 129.85      | 124.48   |
| 21  | K     | 483 | CLA  | C4D-C3D-CAD | 4.91  | 113.44      | 108.11   |
| 22  | D     | 355 | PHO  | C4A-C3A-C2A | 4.90  | 107.50      | 102.84   |
| 28  | D     | 362 | DGD  | C6D-O5D-C1E | -4.88 | 103.33      | 113.80   |
| 21  | B     | 524 | CLA  | C4D-C3D-CAD | 4.88  | 113.41      | 108.11   |
| 21  | B     | 517 | CLA  | C3B-C4B-NB  | -4.87 | 106.18      | 110.53   |
| 21  | C     | 487 | CLA  | C4D-C3D-CAD | 4.84  | 113.37      | 108.11   |
| 21  | C     | 479 | CLA  | C4D-C3D-CAD | 4.84  | 113.36      | 108.11   |
| 28  | C     | 474 | DGD  | C3G-O3G-C1D | 4.84  | 124.17      | 113.80   |
| 28  | A     | 375 | DGD  | C3G-O3G-C1D | 4.84  | 124.17      | 113.80   |
| 21  | B     | 519 | CLA  | C4D-C3D-CAD | 4.84  | 113.36      | 108.11   |
| 28  | C     | 474 | DGD  | C1D-O6D-C5D | -4.83 | 104.28      | 113.72   |
| 22  | A     | 365 | PHO  | C3D-C4D-ND  | 4.82  | 113.88      | 107.71   |
| 21  | B     | 524 | CLA  | CBA-CAA-C2A | 4.81  | 128.10      | 113.79   |
| 28  | C     | 492 | DGD  | C1D-O6D-C5D | -4.81 | 104.33      | 113.72   |
| 21  | B     | 518 | CLA  | C4D-C3D-CAD | 4.80  | 113.31      | 108.11   |
| 27  | B     | 531 | LMG  | O7-C8-C7    | 4.79  | 125.52      | 108.34   |
| 21  | B     | 516 | CLA  | C2A-C1A-CHA | 4.78  | 132.16      | 123.87   |
| 25  | J     | 112 | BCR  | C2-C1-C6    | 4.77  | 117.37      | 110.44   |
| 21  | C     | 477 | CLA  | C4D-C3D-CAD | 4.76  | 113.27      | 108.11   |
| 21  | K     | 483 | CLA  | O2D-CGD-CBD | 4.75  | 119.54      | 111.23   |
| 21  | B     | 523 | CLA  | C3B-C4B-NB  | -4.75 | 106.29      | 110.53   |
| 21  | A     | 363 | CLA  | C4D-C3D-CAD | 4.75  | 113.27      | 108.11   |
| 21  | C     | 483 | CLA  | C3B-C4B-NB  | -4.75 | 106.29      | 110.53   |
| 25  | B     | 530 | BCR  | C7-C8-C9    | 4.75  | 133.26      | 126.23   |
| 21  | C     | 488 | CLA  | C3B-C4B-NB  | -4.74 | 106.30      | 110.53   |
| 21  | C     | 482 | CLA  | C3B-C4B-NB  | -4.73 | 106.31      | 110.53   |
| 22  | D     | 355 | PHO  | C4D-CHA-CBD | -4.73 | 106.19      | 108.45   |
| 21  | C     | 480 | CLA  | C4D-C3D-CAD | 4.71  | 113.22      | 108.11   |
| 22  | A     | 365 | PHO  | C4A-C3A-C2A | 4.70  | 107.31      | 102.84   |
| 30  | L     | 213 | SQD  | C44-O6-C1   | 4.70  | 123.87      | 113.80   |
| 21  | C     | 488 | CLA  | C3A-C2A-C1A | 4.68  | 108.35      | 101.34   |
| 22  | D     | 355 | PHO  | C3D-C4D-ND  | 4.67  | 113.69      | 107.71   |
| 25  | J     | 115 | BCR  | C8-C7-C6    | 4.66  | 139.45      | 127.00   |
| 30  | F     | 224 | SQD  | O8-S-C6     | -4.66 | 96.97       | 105.97   |
| 27  | B     | 531 | LMG  | C22-C21-C20 | -4.66 | 90.81       | 114.37   |
| 21  | B     | 514 | CLA  | C4D-C3D-CAD | 4.66  | 113.17      | 108.11   |
| 27  | B     | 531 | LMG  | C9-C8-C7    | -4.65 | 100.95      | 111.78   |
| 25  | J     | 115 | BCR  | C1-C6-C5    | -4.64 | 116.29      | 122.64   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 27  | C     | 494 | LMG  | C9-O8-C28   | 4.63  | 134.05      | 117.12   |
| 25  | C     | 489 | BCR  | C24-C23-C22 | 4.61  | 133.06      | 126.23   |
| 28  | C     | 492 | DGD  | C3G-O3G-C1D | -4.60 | 103.94      | 113.80   |
| 21  | B     | 522 | CLA  | C3B-C4B-NB  | -4.58 | 106.44      | 110.53   |
| 21  | C     | 488 | CLA  | C4D-C3D-CAD | 4.58  | 113.08      | 108.11   |
| 21  | B     | 521 | CLA  | CBA-CAA-C2A | 4.58  | 127.41      | 113.79   |
| 28  | C     | 492 | DGD  | C8A-C7A-C6A | -4.57 | 91.25       | 114.37   |
| 28  | C     | 474 | DGD  | O3G-C3G-C2G | -4.55 | 99.74       | 110.82   |
| 21  | C     | 478 | CLA  | C4D-C3D-CAD | 4.55  | 113.05      | 108.11   |
| 25  | X     | 107 | BCR  | C12-C13-C14 | -4.55 | 111.86      | 119.01   |
| 21  | B     | 516 | CLA  | C4D-C3D-CAD | 4.54  | 113.04      | 108.11   |
| 21  | B     | 521 | CLA  | C4D-C3D-CAD | 4.54  | 113.04      | 108.11   |
| 21  | A     | 363 | CLA  | CBA-CAA-C2A | 4.54  | 127.31      | 113.79   |
| 25  | X     | 107 | BCR  | C29-C30-C25 | 4.54  | 117.03      | 110.44   |
| 33  | V     | 164 | HEM  | CHA-C4D-C3D | -4.54 | 116.86      | 125.23   |
| 21  | B     | 520 | CLA  | O2D-CGD-CBD | 4.52  | 119.13      | 111.23   |
| 21  | B     | 513 | CLA  | C3B-C4B-NB  | -4.51 | 106.50      | 110.53   |
| 28  | C     | 493 | DGD  | O6E-C1E-O5D | 4.50  | 120.67      | 110.04   |
| 27  | D     | 359 | LMG  | C9-C8-C7    | 4.49  | 122.27      | 111.78   |
| 21  | C     | 485 | CLA  | C4D-C3D-CAD | 4.49  | 112.99      | 108.11   |
| 33  | F     | 85  | HEM  | C4A-C3A-C2A | -4.49 | 101.68      | 106.82   |
| 28  | D     | 362 | DGD  | C1G-O1G-C1A | 4.47  | 133.47      | 117.12   |
| 28  | B     | 533 | DGD  | O6D-C5D-C6D | 4.47  | 115.56      | 106.69   |
| 21  | B     | 524 | CLA  | C3B-C4B-NB  | -4.46 | 106.55      | 110.53   |
| 21  | A     | 363 | CLA  | O2D-CGD-CBD | 4.45  | 119.01      | 111.23   |
| 21  | B     | 512 | CLA  | C4D-C3D-CAD | 4.45  | 112.94      | 108.11   |
| 27  | B     | 531 | LMG  | C15-C14-C13 | -4.44 | 91.91       | 114.37   |
| 21  | B     | 518 | CLA  | CBA-CAA-C2A | 4.44  | 127.00      | 113.79   |
| 21  | C     | 487 | CLA  | C2A-C1A-CHA | 4.44  | 131.57      | 123.87   |
| 21  | C     | 480 | CLA  | O2D-CGD-CBD | 4.44  | 118.98      | 111.23   |
| 21  | C     | 481 | CLA  | C3B-C4B-NB  | -4.43 | 106.57      | 110.53   |
| 28  | C     | 474 | DGD  | C3G-C2G-C1G | 4.43  | 122.12      | 111.78   |
| 21  | B     | 525 | CLA  | C3B-C4B-NB  | -4.43 | 106.58      | 110.53   |
| 28  | C     | 493 | DGD  | O6D-C5D-C4D | 4.43  | 117.68      | 109.70   |
| 28  | C     | 491 | DGD  | C4A-C3A-C2A | -4.43 | 96.86       | 113.13   |
| 32  | D     | 357 | PL9  | C3-C4-C5    | 4.42  | 124.08      | 118.57   |
| 33  | V     | 164 | HEM  | CHA-C4D-ND  | 4.41  | 129.82      | 124.37   |
| 21  | A     | 366 | CLA  | C3B-C4B-NB  | -4.40 | 106.60      | 110.53   |
| 21  | C     | 477 | CLA  | C3A-C2A-C1A | 4.40  | 107.93      | 101.34   |
| 25  | J     | 112 | BCR  | C11-C10-C9  | 4.39  | 133.44      | 127.28   |
| 25  | C     | 490 | BCR  | C24-C23-C22 | 4.39  | 132.72      | 126.23   |
| 21  | C     | 479 | CLA  | C1-C2-C3    | 4.38  | 133.37      | 126.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 28  | B     | 533 | DGD  | O5D-C1E-C2E | 4.37  | 114.91      | 108.27   |
| 21  | C     | 484 | CLA  | C4D-C3D-CAD | 4.37  | 112.85      | 108.11   |
| 29  | D     | 363 | LMT  | C1-O1'-C1'  | 4.36  | 121.13      | 113.68   |
| 29  | D     | 363 | LMT  | C1B-O1B-C4' | -4.36 | 107.65      | 117.98   |
| 21  | B     | 517 | CLA  | C11-C10-C8  | 4.36  | 130.44      | 115.97   |
| 21  | B     | 515 | CLA  | C3B-C4B-NB  | -4.35 | 106.65      | 110.53   |
| 33  | V     | 164 | HEM  | C1B-NB-C4B  | 4.34  | 110.35      | 105.21   |
| 21  | B     | 515 | CLA  | C4D-C3D-CAD | 4.34  | 112.82      | 108.11   |
| 21  | D     | 354 | CLA  | C3B-C4B-NB  | -4.33 | 106.66      | 110.53   |
| 21  | K     | 483 | CLA  | C3B-C4B-NB  | -4.33 | 106.67      | 110.53   |
| 21  | B     | 513 | CLA  | C2A-C1A-CHA | 4.31  | 131.35      | 123.87   |
| 28  | C     | 491 | DGD  | C6D-O5D-C1E | -4.31 | 104.55      | 113.80   |
| 21  | C     | 485 | CLA  | C3B-C4B-NB  | -4.31 | 106.69      | 110.53   |
| 32  | D     | 357 | PL9  | C10-C9-C8   | -4.30 | 112.59      | 123.63   |
| 21  | B     | 526 | CLA  | C4D-C3D-CAD | 4.29  | 112.77      | 108.11   |
| 27  | D     | 359 | LMG  | O7-C8-C7    | 4.28  | 123.71      | 108.34   |
| 21  | B     | 517 | CLA  | O2D-CGD-CBD | 4.27  | 118.69      | 111.23   |
| 25  | Z     | 116 | BCR  | C29-C30-C25 | 4.26  | 116.62      | 110.44   |
| 25  | J     | 112 | BCR  | C7-C8-C9    | 4.25  | 132.52      | 126.23   |
| 28  | A     | 375 | DGD  | O6D-C1D-O3G | 4.24  | 120.06      | 110.04   |
| 27  | C     | 494 | LMG  | C13-C12-C11 | -4.23 | 97.57       | 113.13   |
| 21  | C     | 487 | CLA  | C3B-C4B-NB  | -4.23 | 106.75      | 110.53   |
| 32  | D     | 357 | PL9  | C46-C47-C48 | 4.22  | 132.92      | 112.02   |
| 21  | D     | 356 | CLA  | O2D-CGD-CBD | 4.22  | 118.61      | 111.23   |
| 21  | B     | 521 | CLA  | CAA-C2A-C1A | -4.22 | 98.15       | 111.97   |
| 21  | B     | 526 | CLA  | C3B-C4B-NB  | -4.22 | 106.77      | 110.53   |
| 28  | C     | 474 | DGD  | C3A-C2A-C1A | -4.21 | 98.26       | 113.69   |
| 33  | F     | 85  | HEM  | CHA-C4D-ND  | 4.21  | 129.58      | 124.37   |
| 21  | A     | 364 | CLA  | C3B-C4B-NB  | -4.21 | 106.78      | 110.53   |
| 27  | B     | 531 | LMG  | C18-C17-C16 | 4.20  | 135.58      | 114.37   |
| 25  | C     | 490 | BCR  | C29-C30-C25 | 4.19  | 116.53      | 110.44   |
| 32  | D     | 357 | PL9  | C7-C3-C2    | -4.19 | 118.45      | 123.39   |
| 27  | D     | 359 | LMG  | O8-C9-C8    | -4.19 | 96.31       | 108.40   |
| 30  | L     | 213 | SQD  | O8-S-C6     | -4.19 | 97.88       | 105.97   |
| 25  | D     | 358 | BCR  | C24-C23-C22 | 4.19  | 132.43      | 126.23   |
| 33  | F     | 85  | HEM  | CHA-C4D-C3D | -4.19 | 117.50      | 125.23   |
| 25  | X     | 107 | BCR  | C8-C7-C6    | 4.19  | 138.18      | 127.00   |
| 25  | J     | 112 | BCR  | C23-C24-C25 | 4.18  | 138.17      | 127.00   |
| 30  | F     | 224 | SQD  | C11-C10-C9  | 4.18  | 135.49      | 114.37   |
| 21  | B     | 522 | CLA  | C4D-C3D-CAD | 4.18  | 112.64      | 108.11   |
| 21  | B     | 523 | CLA  | C4D-C3D-CAD | 4.18  | 112.64      | 108.11   |
| 25  | X     | 107 | BCR  | C30-C25-C26 | -4.16 | 116.95      | 122.64   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 29  | A     | 376 | LMT  | O1B-C1B-C2B | 4.16  | 118.33      | 108.09   |
| 21  | C     | 486 | CLA  | C4D-C3D-CAD | 4.15  | 112.61      | 108.11   |
| 21  | D     | 354 | CLA  | O2D-CGD-CBD | 4.13  | 118.45      | 111.23   |
| 25  | D     | 358 | BCR  | C2-C1-C6    | 4.12  | 116.43      | 110.44   |
| 27  | I     | 220 | LMG  | C9-C8-C7    | -4.10 | 102.22      | 111.78   |
| 28  | B     | 533 | DGD  | O6E-C1E-O5D | 4.09  | 119.71      | 110.04   |
| 21  | C     | 483 | CLA  | O2D-CGD-CBD | 4.09  | 118.38      | 111.23   |
| 27  | C     | 494 | LMG  | O1-C7-C8    | -4.08 | 100.90      | 110.82   |
| 21  | A     | 363 | CLA  | C3B-C4B-NB  | -4.07 | 106.90      | 110.53   |
| 32  | D     | 357 | PL9  | C20-C19-C21 | 4.06  | 122.28      | 115.23   |
| 21  | B     | 518 | CLA  | O2D-CGD-CBD | 4.06  | 118.32      | 111.23   |
| 25  | J     | 115 | BCR  | C38-C26-C27 | -4.05 | 104.96      | 113.60   |
| 28  | B     | 533 | DGD  | O1G-C1A-C2A | 4.05  | 124.19      | 111.83   |
| 21  | D     | 356 | CLA  | C3B-C4B-NB  | -4.05 | 106.92      | 110.53   |
| 21  | B     | 525 | CLA  | C2A-C1A-CHA | 4.03  | 130.86      | 123.87   |
| 25  | B     | 527 | BCR  | C29-C30-C25 | 4.03  | 116.29      | 110.44   |
| 21  | C     | 486 | CLA  | CBA-CAA-C2A | 4.02  | 125.75      | 113.79   |
| 30  | C     | 475 | SQD  | O48-C23-C24 | 4.02  | 124.08      | 111.83   |
| 21  | B     | 516 | CLA  | C3A-C2A-C1A | 4.02  | 107.35      | 101.34   |
| 21  | B     | 512 | CLA  | C3B-C4B-NB  | -4.01 | 106.95      | 110.53   |
| 21  | A     | 362 | CLA  | C3B-C4B-NB  | -4.01 | 106.95      | 110.53   |
| 21  | C     | 487 | CLA  | C2A-C3A-C4A | 4.00  | 108.33      | 101.87   |
| 21  | C     | 480 | CLA  | C3A-C2A-C1A | 4.00  | 107.33      | 101.34   |
| 21  | C     | 485 | CLA  | C2A-C1A-CHA | 3.99  | 130.80      | 123.87   |
| 32  | D     | 357 | PL9  | C15-C14-C16 | 3.98  | 122.13      | 115.23   |
| 25  | J     | 112 | BCR  | C29-C30-C25 | 3.98  | 116.22      | 110.44   |
| 21  | B     | 525 | CLA  | O2D-CGD-CBD | 3.98  | 118.18      | 111.23   |
| 21  | C     | 480 | CLA  | C3B-C4B-NB  | -3.98 | 106.98      | 110.53   |
| 25  | X     | 107 | BCR  | C38-C26-C27 | -3.95 | 105.17      | 113.60   |
| 21  | A     | 363 | CLA  | C1-C2-C3    | 3.95  | 132.67      | 126.20   |
| 32  | D     | 357 | PL9  | C30-C29-C31 | 3.95  | 122.08      | 115.23   |
| 21  | B     | 516 | CLA  | C3B-C4B-NB  | -3.94 | 107.02      | 110.53   |
| 30  | F     | 224 | SQD  | O48-C23-C24 | 3.93  | 123.83      | 111.83   |
| 28  | C     | 493 | DGD  | C6B-C5B-C4B | -3.93 | 94.49       | 114.37   |
| 21  | A     | 366 | CLA  | O2D-CGD-CBD | 3.93  | 118.10      | 111.23   |
| 25  | B     | 529 | BCR  | C33-C5-C4   | -3.92 | 105.23      | 113.60   |
| 33  | V     | 164 | HEM  | CAD-C3D-C2D | 3.92  | 135.21      | 127.87   |
| 21  | C     | 486 | CLA  | C1-C2-C3    | 3.92  | 132.61      | 126.20   |
| 28  | C     | 492 | DGD  | O2G-C2G-C1G | 3.91  | 122.38      | 108.34   |
| 28  | B     | 533 | DGD  | C3A-C2A-C1A | -3.91 | 99.36       | 113.69   |
| 21  | B     | 526 | CLA  | C1-C2-C3    | 3.91  | 132.60      | 126.20   |
| 21  | K     | 483 | CLA  | C1-C2-C3    | 3.90  | 132.59      | 126.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | A     | 364 | CLA  | C2A-C1A-CHA | 3.90  | 130.64      | 123.87   |
| 28  | D     | 362 | DGD  | C6D-C5D-C4D | -3.90 | 103.88      | 112.07   |
| 21  | C     | 477 | CLA  | O2D-CGD-CBD | 3.90  | 118.05      | 111.23   |
| 30  | D     | 361 | SQD  | C44-O6-C1   | 3.90  | 122.15      | 113.80   |
| 21  | C     | 480 | CLA  | CAA-CBA-CGA | -3.90 | 102.15      | 113.21   |
| 25  | B     | 527 | BCR  | C2-C1-C6    | 3.89  | 116.09      | 110.44   |
| 25  | B     | 530 | BCR  | C29-C30-C25 | 3.89  | 116.09      | 110.44   |
| 21  | C     | 481 | CLA  | C3A-C2A-C1A | 3.89  | 107.17      | 101.34   |
| 33  | F     | 85  | HEM  | C4B-C3B-C2B | -3.89 | 103.70      | 107.28   |
| 27  | M     | 217 | LMG  | C9-O8-C28   | 3.89  | 131.33      | 117.12   |
| 21  | A     | 362 | CLA  | O2D-CGD-CBD | 3.88  | 118.02      | 111.23   |
| 25  | C     | 489 | BCR  | C33-C5-C6   | 3.88  | 128.72      | 124.48   |
| 25  | D     | 358 | BCR  | C38-C26-C27 | -3.88 | 105.33      | 113.60   |
| 25  | B     | 530 | BCR  | C23-C24-C25 | 3.87  | 137.34      | 127.00   |
| 30  | D     | 361 | SQD  | C11-C10-C9  | 3.87  | 133.93      | 114.37   |
| 21  | C     | 487 | CLA  | O2D-CGD-CBD | 3.87  | 117.99      | 111.23   |
| 27  | I     | 220 | LMG  | O7-C8-C7    | 3.87  | 122.21      | 108.34   |
| 25  | X     | 107 | BCR  | C2-C1-C6    | 3.86  | 116.05      | 110.44   |
| 27  | B     | 531 | LMG  | C20-C19-C18 | 3.86  | 133.89      | 114.37   |
| 21  | C     | 482 | CLA  | CBA-CAA-C2A | 3.86  | 125.28      | 113.79   |
| 25  | B     | 527 | BCR  | C16-C17-C18 | 3.86  | 132.69      | 127.28   |
| 21  | B     | 514 | CLA  | C3B-C4B-NB  | -3.86 | 107.09      | 110.53   |
| 21  | C     | 478 | CLA  | O2D-CGD-CBD | 3.85  | 117.96      | 111.23   |
| 21  | B     | 518 | CLA  | C3A-C2A-C1A | 3.85  | 107.10      | 101.34   |
| 25  | D     | 358 | BCR  | C1-C6-C5    | -3.84 | 117.39      | 122.64   |
| 25  | J     | 115 | BCR  | C29-C30-C25 | 3.83  | 116.00      | 110.44   |
| 28  | D     | 362 | DGD  | C3G-C2G-C1G | 3.82  | 120.69      | 111.78   |
| 21  | B     | 515 | CLA  | CBA-CAA-C2A | 3.82  | 125.16      | 113.79   |
| 21  | C     | 488 | CLA  | CAA-CBA-CGA | -3.81 | 102.38      | 113.21   |
| 21  | C     | 478 | CLA  | C3B-C4B-NB  | -3.80 | 107.13      | 110.53   |
| 32  | D     | 357 | PL9  | C35-C34-C36 | 3.80  | 121.83      | 115.23   |
| 22  | A     | 365 | PHO  | C1A-C2A-C3A | 3.80  | 106.45      | 102.84   |
| 21  | B     | 519 | CLA  | CBA-CAA-C2A | 3.80  | 125.10      | 113.79   |
| 30  | L     | 213 | SQD  | C11-C10-C9  | 3.80  | 133.57      | 114.37   |
| 28  | D     | 362 | DGD  | C2G-O2G-C1B | 3.80  | 126.88      | 117.80   |
| 21  | B     | 521 | CLA  | C3B-C4B-NB  | -3.79 | 107.15      | 110.53   |
| 21  | B     | 517 | CLA  | C1-C2-C3    | 3.79  | 132.40      | 126.20   |
| 21  | B     | 515 | CLA  | CAA-C2A-C1A | -3.78 | 99.59       | 111.97   |
| 21  | A     | 366 | CLA  | C2A-C1A-CHA | 3.77  | 130.42      | 123.87   |
| 27  | A     | 373 | LMG  | O7-C10-C11  | 3.77  | 119.64      | 111.48   |
| 28  | C     | 474 | DGD  | O6E-C1E-O5D | 3.77  | 118.95      | 110.04   |
| 30  | D     | 361 | SQD  | O8-S-C6     | -3.77 | 98.69       | 105.97   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 28  | B     | 528 | DGD  | O2G-C1B-C2B | 3.77  | 119.63      | 111.48   |
| 21  | C     | 477 | CLA  | C2A-C1A-CHA | 3.76  | 130.40      | 123.87   |
| 25  | J     | 112 | BCR  | C33-C5-C4   | -3.76 | 105.58      | 113.60   |
| 28  | A     | 375 | DGD  | O5D-C6D-C5D | 3.75  | 117.87      | 109.42   |
| 29  | D     | 536 | LMT  | O1'-C1-C2   | -3.73 | 96.70       | 109.37   |
| 27  | D     | 360 | LMG  | O7-C10-C11  | 3.73  | 119.55      | 111.48   |
| 25  | Z     | 116 | BCR  | C23-C24-C25 | 3.73  | 136.96      | 127.00   |
| 21  | B     | 513 | CLA  | C2A-C3A-C4A | 3.73  | 107.89      | 101.87   |
| 21  | B     | 519 | CLA  | C1-C2-C3    | 3.72  | 132.30      | 126.20   |
| 21  | B     | 526 | CLA  | O2D-CGD-CBD | 3.72  | 117.74      | 111.23   |
| 28  | D     | 362 | DGD  | O2G-C1B-C2B | 3.72  | 119.53      | 111.48   |
| 21  | C     | 487 | CLA  | C1-C2-C3    | 3.71  | 132.28      | 126.20   |
| 30  | C     | 475 | SQD  | C31-C30-C29 | 3.71  | 133.12      | 114.37   |
| 25  | A     | 369 | BCR  | C38-C26-C27 | -3.71 | 105.69      | 113.60   |
| 30  | C     | 475 | SQD  | C11-C10-C9  | 3.71  | 133.11      | 114.37   |
| 30  | C     | 475 | SQD  | C44-O6-C1   | 3.71  | 121.75      | 113.80   |
| 25  | B     | 530 | BCR  | C2-C1-C6    | 3.71  | 115.82      | 110.44   |
| 25  | C     | 489 | BCR  | C29-C30-C25 | 3.70  | 115.82      | 110.44   |
| 21  | B     | 511 | CLA  | C2A-C3A-C4A | 3.70  | 107.85      | 101.87   |
| 21  | B     | 519 | CLA  | C3B-C4B-NB  | -3.70 | 107.23      | 110.53   |
| 21  | B     | 517 | CLA  | C3A-C2A-C1A | 3.68  | 106.85      | 101.34   |
| 30  | C     | 475 | SQD  | O8-S-C6     | -3.67 | 98.88       | 105.97   |
| 21  | B     | 513 | CLA  | C3A-C2A-C1A | 3.67  | 106.84      | 101.34   |
| 29  | O     | 274 | LMT  | C3B-C4B-C5B | 3.66  | 116.88      | 110.23   |
| 25  | C     | 489 | BCR  | C38-C26-C27 | -3.66 | 105.78      | 113.60   |
| 25  | D     | 358 | BCR  | C29-C30-C25 | 3.66  | 115.76      | 110.44   |
| 21  | B     | 515 | CLA  | O2D-CGD-CBD | 3.66  | 117.63      | 111.23   |
| 21  | B     | 518 | CLA  | C2A-C3A-C4A | 3.66  | 107.78      | 101.87   |
| 32  | D     | 357 | PL9  | C25-C24-C26 | 3.66  | 121.58      | 115.23   |
| 25  | B     | 529 | BCR  | C29-C30-C25 | 3.65  | 115.75      | 110.44   |
| 26  | A     | 371 | LHG  | O8-C23-C24  | 3.65  | 122.97      | 111.83   |
| 21  | B     | 518 | CLA  | C3B-C4B-NB  | -3.65 | 107.27      | 110.53   |
| 21  | C     | 477 | CLA  | C3B-C4B-NB  | -3.64 | 107.28      | 110.53   |
| 27  | I     | 220 | LMG  | C12-C11-C10 | 3.63  | 127.00      | 113.69   |
| 25  | D     | 358 | BCR  | C33-C5-C4   | -3.63 | 105.86      | 113.60   |
| 25  | B     | 529 | BCR  | C38-C26-C27 | -3.62 | 105.89      | 113.60   |
| 29  | B     | 535 | LMT  | C3B-C4B-C5B | 3.62  | 116.79      | 110.23   |
| 27  | B     | 531 | LMG  | C38-C37-C36 | 3.61  | 132.64      | 114.37   |
| 25  | C     | 490 | BCR  | C8-C7-C6    | 3.61  | 136.63      | 127.00   |
| 21  | C     | 479 | CLA  | C3B-C4B-NB  | -3.61 | 107.31      | 110.53   |
| 27  | I     | 220 | LMG  | C15-C14-C13 | -3.60 | 96.16       | 114.37   |
| 27  | D     | 359 | LMG  | C9-O8-C28   | 3.60  | 130.28      | 117.12   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | J     | 112 | BCR  | C30-C25-C26 | -3.60 | 117.72      | 122.64   |
| 25  | J     | 115 | BCR  | C33-C5-C4   | -3.59 | 105.94      | 113.60   |
| 21  | B     | 512 | CLA  | O2D-CGD-CBD | 3.59  | 117.50      | 111.23   |
| 29  | A     | 376 | LMT  | C3B-C4B-C5B | 3.59  | 116.73      | 110.23   |
| 28  | C     | 492 | DGD  | C3G-C2G-C1G | -3.58 | 103.43      | 111.78   |
| 32  | D     | 357 | PL9  | C20-C19-C18 | -3.58 | 114.43      | 123.63   |
| 25  | J     | 112 | BCR  | C8-C9-C10   | -3.58 | 113.38      | 119.01   |
| 29  | I     | 274 | LMT  | C3B-C4B-C5B | 3.58  | 116.72      | 110.23   |
| 21  | C     | 479 | CLA  | CBA-CAA-C2A | 3.58  | 124.43      | 113.79   |
| 27  | J     | 492 | LMG  | C38-C37-C36 | 3.57  | 132.44      | 114.37   |
| 21  | A     | 364 | CLA  | CBA-CAA-C2A | 3.57  | 124.42      | 113.79   |
| 33  | F     | 85  | HEM  | CAD-C3D-C4D | -3.57 | 118.48      | 124.70   |
| 25  | B     | 530 | BCR  | C33-C5-C4   | -3.57 | 105.99      | 113.60   |
| 33  | V     | 164 | HEM  | C3B-C4B-NB  | -3.57 | 106.91      | 109.47   |
| 28  | B     | 533 | DGD  | C1D-O6D-C5D | -3.56 | 106.76      | 113.72   |
| 25  | Z     | 116 | BCR  | C8-C7-C6    | 3.55  | 136.49      | 127.00   |
| 28  | C     | 492 | DGD  | O6D-C5D-C4D | 3.55  | 116.10      | 109.70   |
| 25  | D     | 358 | BCR  | C30-C25-C26 | -3.55 | 117.78      | 122.64   |
| 30  | F     | 224 | SQD  | C44-O6-C1   | 3.55  | 121.41      | 113.80   |
| 21  | B     | 522 | CLA  | C3A-C2A-C1A | 3.55  | 106.65      | 101.34   |
| 21  | C     | 488 | CLA  | C2A-C1A-CHA | 3.55  | 130.02      | 123.87   |
| 25  | C     | 490 | BCR  | C33-C5-C4   | -3.55 | 106.04      | 113.60   |
| 27  | J     | 492 | LMG  | C8-O7-C10   | 3.54  | 126.27      | 117.80   |
| 27  | C     | 494 | LMG  | O7-C8-C7    | 3.54  | 121.04      | 108.34   |
| 25  | B     | 530 | BCR  | C30-C25-C26 | -3.54 | 117.80      | 122.64   |
| 25  | A     | 369 | BCR  | C30-C25-C26 | -3.54 | 117.80      | 122.64   |
| 25  | J     | 112 | BCR  | C1-C6-C5    | -3.53 | 117.81      | 122.64   |
| 21  | C     | 478 | CLA  | C3A-C2A-C1A | 3.53  | 106.63      | 101.34   |
| 30  | L     | 213 | SQD  | O48-C23-C24 | 3.53  | 122.59      | 111.83   |
| 25  | C     | 490 | BCR  | C23-C22-C21 | -3.53 | 113.46      | 119.01   |
| 21  | B     | 513 | CLA  | O2D-CGD-CBD | 3.53  | 117.39      | 111.23   |
| 21  | B     | 519 | CLA  | C3A-C2A-C1A | 3.52  | 106.61      | 101.34   |
| 26  | C     | 476 | LHG  | O7-C7-C8    | 3.52  | 119.10      | 111.48   |
| 21  | B     | 516 | CLA  | CBA-CAA-C2A | 3.52  | 124.26      | 113.79   |
| 25  | B     | 527 | BCR  | C33-C5-C4   | -3.52 | 106.10      | 113.60   |
| 25  | A     | 369 | BCR  | C29-C30-C25 | 3.50  | 115.53      | 110.44   |
| 21  | B     | 526 | CLA  | C2A-C1A-CHA | 3.50  | 129.95      | 123.87   |
| 21  | B     | 520 | CLA  | C2A-C3A-C4A | 3.50  | 107.53      | 101.87   |
| 27  | D     | 359 | LMG  | C12-C11-C10 | 3.50  | 126.50      | 113.69   |
| 27  | B     | 531 | LMG  | C12-C11-C10 | 3.48  | 126.46      | 113.69   |
| 21  | B     | 517 | CLA  | C2A-C1A-CHA | 3.48  | 129.91      | 123.87   |
| 28  | A     | 375 | DGD  | O6D-C5D-C6D | 3.48  | 113.59      | 106.69   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | A     | 362 | CLA  | C2A-C3A-C4A | 3.48  | 107.49      | 101.87   |
| 27  | D     | 360 | LMG  | C8-O7-C10   | -3.48 | 109.47      | 117.80   |
| 29  | D     | 536 | LMT  | C3B-C4B-C5B | 3.48  | 116.54      | 110.23   |
| 30  | D     | 361 | SQD  | O48-C23-C24 | 3.48  | 122.44      | 111.83   |
| 21  | C     | 483 | CLA  | C2A-C1A-CHA | 3.48  | 129.90      | 123.87   |
| 28  | C     | 491 | DGD  | C3G-O3G-C1D | -3.47 | 106.35      | 113.80   |
| 27  | C     | 494 | LMG  | C38-C37-C36 | 3.47  | 131.93      | 114.37   |
| 21  | C     | 484 | CLA  | C1-C2-C3    | 3.47  | 131.89      | 126.20   |
| 21  | B     | 525 | CLA  | C2A-C3A-C4A | 3.47  | 107.48      | 101.87   |
| 21  | C     | 485 | CLA  | C3A-C2A-C1A | 3.47  | 106.54      | 101.34   |
| 21  | B     | 526 | CLA  | C2A-C3A-C4A | 3.47  | 107.47      | 101.87   |
| 22  | A     | 365 | PHO  | C4D-ND-C1D  | -3.47 | 104.72      | 108.87   |
| 21  | C     | 484 | CLA  | C3A-C2A-C1A | 3.46  | 106.53      | 101.34   |
| 28  | B     | 528 | DGD  | C2G-O2G-C1B | -3.46 | 109.50      | 117.80   |
| 27  | J     | 492 | LMG  | C12-C11-C10 | -3.46 | 101.00      | 113.69   |
| 21  | A     | 366 | CLA  | C3A-C2A-C1A | 3.46  | 106.53      | 101.34   |
| 27  | A     | 373 | LMG  | C8-O7-C10   | -3.46 | 109.51      | 117.80   |
| 21  | D     | 356 | CLA  | C2A-C3A-C4A | 3.46  | 107.46      | 101.87   |
| 21  | B     | 526 | CLA  | C3A-C2A-C1A | 3.45  | 106.51      | 101.34   |
| 21  | B     | 521 | CLA  | O2D-CGD-CBD | 3.45  | 117.27      | 111.23   |
| 21  | C     | 479 | CLA  | C2A-C3A-C4A | 3.45  | 107.44      | 101.87   |
| 25  | J     | 115 | BCR  | C30-C25-C26 | -3.45 | 117.92      | 122.64   |
| 27  | B     | 531 | LMG  | C16-C15-C14 | 3.45  | 131.80      | 114.37   |
| 25  | X     | 107 | BCR  | C16-C17-C18 | 3.45  | 132.11      | 127.28   |
| 21  | K     | 483 | CLA  | C3A-C2A-C1A | 3.44  | 106.50      | 101.34   |
| 25  | X     | 107 | BCR  | C35-C13-C12 | 3.44  | 123.34      | 118.09   |
| 21  | D     | 354 | CLA  | C12-C11-C10 | -3.44 | 97.88       | 113.28   |
| 21  | B     | 524 | CLA  | CAA-C2A-C1A | -3.43 | 100.72      | 111.97   |
| 29  | D     | 363 | LMT  | C3B-C4B-C5B | 3.43  | 116.45      | 110.23   |
| 21  | A     | 363 | CLA  | CAA-C2A-C1A | -3.43 | 100.73      | 111.97   |
| 21  | C     | 481 | CLA  | O2D-CGD-CBD | 3.42  | 117.21      | 111.23   |
| 29  | O     | 274 | LMT  | O1'-C1-C2   | -3.42 | 97.76       | 109.37   |
| 25  | B     | 527 | BCR  | C38-C26-C27 | -3.42 | 106.30      | 113.60   |
| 21  | B     | 515 | CLA  | C3A-C2A-C1A | 3.42  | 106.46      | 101.34   |
| 25  | D     | 358 | BCR  | C23-C24-C25 | 3.41  | 136.11      | 127.00   |
| 29  | B     | 535 | LMT  | C1-O1'-C1'  | -3.41 | 107.86      | 113.68   |
| 21  | B     | 518 | CLA  | CAA-CBA-CGA | -3.41 | 103.54      | 113.21   |
| 25  | C     | 490 | BCR  | C2-C1-C6    | 3.39  | 115.37      | 110.44   |
| 21  | C     | 486 | CLA  | CAA-C2A-C1A | -3.39 | 100.86      | 111.97   |
| 21  | D     | 356 | CLA  | C2A-C1A-CHA | 3.39  | 129.75      | 123.87   |
| 21  | C     | 478 | CLA  | C2A-C3A-C4A | 3.38  | 107.33      | 101.87   |
| 25  | B     | 529 | BCR  | C8-C7-C6    | 3.38  | 136.03      | 127.00   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | B     | 527 | BCR  | C12-C13-C14 | -3.38 | 113.69      | 119.01   |
| 21  | C     | 484 | CLA  | O2D-CGD-CBD | 3.38  | 117.14      | 111.23   |
| 21  | C     | 488 | CLA  | C1-C2-C3    | 3.37  | 131.72      | 126.20   |
| 21  | B     | 517 | CLA  | C2A-C3A-C4A | 3.37  | 107.32      | 101.87   |
| 33  | F     | 85  | HEM  | C1B-NB-C4B  | 3.37  | 109.20      | 105.21   |
| 21  | B     | 519 | CLA  | O2D-CGD-CBD | 3.37  | 117.12      | 111.23   |
| 33  | V     | 164 | HEM  | CBA-CAA-C2A | 3.37  | 121.85      | 112.53   |
| 25  | Z     | 116 | BCR  | C16-C17-C18 | 3.37  | 132.00      | 127.28   |
| 25  | C     | 489 | BCR  | C35-C13-C12 | 3.36  | 123.23      | 118.09   |
| 21  | C     | 484 | CLA  | CBA-CAA-C2A | 3.36  | 123.80      | 113.79   |
| 22  | A     | 365 | PHO  | O1D-CGD-CBD | -3.36 | 119.63      | 124.72   |
| 21  | D     | 356 | CLA  | CBA-CAA-C2A | 3.35  | 123.77      | 113.79   |
| 21  | A     | 364 | CLA  | C3A-C2A-C1A | 3.35  | 106.35      | 101.34   |
| 21  | A     | 364 | CLA  | C2A-C3A-C4A | 3.34  | 107.27      | 101.87   |
| 21  | C     | 484 | CLA  | CAA-C2A-C1A | -3.34 | 101.02      | 111.97   |
| 25  | X     | 107 | BCR  | C23-C24-C25 | 3.34  | 135.93      | 127.00   |
| 21  | C     | 477 | CLA  | CAA-C2A-C1A | -3.34 | 101.03      | 111.97   |
| 21  | A     | 364 | CLA  | O2D-CGD-CBD | 3.34  | 117.06      | 111.23   |
| 21  | C     | 482 | CLA  | C2A-C3A-C4A | 3.33  | 107.25      | 101.87   |
| 28  | C     | 492 | DGD  | O6E-C1E-O5D | 3.33  | 117.92      | 110.04   |
| 28  | A     | 375 | DGD  | O2G-C2G-C3G | 3.33  | 120.30      | 108.34   |
| 25  | B     | 529 | BCR  | C23-C24-C25 | 3.32  | 135.88      | 127.00   |
| 21  | B     | 524 | CLA  | C2A-C3A-C4A | 3.32  | 107.24      | 101.87   |
| 25  | Z     | 116 | BCR  | C33-C5-C4   | -3.32 | 106.51      | 113.60   |
| 25  | C     | 490 | BCR  | C38-C26-C27 | -3.32 | 106.52      | 113.60   |
| 21  | A     | 362 | CLA  | C3A-C2A-C1A | 3.32  | 106.31      | 101.34   |
| 21  | B     | 515 | CLA  | C2A-C3A-C4A | 3.32  | 107.23      | 101.87   |
| 21  | K     | 483 | CLA  | C2A-C3A-C4A | 3.31  | 107.22      | 101.87   |
| 21  | B     | 525 | CLA  | C3A-C2A-C1A | 3.31  | 106.30      | 101.34   |
| 28  | A     | 375 | DGD  | C3G-C2G-C1G | -3.31 | 104.07      | 111.78   |
| 25  | X     | 107 | BCR  | C1-C6-C5    | -3.31 | 118.12      | 122.64   |
| 21  | B     | 516 | CLA  | C2A-C3A-C4A | 3.30  | 107.20      | 101.87   |
| 21  | B     | 519 | CLA  | C2A-C1A-CHA | 3.30  | 129.59      | 123.87   |
| 25  | D     | 358 | BCR  | C8-C7-C6    | 3.29  | 135.80      | 127.00   |
| 27  | J     | 492 | LMG  | C14-C13-C12 | -3.29 | 97.72       | 114.37   |
| 21  | A     | 363 | CLA  | C3A-C2A-C1A | 3.29  | 106.27      | 101.34   |
| 21  | D     | 354 | CLA  | C2A-C3A-C4A | 3.29  | 107.19      | 101.87   |
| 21  | B     | 521 | CLA  | C2A-C3A-C4A | 3.29  | 107.18      | 101.87   |
| 33  | F     | 85  | HEM  | CBC-CAC-C3C | -3.29 | 111.09      | 127.53   |
| 27  | B     | 531 | LMG  | O1-C7-C8    | 3.29  | 118.81      | 110.82   |
| 21  | A     | 363 | CLA  | C2A-C3A-C4A | 3.28  | 107.17      | 101.87   |
| 21  | C     | 477 | CLA  | C2A-C3A-C4A | 3.28  | 107.17      | 101.87   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | B     | 524 | CLA  | C1-C2-C3    | 3.28  | 131.57      | 126.20   |
| 29  | T     | 226 | LMT  | C3B-C4B-C5B | 3.28  | 116.18      | 110.23   |
| 21  | C     | 482 | CLA  | CED-O2D-CGD | 3.27  | 123.33      | 115.92   |
| 28  | C     | 493 | DGD  | O1G-C1G-C2G | -3.27 | 98.97       | 108.40   |
| 25  | C     | 489 | BCR  | C2-C1-C6    | 3.27  | 115.18      | 110.44   |
| 21  | C     | 483 | CLA  | C1-C2-C3    | 3.26  | 131.55      | 126.20   |
| 21  | B     | 522 | CLA  | CED-O2D-CGD | 3.26  | 123.32      | 115.92   |
| 25  | B     | 530 | BCR  | C24-C23-C22 | 3.26  | 131.06      | 126.23   |
| 21  | C     | 479 | CLA  | O1D-CGD-CBD | -3.26 | 118.09      | 124.52   |
| 21  | B     | 522 | CLA  | C2A-C1A-CHA | 3.26  | 129.53      | 123.87   |
| 21  | B     | 519 | CLA  | CAA-CBA-CGA | -3.25 | 103.97      | 113.21   |
| 25  | B     | 529 | BCR  | C2-C1-C6    | 3.25  | 115.16      | 110.44   |
| 28  | A     | 375 | DGD  | C6B-C5B-C4B | -3.24 | 97.98       | 114.37   |
| 21  | C     | 481 | CLA  | C2A-C3A-C4A | 3.24  | 107.11      | 101.87   |
| 21  | B     | 514 | CLA  | C2A-C3A-C4A | 3.24  | 107.10      | 101.87   |
| 21  | A     | 366 | CLA  | C2A-C3A-C4A | 3.24  | 107.10      | 101.87   |
| 21  | C     | 484 | CLA  | CED-O2D-CGD | 3.24  | 123.26      | 115.92   |
| 26  | C     | 476 | LHG  | O8-C23-C24  | 3.24  | 121.71      | 111.83   |
| 28  | C     | 474 | DGD  | O2G-C2G-C1G | 3.24  | 119.96      | 108.34   |
| 25  | X     | 107 | BCR  | C24-C23-C22 | 3.24  | 131.03      | 126.23   |
| 21  | D     | 356 | CLA  | C3A-C2A-C1A | 3.23  | 106.18      | 101.34   |
| 21  | B     | 520 | CLA  | C3B-C4B-NB  | -3.22 | 107.66      | 110.53   |
| 25  | C     | 490 | BCR  | C30-C25-C26 | -3.22 | 118.24      | 122.64   |
| 21  | B     | 516 | CLA  | CED-O2D-CGD | 3.21  | 123.20      | 115.92   |
| 28  | C     | 474 | DGD  | O1G-C1A-O1A | -3.20 | 115.62      | 123.63   |
| 27  | I     | 220 | LMG  | C17-C16-C15 | -3.19 | 98.22       | 114.37   |
| 25  | A     | 369 | BCR  | C33-C5-C4   | -3.19 | 106.79      | 113.60   |
| 28  | C     | 491 | DGD  | C3B-C2B-C1B | 3.19  | 125.36      | 113.69   |
| 21  | C     | 486 | CLA  | C3A-C2A-C1A | 3.18  | 106.11      | 101.34   |
| 25  | B     | 527 | BCR  | C35-C13-C12 | 3.18  | 122.95      | 118.09   |
| 25  | B     | 530 | BCR  | C1-C6-C5    | -3.18 | 118.29      | 122.64   |
| 21  | C     | 478 | CLA  | CBA-CAA-C2A | 3.18  | 123.26      | 113.79   |
| 21  | B     | 521 | CLA  | C3A-C2A-C1A | 3.18  | 106.09      | 101.34   |
| 21  | C     | 485 | CLA  | C2A-C3A-C4A | 3.17  | 107.00      | 101.87   |
| 25  | B     | 527 | BCR  | C30-C25-C26 | -3.17 | 118.30      | 122.64   |
| 21  | C     | 486 | CLA  | C2A-C3A-C4A | 3.17  | 106.99      | 101.87   |
| 29  | O     | 274 | LMT  | C1-O1'-C1'  | 3.17  | 119.09      | 113.68   |
| 21  | C     | 483 | CLA  | C2A-C3A-C4A | 3.17  | 106.99      | 101.87   |
| 21  | B     | 512 | CLA  | C2A-C3A-C4A | 3.17  | 106.98      | 101.87   |
| 21  | C     | 483 | CLA  | C3A-C2A-C1A | 3.16  | 106.08      | 101.34   |
| 25  | J     | 112 | BCR  | C24-C23-C22 | 3.16  | 130.91      | 126.23   |
| 25  | B     | 530 | BCR  | C38-C26-C27 | -3.16 | 106.86      | 113.60   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | Z     | 116 | BCR  | C38-C26-C27 | -3.16 | 106.87      | 113.60   |
| 21  | B     | 524 | CLA  | O1D-CGD-CBD | -3.15 | 118.30      | 124.52   |
| 21  | B     | 511 | CLA  | C3B-C4B-NB  | -3.15 | 107.72      | 110.53   |
| 28  | C     | 491 | DGD  | C6B-C5B-C4B | -3.15 | 98.44       | 114.37   |
| 25  | C     | 489 | BCR  | C1-C6-C5    | -3.15 | 118.33      | 122.64   |
| 25  | J     | 112 | BCR  | C30-C25-C24 | 3.15  | 124.18      | 115.65   |
| 25  | J     | 112 | BCR  | C38-C26-C27 | -3.14 | 106.89      | 113.60   |
| 28  | D     | 362 | DGD  | O6D-C5D-C4D | 3.14  | 115.36      | 109.70   |
| 27  | I     | 220 | LMG  | O8-C28-C29  | 3.14  | 121.42      | 111.83   |
| 21  | B     | 514 | CLA  | CBA-CAA-C2A | 3.14  | 123.13      | 113.79   |
| 25  | Z     | 116 | BCR  | C2-C1-C6    | 3.14  | 115.00      | 110.44   |
| 25  | B     | 527 | BCR  | C23-C24-C25 | 3.14  | 135.37      | 127.00   |
| 21  | B     | 523 | CLA  | O2D-CGD-CBD | 3.13  | 116.71      | 111.23   |
| 25  | C     | 490 | BCR  | C1-C6-C5    | -3.12 | 118.38      | 122.64   |
| 25  | B     | 527 | BCR  | C1-C6-C5    | -3.12 | 118.38      | 122.64   |
| 25  | C     | 489 | BCR  | C30-C25-C26 | -3.12 | 118.38      | 122.64   |
| 21  | C     | 482 | CLA  | C3A-C2A-C1A | 3.11  | 106.00      | 101.34   |
| 29  | D     | 536 | LMT  | C4-C3-C2    | -3.11 | 98.62       | 114.37   |
| 25  | Z     | 116 | BCR  | C30-C25-C26 | -3.11 | 118.38      | 122.64   |
| 21  | B     | 516 | CLA  | C1-C2-C3    | 3.11  | 131.29      | 126.20   |
| 25  | X     | 107 | BCR  | C33-C5-C4   | -3.11 | 106.97      | 113.60   |
| 33  | V     | 164 | HEM  | CAB-C3B-C2B | -3.11 | 118.33      | 128.43   |
| 21  | B     | 520 | CLA  | C3A-C2A-C1A | 3.11  | 105.99      | 101.34   |
| 21  | K     | 483 | CLA  | C2A-C1A-CHA | 3.10  | 129.25      | 123.87   |
| 28  | C     | 492 | DGD  | C5A-C4A-C3A | 3.10  | 130.04      | 114.37   |
| 27  | D     | 359 | LMG  | C15-C14-C13 | -3.10 | 98.70       | 114.37   |
| 30  | D     | 361 | SQD  | C3-C4-C5    | -3.10 | 104.62      | 110.23   |
| 21  | B     | 519 | CLA  | C2A-C3A-C4A | 3.10  | 106.87      | 101.87   |
| 30  | C     | 475 | SQD  | C3-C4-C5    | -3.10 | 104.62      | 110.23   |
| 28  | A     | 375 | DGD  | O6D-C5D-C4D | -3.09 | 104.12      | 109.70   |
| 30  | D     | 361 | SQD  | O9-S-C6     | -3.09 | 102.15      | 106.76   |
| 25  | C     | 489 | BCR  | C32-C1-C6   | 3.09  | 115.08      | 110.24   |
| 21  | B     | 520 | CLA  | C1-C2-C3    | 3.08  | 131.25      | 126.20   |
| 21  | C     | 479 | CLA  | CAA-C2A-C1A | -3.08 | 101.88      | 111.97   |
| 30  | F     | 224 | SQD  | C45-O47-C7  | 3.08  | 125.16      | 117.80   |
| 21  | B     | 518 | CLA  | C11-C10-C8  | 3.08  | 126.19      | 115.97   |
| 21  | B     | 514 | CLA  | O2D-CGD-CBD | 3.08  | 116.61      | 111.23   |
| 28  | A     | 375 | DGD  | C3B-C2B-C1B | 3.07  | 124.96      | 113.69   |
| 21  | C     | 482 | CLA  | O2D-CGD-CBD | 3.07  | 116.60      | 111.23   |
| 25  | B     | 529 | BCR  | C1-C6-C5    | -3.06 | 118.45      | 122.64   |
| 30  | D     | 361 | SQD  | C45-O47-C7  | 3.06  | 125.11      | 117.80   |
| 27  | B     | 531 | LMG  | C21-C20-C19 | 3.05  | 129.81      | 114.37   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | B     | 523 | CLA  | C3A-C2A-C1A | 3.05  | 105.91      | 101.34   |
| 27  | C     | 494 | LMG  | C31-C30-C29 | -3.05 | 101.93      | 113.13   |
| 28  | C     | 474 | DGD  | O1A-C1A-C2A | -3.05 | 111.86      | 123.78   |
| 21  | C     | 485 | CLA  | CED-O2D-CGD | 3.05  | 122.83      | 115.92   |
| 25  | B     | 529 | BCR  | C21-C20-C19 | 3.05  | 132.02      | 123.20   |
| 21  | B     | 512 | CLA  | C3A-C2A-C1A | 3.04  | 105.90      | 101.34   |
| 21  | B     | 511 | CLA  | C4B-C3B-C2B | -3.03 | 103.53      | 107.30   |
| 32  | D     | 357 | PL9  | C35-C34-C33 | -3.03 | 115.84      | 123.63   |
| 21  | B     | 516 | CLA  | CAA-CBA-CGA | -3.02 | 104.62      | 113.21   |
| 21  | C     | 484 | CLA  | C2A-C3A-C4A | 3.02  | 106.75      | 101.87   |
| 29  | I     | 274 | LMT  | O1B-C4'-C3' | 3.02  | 114.92      | 107.23   |
| 21  | B     | 523 | CLA  | C4D-CHA-C1A | 3.02  | 124.84      | 121.24   |
| 27  | I     | 220 | LMG  | O8-C9-C8    | 3.02  | 117.09      | 108.40   |
| 21  | B     | 522 | CLA  | C2A-C3A-C4A | 3.01  | 106.73      | 101.87   |
| 28  | C     | 493 | DGD  | O3G-C3G-C2G | 3.01  | 118.14      | 110.82   |
| 29  | D     | 536 | LMT  | C1-O1'-C1'  | 3.01  | 118.82      | 113.68   |
| 33  | V     | 164 | HEM  | CBC-CAC-C3C | -3.00 | 112.52      | 127.53   |
| 21  | A     | 363 | CLA  | C2A-C1A-CHA | 3.00  | 129.07      | 123.87   |
| 25  | D     | 358 | BCR  | C37-C22-C23 | 3.00  | 122.67      | 118.09   |
| 21  | C     | 477 | CLA  | CED-O2D-CGD | 3.00  | 122.71      | 115.92   |
| 28  | C     | 491 | DGD  | O6E-C1E-O5D | 3.00  | 117.12      | 110.04   |
| 30  | C     | 475 | SQD  | C32-C31-C30 | 3.00  | 129.51      | 114.37   |
| 25  | Z     | 116 | BCR  | C32-C1-C6   | 2.99  | 114.93      | 110.24   |
| 21  | B     | 523 | CLA  | C2A-C1A-CHA | 2.99  | 129.05      | 123.87   |
| 30  | L     | 213 | SQD  | C31-C30-C29 | 2.98  | 133.51      | 113.36   |
| 21  | C     | 477 | CLA  | CAA-CBA-CGA | -2.98 | 104.75      | 113.21   |
| 25  | C     | 489 | BCR  | C23-C22-C21 | -2.98 | 114.33      | 119.01   |
| 28  | C     | 491 | DGD  | C1D-O6D-C5D | -2.98 | 107.91      | 113.72   |
| 21  | C     | 486 | CLA  | CED-O2D-CGD | 2.97  | 122.64      | 115.92   |
| 28  | C     | 493 | DGD  | C3B-C2B-C1B | 2.97  | 124.56      | 113.69   |
| 28  | C     | 493 | DGD  | O3D-C3D-C2D | 2.96  | 117.35      | 110.38   |
| 21  | B     | 523 | CLA  | C2A-C3A-C4A | 2.96  | 106.64      | 101.87   |
| 32  | D     | 357 | PL9  | C15-C14-C13 | -2.95 | 116.04      | 123.63   |
| 25  | C     | 490 | BCR  | C20-C21-C22 | 2.95  | 131.42      | 127.28   |
| 30  | F     | 224 | SQD  | C3-C4-C5    | -2.95 | 104.88      | 110.23   |
| 25  | C     | 489 | BCR  | C37-C22-C23 | 2.95  | 122.59      | 118.09   |
| 27  | J     | 492 | LMG  | C9-C8-C7    | -2.94 | 104.93      | 111.78   |
| 21  | B     | 519 | CLA  | CED-O2D-CGD | 2.93  | 122.56      | 115.92   |
| 29  | I     | 274 | LMT  | O1'-C1-C2   | -2.93 | 99.42       | 109.37   |
| 25  | B     | 529 | BCR  | C30-C25-C26 | -2.92 | 118.64      | 122.64   |
| 21  | B     | 519 | CLA  | CAA-C2A-C1A | -2.92 | 102.40      | 111.97   |
| 21  | B     | 521 | CLA  | C4B-C3B-C2B | -2.92 | 103.67      | 107.30   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | C     | 478 | CLA  | CAA-C2A-C1A | -2.91 | 102.42      | 111.97   |
| 25  | J     | 112 | BCR  | C8-C7-C6    | 2.91  | 134.78      | 127.00   |
| 21  | C     | 480 | CLA  | C2A-C3A-C4A | 2.91  | 106.57      | 101.87   |
| 25  | C     | 490 | BCR  | C15-C14-C13 | 2.91  | 131.36      | 127.28   |
| 21  | B     | 523 | CLA  | C1-C2-C3    | 2.91  | 130.96      | 126.20   |
| 21  | B     | 513 | CLA  | C4B-C3B-C2B | -2.91 | 103.69      | 107.30   |
| 25  | C     | 489 | BCR  | C33-C5-C4   | -2.90 | 107.40      | 113.60   |
| 21  | B     | 518 | CLA  | C3D-C4D-ND  | 2.90  | 114.70      | 109.99   |
| 21  | C     | 485 | CLA  | O2D-CGD-CBD | 2.90  | 116.30      | 111.23   |
| 32  | D     | 357 | PL9  | O1-C4-C3    | -2.90 | 117.67      | 120.73   |
| 21  | B     | 515 | CLA  | C3D-C4D-ND  | 2.90  | 114.70      | 109.99   |
| 22  | D     | 355 | PHO  | OBD-CAD-C3D | 2.90  | 132.41      | 127.89   |
| 25  | B     | 527 | BCR  | C19-C18-C17 | -2.90 | 114.45      | 119.01   |
| 21  | B     | 521 | CLA  | CAA-CBA-CGA | -2.89 | 104.99      | 113.21   |
| 27  | J     | 492 | LMG  | O8-C9-C8    | 2.89  | 116.73      | 108.40   |
| 25  | D     | 358 | BCR  | C20-C21-C22 | 2.89  | 131.33      | 127.28   |
| 25  | C     | 490 | BCR  | C35-C13-C12 | 2.89  | 122.50      | 118.09   |
| 21  | C     | 488 | CLA  | O2D-CGD-CBD | 2.89  | 116.28      | 111.23   |
| 29  | D     | 363 | LMT  | O1'-C1-C2   | -2.89 | 99.57       | 109.37   |
| 25  | B     | 527 | BCR  | C11-C10-C9  | 2.88  | 131.32      | 127.28   |
| 21  | B     | 522 | CLA  | O2D-CGD-CBD | 2.88  | 116.26      | 111.23   |
| 25  | C     | 490 | BCR  | C30-C25-C24 | 2.88  | 123.46      | 115.65   |
| 27  | C     | 494 | LMG  | C7-O1-C1    | 2.88  | 119.97      | 113.80   |
| 28  | C     | 491 | DGD  | O3G-C3G-C2G | 2.88  | 117.81      | 110.82   |
| 21  | B     | 524 | CLA  | C3A-C2A-C1A | 2.87  | 105.64      | 101.34   |
| 29  | A     | 376 | LMT  | C7-C6-C5    | -2.87 | 99.88       | 114.37   |
| 28  | C     | 474 | DGD  | C4A-C3A-C2A | 2.87  | 123.66      | 113.13   |
| 28  | C     | 493 | DGD  | C1G-O1G-C1A | 2.86  | 127.59      | 117.12   |
| 33  | V     | 164 | HEM  | C3D-C4D-ND  | 2.86  | 113.31      | 110.17   |
| 28  | C     | 492 | DGD  | CBA-CAA-C9A | -2.86 | 99.90       | 114.37   |
| 33  | F     | 85  | HEM  | CAB-C3B-C4B | 2.86  | 137.03      | 124.39   |
| 22  | A     | 365 | PHO  | CMA-C3A-C4A | -2.86 | 108.46      | 114.61   |
| 25  | B     | 529 | BCR  | C24-C23-C22 | 2.85  | 130.46      | 126.23   |
| 21  | B     | 525 | CLA  | C1-C2-C3    | 2.85  | 130.87      | 126.20   |
| 21  | B     | 517 | CLA  | CAA-C2A-C1A | -2.85 | 102.65      | 111.97   |
| 32  | D     | 357 | PL9  | C10-C9-C11  | -2.84 | 110.29      | 115.23   |
| 21  | B     | 521 | CLA  | C2A-C1A-CHA | 2.84  | 128.80      | 123.87   |
| 21  | B     | 521 | CLA  | CED-O2D-CGD | 2.84  | 122.36      | 115.92   |
| 28  | C     | 493 | DGD  | C8B-C7B-C6B | -2.84 | 100.02      | 114.37   |
| 21  | C     | 484 | CLA  | C3D-C4D-ND  | 2.84  | 114.60      | 109.99   |
| 30  | D     | 361 | SQD  | O47-C7-C8   | 2.84  | 117.62      | 111.48   |
| 30  | D     | 361 | SQD  | C31-C30-C29 | 2.84  | 132.52      | 113.36   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | A     | 364 | CLA  | C1-C2-C3    | 2.82  | 130.82      | 126.20   |
| 33  | F     | 85  | HEM  | CAB-C3B-C2B | -2.82 | 119.26      | 128.43   |
| 21  | B     | 521 | CLA  | C3D-C4D-ND  | 2.82  | 114.57      | 109.99   |
| 21  | C     | 488 | CLA  | C2A-C3A-C4A | 2.82  | 106.42      | 101.87   |
| 21  | B     | 526 | CLA  | CED-O2D-CGD | 2.82  | 122.31      | 115.92   |
| 28  | D     | 362 | DGD  | O2G-C2G-C1G | 2.81  | 118.44      | 108.34   |
| 21  | A     | 363 | CLA  | C3D-C4D-ND  | 2.81  | 114.56      | 109.99   |
| 21  | B     | 520 | CLA  | C2A-C1A-CHA | 2.81  | 128.74      | 123.87   |
| 25  | B     | 529 | BCR  | C11-C10-C9  | 2.81  | 131.21      | 127.28   |
| 25  | A     | 369 | BCR  | C37-C22-C23 | 2.80  | 122.37      | 118.09   |
| 25  | J     | 112 | BCR  | C32-C1-C2   | -2.80 | 98.19       | 108.95   |
| 22  | D     | 355 | PHO  | C4D-ND-C1D  | -2.80 | 105.52      | 108.87   |
| 28  | B     | 533 | DGD  | O1G-C1A-O1A | -2.79 | 116.65      | 123.63   |
| 21  | B     | 514 | CLA  | C3A-C2A-C1A | 2.78  | 105.50      | 101.34   |
| 33  | V     | 164 | HEM  | CAB-C3B-C4B | 2.78  | 136.67      | 124.39   |
| 21  | B     | 513 | CLA  | CHB-C4A-NA  | 2.78  | 128.41      | 124.40   |
| 30  | L     | 213 | SQD  | C3-C4-C5    | -2.78 | 105.20      | 110.23   |
| 21  | C     | 478 | CLA  | O1D-CGD-CBD | -2.78 | 119.04      | 124.52   |
| 28  | A     | 375 | DGD  | O3G-C3G-C2G | -2.78 | 104.07      | 110.82   |
| 29  | O     | 274 | LMT  | C4-C3-C2    | -2.78 | 100.34      | 114.37   |
| 21  | A     | 363 | CLA  | C4B-C3B-C2B | -2.77 | 103.85      | 107.30   |
| 25  | C     | 490 | BCR  | C37-C22-C23 | 2.77  | 122.32      | 118.09   |
| 25  | C     | 490 | BCR  | C40-C30-C29 | -2.77 | 98.31       | 108.95   |
| 25  | J     | 112 | BCR  | C35-C13-C12 | 2.77  | 122.32      | 118.09   |
| 28  | C     | 493 | DGD  | C8A-C7A-C6A | -2.77 | 100.37      | 114.37   |
| 21  | B     | 511 | CLA  | C1-C2-C3    | 2.77  | 130.73      | 126.20   |
| 25  | C     | 489 | BCR  | C1-C6-C7    | 2.77  | 123.15      | 115.65   |
| 30  | L     | 213 | SQD  | O9-S-C6     | -2.77 | 102.63      | 106.76   |
| 33  | V     | 164 | HEM  | CAA-C2A-C1A | -2.76 | 119.55      | 124.94   |
| 21  | B     | 512 | CLA  | C4B-C3B-C2B | -2.76 | 103.87      | 107.30   |
| 32  | D     | 357 | PL9  | C2-C1-C6    | 2.76  | 122.27      | 119.00   |
| 25  | D     | 358 | BCR  | C23-C22-C21 | -2.75 | 114.68      | 119.01   |
| 29  | I     | 274 | LMT  | C4-C3-C2    | -2.75 | 100.44      | 114.37   |
| 21  | C     | 478 | CLA  | C2A-C1A-CHA | 2.75  | 128.65      | 123.87   |
| 21  | A     | 366 | CLA  | C4B-C3B-C2B | -2.75 | 103.88      | 107.30   |
| 25  | J     | 115 | BCR  | C21-C20-C19 | 2.75  | 131.17      | 123.20   |
| 27  | J     | 492 | LMG  | O7-C8-C9    | 2.75  | 118.21      | 108.34   |
| 21  | B     | 517 | CLA  | O2A-CGA-CBA | 2.75  | 120.22      | 111.83   |
| 21  | B     | 511 | CLA  | C2A-C1A-CHA | 2.75  | 128.64      | 123.87   |
| 21  | C     | 488 | CLA  | CED-O2D-CGD | 2.75  | 122.15      | 115.92   |
| 21  | C     | 478 | CLA  | C3D-C4D-ND  | 2.75  | 114.45      | 109.99   |
| 25  | J     | 112 | BCR  | C34-C9-C8   | 2.75  | 122.28      | 118.09   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | C     | 478 | CLA  | C4B-C3B-C2B | -2.75 | 103.89      | 107.30   |
| 21  | B     | 524 | CLA  | C3D-C4D-ND  | 2.74  | 114.45      | 109.99   |
| 21  | C     | 478 | CLA  | CED-O2D-CGD | 2.74  | 122.13      | 115.92   |
| 21  | B     | 515 | CLA  | CED-O2D-CGD | 2.74  | 122.12      | 115.92   |
| 21  | B     | 521 | CLA  | C5-C3-C2    | 2.73  | 127.30      | 121.17   |
| 21  | B     | 513 | CLA  | CAA-C2A-C3A | -2.73 | 105.61      | 113.00   |
| 27  | D     | 359 | LMG  | C38-C37-C36 | 2.73  | 128.16      | 114.37   |
| 21  | B     | 516 | CLA  | CAA-C2A-C3A | -2.73 | 105.63      | 113.00   |
| 29  | D     | 536 | LMT  | O1'-C1'-C2' | -2.72 | 104.14      | 108.27   |
| 21  | C     | 479 | CLA  | C3A-C2A-C1A | 2.72  | 105.41      | 101.34   |
| 29  | I     | 274 | LMT  | C1-O1'-C1'  | 2.71  | 118.32      | 113.68   |
| 30  | L     | 213 | SQD  | C15-C14-C13 | 2.71  | 128.09      | 114.37   |
| 25  | B     | 527 | BCR  | C36-C18-C19 | 2.71  | 122.23      | 118.09   |
| 27  | D     | 359 | LMG  | C17-C16-C15 | -2.71 | 100.66      | 114.37   |
| 21  | C     | 480 | CLA  | C3D-C4D-ND  | 2.71  | 114.39      | 109.99   |
| 21  | A     | 364 | CLA  | CED-O2D-CGD | 2.71  | 122.07      | 115.92   |
| 21  | B     | 511 | CLA  | CED-O2D-CGD | 2.71  | 122.06      | 115.92   |
| 28  | C     | 492 | DGD  | O2G-C2G-C3G | 2.70  | 118.04      | 108.34   |
| 22  | D     | 355 | PHO  | O1D-CGD-CBD | -2.70 | 120.62      | 124.72   |
| 21  | B     | 519 | CLA  | C4B-C3B-C2B | -2.70 | 103.95      | 107.30   |
| 21  | B     | 517 | CLA  | C3D-C4D-ND  | 2.69  | 114.36      | 109.99   |
| 21  | B     | 523 | CLA  | CED-O2D-CGD | 2.69  | 122.02      | 115.92   |
| 21  | A     | 362 | CLA  | C2A-C1A-CHA | 2.69  | 128.53      | 123.87   |
| 21  | B     | 517 | CLA  | CBA-CAA-C2A | 2.69  | 121.79      | 113.79   |
| 28  | B     | 533 | DGD  | C6D-C5D-C4D | -2.69 | 106.42      | 112.07   |
| 21  | B     | 514 | CLA  | C3D-C4D-ND  | 2.69  | 114.36      | 109.99   |
| 21  | B     | 519 | CLA  | C3D-C4D-ND  | 2.69  | 114.36      | 109.99   |
| 29  | A     | 376 | LMT  | C4-C3-C2    | -2.69 | 100.79      | 114.37   |
| 22  | D     | 355 | PHO  | CMA-C3A-C4A | -2.68 | 108.83      | 114.61   |
| 21  | C     | 481 | CLA  | C3D-C4D-ND  | 2.68  | 114.35      | 109.99   |
| 25  | D     | 358 | BCR  | C35-C13-C12 | 2.68  | 122.19      | 118.09   |
| 21  | C     | 479 | CLA  | C4B-C3B-C2B | -2.68 | 103.97      | 107.30   |
| 21  | A     | 362 | CLA  | CED-O2D-CGD | 2.67  | 121.97      | 115.92   |
| 29  | O     | 274 | LMT  | O1'-C1'-C2' | -2.67 | 104.22      | 108.27   |
| 30  | C     | 475 | SQD  | O8-S-O9     | -2.67 | 104.72      | 111.40   |
| 21  | C     | 483 | CLA  | CED-O2D-CGD | 2.67  | 121.96      | 115.92   |
| 21  | C     | 487 | CLA  | CHA-C1A-NA  | -2.66 | 120.36      | 126.39   |
| 25  | C     | 490 | BCR  | C23-C24-C25 | 2.66  | 134.09      | 127.00   |
| 29  | I     | 274 | LMT  | C7-C6-C5    | -2.66 | 100.94      | 114.37   |
| 28  | C     | 493 | DGD  | O6E-C1E-C2E | 2.65  | 115.83      | 110.37   |
| 21  | C     | 477 | CLA  | CBA-CAA-C2A | 2.65  | 121.68      | 113.79   |
| 21  | D     | 356 | CLA  | CAA-C2A-C1A | -2.65 | 103.29      | 111.97   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | C     | 489 | BCR  | C40-C30-C25 | 2.65  | 114.40      | 110.24   |
| 21  | C     | 485 | CLA  | C1-C2-C3    | 2.65  | 130.54      | 126.20   |
| 21  | B     | 522 | CLA  | O1D-CGD-CBD | -2.65 | 119.29      | 124.52   |
| 21  | C     | 479 | CLA  | C3D-C4D-ND  | 2.65  | 114.29      | 109.99   |
| 21  | D     | 356 | CLA  | C4B-C3B-C2B | -2.64 | 104.01      | 107.30   |
| 21  | B     | 522 | CLA  | C1-C2-C3    | 2.64  | 130.52      | 126.20   |
| 21  | B     | 520 | CLA  | O1D-CGD-CBD | -2.64 | 119.31      | 124.52   |
| 27  | B     | 531 | LMG  | C14-C13-C12 | 2.64  | 127.69      | 114.37   |
| 29  | D     | 536 | LMT  | C7-C6-C5    | -2.63 | 101.07      | 114.37   |
| 21  | C     | 486 | CLA  | O2D-CGD-CBD | 2.63  | 115.82      | 111.23   |
| 27  | C     | 494 | LMG  | C9-C8-C7    | 2.61  | 117.88      | 111.78   |
| 25  | B     | 529 | BCR  | C16-C17-C18 | 2.61  | 130.94      | 127.28   |
| 26  | A     | 371 | LHG  | O7-C7-C8    | 2.61  | 117.12      | 111.48   |
| 27  | I     | 220 | LMG  | C19-C18-C17 | -2.60 | 101.21      | 114.37   |
| 21  | D     | 354 | CLA  | C4B-C3B-C2B | -2.60 | 104.07      | 107.30   |
| 21  | A     | 362 | CLA  | C3D-C4D-ND  | 2.60  | 114.22      | 109.99   |
| 28  | C     | 492 | DGD  | O6E-C1E-C2E | 2.60  | 115.71      | 110.37   |
| 25  | B     | 527 | BCR  | C24-C23-C22 | 2.60  | 130.08      | 126.23   |
| 27  | J     | 492 | LMG  | C39-C38-C37 | 2.59  | 127.48      | 114.37   |
| 28  | B     | 533 | DGD  | C4A-C3A-C2A | 2.59  | 122.66      | 113.13   |
| 27  | D     | 359 | LMG  | O7-C8-C9    | -2.59 | 99.04       | 108.34   |
| 21  | D     | 356 | CLA  | C1-C2-C3    | 2.59  | 130.44      | 126.20   |
| 21  | C     | 481 | CLA  | C4B-C3B-C2B | -2.59 | 104.08      | 107.30   |
| 21  | B     | 513 | CLA  | CED-O2D-CGD | 2.58  | 121.77      | 115.92   |
| 21  | B     | 518 | CLA  | C4B-C3B-C2B | -2.58 | 104.09      | 107.30   |
| 28  | B     | 533 | DGD  | O2G-C1B-O1B | -2.58 | 117.68      | 123.70   |
| 27  | D     | 360 | LMG  | O8-C28-C29  | 2.57  | 119.69      | 111.83   |
| 21  | B     | 518 | CLA  | C2A-C1A-CHA | 2.57  | 128.34      | 123.87   |
| 28  | D     | 362 | DGD  | O6E-C1E-O5D | 2.57  | 116.13      | 110.04   |
| 25  | Z     | 116 | BCR  | C15-C14-C13 | 2.57  | 130.88      | 127.28   |
| 21  | C     | 488 | CLA  | CAA-C2A-C1A | -2.57 | 103.55      | 111.97   |
| 21  | A     | 362 | CLA  | C4B-C3B-C2B | -2.57 | 104.11      | 107.30   |
| 27  | A     | 373 | LMG  | O8-C28-C29  | 2.57  | 119.67      | 111.83   |
| 21  | C     | 477 | CLA  | C4B-C3B-C2B | -2.57 | 104.11      | 107.30   |
| 21  | B     | 517 | CLA  | C4B-C3B-C2B | -2.56 | 104.11      | 107.30   |
| 25  | B     | 529 | BCR  | C40-C30-C25 | 2.56  | 114.26      | 110.24   |
| 33  | F     | 85  | HEM  | CAA-CBA-CGA | 2.56  | 120.45      | 113.67   |
| 21  | C     | 486 | CLA  | C2A-C1A-CHA | 2.56  | 128.31      | 123.87   |
| 21  | B     | 522 | CLA  | C3D-C4D-ND  | 2.56  | 114.14      | 109.99   |
| 29  | A     | 376 | LMT  | C1B-O1B-C4' | -2.56 | 111.92      | 117.98   |
| 30  | C     | 475 | SQD  | C15-C14-C13 | 2.56  | 127.29      | 114.37   |
| 21  | B     | 521 | CLA  | C6-C5-C3    | 2.55  | 119.69      | 113.47   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 28  | B     | 528 | DGD  | O1G-C1A-C2A | 2.55  | 119.62      | 111.83   |
| 28  | C     | 474 | DGD  | C4D-C3D-C2D | 2.55  | 115.31      | 110.83   |
| 25  | Z     | 116 | BCR  | C19-C18-C17 | -2.55 | 115.00      | 119.01   |
| 21  | C     | 482 | CLA  | CAA-C2A-C1A | -2.55 | 103.62      | 111.97   |
| 28  | C     | 491 | DGD  | O2G-C2G-C3G | 2.55  | 117.48      | 108.34   |
| 21  | C     | 485 | CLA  | C4B-C3B-C2B | -2.55 | 104.14      | 107.30   |
| 25  | D     | 358 | BCR  | C16-C17-C18 | 2.54  | 130.84      | 127.28   |
| 29  | D     | 363 | LMT  | O1'-C1'-C2' | -2.54 | 104.42      | 108.27   |
| 21  | B     | 518 | CLA  | C5-C3-C2    | 2.53  | 126.86      | 121.17   |
| 25  | A     | 369 | BCR  | C7-C8-C9    | 2.53  | 129.98      | 126.23   |
| 21  | B     | 513 | CLA  | O1D-CGD-CBD | -2.53 | 119.53      | 124.52   |
| 27  | C     | 494 | LMG  | C6-C5-C4    | -2.53 | 106.81      | 113.02   |
| 27  | M     | 217 | LMG  | O7-C10-O9   | -2.53 | 117.79      | 123.70   |
| 28  | C     | 493 | DGD  | CBA-CAA-C9A | -2.53 | 101.60      | 114.37   |
| 25  | A     | 369 | BCR  | C30-C25-C24 | 2.52  | 122.50      | 115.65   |
| 21  | B     | 512 | CLA  | C3D-C4D-ND  | 2.52  | 114.09      | 109.99   |
| 27  | J     | 492 | LMG  | C34-C33-C32 | -2.52 | 101.63      | 114.37   |
| 25  | B     | 530 | BCR  | C30-C25-C24 | 2.52  | 122.48      | 115.65   |
| 21  | C     | 483 | CLA  | O1D-CGD-CBD | -2.52 | 119.55      | 124.52   |
| 21  | B     | 520 | CLA  | C3D-C4D-ND  | 2.52  | 114.08      | 109.99   |
| 28  | C     | 491 | DGD  | O6D-C1D-O3G | 2.51  | 115.99      | 110.04   |
| 21  | B     | 523 | CLA  | C3D-C4D-ND  | 2.51  | 114.07      | 109.99   |
| 25  | B     | 530 | BCR  | C35-C13-C12 | 2.51  | 121.92      | 118.09   |
| 30  | C     | 475 | SQD  | C45-O47-C7  | 2.51  | 123.80      | 117.80   |
| 32  | D     | 357 | PL9  | C25-C24-C23 | -2.51 | 117.19      | 123.63   |
| 21  | C     | 484 | CLA  | C4B-C3B-C2B | -2.51 | 104.19      | 107.30   |
| 33  | F     | 85  | HEM  | C3D-C4D-ND  | 2.50  | 112.92      | 110.17   |
| 21  | C     | 481 | CLA  | C1D-ND-C4D  | -2.50 | 104.56      | 106.31   |
| 21  | D     | 354 | CLA  | C3A-C2A-C1A | 2.50  | 105.09      | 101.34   |
| 21  | A     | 363 | CLA  | O1D-CGD-CBD | -2.50 | 119.58      | 124.52   |
| 21  | B     | 514 | CLA  | C4B-C3B-C2B | -2.50 | 104.19      | 107.30   |
| 25  | A     | 369 | BCR  | C2-C1-C6    | 2.49  | 114.06      | 110.44   |
| 25  | J     | 112 | BCR  | C40-C30-C25 | 2.49  | 114.16      | 110.24   |
| 21  | A     | 364 | CLA  | C4B-C3B-C2B | -2.49 | 104.20      | 107.30   |
| 28  | A     | 375 | DGD  | O1G-C1A-C2A | 2.49  | 119.43      | 111.83   |
| 21  | C     | 477 | CLA  | C3D-C4D-ND  | 2.49  | 114.03      | 109.99   |
| 33  | V     | 164 | HEM  | C4B-C3B-C2B | -2.49 | 104.99      | 107.28   |
| 21  | A     | 364 | CLA  | CAA-C2A-C1A | -2.49 | 103.83      | 111.97   |
| 32  | D     | 357 | PL9  | C40-C39-C41 | 2.49  | 119.54      | 115.23   |
| 29  | D     | 536 | LMT  | O1B-C1B-C2B | 2.49  | 114.20      | 108.09   |
| 30  | F     | 224 | SQD  | C32-C31-C30 | 2.48  | 130.13      | 113.36   |
| 21  | D     | 354 | CLA  | CED-O2D-CGD | 2.48  | 121.53      | 115.92   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | B     | 526 | CLA  | C4B-C3B-C2B | -2.47 | 104.23      | 107.30   |
| 22  | A     | 365 | PHO  | C2B-C1B-NB  | 2.47  | 111.22      | 109.43   |
| 27  | J     | 492 | LMG  | C13-C12-C11 | 2.47  | 122.20      | 113.13   |
| 25  | B     | 530 | BCR  | C37-C22-C23 | 2.47  | 121.86      | 118.09   |
| 21  | C     | 485 | CLA  | C3D-C4D-ND  | 2.46  | 113.99      | 109.99   |
| 21  | B     | 517 | CLA  | C11-C12-C13 | 2.46  | 124.15      | 115.97   |
| 21  | C     | 480 | CLA  | C2A-C1A-CHA | 2.46  | 128.14      | 123.87   |
| 25  | A     | 369 | BCR  | C35-C13-C12 | 2.46  | 121.85      | 118.09   |
| 25  | B     | 530 | BCR  | C34-C9-C8   | 2.46  | 121.85      | 118.09   |
| 27  | M     | 217 | LMG  | C12-C11-C10 | -2.46 | 104.68      | 113.69   |
| 21  | D     | 356 | CLA  | C3D-C4D-ND  | 2.46  | 113.98      | 109.99   |
| 33  | F     | 85  | HEM  | C3B-C4B-NB  | -2.45 | 107.70      | 109.47   |
| 22  | A     | 365 | PHO  | CED-O2D-CGD | 2.45  | 121.48      | 115.92   |
| 21  | B     | 516 | CLA  | C12-C11-C10 | -2.45 | 102.30      | 113.28   |
| 21  | B     | 511 | CLA  | C3A-C2A-C1A | 2.45  | 105.00      | 101.34   |
| 28  | A     | 375 | DGD  | C1D-O6D-C5D | -2.45 | 108.94      | 113.72   |
| 30  | L     | 213 | SQD  | C45-O47-C7  | 2.44  | 123.65      | 117.80   |
| 25  | X     | 107 | BCR  | C37-C22-C23 | 2.44  | 121.82      | 118.09   |
| 21  | C     | 482 | CLA  | C3D-C4D-ND  | 2.43  | 113.94      | 109.99   |
| 29  | A     | 376 | LMT  | O1'-C1'-C2' | -2.43 | 104.58      | 108.27   |
| 25  | B     | 530 | BCR  | C3-C4-C5    | 2.43  | 118.39      | 114.06   |
| 27  | C     | 494 | LMG  | O8-C9-C8    | -2.43 | 101.40      | 108.40   |
| 21  | K     | 483 | CLA  | CED-O2D-CGD | 2.43  | 121.42      | 115.92   |
| 29  | T     | 226 | LMT  | C1-O1'-C1'  | -2.42 | 109.54      | 113.68   |
| 28  | C     | 493 | DGD  | O6E-C5E-C4E | 2.42  | 114.07      | 109.70   |
| 25  | C     | 490 | BCR  | C32-C1-C6   | 2.42  | 114.04      | 110.24   |
| 30  | F     | 224 | SQD  | C15-C14-C13 | 2.42  | 126.60      | 114.37   |
| 21  | C     | 486 | CLA  | C2C-C1C-NC  | -2.42 | 107.44      | 109.98   |
| 25  | B     | 527 | BCR  | C32-C1-C6   | 2.42  | 114.03      | 110.24   |
| 32  | D     | 357 | PL9  | C3-C2-C1    | -2.41 | 118.52      | 122.59   |
| 25  | Z     | 116 | BCR  | C35-C13-C12 | 2.41  | 121.78      | 118.09   |
| 21  | B     | 514 | CLA  | C2A-C1A-CHA | 2.41  | 128.06      | 123.87   |
| 21  | D     | 354 | CLA  | C2A-C1A-CHA | 2.41  | 128.06      | 123.87   |
| 21  | K     | 483 | CLA  | O1D-CGD-CBD | -2.41 | 119.76      | 124.52   |
| 25  | J     | 115 | BCR  | C40-C30-C25 | 2.41  | 114.03      | 110.24   |
| 21  | D     | 356 | CLA  | O1D-CGD-CBD | -2.41 | 119.77      | 124.52   |
| 21  | C     | 485 | CLA  | O1D-CGD-CBD | -2.41 | 119.77      | 124.52   |
| 25  | B     | 530 | BCR  | C16-C17-C18 | 2.40  | 130.64      | 127.28   |
| 21  | B     | 512 | CLA  | C2A-C1A-CHA | 2.40  | 128.03      | 123.87   |
| 28  | C     | 474 | DGD  | O1B-C1B-C2B | -2.39 | 114.42      | 123.78   |
| 28  | C     | 491 | DGD  | C3A-C2A-C1A | 2.39  | 122.47      | 113.69   |
| 26  | A     | 371 | LHG  | O8-C6-C5    | 2.39  | 115.29      | 108.40   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 33  | V     | 164 | HEM  | C4C-NC-C1C  | 2.39  | 109.72      | 105.82   |
| 32  | D     | 357 | PL9  | C26-C27-C28 | 2.39  | 123.82      | 112.02   |
| 30  | L     | 213 | SQD  | C17-C16-C15 | 2.38  | 126.41      | 114.37   |
| 28  | C     | 493 | DGD  | CFB-CEB-CDB | -2.38 | 102.33      | 114.37   |
| 25  | J     | 112 | BCR  | C37-C22-C23 | 2.38  | 121.73      | 118.09   |
| 25  | B     | 530 | BCR  | C40-C30-C25 | 2.38  | 113.98      | 110.24   |
| 21  | C     | 478 | CLA  | C1-C2-C3    | 2.38  | 130.09      | 126.20   |
| 33  | V     | 164 | HEM  | C4D-C3D-C2D | -2.37 | 103.44      | 106.89   |
| 21  | A     | 364 | CLA  | C3D-C4D-ND  | 2.37  | 113.84      | 109.99   |
| 21  | C     | 483 | CLA  | C4B-C3B-C2B | -2.37 | 104.36      | 107.30   |
| 30  | L     | 213 | SQD  | O47-C7-C8   | 2.37  | 116.60      | 111.48   |
| 28  | B     | 533 | DGD  | O3G-C3G-C2G | -2.37 | 105.06      | 110.82   |
| 21  | C     | 481 | CLA  | C2C-C1C-NC  | -2.37 | 107.50      | 109.98   |
| 25  | B     | 527 | BCR  | C15-C14-C13 | 2.36  | 130.59      | 127.28   |
| 21  | B     | 516 | CLA  | CAA-C2A-C1A | -2.36 | 104.24      | 111.97   |
| 21  | C     | 480 | CLA  | O1D-CGD-CBD | -2.36 | 119.86      | 124.52   |
| 21  | B     | 525 | CLA  | C4B-C3B-C2B | -2.36 | 104.37      | 107.30   |
| 25  | Z     | 116 | BCR  | C36-C18-C19 | 2.36  | 121.69      | 118.09   |
| 25  | J     | 112 | BCR  | C16-C17-C18 | 2.36  | 130.59      | 127.28   |
| 27  | J     | 492 | LMG  | O7-C10-O9   | -2.36 | 118.19      | 123.70   |
| 21  | C     | 482 | CLA  | C2A-C1A-CHA | 2.36  | 127.96      | 123.87   |
| 21  | K     | 483 | CLA  | C3D-C4D-ND  | 2.36  | 113.82      | 109.99   |
| 28  | D     | 362 | DGD  | CBA-CAA-C9A | -2.35 | 102.47      | 114.37   |
| 21  | B     | 516 | CLA  | C4B-C3B-C2B | -2.35 | 104.38      | 107.30   |
| 25  | J     | 112 | BCR  | C12-C13-C14 | -2.35 | 115.31      | 119.01   |
| 21  | C     | 482 | CLA  | C4B-C3B-C2B | -2.35 | 104.38      | 107.30   |
| 21  | B     | 518 | CLA  | CED-O2D-CGD | 2.35  | 121.24      | 115.92   |
| 28  | A     | 375 | DGD  | C6E-C5E-C4E | -2.35 | 107.26      | 113.02   |
| 25  | J     | 115 | BCR  | C31-C1-C2   | 2.34  | 117.95      | 108.95   |
| 27  | C     | 494 | LMG  | C19-C18-C17 | -2.34 | 102.52      | 114.37   |
| 22  | D     | 355 | PHO  | CBC-CAC-C3C | -2.34 | 109.52      | 112.87   |
| 21  | B     | 513 | CLA  | C3D-C4D-ND  | 2.34  | 113.79      | 109.99   |
| 33  | V     | 164 | HEM  | C2A-C1A-NA  | 2.34  | 112.75      | 110.15   |
| 21  | C     | 487 | CLA  | C3A-C2A-C1A | 2.34  | 104.84      | 101.34   |
| 22  | A     | 365 | PHO  | OBD-CAD-C3D | 2.33  | 131.53      | 127.89   |
| 21  | B     | 520 | CLA  | C4B-C3B-C2B | -2.33 | 104.40      | 107.30   |
| 22  | D     | 355 | PHO  | OBD-CAD-CBD | -2.33 | 122.40      | 125.82   |
| 25  | D     | 358 | BCR  | C40-C30-C25 | 2.33  | 113.90      | 110.24   |
| 25  | B     | 527 | BCR  | C34-C9-C8   | 2.33  | 121.64      | 118.09   |
| 21  | A     | 362 | CLA  | C7-C6-C5    | -2.33 | 107.06      | 113.26   |
| 21  | D     | 354 | CLA  | CHB-C1B-NB  | 2.32  | 127.53      | 124.05   |
| 28  | A     | 375 | DGD  | C8B-C7B-C6B | -2.32 | 102.64      | 114.37   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | C     | 483 | CLA  | C3D-C4D-ND  | 2.32  | 113.75      | 109.99   |
| 25  | B     | 529 | BCR  | C32-C1-C6   | 2.31  | 113.87      | 110.24   |
| 25  | A     | 369 | BCR  | C32-C1-C6   | 2.31  | 113.87      | 110.24   |
| 21  | B     | 525 | CLA  | CED-O2D-CGD | 2.31  | 121.16      | 115.92   |
| 21  | C     | 487 | CLA  | C4B-C3B-C2B | -2.31 | 104.43      | 107.30   |
| 25  | X     | 107 | BCR  | C19-C18-C17 | -2.30 | 115.39      | 119.01   |
| 21  | K     | 483 | CLA  | C12-C11-C10 | -2.30 | 102.97      | 113.28   |
| 21  | C     | 482 | CLA  | C5-C3-C2    | 2.30  | 126.33      | 121.17   |
| 21  | D     | 356 | CLA  | CED-O2D-CGD | 2.30  | 121.13      | 115.92   |
| 21  | C     | 482 | CLA  | O1D-CGD-CBD | -2.30 | 119.99      | 124.52   |
| 25  | X     | 107 | BCR  | C1-C6-C7    | 2.29  | 121.88      | 115.65   |
| 28  | C     | 491 | DGD  | C4E-C3E-C2E | -2.29 | 106.81      | 110.83   |
| 25  | Z     | 116 | BCR  | C1-C6-C5    | -2.29 | 119.50      | 122.64   |
| 28  | D     | 362 | DGD  | C8A-C7A-C6A | -2.29 | 102.80      | 114.37   |
| 27  | B     | 531 | LMG  | O8-C28-C29  | 2.29  | 118.81      | 111.83   |
| 28  | D     | 362 | DGD  | O2G-C2G-C3G | -2.28 | 100.15      | 108.34   |
| 30  | C     | 475 | SQD  | C17-C16-C15 | 2.28  | 125.89      | 114.37   |
| 33  | V     | 164 | HEM  | CAA-C2A-C3A | 2.28  | 132.18      | 127.07   |
| 33  | F     | 85  | HEM  | CHD-C4C-NC  | 2.28  | 126.93      | 124.45   |
| 27  | J     | 492 | LMG  | O8-C28-C29  | 2.28  | 118.77      | 111.83   |
| 21  | B     | 524 | CLA  | CAA-CBA-CGA | -2.27 | 106.75      | 113.21   |
| 25  | B     | 530 | BCR  | C32-C1-C6   | 2.27  | 113.81      | 110.24   |
| 28  | C     | 491 | DGD  | O6E-C5E-C4E | 2.27  | 113.79      | 109.70   |
| 25  | B     | 529 | BCR  | C16-C15-C14 | 2.27  | 128.17      | 123.52   |
| 25  | Z     | 116 | BCR  | C1-C6-C7    | 2.27  | 121.81      | 115.65   |
| 21  | B     | 526 | CLA  | C3D-C4D-ND  | 2.27  | 113.68      | 109.99   |
| 26  | C     | 476 | LHG  | C6-C5-C4    | 2.27  | 117.08      | 111.78   |
| 28  | C     | 492 | DGD  | C7A-C6A-C5A | 2.27  | 125.83      | 114.37   |
| 25  | D     | 358 | BCR  | C12-C13-C14 | -2.27 | 115.44      | 119.01   |
| 21  | B     | 515 | CLA  | O1D-CGD-CBD | -2.26 | 120.05      | 124.52   |
| 21  | B     | 512 | CLA  | CED-O2D-CGD | 2.26  | 121.04      | 115.92   |
| 27  | M     | 217 | LMG  | C14-C13-C12 | -2.26 | 102.95      | 114.37   |
| 27  | I     | 220 | LMG  | C14-C13-C12 | 2.25  | 125.76      | 114.37   |
| 21  | B     | 511 | CLA  | O2D-CGD-O1D | -2.25 | 119.46      | 123.85   |
| 25  | A     | 369 | BCR  | C21-C20-C19 | 2.25  | 129.73      | 123.20   |
| 21  | C     | 488 | CLA  | CBA-CAA-C2A | 2.25  | 120.49      | 113.79   |
| 25  | A     | 369 | BCR  | C40-C30-C25 | 2.25  | 113.77      | 110.24   |
| 25  | B     | 530 | BCR  | C1-C6-C7    | 2.25  | 121.74      | 115.65   |
| 25  | C     | 489 | BCR  | C7-C8-C9    | 2.24  | 129.55      | 126.23   |
| 21  | C     | 488 | CLA  | C3D-C4D-ND  | 2.24  | 113.62      | 109.99   |
| 27  | D     | 359 | LMG  | C6-C5-C4    | -2.24 | 107.53      | 113.02   |
| 21  | B     | 511 | CLA  | O1D-CGD-CBD | -2.24 | 120.11      | 124.52   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | B     | 515 | CLA  | C4B-C3B-C2B | -2.23 | 104.52      | 107.30   |
| 21  | C     | 488 | CLA  | C2C-C1C-NC  | -2.23 | 107.64      | 109.98   |
| 21  | C     | 486 | CLA  | C3D-C4D-ND  | 2.23  | 113.62      | 109.99   |
| 28  | B     | 533 | DGD  | C7A-C6A-C5A | -2.23 | 103.10      | 114.37   |
| 25  | A     | 369 | BCR  | C23-C22-C21 | -2.23 | 115.50      | 119.01   |
| 27  | C     | 494 | LMG  | C17-C16-C15 | -2.23 | 103.11      | 114.37   |
| 21  | B     | 523 | CLA  | C4B-C3B-C2B | -2.23 | 104.53      | 107.30   |
| 32  | D     | 357 | PL9  | C53-C6-C1   | 2.22  | 119.84      | 115.28   |
| 25  | B     | 529 | BCR  | C7-C8-C9    | 2.22  | 129.52      | 126.23   |
| 25  | X     | 107 | BCR  | C36-C18-C19 | 2.22  | 121.48      | 118.09   |
| 21  | B     | 511 | CLA  | C3D-C4D-ND  | 2.22  | 113.60      | 109.99   |
| 25  | Z     | 116 | BCR  | C40-C30-C25 | 2.22  | 113.73      | 110.24   |
| 28  | C     | 474 | DGD  | O6E-C5E-C4E | 2.22  | 113.70      | 109.70   |
| 28  | C     | 493 | DGD  | C6A-C5A-C4A | -2.22 | 103.15      | 114.37   |
| 30  | F     | 224 | SQD  | C17-C16-C15 | 2.22  | 125.58      | 114.37   |
| 25  | A     | 369 | BCR  | C8-C7-C6    | 2.22  | 132.92      | 127.00   |
| 28  | B     | 533 | DGD  | C3G-C2G-C1G | -2.21 | 106.62      | 111.78   |
| 21  | B     | 516 | CLA  | C3D-C4D-ND  | 2.21  | 113.58      | 109.99   |
| 21  | B     | 519 | CLA  | O1D-CGD-CBD | -2.21 | 120.16      | 124.52   |
| 28  | A     | 375 | DGD  | O6E-C5E-C6E | 2.21  | 111.92      | 106.44   |
| 21  | C     | 488 | CLA  | C4B-C3B-C2B | -2.21 | 104.55      | 107.30   |
| 25  | J     | 112 | BCR  | C36-C18-C19 | 2.21  | 121.46      | 118.09   |
| 28  | B     | 533 | DGD  | C5B-C4B-C3B | -2.21 | 103.21      | 114.37   |
| 30  | D     | 361 | SQD  | C15-C14-C13 | 2.20  | 125.51      | 114.37   |
| 21  | B     | 517 | CLA  | C12-C11-C10 | -2.20 | 103.41      | 113.28   |
| 28  | C     | 493 | DGD  | CDB-CCB-CBB | -2.20 | 103.24      | 114.37   |
| 33  | F     | 85  | HEM  | C4C-NC-C1C  | 2.20  | 109.41      | 105.82   |
| 27  | C     | 494 | LMG  | O1-C1-C2    | -2.20 | 104.93      | 108.27   |
| 21  | B     | 524 | CLA  | C4B-C3B-C2B | -2.20 | 104.57      | 107.30   |
| 28  | A     | 375 | DGD  | C1G-O1G-C1A | 2.20  | 125.14      | 117.12   |
| 21  | C     | 479 | CLA  | C2A-C1A-CHA | 2.19  | 127.67      | 123.87   |
| 22  | D     | 355 | PHO  | C1-C2-C3    | 2.19  | 129.78      | 126.20   |
| 21  | A     | 364 | CLA  | CMD-C2D-C1D | 2.19  | 128.58      | 124.73   |
| 25  | J     | 112 | BCR  | C40-C30-C29 | -2.18 | 100.56      | 108.95   |
| 21  | B     | 524 | CLA  | C1D-ND-C4D  | -2.18 | 104.78      | 106.31   |
| 21  | B     | 521 | CLA  | CHD-C1D-ND  | -2.18 | 121.73      | 124.80   |
| 21  | C     | 484 | CLA  | C12-C11-C10 | -2.18 | 103.50      | 113.28   |
| 21  | C     | 481 | CLA  | CED-O2D-CGD | 2.18  | 120.86      | 115.92   |
| 25  | Z     | 116 | BCR  | C12-C13-C14 | -2.18 | 115.58      | 119.01   |
| 21  | A     | 366 | CLA  | C3D-C4D-ND  | 2.18  | 113.53      | 109.99   |
| 28  | C     | 491 | DGD  | C5A-C4A-C3A | 2.17  | 125.36      | 114.37   |
| 25  | C     | 489 | BCR  | C23-C24-C25 | 2.17  | 132.80      | 127.00   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 29  | D     | 363 | LMT  | C4-C3-C2    | -2.17 | 103.39      | 114.37   |
| 21  | D     | 354 | CLA  | O1D-CGD-CBD | -2.17 | 120.24      | 124.52   |
| 21  | C     | 486 | CLA  | C12-C11-C10 | -2.17 | 103.57      | 113.28   |
| 27  | D     | 360 | LMG  | C1-O6-C5    | -2.16 | 109.49      | 113.72   |
| 25  | B     | 530 | BCR  | C28-C27-C26 | 2.16  | 117.91      | 114.06   |
| 21  | B     | 511 | CLA  | CHA-C1A-NA  | -2.16 | 121.49      | 126.39   |
| 27  | C     | 494 | LMG  | C12-C11-C10 | 2.16  | 121.62      | 113.69   |
| 21  | B     | 517 | CLA  | O1D-CGD-CBD | -2.16 | 120.26      | 124.52   |
| 27  | A     | 373 | LMG  | C1-O6-C5    | -2.16 | 109.50      | 113.72   |
| 30  | F     | 224 | SQD  | O9-S-C6     | -2.16 | 103.53      | 106.76   |
| 29  | A     | 376 | LMT  | C9-C8-C7    | -2.16 | 103.46      | 114.37   |
| 33  | F     | 85  | HEM  | C2A-C1A-NA  | 2.16  | 112.55      | 110.15   |
| 21  | C     | 487 | CLA  | O1D-CGD-CBD | -2.16 | 120.26      | 124.52   |
| 28  | B     | 533 | DGD  | CDA-CCA-CBA | -2.16 | 103.47      | 114.37   |
| 21  | B     | 523 | CLA  | O1D-CGD-CBD | -2.15 | 120.27      | 124.52   |
| 28  | B     | 528 | DGD  | C1D-O6D-C5D | -2.15 | 109.51      | 113.72   |
| 25  | B     | 530 | BCR  | C12-C13-C14 | -2.15 | 115.62      | 119.01   |
| 29  | I     | 274 | LMT  | O1'-C1'-C2' | -2.15 | 105.01      | 108.27   |
| 21  | B     | 516 | CLA  | O2D-CGD-CBD | 2.15  | 114.99      | 111.23   |
| 21  | B     | 521 | CLA  | C4-C3-C5    | -2.15 | 111.50      | 115.23   |
| 28  | B     | 528 | DGD  | C1E-O6E-C5E | -2.15 | 109.52      | 113.72   |
| 27  | I     | 220 | LMG  | O6-C1-O1    | 2.15  | 115.12      | 110.04   |
| 21  | A     | 363 | CLA  | CHD-C4C-NC  | 2.15  | 127.56      | 124.23   |
| 21  | C     | 484 | CLA  | O1D-CGD-CBD | -2.15 | 120.29      | 124.52   |
| 30  | C     | 475 | SQD  | O47-C7-C8   | 2.14  | 116.12      | 111.48   |
| 28  | B     | 533 | DGD  | C3G-O3G-C1D | -2.14 | 109.20      | 113.80   |
| 27  | D     | 359 | LMG  | O7-C10-C11  | -2.14 | 106.85      | 111.48   |
| 25  | C     | 490 | BCR  | C12-C13-C14 | -2.14 | 115.64      | 119.01   |
| 21  | C     | 477 | CLA  | C1-C2-C3    | 2.14  | 129.70      | 126.20   |
| 27  | J     | 492 | LMG  | O9-C10-C11  | -2.14 | 115.42      | 123.78   |
| 28  | D     | 362 | DGD  | O3D-C3D-C2D | 2.14  | 115.42      | 110.38   |
| 21  | A     | 366 | CLA  | CED-O2D-CGD | 2.13  | 120.75      | 115.92   |
| 21  | D     | 354 | CLA  | C11-C10-C8  | 2.13  | 123.04      | 115.97   |
| 30  | F     | 224 | SQD  | C31-C30-C29 | 2.13  | 133.91      | 115.25   |
| 30  | L     | 213 | SQD  | O8-S-O7     | 2.13  | 116.72      | 111.40   |
| 28  | C     | 493 | DGD  | C5B-C4B-C3B | 2.13  | 125.11      | 114.37   |
| 25  | A     | 369 | BCR  | C1-C6-C7    | 2.12  | 121.41      | 115.65   |
| 21  | B     | 514 | CLA  | CAA-C2A-C1A | -2.12 | 105.02      | 111.97   |
| 21  | B     | 526 | CLA  | CBA-CAA-C2A | 2.12  | 120.10      | 113.79   |
| 25  | B     | 530 | BCR  | C36-C18-C19 | 2.12  | 121.32      | 118.09   |
| 28  | C     | 491 | DGD  | O3G-C1D-C2D | -2.12 | 105.06      | 108.27   |
| 27  | J     | 492 | LMG  | C9-O8-C28   | 2.11  | 124.81      | 117.12   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | A     | 369 | BCR  | C12-C13-C14 | -2.11 | 115.70      | 119.01   |
| 30  | F     | 224 | SQD  | O48-C23-O10 | -2.10 | 118.36      | 123.63   |
| 25  | A     | 369 | BCR  | C10-C11-C12 | 2.10  | 129.29      | 123.20   |
| 21  | B     | 517 | CLA  | C9-C8-C7    | -2.10 | 103.78      | 111.27   |
| 28  | C     | 493 | DGD  | C4D-C3D-C2D | 2.10  | 114.52      | 110.83   |
| 28  | B     | 533 | DGD  | C4B-C3B-C2B | 2.10  | 120.85      | 113.13   |
| 21  | C     | 478 | CLA  | C1D-ND-C4D  | -2.09 | 104.84      | 106.31   |
| 28  | B     | 528 | DGD  | C1G-O1G-C1A | -2.09 | 109.47      | 117.12   |
| 25  | X     | 107 | BCR  | C23-C22-C21 | -2.09 | 115.72      | 119.01   |
| 27  | J     | 492 | LMG  | C35-C34-C33 | 2.09  | 124.95      | 114.37   |
| 28  | D     | 362 | DGD  | C4A-C3A-C2A | -2.09 | 105.44      | 113.13   |
| 21  | B     | 525 | CLA  | O1D-CGD-CBD | -2.09 | 120.40      | 124.52   |
| 21  | C     | 481 | CLA  | OBD-CAD-C3D | 2.09  | 133.30      | 128.42   |
| 27  | M     | 217 | LMG  | O8-C9-C8    | -2.08 | 102.39      | 108.40   |
| 21  | C     | 477 | CLA  | O1D-CGD-CBD | -2.08 | 120.41      | 124.52   |
| 27  | D     | 360 | LMG  | C9-O8-C28   | -2.08 | 109.50      | 117.12   |
| 27  | C     | 494 | LMG  | C30-C29-C28 | 2.08  | 121.33      | 113.69   |
| 21  | C     | 485 | CLA  | C4D-CHA-C1A | 2.08  | 123.73      | 121.24   |
| 25  | Z     | 116 | BCR  | C30-C25-C24 | 2.08  | 121.29      | 115.65   |
| 25  | B     | 527 | BCR  | C37-C22-C23 | 2.08  | 121.26      | 118.09   |
| 27  | I     | 220 | LMG  | C16-C15-C14 | 2.08  | 124.87      | 114.37   |
| 25  | B     | 529 | BCR  | C28-C27-C26 | 2.08  | 117.76      | 114.06   |
| 27  | A     | 373 | LMG  | C9-O8-C28   | -2.08 | 109.53      | 117.12   |
| 21  | B     | 514 | CLA  | CED-O2D-CGD | 2.07  | 120.62      | 115.92   |
| 25  | D     | 358 | BCR  | C11-C10-C9  | 2.07  | 130.18      | 127.28   |
| 21  | B     | 513 | CLA  | CAA-C2A-C1A | -2.07 | 105.19      | 111.97   |
| 21  | B     | 518 | CLA  | O1D-CGD-CBD | -2.07 | 120.44      | 124.52   |
| 28  | B     | 533 | DGD  | O1B-C1B-C2B | -2.07 | 115.69      | 123.78   |
| 25  | X     | 107 | BCR  | C11-C12-C13 | 2.07  | 132.03      | 126.36   |
| 25  | C     | 490 | BCR  | C28-C27-C26 | 2.07  | 117.74      | 114.06   |
| 25  | C     | 490 | BCR  | C1-C6-C7    | 2.06  | 121.25      | 115.65   |
| 30  | F     | 224 | SQD  | O47-C7-C8   | 2.06  | 115.94      | 111.48   |
| 30  | L     | 213 | SQD  | C13-C12-C11 | 2.06  | 124.80      | 114.37   |
| 27  | D     | 359 | LMG  | C32-C31-C30 | -2.06 | 103.95      | 114.37   |
| 25  | D     | 358 | BCR  | C36-C18-C19 | 2.06  | 121.24      | 118.09   |
| 21  | C     | 482 | CLA  | CMD-C2D-C1D | 2.06  | 128.36      | 124.73   |
| 30  | L     | 213 | SQD  | C19-C18-C17 | 2.06  | 124.78      | 114.37   |
| 29  | O     | 274 | LMT  | O1B-C1B-C2B | 2.06  | 113.15      | 108.09   |
| 28  | D     | 362 | DGD  | C5A-C4A-C3A | 2.06  | 124.77      | 114.37   |
| 28  | C     | 493 | DGD  | O2G-C2G-C3G | 2.06  | 115.72      | 108.34   |
| 21  | C     | 477 | CLA  | CHC-C1C-NC  | 2.06  | 127.41      | 124.31   |
| 29  | O     | 274 | LMT  | O5B-C5B-C6B | 2.05  | 111.53      | 106.44   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | A     | 369 | BCR  | C1-C6-C5    | -2.05 | 119.83      | 122.64   |
| 21  | B     | 515 | CLA  | C1D-ND-C4D  | -2.05 | 104.87      | 106.31   |
| 21  | A     | 366 | CLA  | C1-C2-C3    | 2.05  | 129.56      | 126.20   |
| 21  | B     | 525 | CLA  | CHA-C1A-NA  | -2.05 | 121.74      | 126.39   |
| 33  | F     | 85  | HEM  | C4D-C3D-C2D | -2.05 | 103.91      | 106.89   |
| 25  | A     | 369 | BCR  | C36-C18-C19 | 2.05  | 121.22      | 118.09   |
| 21  | A     | 364 | CLA  | CAA-C2A-C3A | -2.04 | 107.49      | 113.00   |
| 25  | C     | 489 | BCR  | C8-C7-C6    | 2.04  | 132.44      | 127.00   |
| 21  | A     | 364 | CLA  | O1D-CGD-CBD | -2.04 | 120.50      | 124.52   |
| 21  | C     | 480 | CLA  | CHC-C1C-NC  | 2.03  | 127.38      | 124.31   |
| 21  | K     | 483 | CLA  | C4B-C3B-C2B | -2.03 | 104.77      | 107.30   |
| 21  | C     | 481 | CLA  | C12-C11-C10 | -2.03 | 104.18      | 113.28   |
| 29  | A     | 376 | LMT  | C1'-O5'-C5' | -2.03 | 109.76      | 113.72   |
| 21  | B     | 521 | CLA  | CMD-C2D-C1D | 2.03  | 128.30      | 124.73   |
| 25  | A     | 369 | BCR  | C34-C9-C8   | 2.03  | 121.19      | 118.09   |
| 30  | F     | 224 | SQD  | O8-S-O7     | 2.03  | 116.47      | 111.40   |
| 27  | D     | 360 | LMG  | C7-O1-C1    | -2.03 | 109.45      | 113.80   |
| 21  | B     | 517 | CLA  | C9-C8-C10   | -2.03 | 104.05      | 111.27   |
| 21  | B     | 521 | CLA  | C1-C2-C3    | 2.02  | 129.51      | 126.20   |
| 25  | C     | 490 | BCR  | C32-C1-C2   | -2.02 | 101.18      | 108.95   |
| 25  | D     | 358 | BCR  | C1-C6-C7    | 2.02  | 121.13      | 115.65   |
| 21  | D     | 354 | CLA  | C3D-C4D-ND  | 2.02  | 113.27      | 109.99   |
| 21  | B     | 524 | CLA  | C2A-C1A-CHA | 2.02  | 127.37      | 123.87   |
| 21  | B     | 512 | CLA  | CAA-CBA-CGA | -2.02 | 107.49      | 113.21   |
| 21  | B     | 521 | CLA  | C11-C12-C13 | 2.02  | 122.66      | 115.97   |
| 28  | B     | 528 | DGD  | C6D-O5D-C1E | -2.01 | 109.48      | 113.80   |
| 29  | O     | 274 | LMT  | C7-C6-C5    | -2.01 | 104.19      | 114.37   |
| 28  | C     | 474 | DGD  | O2D-C2D-C1D | 2.01  | 114.87      | 110.08   |
| 33  | F     | 85  | HEM  | C2B-C1B-NB  | 2.01  | 112.15      | 109.84   |
| 25  | C     | 489 | BCR  | C30-C25-C24 | 2.01  | 121.11      | 115.65   |
| 30  | F     | 224 | SQD  | C13-C12-C11 | 2.01  | 124.54      | 114.37   |
| 21  | B     | 515 | CLA  | C12-C11-C10 | -2.01 | 104.27      | 113.28   |
| 27  | M     | 217 | LMG  | C7-O1-C1    | -2.01 | 109.49      | 113.80   |
| 27  | D     | 359 | LMG  | C34-C33-C32 | -2.01 | 104.22      | 114.37   |
| 28  | B     | 528 | DGD  | C3G-O3G-C1D | -2.01 | 109.49      | 113.80   |
| 28  | D     | 362 | DGD  | C3A-C2A-C1A | 2.01  | 121.05      | 113.69   |
| 25  | Z     | 116 | BCR  | C37-C22-C23 | 2.01  | 121.15      | 118.09   |
| 30  | D     | 361 | SQD  | O8-S-O9     | -2.00 | 106.39      | 111.40   |
| 21  | B     | 517 | CLA  | OBD-CAD-C3D | 2.00  | 133.10      | 128.42   |
| 21  | B     | 516 | CLA  | O1D-CGD-CBD | -2.00 | 120.57      | 124.52   |
| 28  | C     | 491 | DGD  | C3G-C2G-C1G | 2.00  | 116.45      | 111.78   |
| 25  | C     | 490 | BCR  | C10-C11-C12 | 2.00  | 129.00      | 123.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | C     | 483 | CLA  | C12-C11-C10 | -2.00 | 104.31      | 113.28   |
| 27  | J     | 492 | LMG  | C32-C31-C30 | -2.00 | 104.25      | 114.37   |
| 21  | C     | 486 | CLA  | C4B-C3B-C2B | -2.00 | 104.81      | 107.30   |

All (39) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 21  | A     | 362 | CLA  | C8   |
| 21  | A     | 363 | CLA  | C8   |
| 21  | A     | 366 | CLA  | C8   |
| 21  | A     | 364 | CLA  | C8   |
| 21  | B     | 511 | CLA  | C8   |
| 21  | B     | 512 | CLA  | C8   |
| 21  | B     | 513 | CLA  | C8   |
| 21  | B     | 514 | CLA  | C8   |
| 21  | B     | 515 | CLA  | C8   |
| 21  | B     | 516 | CLA  | C8   |
| 21  | B     | 517 | CLA  | C8   |
| 21  | B     | 518 | CLA  | C8   |
| 21  | B     | 519 | CLA  | C8   |
| 21  | B     | 520 | CLA  | C8   |
| 21  | B     | 521 | CLA  | C8   |
| 21  | B     | 522 | CLA  | C8   |
| 21  | B     | 523 | CLA  | C8   |
| 21  | B     | 524 | CLA  | C8   |
| 21  | B     | 525 | CLA  | C8   |
| 21  | B     | 526 | CLA  | C8   |
| 21  | C     | 477 | CLA  | C8   |
| 21  | C     | 478 | CLA  | C8   |
| 21  | C     | 479 | CLA  | C8   |
| 21  | C     | 480 | CLA  | C8   |
| 21  | C     | 481 | CLA  | C8   |
| 21  | C     | 482 | CLA  | C8   |
| 21  | C     | 483 | CLA  | C8   |
| 21  | C     | 484 | CLA  | C8   |
| 21  | C     | 485 | CLA  | C8   |
| 21  | C     | 486 | CLA  | C8   |
| 21  | C     | 487 | CLA  | C8   |
| 21  | C     | 488 | CLA  | C8   |
| 21  | D     | 354 | CLA  | C8   |
| 21  | D     | 356 | CLA  | C8   |
| 21  | K     | 483 | CLA  | C8   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 22  | A     | 365 | PHO  | C8   |
| 22  | D     | 355 | PHO  | C8   |
| 28  | C     | 492 | DGD  | C1E  |
| 28  | C     | 493 | DGD  | C1E  |

All (685) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 21  | B     | 511 | CLA  | C11-C12-C13-C14 |
| 21  | B     | 516 | CLA  | C4-C3-C5-C6     |
| 21  | B     | 524 | CLA  | CAD-CBD-CGD-O2D |
| 21  | C     | 477 | CLA  | CAD-CBD-CGD-O1D |
| 21  | C     | 477 | CLA  | CAD-CBD-CGD-O2D |
| 21  | C     | 480 | CLA  | CHA-CBD-CGD-O1D |
| 21  | C     | 480 | CLA  | CHA-CBD-CGD-O2D |
| 21  | C     | 483 | CLA  | C4-C3-C5-C6     |
| 21  | K     | 483 | CLA  | CHA-CBD-CGD-O1D |
| 21  | K     | 483 | CLA  | CHA-CBD-CGD-O2D |
| 23  | A     | 367 | MES  | C7-C8-S-O2S     |
| 23  | A     | 367 | MES  | C7-C8-S-O3S     |
| 25  | A     | 369 | BCR  | C6-C7-C8-C9     |
| 25  | B     | 527 | BCR  | C1-C6-C7-C8     |
| 25  | B     | 527 | BCR  | C5-C6-C7-C8     |
| 25  | B     | 527 | BCR  | C6-C7-C8-C9     |
| 25  | C     | 489 | BCR  | C6-C7-C8-C9     |
| 25  | C     | 490 | BCR  | C6-C7-C8-C9     |
| 25  | C     | 490 | BCR  | C23-C24-C25-C26 |
| 25  | C     | 490 | BCR  | C23-C24-C25-C30 |
| 25  | D     | 358 | BCR  | C1-C6-C7-C8     |
| 25  | D     | 358 | BCR  | C5-C6-C7-C8     |
| 25  | D     | 358 | BCR  | C6-C7-C8-C9     |
| 25  | J     | 115 | BCR  | C6-C7-C8-C9     |
| 25  | J     | 112 | BCR  | C6-C7-C8-C9     |
| 25  | X     | 107 | BCR  | C1-C6-C7-C8     |
| 25  | X     | 107 | BCR  | C5-C6-C7-C8     |
| 25  | Z     | 116 | BCR  | C1-C6-C7-C8     |
| 25  | Z     | 116 | BCR  | C5-C6-C7-C8     |
| 26  | C     | 476 | LHG  | O1-C1-C2-C3     |
| 26  | C     | 476 | LHG  | C8-C7-O7-C5     |
| 27  | B     | 531 | LMG  | C7-C8-O7-C10    |
| 27  | D     | 360 | LMG  | C11-C10-O7-C8   |
| 27  | J     | 492 | LMG  | O7-C8-C9-O8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 28  | C     | 474 | DGD  | O6E-C1E-O5D-C6D |
| 28  | C     | 491 | DGD  | O6E-C1E-O5D-C6D |
| 28  | C     | 492 | DGD  | O6E-C1E-O5D-C6D |
| 28  | C     | 493 | DGD  | O2G-C2G-C3G-O3G |
| 28  | C     | 493 | DGD  | O6E-C1E-O5D-C6D |
| 28  | D     | 362 | DGD  | O1G-C1G-C2G-O2G |
| 28  | D     | 362 | DGD  | O6E-C1E-O5D-C6D |
| 30  | C     | 475 | SQD  | C8-C7-O47-C45   |
| 30  | D     | 361 | SQD  | O49-C7-O47-C45  |
| 30  | D     | 361 | SQD  | C8-C7-O47-C45   |
| 30  | D     | 361 | SQD  | C5-C6-S-O7      |
| 30  | D     | 361 | SQD  | C5-C6-S-O8      |
| 30  | D     | 361 | SQD  | C5-C6-S-O9      |
| 30  | F     | 224 | SQD  | O5-C1-O6-C44    |
| 30  | F     | 224 | SQD  | O5-C5-C6-S      |
| 30  | F     | 224 | SQD  | C5-C6-S-O8      |
| 30  | L     | 213 | SQD  | C2-C1-O6-C44    |
| 30  | L     | 213 | SQD  | O49-C7-O47-C45  |
| 30  | L     | 213 | SQD  | C8-C7-O47-C45   |
| 32  | D     | 357 | PL9  | C26-C27-C28-C29 |
| 32  | D     | 357 | PL9  | C39-C41-C42-C43 |
| 32  | D     | 357 | PL9  | C46-C47-C48-C49 |
| 33  | F     | 85  | HEM  | C2B-C3B-CAB-CBB |
| 33  | F     | 85  | HEM  | C4B-C3B-CAB-CBB |
| 33  | F     | 85  | HEM  | C2C-C3C-CAC-CBC |
| 33  | F     | 85  | HEM  | C4C-C3C-CAC-CBC |
| 33  | V     | 164 | HEM  | C3A-C2A-CAA-CBA |
| 33  | V     | 164 | HEM  | C2B-C3B-CAB-CBB |
| 33  | V     | 164 | HEM  | C4B-C3B-CAB-CBB |
| 29  | I     | 274 | LMT  | C3'-C4'-O1B-C1B |
| 22  | D     | 355 | PHO  | CBD-CGD-O2D-CED |
| 21  | B     | 517 | CLA  | C13-C15-C16-C17 |
| 21  | B     | 522 | CLA  | C10-C11-C12-C13 |
| 30  | F     | 224 | SQD  | O10-C23-O48-C46 |
| 28  | B     | 528 | DGD  | O6D-C5D-C6D-O5D |
| 28  | C     | 493 | DGD  | O6D-C5D-C6D-O5D |
| 26  | C     | 476 | LHG  | O9-C7-O7-C5     |
| 27  | D     | 360 | LMG  | O9-C10-O7-C8    |
| 30  | C     | 475 | SQD  | O49-C7-O47-C45  |
| 21  | A     | 362 | CLA  | C3-C5-C6-C7     |
| 21  | A     | 364 | CLA  | C3-C5-C6-C7     |
| 21  | B     | 511 | CLA  | C3-C5-C6-C7     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 21  | B     | 514 | CLA  | C3-C5-C6-C7     |
| 21  | B     | 519 | CLA  | C3-C5-C6-C7     |
| 21  | C     | 478 | CLA  | C3-C5-C6-C7     |
| 21  | C     | 484 | CLA  | C3-C5-C6-C7     |
| 29  | B     | 535 | LMT  | C5'-C4'-O1B-C1B |
| 21  | A     | 366 | CLA  | CBA-CGA-O2A-C1  |
| 30  | F     | 224 | SQD  | C24-C23-O48-C46 |
| 28  | B     | 528 | DGD  | C4E-C5E-C6E-O5E |
| 29  | A     | 376 | LMT  | C5'-C4'-O1B-C1B |
| 21  | B     | 515 | CLA  | C4-C3-C5-C6     |
| 21  | B     | 517 | CLA  | C4-C3-C5-C6     |
| 21  | B     | 525 | CLA  | C4-C3-C5-C6     |
| 21  | C     | 484 | CLA  | C4-C3-C5-C6     |
| 21  | B     | 515 | CLA  | C2-C3-C5-C6     |
| 21  | B     | 516 | CLA  | C2-C3-C5-C6     |
| 21  | B     | 517 | CLA  | C2-C3-C5-C6     |
| 21  | B     | 525 | CLA  | C2-C3-C5-C6     |
| 21  | C     | 483 | CLA  | C2-C3-C5-C6     |
| 21  | C     | 484 | CLA  | C2-C3-C5-C6     |
| 21  | B     | 520 | CLA  | C2A-CAA-CBA-CGA |
| 21  | B     | 522 | CLA  | C2A-CAA-CBA-CGA |
| 21  | B     | 517 | CLA  | C3-C5-C6-C7     |
| 21  | C     | 479 | CLA  | C3-C5-C6-C7     |
| 21  | C     | 481 | CLA  | C3-C5-C6-C7     |
| 21  | C     | 485 | CLA  | C3-C5-C6-C7     |
| 21  | A     | 363 | CLA  | CBA-CGA-O2A-C1  |
| 21  | B     | 524 | CLA  | CBA-CGA-O2A-C1  |
| 21  | C     | 483 | CLA  | CBA-CGA-O2A-C1  |
| 27  | I     | 220 | LMG  | C18-C19-C20-C21 |
| 28  | C     | 491 | DGD  | C7A-C8A-C9A-CAA |
| 32  | D     | 357 | PL9  | C7-C8-C9-C10    |
| 21  | A     | 363 | CLA  | O1A-CGA-O2A-C1  |
| 21  | A     | 366 | CLA  | O1A-CGA-O2A-C1  |
| 21  | C     | 483 | CLA  | O1A-CGA-O2A-C1  |
| 21  | D     | 354 | CLA  | O1A-CGA-O2A-C1  |
| 26  | A     | 371 | LHG  | O10-C23-O8-C6   |
| 27  | B     | 531 | LMG  | C36-C37-C38-C39 |
| 27  | C     | 494 | LMG  | C18-C19-C20-C21 |
| 27  | C     | 494 | LMG  | C36-C37-C38-C39 |
| 27  | D     | 359 | LMG  | C36-C37-C38-C39 |
| 27  | D     | 360 | LMG  | C36-C37-C38-C39 |
| 27  | J     | 492 | LMG  | C36-C37-C38-C39 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 27  | M     | 217 | LMG  | C18-C19-C20-C21 |
| 28  | B     | 533 | DGD  | C7B-C8B-C9B-CAB |
| 29  | D     | 536 | LMT  | C3-C4-C5-C6     |
| 21  | C     | 482 | CLA  | C3-C5-C6-C7     |
| 27  | B     | 531 | LMG  | C18-C19-C20-C21 |
| 27  | D     | 359 | LMG  | C18-C19-C20-C21 |
| 27  | J     | 492 | LMG  | C18-C19-C20-C21 |
| 28  | C     | 474 | DGD  | C7A-C8A-C9A-CAA |
| 28  | C     | 492 | DGD  | C7B-C8B-C9B-CAB |
| 28  | C     | 493 | DGD  | C7B-C8B-C9B-CAB |
| 28  | D     | 362 | DGD  | C7A-C8A-C9A-CAA |
| 29  | A     | 376 | LMT  | C3-C4-C5-C6     |
| 29  | D     | 363 | LMT  | C3-C4-C5-C6     |
| 29  | I     | 274 | LMT  | C3-C4-C5-C6     |
| 29  | T     | 226 | LMT  | C3-C4-C5-C6     |
| 21  | B     | 522 | CLA  | CBA-CGA-O2A-C1  |
| 27  | A     | 373 | LMG  | C29-C28-O8-C9   |
| 21  | B     | 524 | CLA  | O1A-CGA-O2A-C1  |
| 21  | B     | 511 | CLA  | C2C-C3C-CAC-CBC |
| 27  | A     | 373 | LMG  | O10-C28-O8-C9   |
| 28  | B     | 528 | DGD  | C7B-C8B-C9B-CAB |
| 29  | O     | 274 | LMT  | C3-C4-C5-C6     |
| 28  | B     | 528 | DGD  | C4D-C5D-C6D-O5D |
| 28  | B     | 533 | DGD  | C7A-C8A-C9A-CAA |
| 28  | C     | 474 | DGD  | C7B-C8B-C9B-CAB |
| 28  | D     | 362 | DGD  | C7B-C8B-C9B-CAB |
| 27  | A     | 373 | LMG  | O6-C5-C6-O5     |
| 22  | D     | 355 | PHO  | O1D-CGD-O2D-CED |
| 21  | A     | 362 | CLA  | CBA-CGA-O2A-C1  |
| 21  | D     | 354 | CLA  | CBA-CGA-O2A-C1  |
| 26  | A     | 371 | LHG  | C24-C23-O8-C6   |
| 21  | C     | 479 | CLA  | C4-C3-C5-C6     |
| 21  | C     | 479 | CLA  | C2-C3-C5-C6     |
| 32  | D     | 357 | PL9  | C24-C26-C27-C28 |
| 28  | A     | 375 | DGD  | C7B-C8B-C9B-CAB |
| 28  | C     | 492 | DGD  | C7A-C8A-C9A-CAA |
| 28  | C     | 493 | DGD  | C7A-C8A-C9A-CAA |
| 33  | V     | 164 | HEM  | C1A-C2A-CAA-CBA |
| 28  | B     | 528 | DGD  | O6E-C5E-C6E-O5E |
| 21  | C     | 481 | CLA  | C2A-CAA-CBA-CGA |
| 21  | A     | 362 | CLA  | O1A-CGA-O2A-C1  |
| 21  | B     | 522 | CLA  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 28  | B     | 533 | DGD  | O6E-C1E-O5D-C6D |
| 29  | B     | 535 | LMT  | C3-C4-C5-C6     |
| 21  | C     | 485 | CLA  | CBA-CGA-O2A-C1  |
| 30  | D     | 361 | SQD  | C24-C23-O48-C46 |
| 28  | B     | 528 | DGD  | C7A-C8A-C9A-CAA |
| 30  | D     | 361 | SQD  | O10-C23-O48-C46 |
| 21  | B     | 518 | CLA  | CBA-CGA-O2A-C1  |
| 21  | C     | 478 | CLA  | CBA-CGA-O2A-C1  |
| 21  | C     | 488 | CLA  | CBA-CGA-O2A-C1  |
| 27  | D     | 360 | LMG  | C29-C28-O8-C9   |
| 26  | C     | 476 | LHG  | C23-C24-C25-C26 |
| 21  | B     | 523 | CLA  | C4-C3-C5-C6     |
| 21  | B     | 523 | CLA  | C2-C3-C5-C6     |
| 21  | C     | 480 | CLA  | C3-C5-C6-C7     |
| 21  | B     | 518 | CLA  | C11-C12-C13-C14 |
| 21  | B     | 520 | CLA  | C14-C13-C15-C16 |
| 21  | B     | 523 | CLA  | C11-C12-C13-C14 |
| 21  | C     | 477 | CLA  | C6-C7-C8-C9     |
| 21  | C     | 480 | CLA  | C11-C12-C13-C14 |
| 21  | C     | 481 | CLA  | C6-C7-C8-C9     |
| 21  | C     | 482 | CLA  | C6-C7-C8-C9     |
| 21  | C     | 486 | CLA  | C11-C12-C13-C14 |
| 22  | D     | 355 | PHO  | C11-C12-C13-C14 |
| 22  | D     | 355 | PHO  | C14-C13-C15-C16 |
| 27  | A     | 373 | LMG  | C4-C5-C6-O5     |
| 21  | B     | 521 | CLA  | C2A-CAA-CBA-CGA |
| 21  | C     | 488 | CLA  | O1A-CGA-O2A-C1  |
| 27  | D     | 360 | LMG  | O10-C28-O8-C9   |
| 29  | O     | 274 | LMT  | C5'-C4'-O1B-C1B |
| 28  | C     | 474 | DGD  | O2G-C2G-C3G-O3G |
| 22  | A     | 365 | PHO  | C13-C15-C16-C17 |
| 21  | A     | 363 | CLA  | C10-C11-C12-C13 |
| 22  | A     | 365 | PHO  | C15-C16-C17-C18 |
| 21  | B     | 516 | CLA  | C11-C12-C13-C15 |
| 21  | B     | 518 | CLA  | C12-C13-C15-C16 |
| 21  | C     | 488 | CLA  | C11-C12-C13-C15 |
| 21  | B     | 514 | CLA  | CBA-CGA-O2A-C1  |
| 21  | B     | 518 | CLA  | O1A-CGA-O2A-C1  |
| 21  | C     | 478 | CLA  | O1A-CGA-O2A-C1  |
| 21  | A     | 362 | CLA  | C13-C15-C16-C17 |
| 21  | B     | 513 | CLA  | C10-C11-C12-C13 |
| 21  | C     | 480 | CLA  | C13-C15-C16-C17 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | D     | 355 | PHO  | C13-C15-C16-C17 |
| 21  | B     | 516 | CLA  | C2A-CAA-CBA-CGA |
| 21  | B     | 518 | CLA  | C2A-CAA-CBA-CGA |
| 21  | C     | 477 | CLA  | C2A-CAA-CBA-CGA |
| 21  | B     | 511 | CLA  | C4C-C3C-CAC-CBC |
| 21  | B     | 516 | CLA  | C13-C15-C16-C17 |
| 26  | A     | 371 | LHG  | C23-C24-C25-C26 |
| 27  | A     | 373 | LMG  | C10-C11-C12-C13 |
| 27  | D     | 360 | LMG  | C10-C11-C12-C13 |
| 30  | C     | 475 | SQD  | C23-C24-C25-C26 |
| 21  | B     | 523 | CLA  | C3-C5-C6-C7     |
| 21  | B     | 512 | CLA  | C10-C11-C12-C13 |
| 21  | B     | 525 | CLA  | C13-C15-C16-C17 |
| 21  | C     | 480 | CLA  | C10-C11-C12-C13 |
| 21  | C     | 485 | CLA  | O1A-CGA-O2A-C1  |
| 21  | A     | 366 | CLA  | C13-C15-C16-C17 |
| 21  | C     | 479 | CLA  | C13-C15-C16-C17 |
| 28  | D     | 362 | DGD  | CFB-CGB-CHB-CIB |
| 21  | B     | 511 | CLA  | C13-C15-C16-C17 |
| 28  | B     | 533 | DGD  | CFB-CGB-CHB-CIB |
| 28  | C     | 492 | DGD  | CFB-CGB-CHB-CIB |
| 28  | C     | 493 | DGD  | CFB-CGB-CHB-CIB |
| 21  | B     | 513 | CLA  | O1A-CGA-O2A-C1  |
| 21  | C     | 486 | CLA  | C13-C15-C16-C17 |
| 21  | B     | 513 | CLA  | CBA-CGA-O2A-C1  |
| 21  | C     | 487 | CLA  | CBA-CGA-O2A-C1  |
| 21  | B     | 514 | CLA  | O1A-CGA-O2A-C1  |
| 28  | B     | 528 | DGD  | C1B-C2B-C3B-C4B |
| 21  | C     | 488 | CLA  | C2A-CAA-CBA-CGA |
| 21  | B     | 511 | CLA  | CBA-CGA-O2A-C1  |
| 21  | B     | 512 | CLA  | CBA-CGA-O2A-C1  |
| 21  | C     | 479 | CLA  | CBA-CGA-O2A-C1  |
| 21  | C     | 482 | CLA  | CBA-CGA-O2A-C1  |
| 21  | A     | 362 | CLA  | C10-C11-C12-C13 |
| 21  | C     | 482 | CLA  | C10-C11-C12-C13 |
| 21  | B     | 511 | CLA  | O1A-CGA-O2A-C1  |
| 32  | D     | 357 | PL9  | C35-C34-C36-C37 |
| 21  | B     | 526 | CLA  | C3-C5-C6-C7     |
| 27  | D     | 360 | LMG  | C2-C1-O1-C7     |
| 30  | C     | 475 | SQD  | C2-C1-O6-C44    |
| 32  | D     | 357 | PL9  | C34-C36-C37-C38 |
| 21  | D     | 356 | CLA  | C13-C15-C16-C17 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 21  | C     | 487 | CLA  | C2A-CAA-CBA-CGA |
| 28  | B     | 528 | DGD  | C1G-C2G-O2G-C1B |
| 21  | A     | 363 | CLA  | C3-C5-C6-C7     |
| 21  | B     | 514 | CLA  | C10-C11-C12-C13 |
| 27  | D     | 360 | LMG  | O6-C1-O1-C7     |
| 28  | B     | 528 | DGD  | C2B-C1B-O2G-C2G |
| 30  | C     | 475 | SQD  | C24-C23-O48-C46 |
| 28  | C     | 492 | DGD  | O6D-C5D-C6D-O5D |
| 21  | B     | 516 | CLA  | C2-C1-O2A-CGA   |
| 21  | B     | 522 | CLA  | C2-C1-O2A-CGA   |
| 21  | C     | 482 | CLA  | O1A-CGA-O2A-C1  |
| 21  | C     | 487 | CLA  | O1A-CGA-O2A-C1  |
| 30  | F     | 224 | SQD  | C10-C11-C12-C13 |
| 27  | A     | 373 | LMG  | C28-C29-C30-C31 |
| 27  | A     | 373 | LMG  | C30-C31-C32-C33 |
| 26  | C     | 476 | LHG  | O1-C1-C2-O2     |
| 21  | A     | 363 | CLA  | C2A-CAA-CBA-CGA |
| 30  | F     | 224 | SQD  | C11-C12-C13-C14 |
| 22  | D     | 355 | PHO  | C5-C6-C7-C8     |
| 28  | B     | 528 | DGD  | O1B-C1B-O2G-C2G |
| 21  | C     | 487 | CLA  | C10-C11-C12-C13 |
| 27  | D     | 360 | LMG  | C13-C14-C15-C16 |
| 30  | C     | 475 | SQD  | C17-C18-C19-C20 |
| 21  | B     | 512 | CLA  | O1A-CGA-O2A-C1  |
| 21  | C     | 479 | CLA  | O1A-CGA-O2A-C1  |
| 29  | O     | 274 | LMT  | C3'-C4'-O1B-C1B |
| 26  | C     | 476 | LHG  | C13-C14-C15-C16 |
| 30  | F     | 224 | SQD  | C12-C13-C14-C15 |
| 21  | C     | 483 | CLA  | C13-C15-C16-C17 |
| 27  | D     | 360 | LMG  | C11-C12-C13-C14 |
| 30  | F     | 224 | SQD  | C25-C26-C27-C28 |
| 30  | L     | 213 | SQD  | C27-C28-C29-C30 |
| 30  | C     | 475 | SQD  | O10-C23-O48-C46 |
| 25  | A     | 369 | BCR  | C1-C6-C7-C8     |
| 25  | B     | 530 | BCR  | C1-C6-C7-C8     |
| 25  | B     | 530 | BCR  | C5-C6-C7-C8     |
| 25  | B     | 530 | BCR  | C23-C24-C25-C26 |
| 25  | B     | 530 | BCR  | C23-C24-C25-C30 |
| 25  | C     | 489 | BCR  | C1-C6-C7-C8     |
| 25  | C     | 489 | BCR  | C5-C6-C7-C8     |
| 25  | C     | 489 | BCR  | C23-C24-C25-C26 |
| 25  | C     | 489 | BCR  | C23-C24-C25-C30 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 27  | A     | 373 | LMG  | C36-C37-C38-C39 |
| 21  | B     | 524 | CLA  | C13-C15-C16-C17 |
| 25  | B     | 527 | BCR  | C22-C23-C24-C25 |
| 30  | D     | 361 | SQD  | O5-C1-O6-C44    |
| 30  | D     | 361 | SQD  | C2-C1-O6-C44    |
| 21  | A     | 363 | CLA  | C13-C15-C16-C17 |
| 26  | A     | 371 | LHG  | C11-C10-C9-C8   |
| 26  | A     | 371 | LHG  | C28-C29-C30-C31 |
| 21  | C     | 488 | CLA  | C3-C5-C6-C7     |
| 30  | L     | 213 | SQD  | C25-C26-C27-C28 |
| 30  | F     | 224 | SQD  | C27-C28-C29-C30 |
| 21  | D     | 356 | CLA  | C2A-CAA-CBA-CGA |
| 21  | B     | 516 | CLA  | C10-C11-C12-C13 |
| 27  | A     | 373 | LMG  | C15-C16-C17-C18 |
| 21  | C     | 486 | CLA  | C10-C11-C12-C13 |
| 30  | F     | 224 | SQD  | C11-C10-C9-C8   |
| 28  | B     | 528 | DGD  | C1A-C2A-C3A-C4A |
| 27  | D     | 359 | LMG  | O1-C7-C8-O7     |
| 27  | M     | 217 | LMG  | O1-C7-C8-O7     |
| 28  | A     | 375 | DGD  | O1G-C1G-C2G-O2G |
| 27  | D     | 360 | LMG  | C12-C13-C14-C15 |
| 21  | B     | 525 | CLA  | CBA-CGA-O2A-C1  |
| 21  | D     | 356 | CLA  | C3-C5-C6-C7     |
| 21  | B     | 518 | CLA  | C13-C15-C16-C17 |
| 26  | A     | 371 | LHG  | C24-C25-C26-C27 |
| 26  | A     | 371 | LHG  | C26-C27-C28-C29 |
| 27  | A     | 373 | LMG  | C11-C12-C13-C14 |
| 21  | B     | 522 | CLA  | C11-C12-C13-C15 |
| 21  | B     | 525 | CLA  | C6-C7-C8-C10    |
| 21  | B     | 525 | CLA  | C12-C13-C15-C16 |
| 21  | C     | 477 | CLA  | C6-C7-C8-C10    |
| 21  | C     | 477 | CLA  | C12-C13-C15-C16 |
| 21  | C     | 480 | CLA  | C11-C12-C13-C15 |
| 21  | C     | 480 | CLA  | C12-C13-C15-C16 |
| 21  | C     | 485 | CLA  | C6-C7-C8-C10    |
| 21  | D     | 354 | CLA  | C11-C12-C13-C15 |
| 30  | F     | 224 | SQD  | C15-C16-C17-C18 |
| 26  | C     | 476 | LHG  | C12-C13-C14-C15 |
| 26  | C     | 476 | LHG  | C11-C12-C13-C14 |
| 21  | D     | 354 | CLA  | C10-C11-C12-C13 |
| 21  | A     | 362 | CLA  | C6-C7-C8-C9     |
| 21  | A     | 363 | CLA  | C14-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 21  | A     | 364 | CLA  | C11-C12-C13-C14 |
| 21  | B     | 523 | CLA  | C14-C13-C15-C16 |
| 21  | B     | 524 | CLA  | C6-C7-C8-C9     |
| 21  | D     | 354 | CLA  | C11-C12-C13-C14 |
| 21  | B     | 525 | CLA  | O1A-CGA-O2A-C1  |
| 30  | C     | 475 | SQD  | C25-C26-C27-C28 |
| 30  | D     | 361 | SQD  | C10-C11-C12-C13 |
| 26  | A     | 371 | LHG  | C4-C5-C6-O8     |
| 27  | A     | 373 | LMG  | C7-C8-C9-O8     |
| 27  | D     | 359 | LMG  | O1-C7-C8-C9     |
| 27  | I     | 220 | LMG  | O1-C7-C8-C9     |
| 27  | M     | 217 | LMG  | O1-C7-C8-C9     |
| 28  | A     | 375 | DGD  | C1G-C2G-C3G-O3G |
| 28  | D     | 362 | DGD  | O1G-C1G-C2G-C3G |
| 30  | C     | 475 | SQD  | C10-C11-C12-C13 |
| 21  | C     | 480 | CLA  | O1A-CGA-O2A-C1  |
| 28  | D     | 362 | DGD  | O6D-C5D-C6D-O5D |
| 21  | C     | 477 | CLA  | O1A-CGA-O2A-C1  |
| 21  | B     | 521 | CLA  | C13-C15-C16-C17 |
| 21  | C     | 477 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 365 | PHO  | O2A-C1-C2-C3    |
| 27  | C     | 494 | LMG  | C7-C8-O7-C10    |
| 27  | D     | 359 | LMG  | C7-C8-O7-C10    |
| 27  | D     | 360 | LMG  | C7-C8-O7-C10    |
| 27  | J     | 492 | LMG  | C9-C8-O7-C10    |
| 30  | C     | 475 | SQD  | C24-C25-C26-C27 |
| 27  | A     | 373 | LMG  | C37-C38-C39-C40 |
| 30  | C     | 475 | SQD  | C29-C30-C31-C32 |
| 27  | D     | 360 | LMG  | C16-C17-C18-C19 |
| 21  | B     | 521 | CLA  | CBA-CGA-O2A-C1  |
| 21  | C     | 480 | CLA  | CBA-CGA-O2A-C1  |
| 30  | C     | 475 | SQD  | C11-C12-C13-C14 |
| 21  | B     | 524 | CLA  | C4-C3-C5-C6     |
| 32  | D     | 357 | PL9  | C12-C11-C9-C10  |
| 30  | F     | 224 | SQD  | C29-C30-C31-C32 |
| 30  | L     | 213 | SQD  | C19-C20-C21-C22 |
| 27  | A     | 373 | LMG  | C16-C17-C18-C19 |
| 30  | L     | 213 | SQD  | C10-C11-C12-C13 |
| 27  | A     | 373 | LMG  | O7-C8-C9-O8     |
| 30  | C     | 475 | SQD  | O6-C44-C45-O47  |
| 30  | D     | 361 | SQD  | O6-C44-C45-O47  |
| 30  | F     | 224 | SQD  | C24-C25-C26-C27 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 27  | A     | 373 | LMG  | C14-C15-C16-C17 |
| 21  | K     | 483 | CLA  | C4-C3-C5-C6     |
| 32  | D     | 357 | PL9  | C45-C44-C46-C47 |
| 21  | D     | 356 | CLA  | CBA-CGA-O2A-C1  |
| 21  | A     | 362 | CLA  | C14-C13-C15-C16 |
| 21  | B     | 514 | CLA  | C11-C12-C13-C14 |
| 21  | B     | 520 | CLA  | C11-C12-C13-C14 |
| 21  | B     | 522 | CLA  | C6-C7-C8-C9     |
| 21  | B     | 522 | CLA  | C11-C12-C13-C14 |
| 21  | B     | 525 | CLA  | C6-C7-C8-C9     |
| 21  | B     | 525 | CLA  | C14-C13-C15-C16 |
| 21  | C     | 477 | CLA  | C14-C13-C15-C16 |
| 21  | C     | 480 | CLA  | C14-C13-C15-C16 |
| 21  | C     | 483 | CLA  | C14-C13-C15-C16 |
| 22  | D     | 355 | PHO  | C3-C5-C6-C7     |
| 21  | A     | 362 | CLA  | C6-C7-C8-C10    |
| 21  | A     | 362 | CLA  | C12-C13-C15-C16 |
| 21  | A     | 363 | CLA  | C12-C13-C15-C16 |
| 21  | A     | 366 | CLA  | C12-C13-C15-C16 |
| 21  | B     | 511 | CLA  | C11-C12-C13-C15 |
| 21  | B     | 514 | CLA  | C11-C12-C13-C15 |
| 21  | B     | 518 | CLA  | C11-C12-C13-C15 |
| 21  | B     | 520 | CLA  | C11-C12-C13-C15 |
| 21  | B     | 523 | CLA  | C6-C7-C8-C10    |
| 21  | B     | 523 | CLA  | C12-C13-C15-C16 |
| 21  | B     | 524 | CLA  | C6-C7-C8-C10    |
| 21  | C     | 479 | CLA  | C11-C12-C13-C15 |
| 22  | D     | 355 | PHO  | C6-C7-C8-C10    |
| 22  | D     | 355 | PHO  | C12-C13-C15-C16 |
| 26  | A     | 371 | LHG  | C9-C10-C11-C12  |
| 27  | A     | 373 | LMG  | C12-C13-C14-C15 |
| 21  | B     | 521 | CLA  | O1A-CGA-O2A-C1  |
| 21  | B     | 520 | CLA  | C4-C3-C5-C6     |
| 21  | B     | 520 | CLA  | C2-C3-C5-C6     |
| 21  | K     | 483 | CLA  | C2-C3-C5-C6     |
| 21  | B     | 515 | CLA  | CBA-CGA-O2A-C1  |
| 21  | B     | 524 | CLA  | C2C-C3C-CAC-CBC |
| 27  | A     | 373 | LMG  | C29-C30-C31-C32 |
| 28  | A     | 375 | DGD  | O1G-C1G-C2G-C3G |
| 28  | B     | 533 | DGD  | O1G-C1G-C2G-C3G |
| 28  | B     | 528 | DGD  | C1G-C2G-C3G-O3G |
| 28  | C     | 491 | DGD  | C1G-C2G-C3G-O3G |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 28  | C     | 492 | DGD  | C1G-C2G-C3G-O3G |
| 30  | D     | 361 | SQD  | O6-C44-C45-C46  |
| 30  | L     | 213 | SQD  | C17-C18-C19-C20 |
| 29  | A     | 376 | LMT  | C3'-C4'-O1B-C1B |
| 25  | A     | 369 | BCR  | C23-C24-C25-C30 |
| 21  | C     | 485 | CLA  | C10-C11-C12-C13 |
| 28  | B     | 528 | DGD  | C2B-C3B-C4B-C5B |
| 21  | B     | 517 | CLA  | C2A-CAA-CBA-CGA |
| 26  | C     | 476 | LHG  | O7-C5-C6-O8     |
| 27  | B     | 531 | LMG  | O7-C8-C9-O8     |
| 27  | D     | 360 | LMG  | O7-C8-C9-O8     |
| 28  | B     | 533 | DGD  | O2G-C2G-C3G-O3G |
| 28  | C     | 491 | DGD  | O2G-C2G-C3G-O3G |
| 32  | D     | 357 | PL9  | C4-C3-C7-C8     |
| 21  | C     | 482 | CLA  | C4-C3-C5-C6     |
| 21  | A     | 364 | CLA  | CBA-CGA-O2A-C1  |
| 21  | A     | 366 | CLA  | C14-C13-C15-C16 |
| 21  | B     | 521 | CLA  | C6-C7-C8-C9     |
| 25  | J     | 115 | BCR  | C22-C23-C24-C25 |
| 28  | B     | 528 | DGD  | O6E-C1E-O5D-C6D |
| 30  | D     | 361 | SQD  | C12-C13-C14-C15 |
| 26  | C     | 476 | LHG  | C9-C10-C11-C12  |
| 21  | C     | 482 | CLA  | C2-C3-C5-C6     |
| 23  | A     | 367 | MES  | C7-C8-S-O1S     |
| 21  | B     | 511 | CLA  | C12-C13-C15-C16 |
| 21  | C     | 478 | CLA  | C12-C13-C15-C16 |
| 21  | C     | 481 | CLA  | C11-C12-C13-C15 |
| 21  | C     | 486 | CLA  | C12-C13-C15-C16 |
| 27  | D     | 360 | LMG  | C15-C16-C17-C18 |
| 21  | A     | 364 | CLA  | O1A-CGA-O2A-C1  |
| 21  | B     | 515 | CLA  | O1A-CGA-O2A-C1  |
| 21  | B     | 517 | CLA  | C10-C11-C12-C13 |
| 21  | C     | 479 | CLA  | C10-C11-C12-C13 |
| 21  | B     | 511 | CLA  | C4-C3-C5-C6     |
| 32  | D     | 357 | PL9  | C43-C44-C46-C47 |
| 33  | V     | 164 | HEM  | C2C-C3C-CAC-CBC |
| 22  | A     | 365 | PHO  | C3-C5-C6-C7     |
| 27  | I     | 220 | LMG  | C7-C8-O7-C10    |
| 28  | A     | 375 | DGD  | C3G-C2G-O2G-C1B |
| 28  | C     | 491 | DGD  | C3G-C2G-O2G-C1B |
| 28  | C     | 492 | DGD  | C1G-C2G-O2G-C1B |
| 28  | C     | 493 | DGD  | C3G-C2G-O2G-C1B |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 21  | D     | 356 | CLA  | O1A-CGA-O2A-C1  |
| 30  | C     | 475 | SQD  | O5-C1-O6-C44    |
| 26  | C     | 476 | LHG  | C4-C5-C6-O8     |
| 27  | J     | 492 | LMG  | C7-C8-C9-O8     |
| 28  | B     | 533 | DGD  | C1G-C2G-C3G-O3G |
| 28  | C     | 493 | DGD  | C1G-C2G-C3G-O3G |
| 28  | D     | 362 | DGD  | C1G-C2G-C3G-O3G |
| 33  | V     | 164 | HEM  | C4C-C3C-CAC-CBC |
| 28  | B     | 528 | DGD  | O2G-C2G-C3G-O3G |
| 21  | A     | 364 | CLA  | C6-C7-C8-C9     |
| 21  | C     | 485 | CLA  | C6-C7-C8-C9     |
| 21  | C     | 488 | CLA  | C11-C12-C13-C14 |
| 28  | B     | 528 | DGD  | C4B-C5B-C6B-C7B |
| 30  | L     | 213 | SQD  | C16-C17-C18-C19 |
| 21  | B     | 513 | CLA  | CAA-CBA-CGA-O2A |
| 21  | C     | 478 | CLA  | C10-C11-C12-C13 |
| 21  | B     | 519 | CLA  | C13-C15-C16-C17 |
| 26  | A     | 371 | LHG  | O2-C2-C3-O3     |
| 26  | A     | 371 | LHG  | C25-C26-C27-C28 |
| 21  | B     | 526 | CLA  | CBA-CGA-O2A-C1  |
| 21  | B     | 519 | CLA  | C10-C11-C12-C13 |
| 21  | B     | 526 | CLA  | O1A-CGA-O2A-C1  |
| 21  | B     | 511 | CLA  | C2-C3-C5-C6     |
| 21  | D     | 354 | CLA  | C2A-CAA-CBA-CGA |
| 30  | C     | 475 | SQD  | C5-C6-S-O9      |
| 21  | B     | 514 | CLA  | C12-C13-C15-C16 |
| 22  | A     | 365 | PHO  | C12-C13-C15-C16 |
| 26  | C     | 476 | LHG  | C26-C27-C28-C29 |
| 28  | B     | 528 | DGD  | C2A-C3A-C4A-C5A |
| 22  | D     | 355 | PHO  | C4-C3-C5-C6     |
| 21  | B     | 511 | CLA  | C2A-CAA-CBA-CGA |
| 21  | B     | 513 | CLA  | C2A-CAA-CBA-CGA |
| 21  | B     | 523 | CLA  | C6-C7-C8-C9     |
| 21  | C     | 478 | CLA  | C14-C13-C15-C16 |
| 21  | C     | 481 | CLA  | C11-C12-C13-C14 |
| 30  | L     | 213 | SQD  | C14-C15-C16-C17 |
| 27  | I     | 220 | LMG  | O1-C7-C8-O7     |
| 28  | A     | 375 | DGD  | O2G-C2G-C3G-O3G |
| 28  | B     | 533 | DGD  | O1G-C1G-C2G-O2G |
| 28  | C     | 474 | DGD  | O1G-C1G-C2G-O2G |
| 28  | D     | 362 | DGD  | O2G-C2G-C3G-O3G |
| 30  | L     | 213 | SQD  | O6-C44-C45-O47  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 27  | D     | 360 | LMG  | C7-C8-C9-O8     |
| 21  | B     | 522 | CLA  | CAD-CBD-CGD-O2D |
| 21  | C     | 485 | CLA  | CAD-CBD-CGD-O2D |
| 21  | C     | 487 | CLA  | CAD-CBD-CGD-O2D |
| 30  | C     | 475 | SQD  | C9-C10-C11-C12  |
| 30  | C     | 475 | SQD  | C12-C13-C14-C15 |
| 21  | B     | 522 | CLA  | CAD-CBD-CGD-O1D |
| 21  | B     | 524 | CLA  | CAD-CBD-CGD-O1D |
| 21  | C     | 484 | CLA  | CHA-CBD-CGD-O1D |
| 21  | C     | 484 | CLA  | CHA-CBD-CGD-O2D |
| 21  | C     | 485 | CLA  | CAD-CBD-CGD-O1D |
| 21  | C     | 487 | CLA  | CAD-CBD-CGD-O1D |
| 26  | C     | 476 | LHG  | C4-O6-P-O4      |
| 25  | J     | 115 | BCR  | C5-C6-C7-C8     |
| 21  | B     | 524 | CLA  | C2-C3-C5-C6     |
| 22  | D     | 355 | PHO  | C2-C3-C5-C6     |
| 26  | A     | 371 | LHG  | C2-C3-O3-P      |
| 21  | B     | 524 | CLA  | C4C-C3C-CAC-CBC |
| 21  | C     | 481 | CLA  | CBA-CGA-O2A-C1  |
| 27  | D     | 360 | LMG  | C30-C31-C32-C33 |
| 28  | C     | 474 | DGD  | C1G-C2G-O2G-C1B |
| 28  | D     | 362 | DGD  | C1G-C2G-O2G-C1B |
| 29  | B     | 535 | LMT  | C3'-C4'-O1B-C1B |
| 21  | C     | 479 | CLA  | C11-C12-C13-C14 |
| 21  | C     | 486 | CLA  | C14-C13-C15-C16 |
| 22  | D     | 355 | PHO  | C6-C7-C8-C9     |
| 21  | B     | 512 | CLA  | C6-C7-C8-C10    |
| 27  | A     | 373 | LMG  | C35-C36-C37-C38 |
| 21  | C     | 485 | CLA  | C4-C3-C5-C6     |
| 27  | A     | 373 | LMG  | C18-C19-C20-C21 |
| 26  | A     | 371 | LHG  | O7-C5-C6-O8     |
| 28  | C     | 493 | DGD  | O1G-C1G-C2G-O2G |
| 21  | A     | 366 | CLA  | C3-C5-C6-C7     |
| 28  | C     | 492 | DGD  | O1G-C1G-C2G-C3G |
| 30  | L     | 213 | SQD  | O6-C44-C45-C46  |
| 21  | B     | 511 | CLA  | C14-C13-C15-C16 |
| 21  | B     | 514 | CLA  | C14-C13-C15-C16 |
| 21  | B     | 517 | CLA  | CBA-CGA-O2A-C1  |
| 27  | D     | 360 | LMG  | C19-C20-C21-C22 |
| 21  | B     | 522 | CLA  | C4-C3-C5-C6     |
| 21  | C     | 485 | CLA  | C2-C3-C5-C6     |
| 21  | B     | 517 | CLA  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 21  | B     | 520 | CLA  | C12-C13-C15-C16 |
| 21  | C     | 482 | CLA  | C6-C7-C8-C10    |
| 21  | C     | 483 | CLA  | C11-C12-C13-C15 |
| 21  | C     | 487 | CLA  | C6-C7-C8-C10    |
| 21  | B     | 520 | CLA  | O1A-CGA-O2A-C1  |
| 30  | L     | 213 | SQD  | C13-C14-C15-C16 |
| 27  | D     | 360 | LMG  | C18-C19-C20-C21 |
| 21  | B     | 526 | CLA  | C13-C15-C16-C17 |
| 21  | C     | 482 | CLA  | C2-C1-O2A-CGA   |
| 21  | B     | 520 | CLA  | C13-C15-C16-C17 |
| 21  | B     | 519 | CLA  | C4-C3-C5-C6     |
| 21  | B     | 512 | CLA  | C14-C13-C15-C16 |
| 21  | B     | 513 | CLA  | C11-C12-C13-C14 |
| 21  | B     | 513 | CLA  | C14-C13-C15-C16 |
| 21  | B     | 515 | CLA  | C11-C12-C13-C14 |
| 21  | B     | 520 | CLA  | C6-C7-C8-C9     |
| 21  | B     | 526 | CLA  | C11-C12-C13-C14 |
| 21  | C     | 483 | CLA  | C11-C12-C13-C14 |
| 26  | C     | 476 | LHG  | C11-C10-C9-C8   |
| 26  | C     | 476 | LHG  | C10-C11-C12-C13 |
| 21  | A     | 364 | CLA  | C13-C15-C16-C17 |
| 28  | B     | 533 | DGD  | C1G-C2G-O2G-C1B |
| 21  | B     | 522 | CLA  | C2-C3-C5-C6     |
| 21  | B     | 516 | CLA  | C3-C5-C6-C7     |
| 21  | C     | 488 | CLA  | C2C-C3C-CAC-CBC |
| 25  | A     | 369 | BCR  | C5-C6-C7-C8     |
| 25  | A     | 369 | BCR  | C23-C24-C25-C26 |
| 33  | F     | 85  | HEM  | CAA-CBA-CGA-O1A |
| 21  | C     | 481 | CLA  | C4-C3-C5-C6     |
| 32  | D     | 357 | PL9  | C30-C29-C31-C32 |
| 21  | B     | 526 | CLA  | C6-C7-C8-C10    |
| 21  | C     | 484 | CLA  | C12-C13-C15-C16 |
| 26  | A     | 371 | LHG  | C1-C2-C3-O3     |
| 21  | B     | 526 | CLA  | C4-C3-C5-C6     |
| 32  | D     | 357 | PL9  | C2-C3-C7-C8     |
| 33  | F     | 85  | HEM  | CAD-CBD-CGD-O2D |
| 21  | A     | 364 | CLA  | C14-C13-C15-C16 |
| 21  | B     | 519 | CLA  | C14-C13-C15-C16 |
| 21  | C     | 484 | CLA  | C14-C13-C15-C16 |
| 30  | D     | 361 | SQD  | C11-C10-C9-C8   |
| 21  | A     | 364 | CLA  | C4-C3-C5-C6     |
| 21  | B     | 519 | CLA  | C2-C3-C5-C6     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 21  | B     | 520 | CLA  | CBA-CGA-O2A-C1  |
| 30  | C     | 475 | SQD  | O6-C44-C45-C46  |
| 30  | L     | 213 | SQD  | C44-C45-C46-O48 |
| 33  | F     | 85  | HEM  | CAA-CBA-CGA-O2A |
| 33  | F     | 85  | HEM  | CAD-CBD-CGD-O1D |
| 21  | C     | 482 | CLA  | CAA-CBA-CGA-O2A |
| 21  | B     | 521 | CLA  | C10-C11-C12-C13 |
| 21  | C     | 484 | CLA  | CAA-CBA-CGA-O2A |
| 21  | B     | 518 | CLA  | CAA-CBA-CGA-O2A |
| 33  | V     | 164 | HEM  | CAD-CBD-CGD-O1D |
| 21  | B     | 526 | CLA  | C2-C3-C5-C6     |
| 21  | B     | 515 | CLA  | C11-C12-C13-C15 |
| 33  | V     | 164 | HEM  | CAA-CBA-CGA-O2A |
| 21  | B     | 516 | CLA  | C11-C12-C13-C14 |
| 21  | B     | 522 | CLA  | C14-C13-C15-C16 |
| 30  | D     | 361 | SQD  | C45-C44-O6-C1   |
| 33  | V     | 164 | HEM  | CAD-CBD-CGD-O2D |
| 21  | B     | 521 | CLA  | C2-C1-O2A-CGA   |
| 21  | B     | 524 | CLA  | C2-C1-O2A-CGA   |
| 21  | C     | 479 | CLA  | C2-C1-O2A-CGA   |
| 30  | C     | 475 | SQD  | C11-C10-C9-C8   |
| 21  | B     | 513 | CLA  | CAA-CBA-CGA-O1A |
| 21  | B     | 515 | CLA  | CAA-CBA-CGA-O2A |
| 25  | X     | 107 | BCR  | C6-C7-C8-C9     |
| 33  | V     | 164 | HEM  | CAA-CBA-CGA-O1A |
| 27  | A     | 373 | LMG  | C32-C33-C34-C35 |
| 30  | F     | 224 | SQD  | O6-C44-C45-C46  |
| 21  | C     | 480 | CLA  | CAA-CBA-CGA-O2A |
| 30  | F     | 224 | SQD  | O47-C45-C46-O48 |
| 21  | B     | 512 | CLA  | C6-C7-C8-C9     |
| 22  | A     | 365 | PHO  | C14-C13-C15-C16 |
| 21  | C     | 483 | CLA  | CAA-CBA-CGA-O2A |
| 21  | B     | 512 | CLA  | C12-C13-C15-C16 |
| 21  | B     | 513 | CLA  | C12-C13-C15-C16 |
| 21  | B     | 519 | CLA  | C12-C13-C15-C16 |
| 21  | B     | 522 | CLA  | C12-C13-C15-C16 |
| 21  | B     | 523 | CLA  | C11-C12-C13-C15 |
| 21  | C     | 481 | CLA  | C6-C7-C8-C10    |
| 21  | C     | 484 | CLA  | C11-C12-C13-C15 |
| 21  | C     | 486 | CLA  | C11-C12-C13-C15 |
| 21  | D     | 354 | CLA  | C6-C7-C8-C10    |
| 21  | C     | 487 | CLA  | C2C-C3C-CAC-CBC |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 21  | B     | 523 | CLA  | C2-C1-O2A-CGA   |
| 21  | B     | 520 | CLA  | CAA-CBA-CGA-O2A |
| 22  | D     | 355 | PHO  | CAA-CBA-CGA-O2A |
| 30  | C     | 475 | SQD  | C15-C16-C17-C18 |
| 21  | C     | 479 | CLA  | CAA-CBA-CGA-O2A |
| 30  | L     | 213 | SQD  | C4-C5-C6-S      |
| 26  | C     | 476 | LHG  | C25-C26-C27-C28 |
| 21  | D     | 356 | CLA  | C6-C7-C8-C9     |
| 28  | C     | 474 | DGD  | O1G-C1G-C2G-C3G |
| 21  | A     | 363 | CLA  | C4B-C3B-CAB-CBB |
| 21  | A     | 364 | CLA  | C4B-C3B-CAB-CBB |
| 21  | B     | 511 | CLA  | C4B-C3B-CAB-CBB |
| 21  | B     | 513 | CLA  | C4B-C3B-CAB-CBB |
| 21  | B     | 515 | CLA  | C4B-C3B-CAB-CBB |
| 21  | B     | 516 | CLA  | C4B-C3B-CAB-CBB |
| 21  | B     | 523 | CLA  | C4B-C3B-CAB-CBB |
| 21  | C     | 477 | CLA  | C4B-C3B-CAB-CBB |
| 21  | C     | 479 | CLA  | C4B-C3B-CAB-CBB |
| 21  | C     | 480 | CLA  | C4B-C3B-CAB-CBB |
| 21  | C     | 481 | CLA  | C4B-C3B-CAB-CBB |
| 21  | C     | 484 | CLA  | C4B-C3B-CAB-CBB |
| 21  | D     | 354 | CLA  | C4B-C3B-CAB-CBB |
| 28  | B     | 528 | DGD  | O6D-C1D-O3G-C3G |
| 21  | B     | 511 | CLA  | CAA-CBA-CGA-O2A |
| 30  | C     | 475 | SQD  | O47-C7-C8-C9    |
| 22  | D     | 355 | PHO  | C15-C16-C17-C18 |
| 30  | D     | 361 | SQD  | C11-C12-C13-C14 |
| 21  | B     | 521 | CLA  | CAA-CBA-CGA-O2A |
| 21  | K     | 483 | CLA  | CAA-CBA-CGA-O2A |
| 21  | B     | 520 | CLA  | C3-C5-C6-C7     |
| 21  | C     | 484 | CLA  | C2-C1-O2A-CGA   |
| 21  | D     | 356 | CLA  | C2-C1-O2A-CGA   |
| 22  | D     | 355 | PHO  | C2-C1-O2A-CGA   |
| 21  | A     | 364 | CLA  | C11-C12-C13-C15 |
| 21  | C     | 481 | CLA  | C12-C13-C15-C16 |
| 21  | D     | 356 | CLA  | C6-C7-C8-C10    |
| 21  | D     | 354 | CLA  | CAA-CBA-CGA-O2A |
| 21  | A     | 364 | CLA  | C2C-C3C-CAC-CBC |
| 32  | D     | 357 | PL9  | C21-C22-C23-C24 |
| 21  | C     | 480 | CLA  | CAA-CBA-CGA-O1A |
| 32  | D     | 357 | PL9  | C28-C29-C31-C32 |
| 21  | B     | 514 | CLA  | C13-C15-C16-C17 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 21  | C     | 483 | CLA  | CAA-CBA-CGA-O1A |
| 30  | C     | 475 | SQD  | O49-C7-C8-C9    |
| 30  | F     | 224 | SQD  | C7-C8-C9-C10    |
| 21  | B     | 526 | CLA  | C6-C7-C8-C9     |
| 21  | K     | 483 | CLA  | C14-C13-C15-C16 |
| 22  | D     | 355 | PHO  | CAA-CBA-CGA-O1A |
| 27  | D     | 360 | LMG  | C8-C7-O1-C1     |
| 21  | C     | 481 | CLA  | O1A-CGA-O2A-C1  |
| 21  | B     | 520 | CLA  | CAA-CBA-CGA-O1A |
| 30  | F     | 224 | SQD  | C44-C45-C46-O48 |
| 21  | B     | 521 | CLA  | CAA-CBA-CGA-O1A |
| 32  | D     | 357 | PL9  | C11-C12-C13-C14 |
| 32  | D     | 357 | PL9  | C41-C42-C43-C44 |
| 26  | A     | 371 | LHG  | O7-C7-C8-C9     |
| 21  | C     | 484 | CLA  | C13-C15-C16-C17 |
| 21  | B     | 511 | CLA  | CAA-CBA-CGA-O1A |
| 21  | B     | 514 | CLA  | CAA-CBA-CGA-O2A |
| 30  | L     | 213 | SQD  | O47-C7-C8-C9    |
| 21  | C     | 478 | CLA  | CAA-CBA-CGA-O2A |
| 21  | D     | 354 | CLA  | CAA-CBA-CGA-O1A |
| 26  | A     | 371 | LHG  | O9-C7-C8-C9     |

There are no ring outliers.

77 monomers are involved in 672 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 26  | A     | 371 | LHG  | 7       | 0            |
| 21  | B     | 522 | CLA  | 10      | 0            |
| 21  | K     | 483 | CLA  | 12      | 0            |
| 28  | C     | 491 | DGD  | 17      | 0            |
| 21  | C     | 479 | CLA  | 19      | 0            |
| 29  | I     | 274 | LMT  | 2       | 0            |
| 21  | C     | 488 | CLA  | 6       | 0            |
| 29  | D     | 536 | LMT  | 1       | 0            |
| 27  | A     | 373 | LMG  | 40      | 0            |
| 25  | A     | 369 | BCR  | 9       | 0            |
| 27  | D     | 359 | LMG  | 6       | 0            |
| 28  | B     | 533 | DGD  | 18      | 0            |
| 25  | J     | 115 | BCR  | 7       | 0            |
| 21  | C     | 480 | CLA  | 14      | 0            |
| 25  | B     | 527 | BCR  | 1       | 0            |
| 21  | B     | 518 | CLA  | 12      | 0            |

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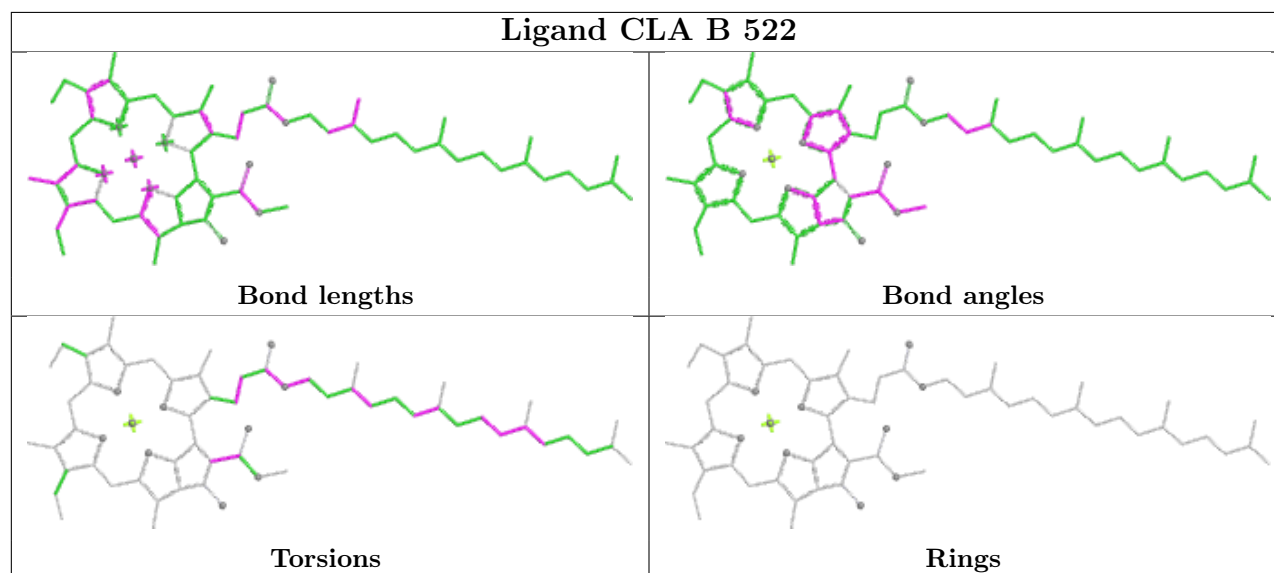
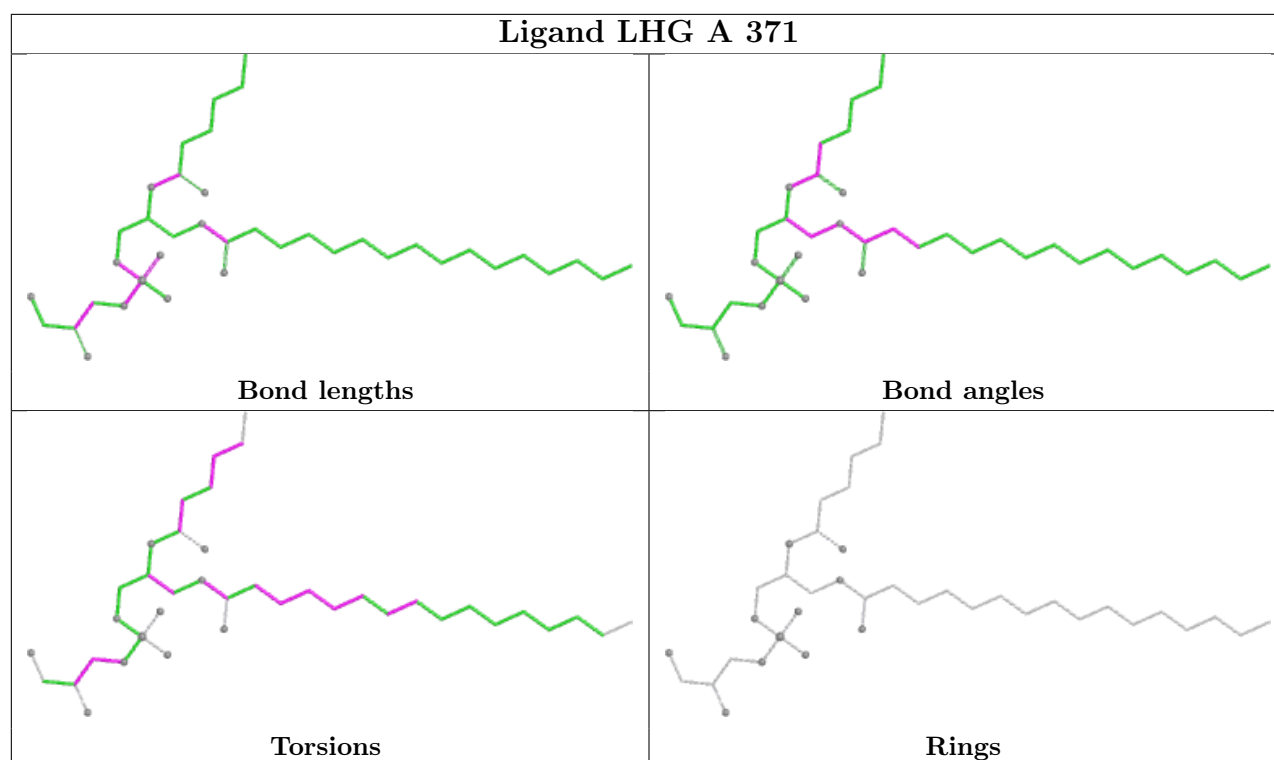
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 21  | B     | 520 | CLA  | 7       | 0            |
| 21  | C     | 483 | CLA  | 11      | 0            |
| 27  | B     | 531 | LMG  | 6       | 0            |
| 21  | B     | 519 | CLA  | 6       | 0            |
| 21  | B     | 524 | CLA  | 5       | 0            |
| 28  | C     | 474 | DGD  | 8       | 0            |
| 21  | A     | 362 | CLA  | 19      | 0            |
| 21  | B     | 514 | CLA  | 9       | 0            |
| 25  | B     | 530 | BCR  | 2       | 0            |
| 25  | Z     | 116 | BCR  | 5       | 0            |
| 21  | B     | 523 | CLA  | 5       | 0            |
| 30  | D     | 361 | SQD  | 9       | 0            |
| 21  | C     | 487 | CLA  | 15      | 0            |
| 21  | B     | 525 | CLA  | 6       | 0            |
| 27  | J     | 492 | LMG  | 4       | 0            |
| 27  | C     | 494 | LMG  | 6       | 0            |
| 21  | C     | 478 | CLA  | 13      | 0            |
| 25  | X     | 107 | BCR  | 5       | 0            |
| 25  | C     | 489 | BCR  | 17      | 0            |
| 21  | C     | 486 | CLA  | 21      | 0            |
| 33  | F     | 85  | HEM  | 6       | 0            |
| 23  | A     | 367 | MES  | 13      | 0            |
| 21  | B     | 515 | CLA  | 9       | 0            |
| 32  | D     | 357 | PL9  | 30      | 0            |
| 21  | C     | 484 | CLA  | 13      | 0            |
| 21  | C     | 485 | CLA  | 2       | 0            |
| 21  | D     | 354 | CLA  | 15      | 0            |
| 28  | B     | 528 | DGD  | 23      | 0            |
| 21  | B     | 513 | CLA  | 23      | 0            |
| 29  | B     | 535 | LMT  | 2       | 0            |
| 21  | B     | 516 | CLA  | 7       | 0            |
| 21  | B     | 517 | CLA  | 19      | 0            |
| 25  | B     | 529 | BCR  | 5       | 0            |
| 28  | C     | 492 | DGD  | 14      | 0            |
| 28  | A     | 375 | DGD  | 1       | 0            |
| 25  | J     | 112 | BCR  | 12      | 0            |
| 30  | C     | 475 | SQD  | 5       | 0            |
| 21  | A     | 363 | CLA  | 14      | 0            |
| 28  | C     | 493 | DGD  | 40      | 0            |
| 21  | B     | 526 | CLA  | 4       | 0            |
| 21  | B     | 512 | CLA  | 9       | 0            |
| 21  | C     | 481 | CLA  | 16      | 0            |

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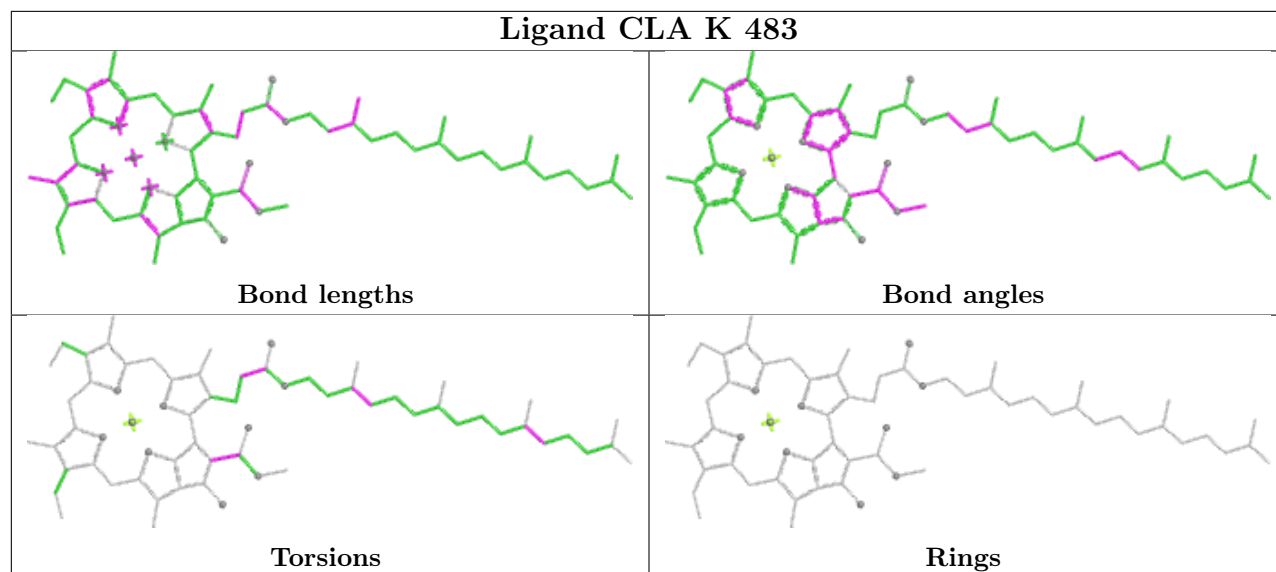
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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 30  | L     | 213 | SQD  | 2       | 0            |
| 26  | C     | 476 | LHG  | 5       | 0            |
| 27  | M     | 217 | LMG  | 3       | 0            |
| 21  | D     | 356 | CLA  | 3       | 0            |
| 33  | V     | 164 | HEM  | 5       | 0            |
| 21  | B     | 511 | CLA  | 3       | 0            |
| 21  | C     | 482 | CLA  | 7       | 0            |
| 21  | C     | 477 | CLA  | 9       | 0            |
| 29  | T     | 226 | LMT  | 1       | 0            |
| 22  | D     | 355 | PHO  | 15      | 0            |
| 21  | B     | 521 | CLA  | 13      | 0            |
| 29  | D     | 363 | LMT  | 2       | 0            |
| 21  | A     | 364 | CLA  | 7       | 0            |
| 25  | D     | 358 | BCR  | 8       | 0            |
| 21  | A     | 366 | CLA  | 9       | 0            |
| 25  | C     | 490 | BCR  | 7       | 0            |
| 29  | O     | 274 | LMT  | 1       | 0            |
| 22  | A     | 365 | PHO  | 6       | 0            |
| 27  | D     | 360 | LMG  | 30      | 0            |

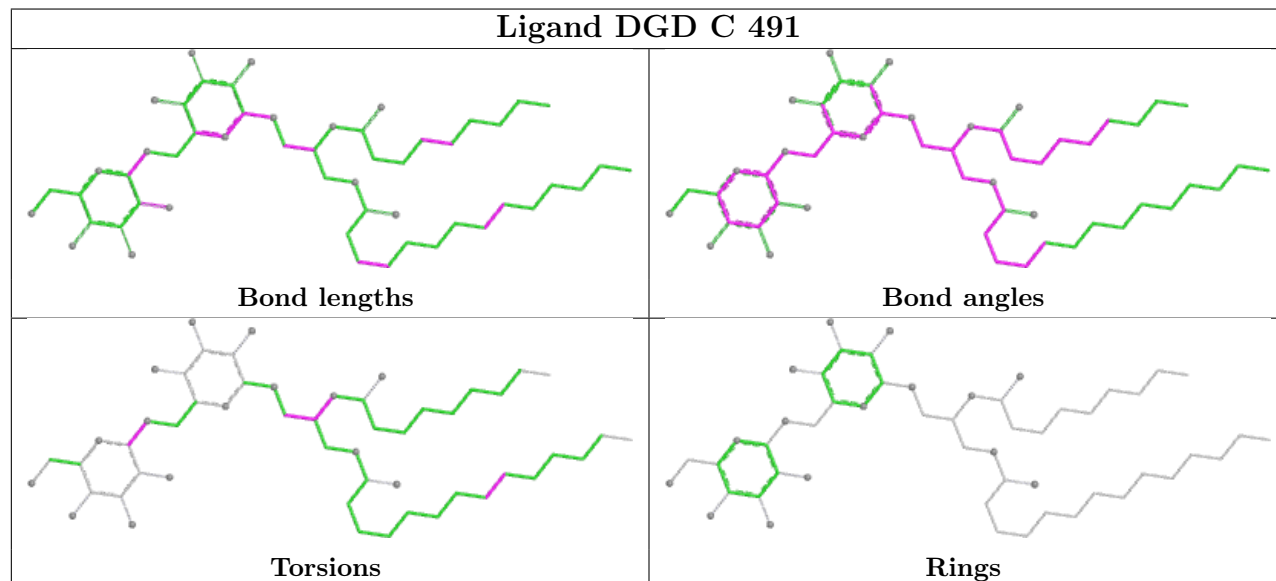
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



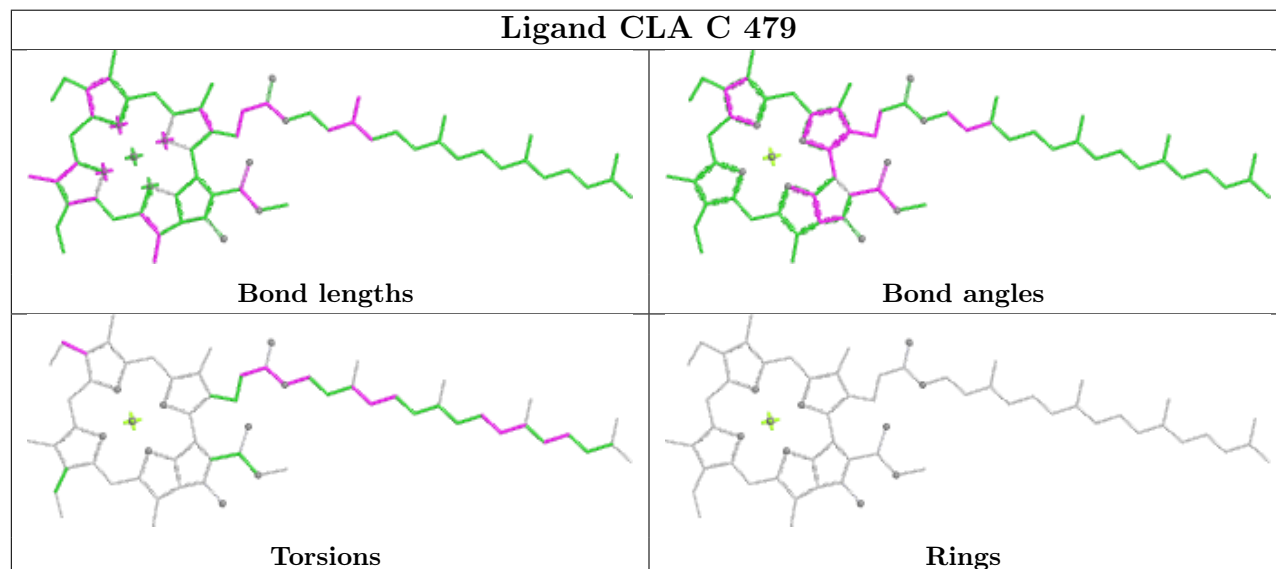
## Ligand CLA K 483

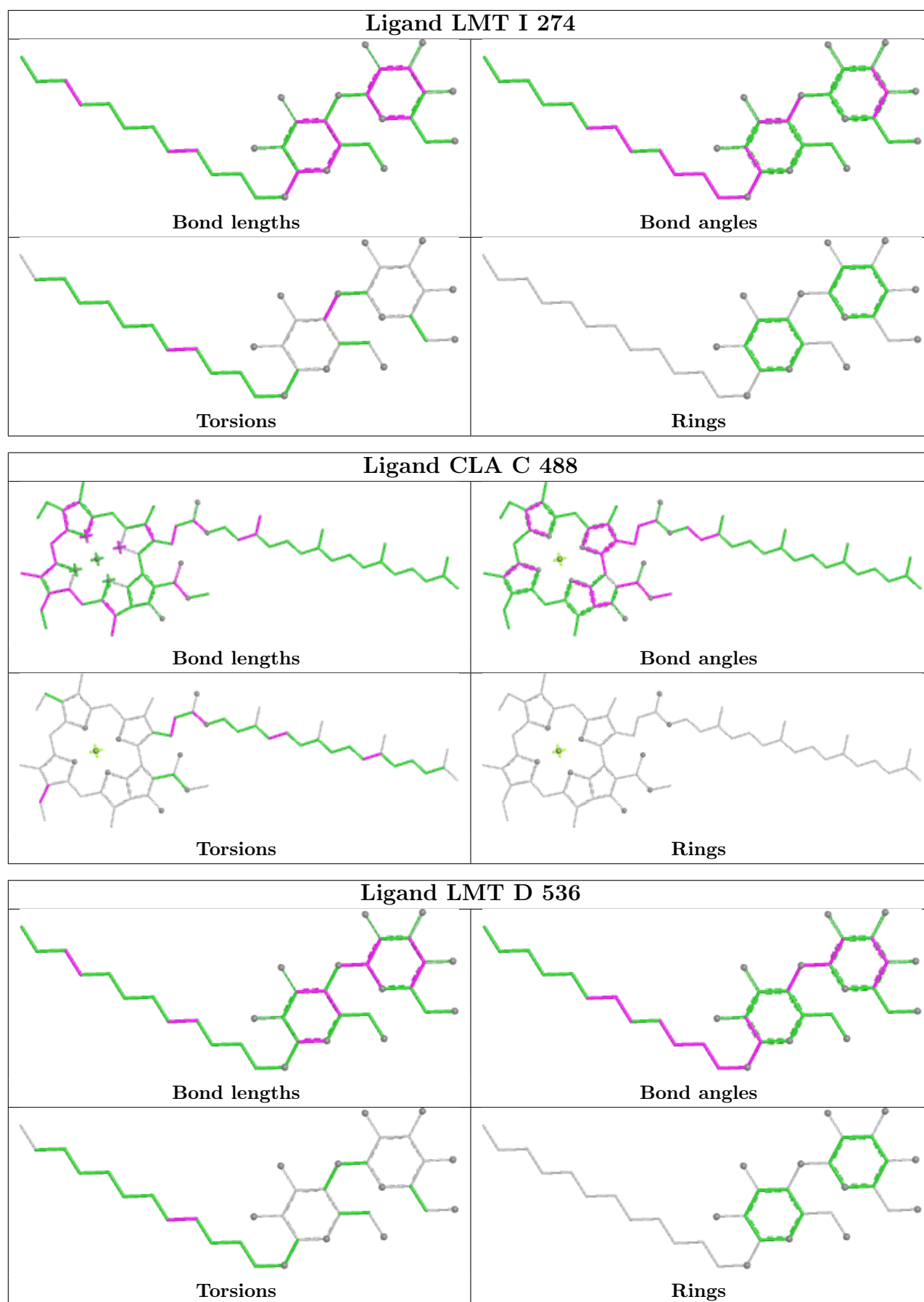


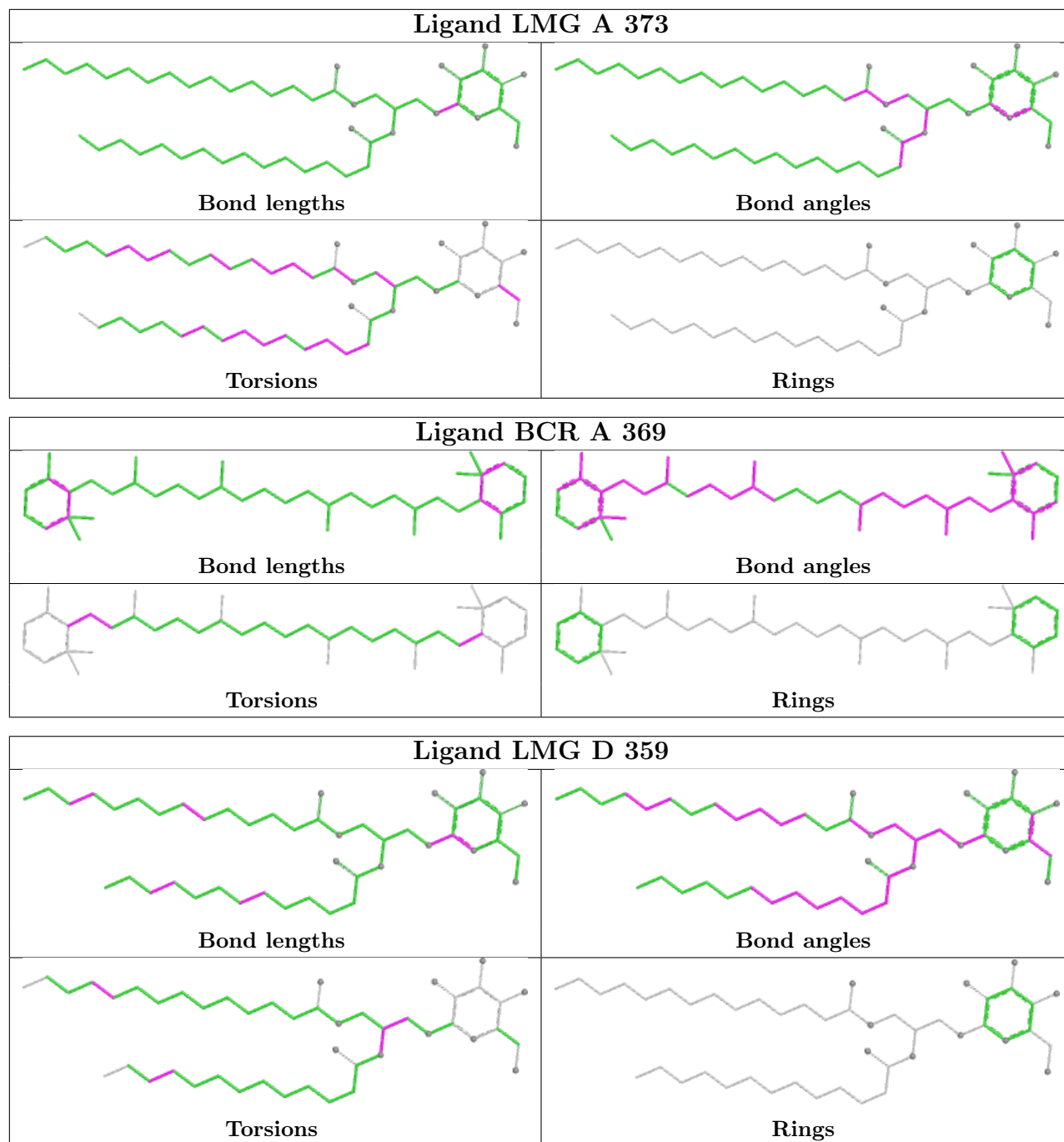
## Ligand DGD C 491

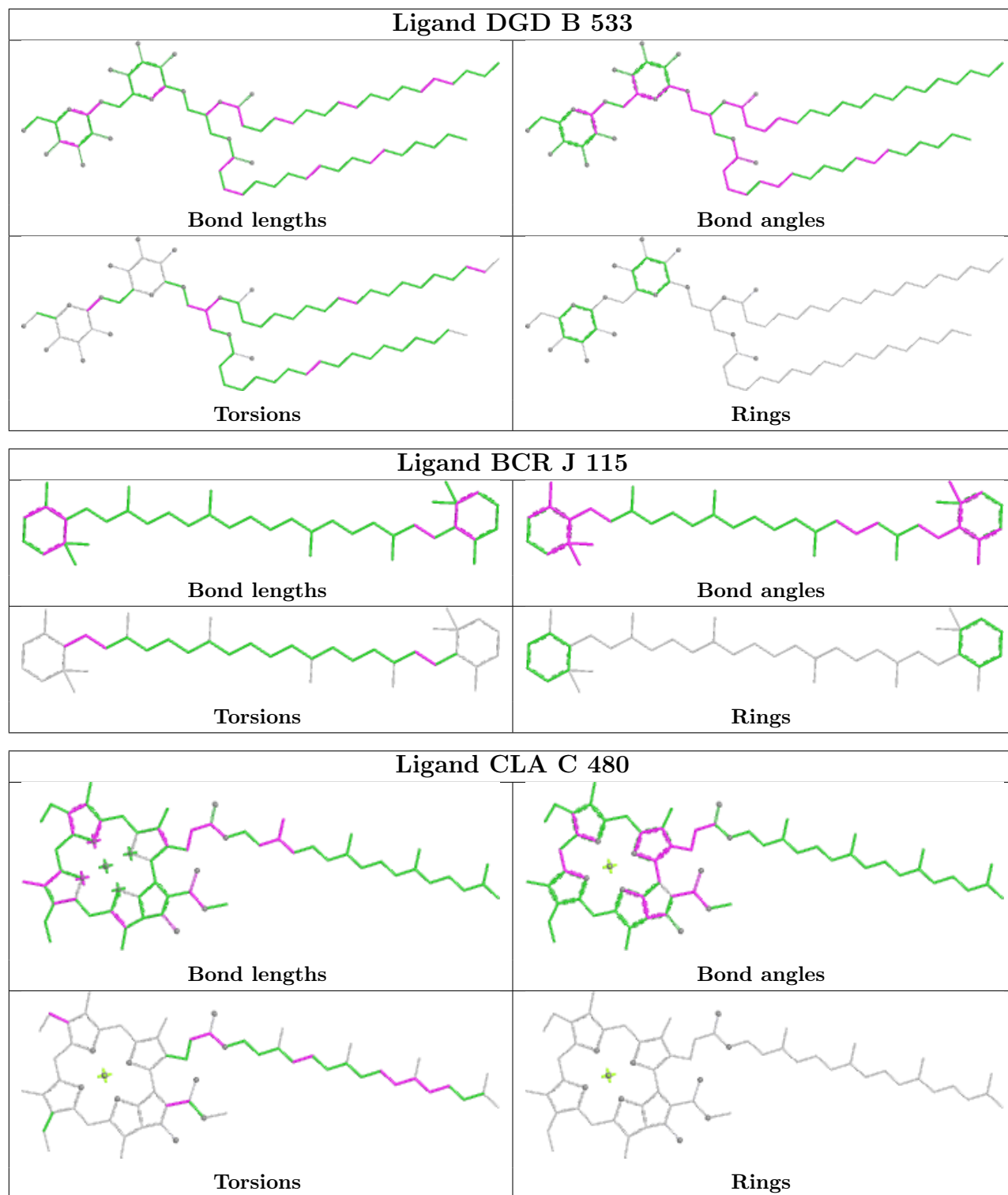


## Ligand CLA C 479

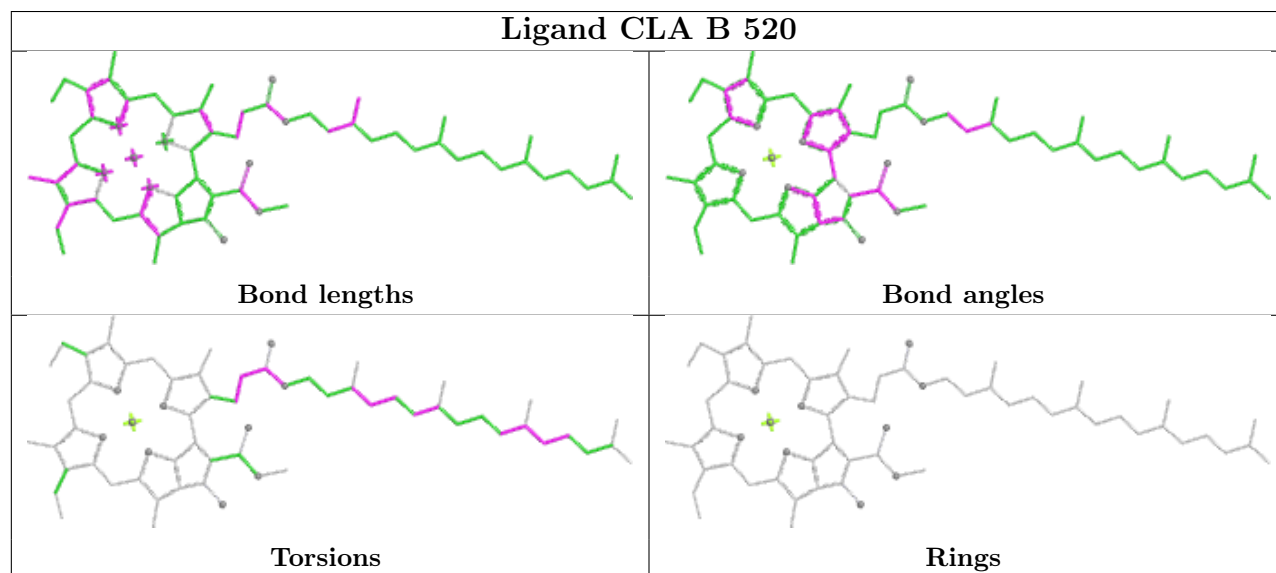
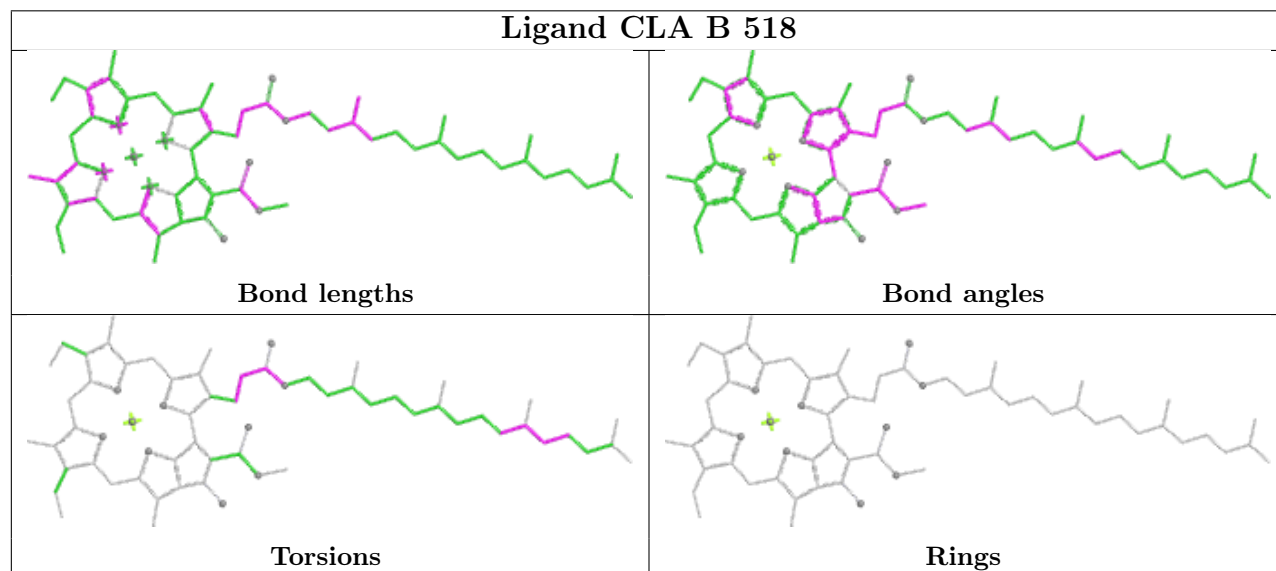
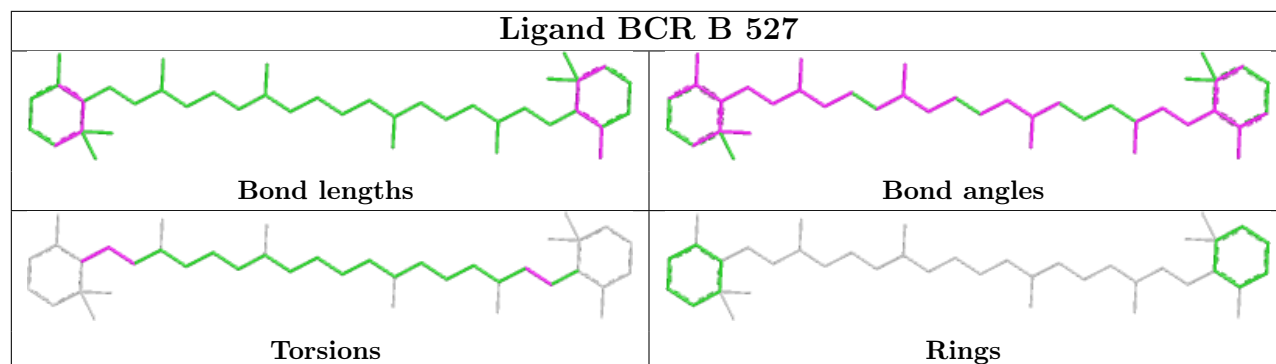




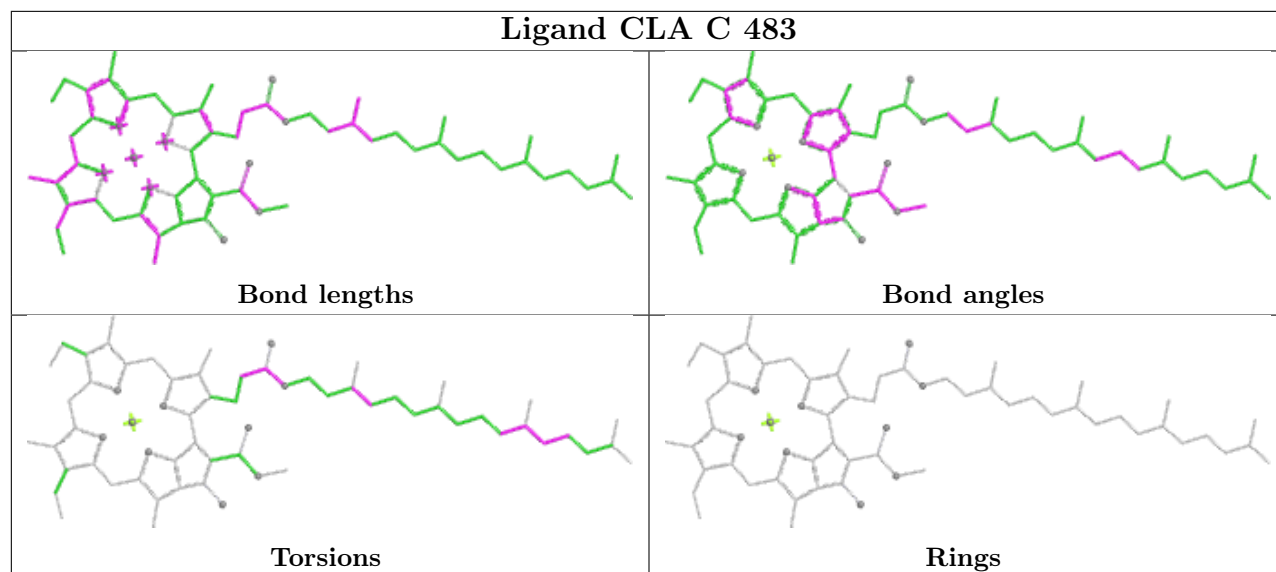




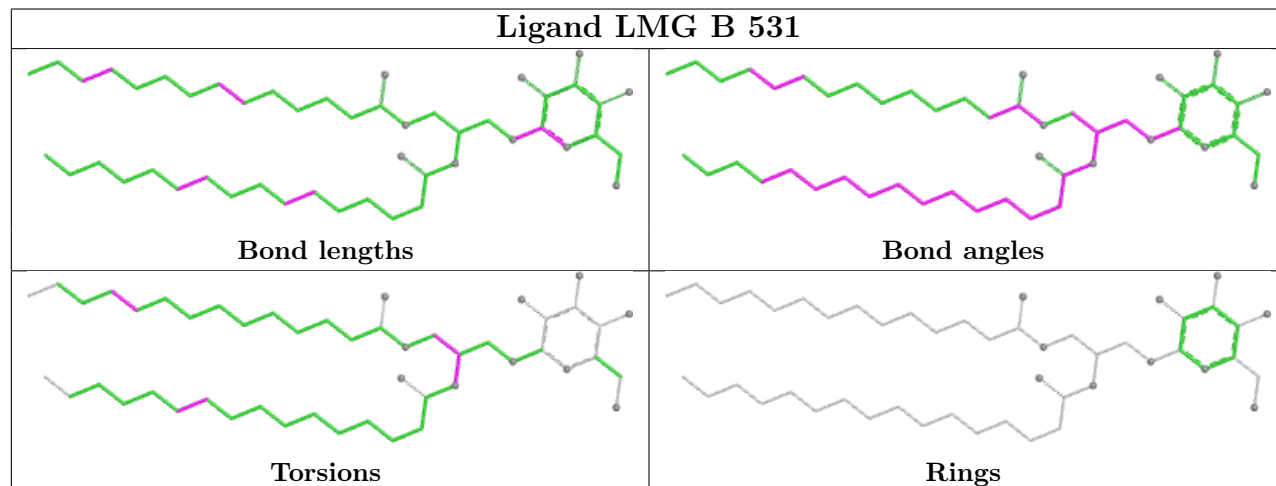




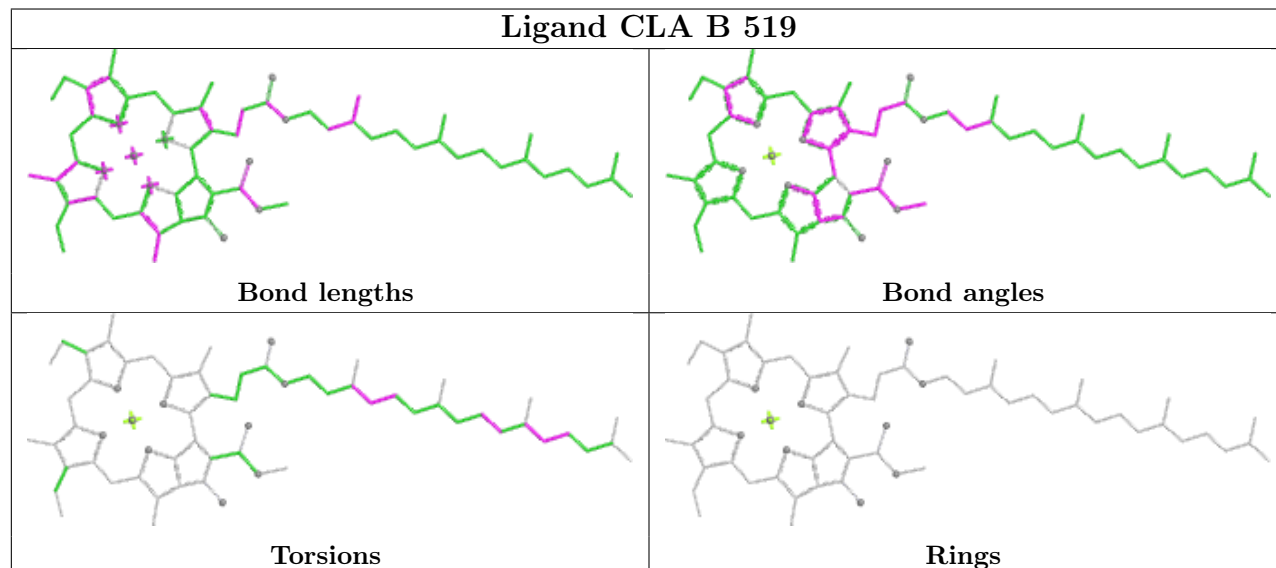
## Ligand CLA C 483



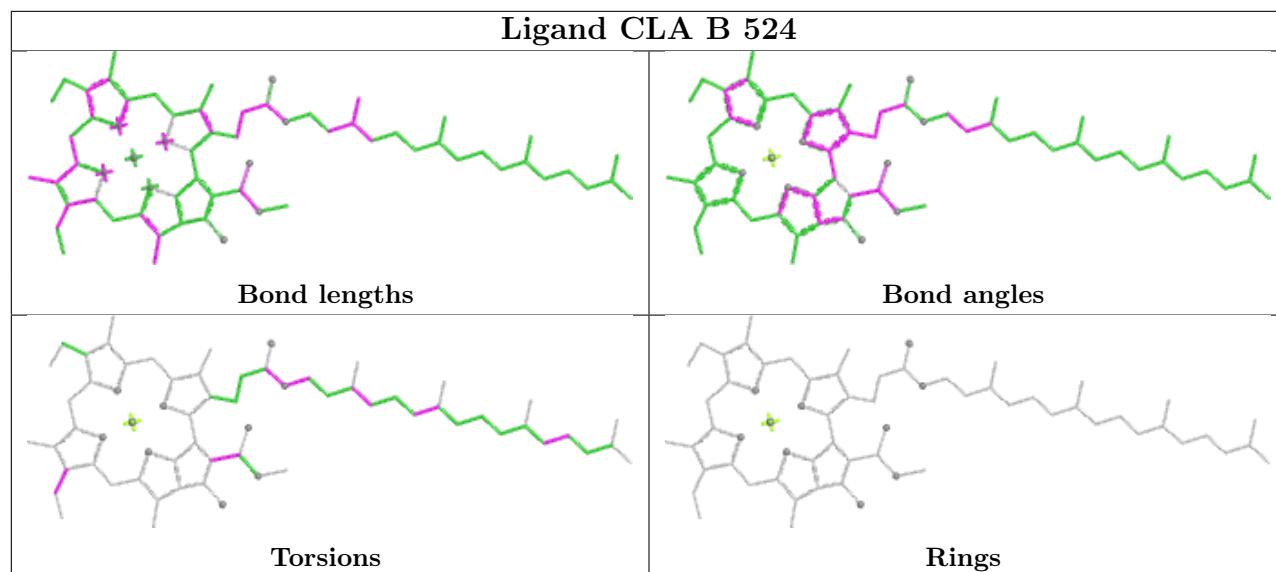
## Ligand LMG B 531



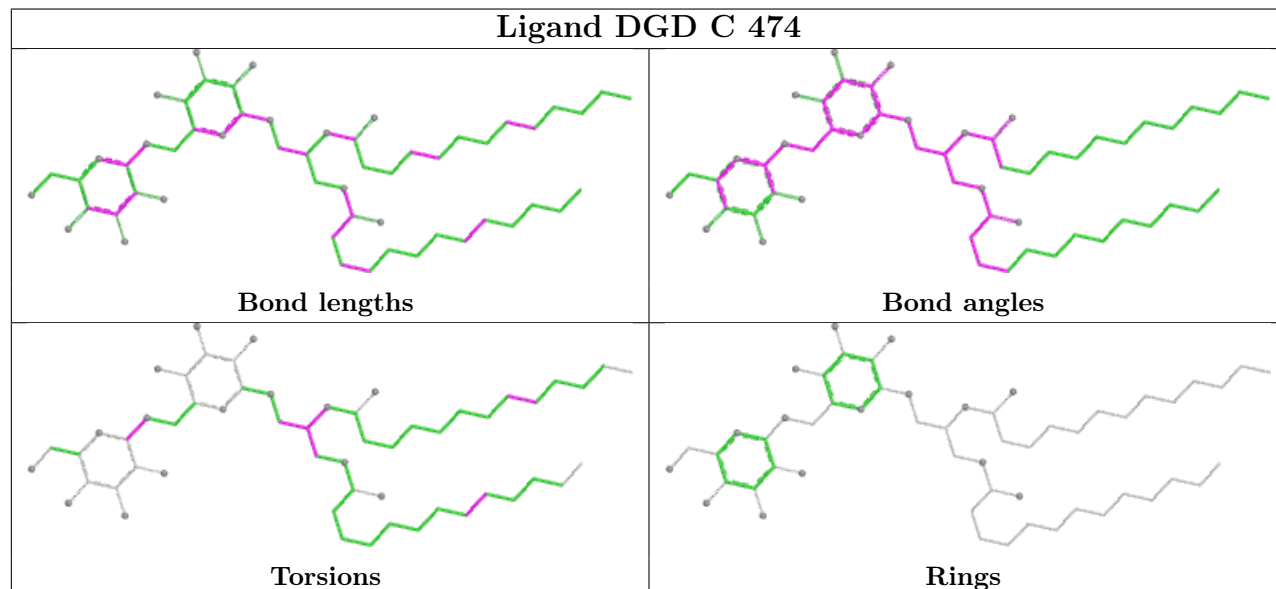
## Ligand CLA B 519



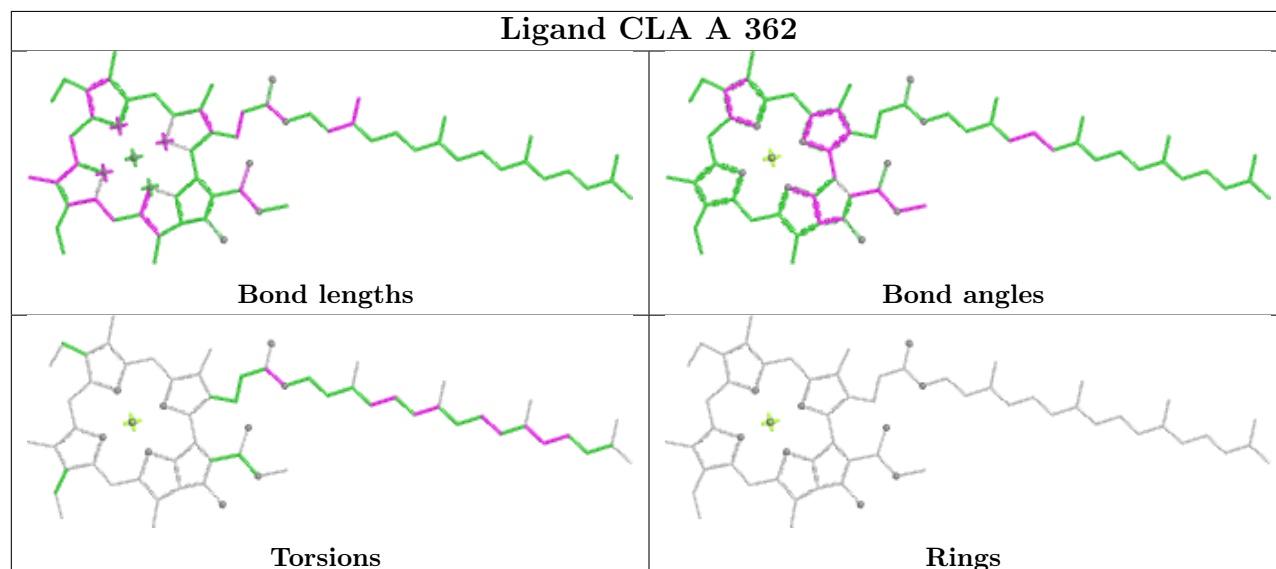
## Ligand CLA B 524

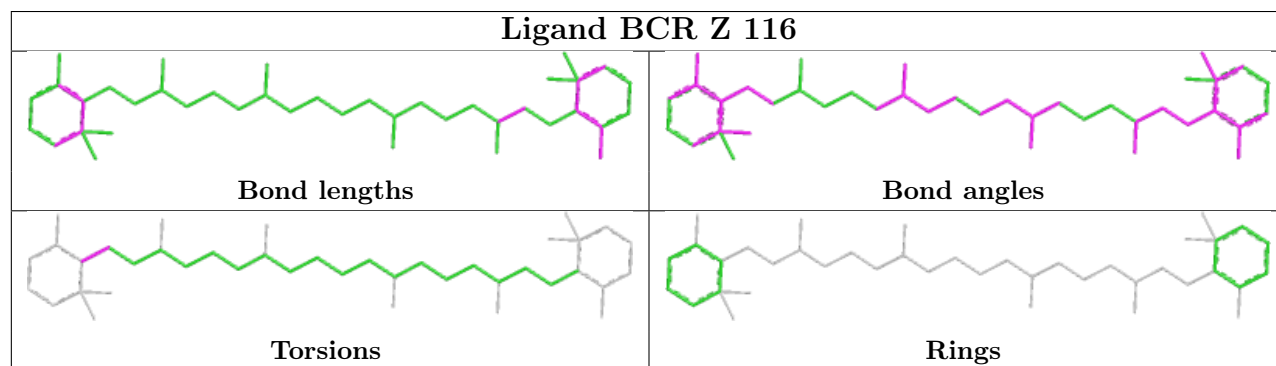
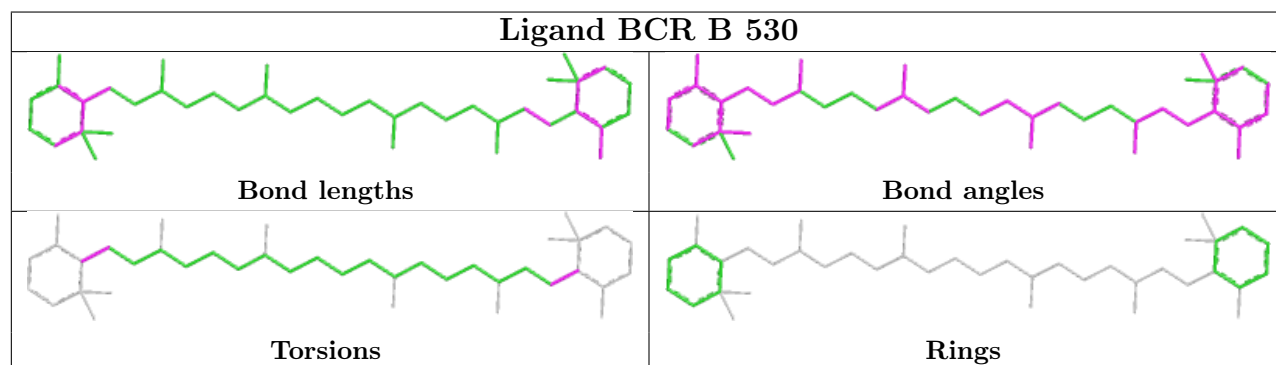
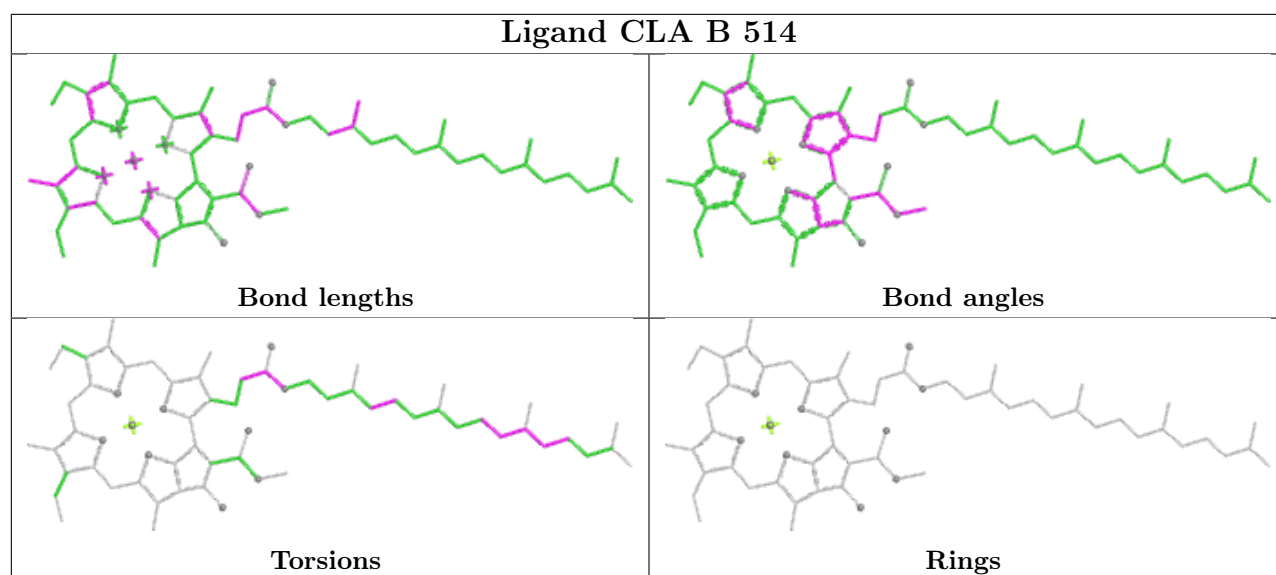


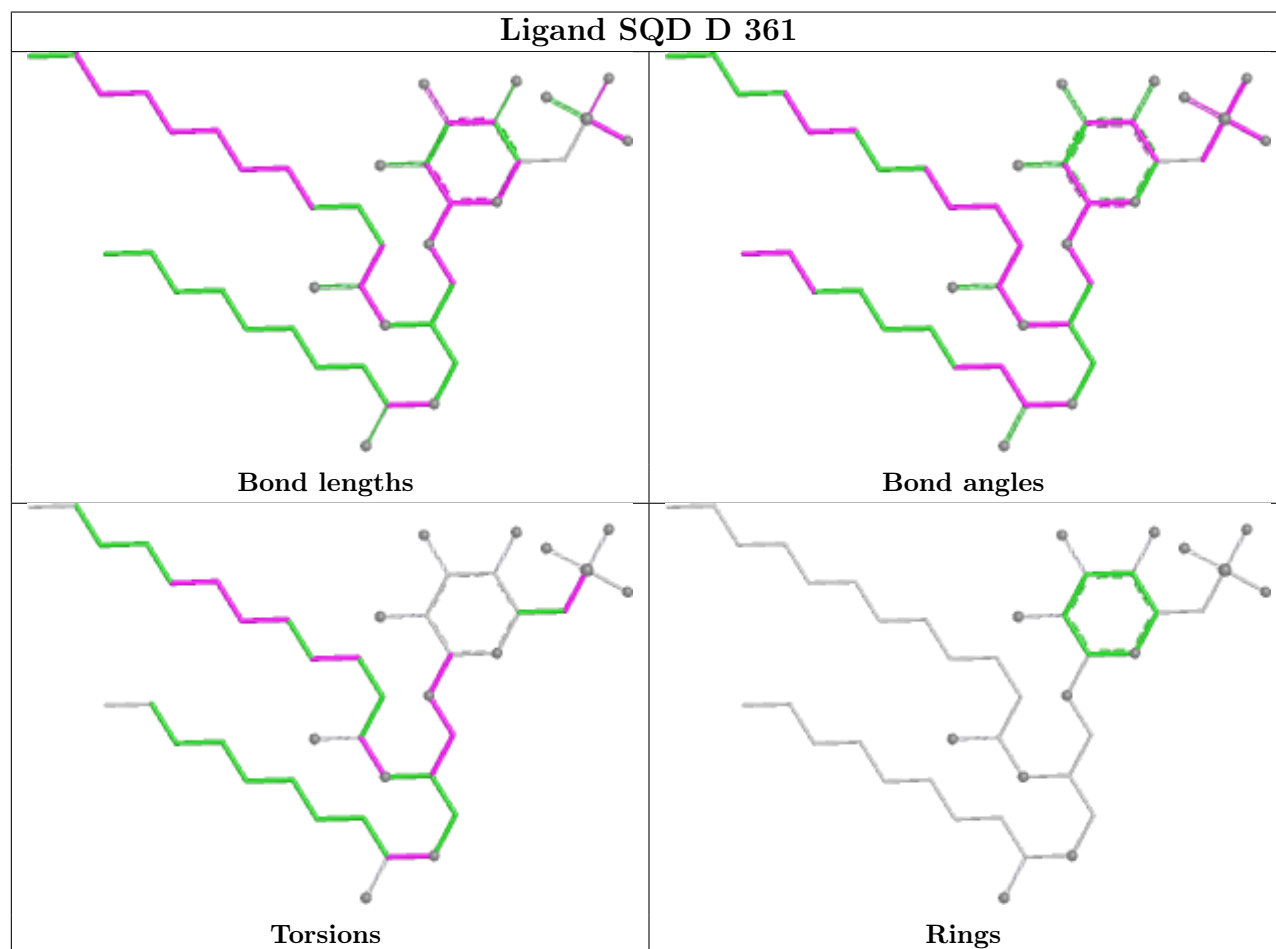
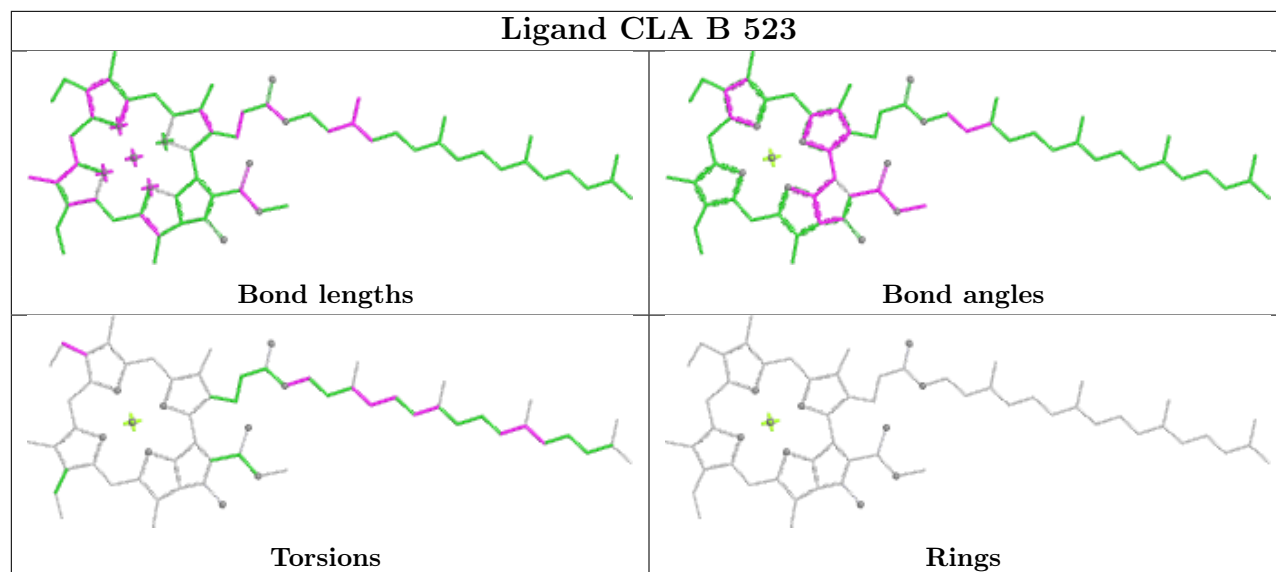
## Ligand DGD C 474



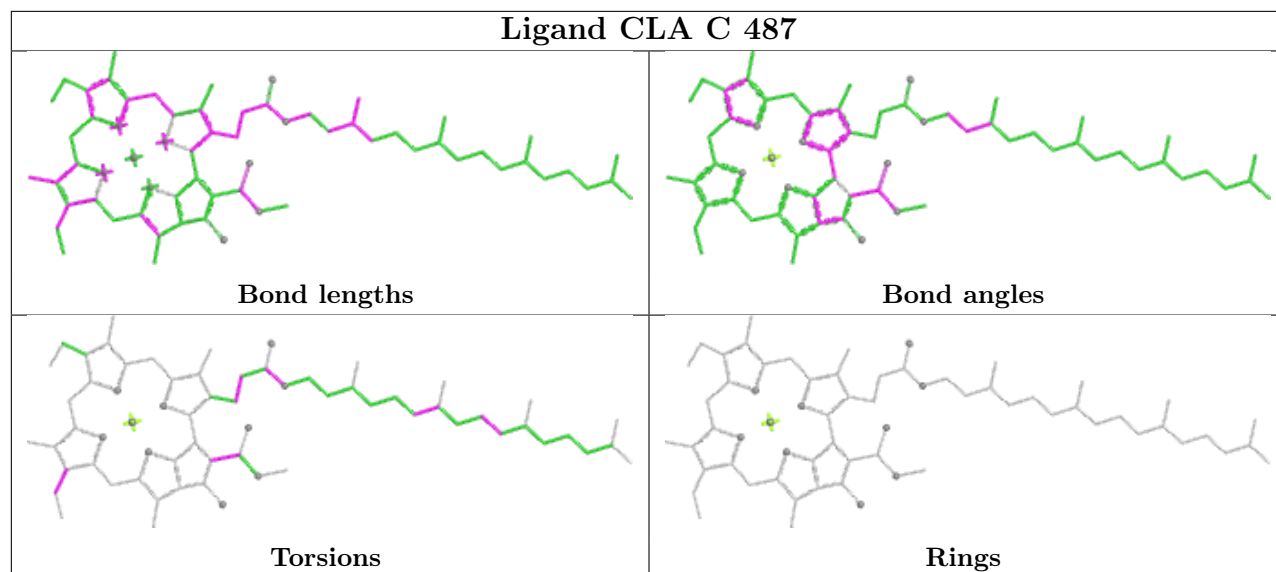
## Ligand CLA A 362



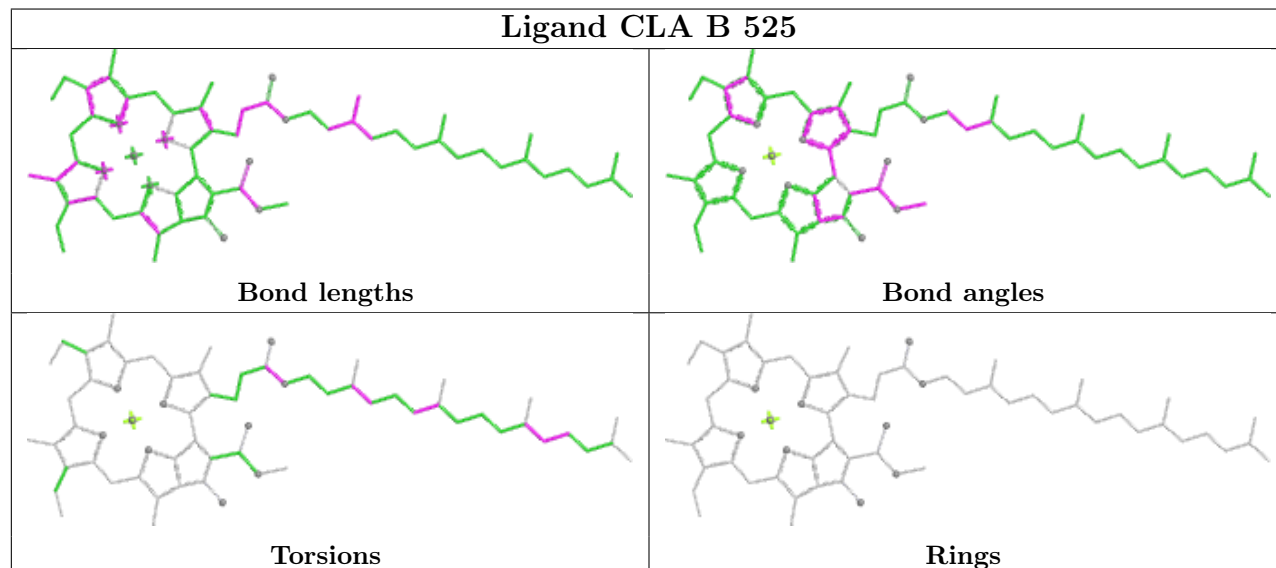




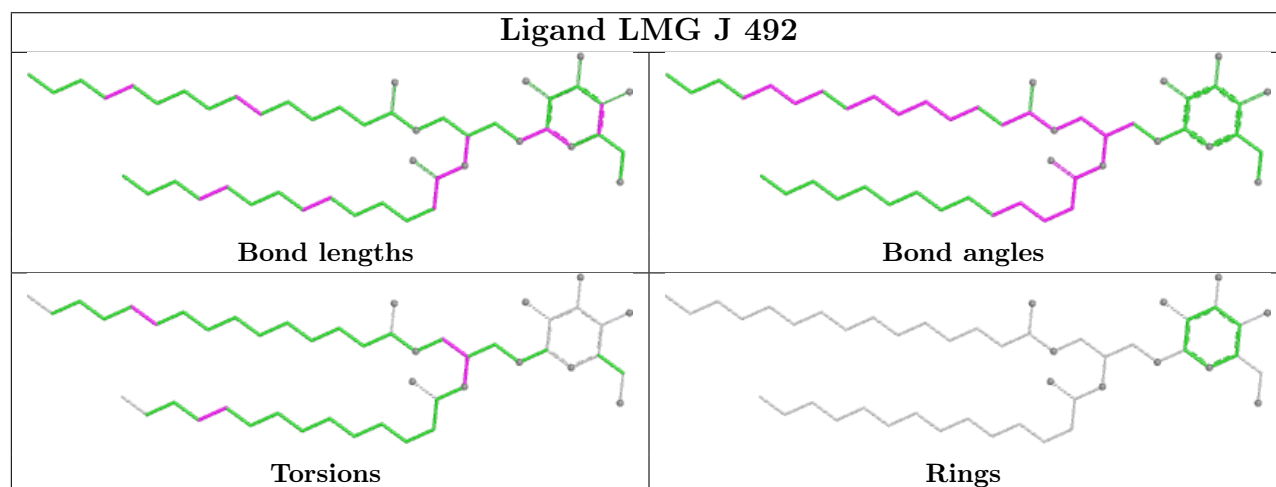
## Ligand CLA C 487

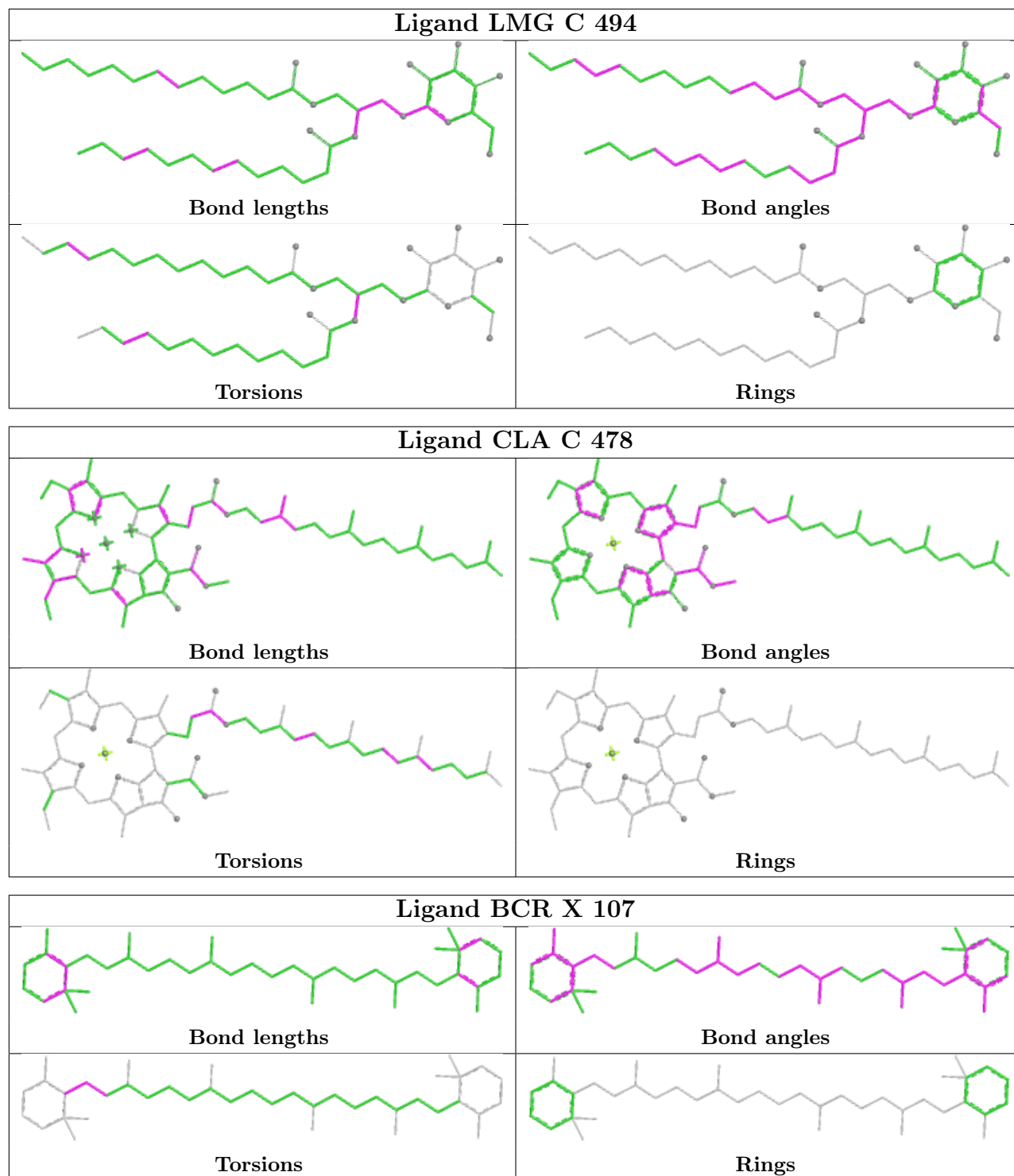


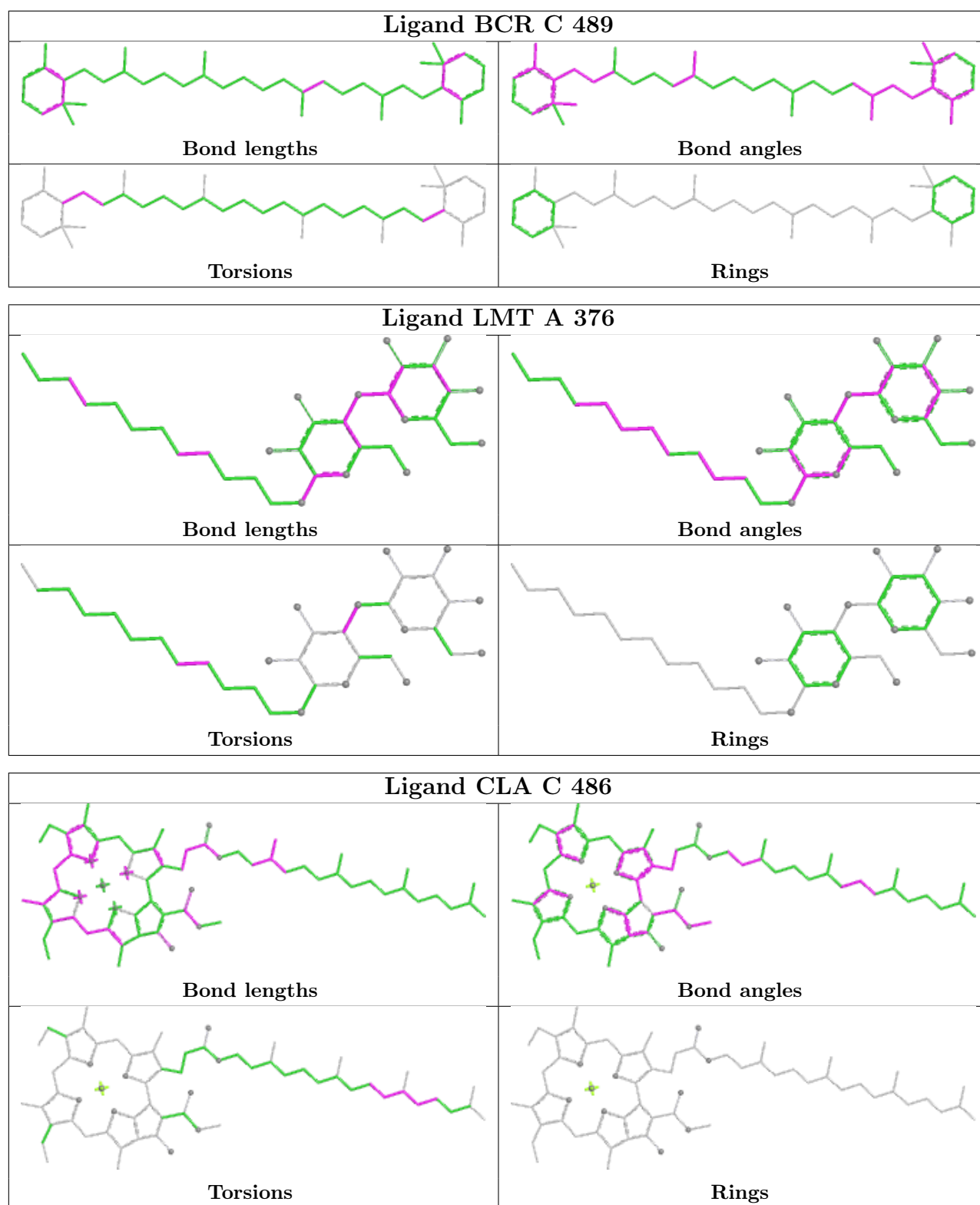
## Ligand CLA B 525



## Ligand LMG J 492

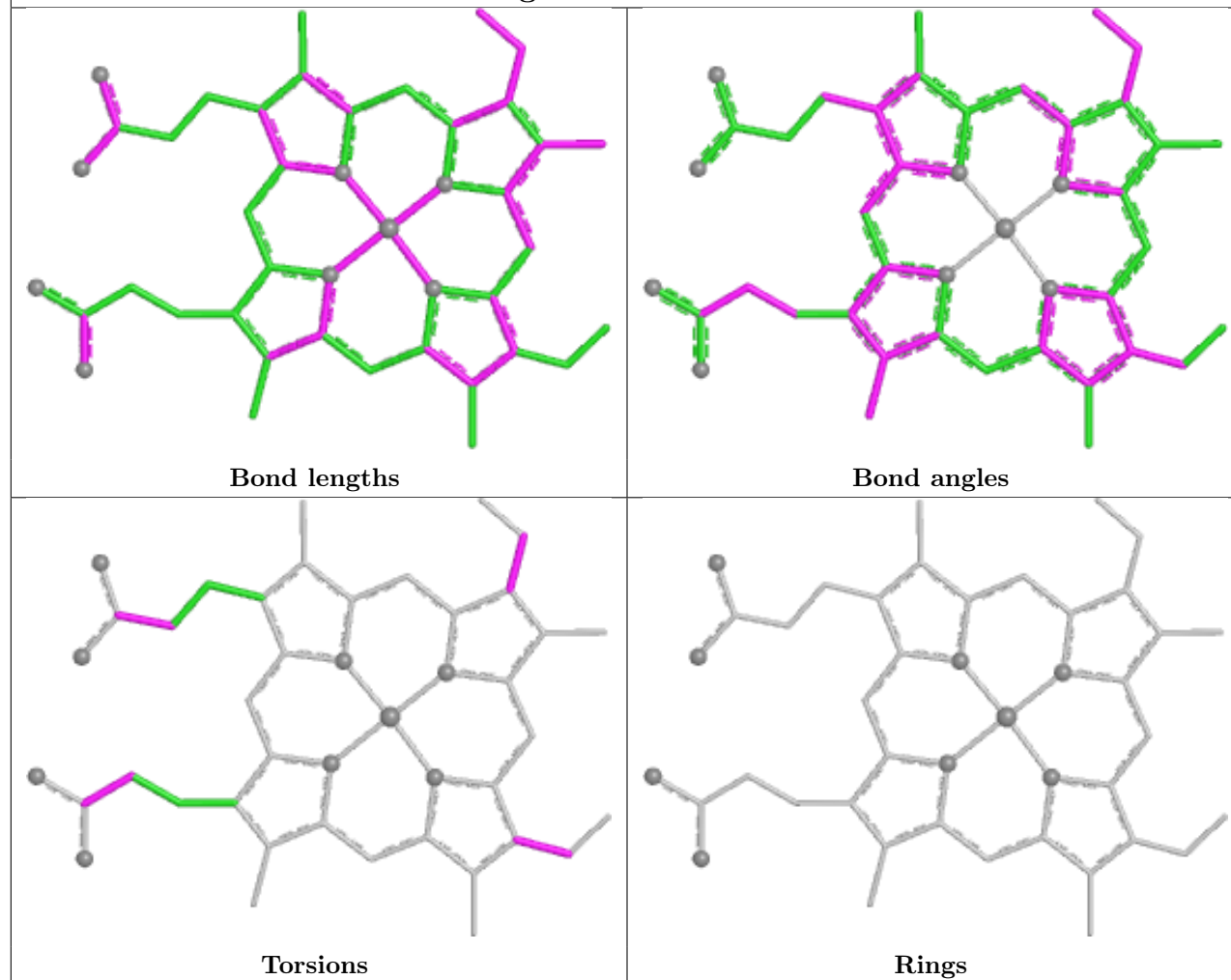




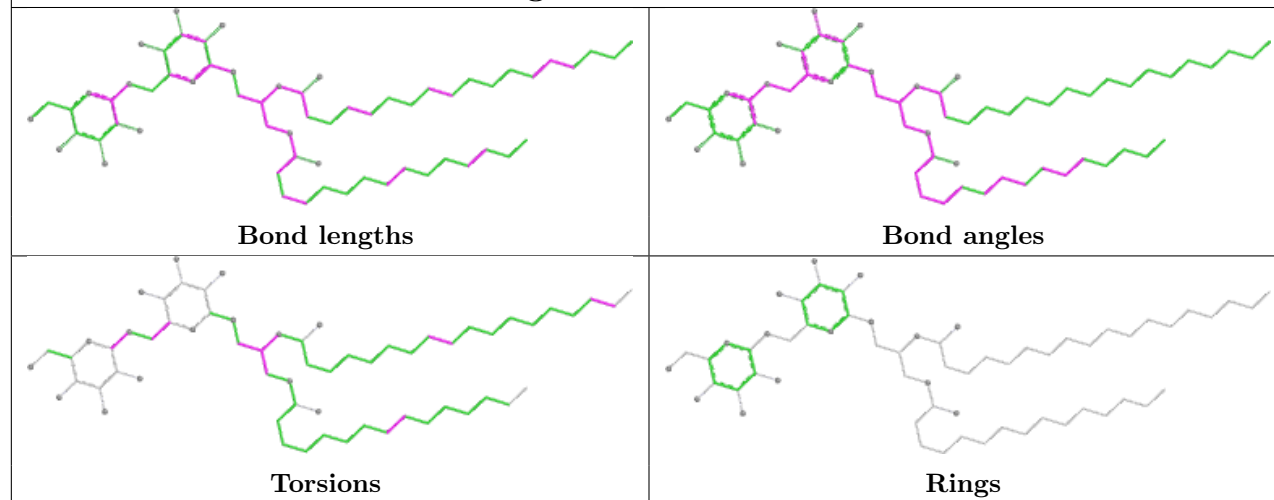


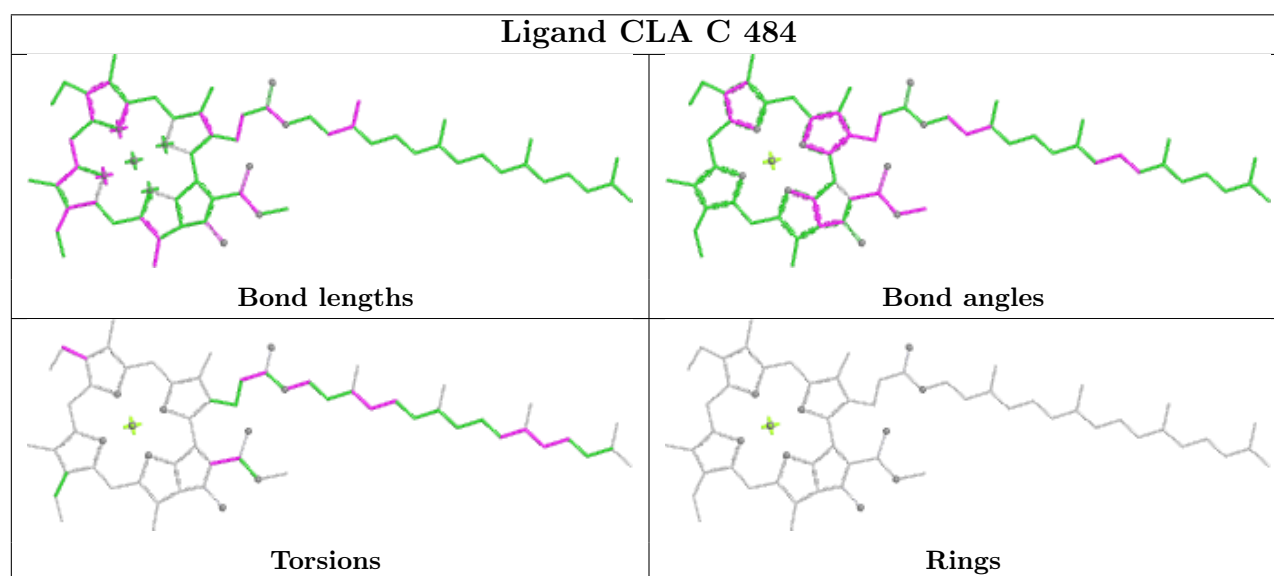
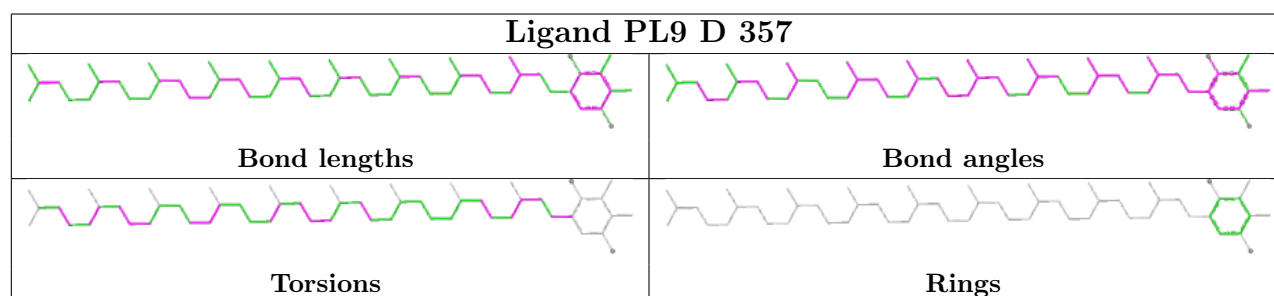
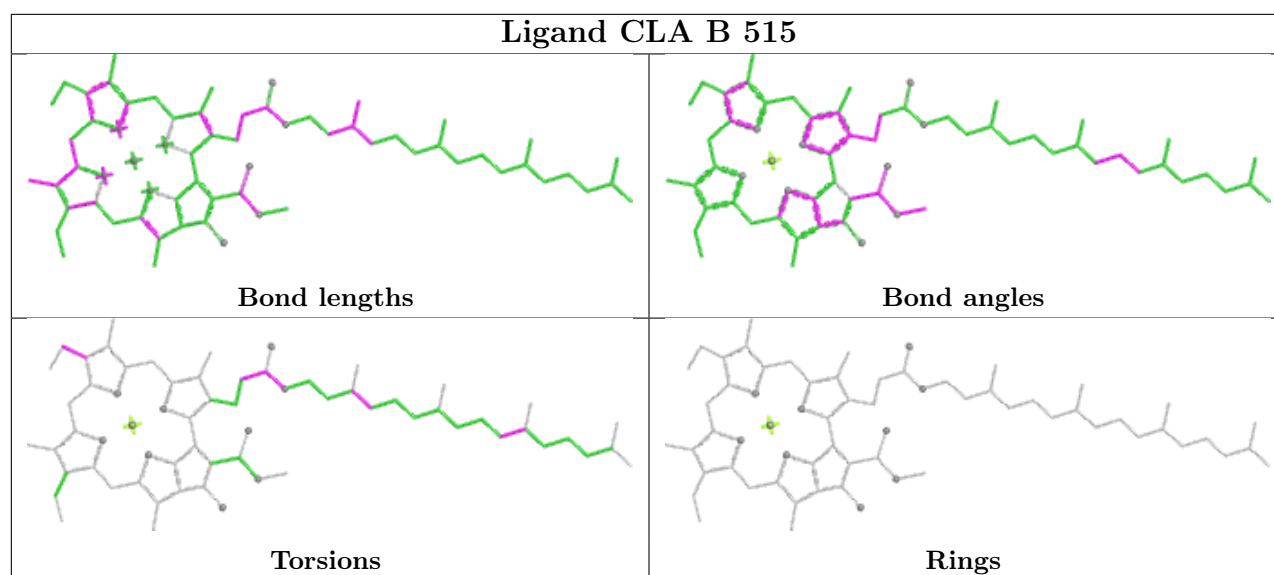


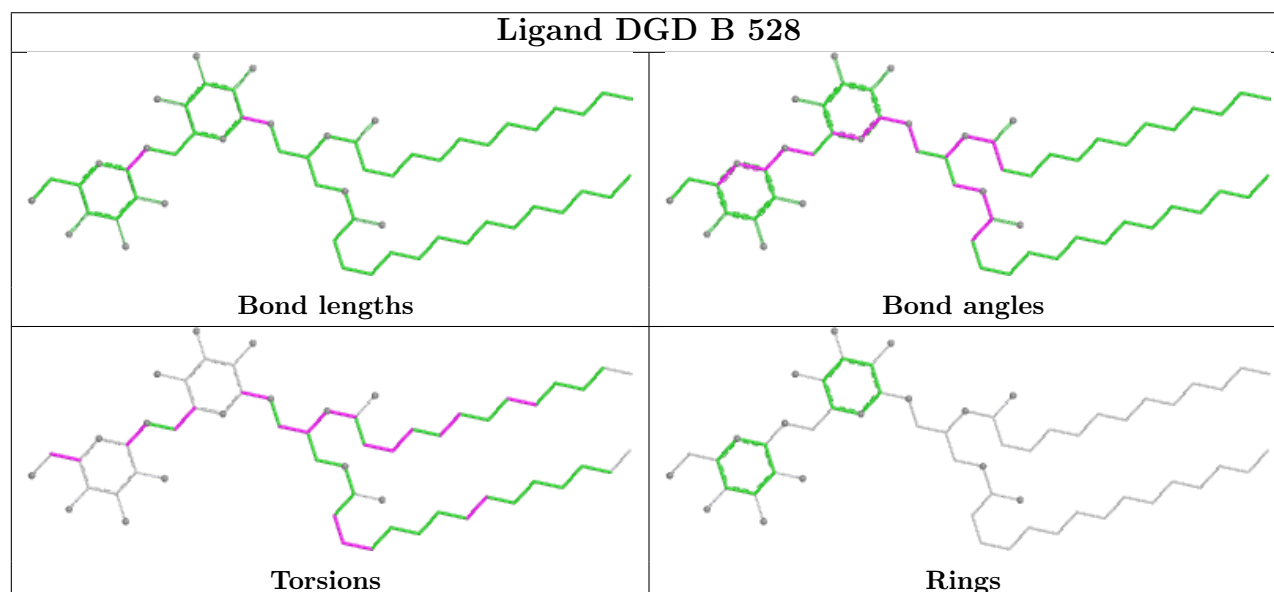
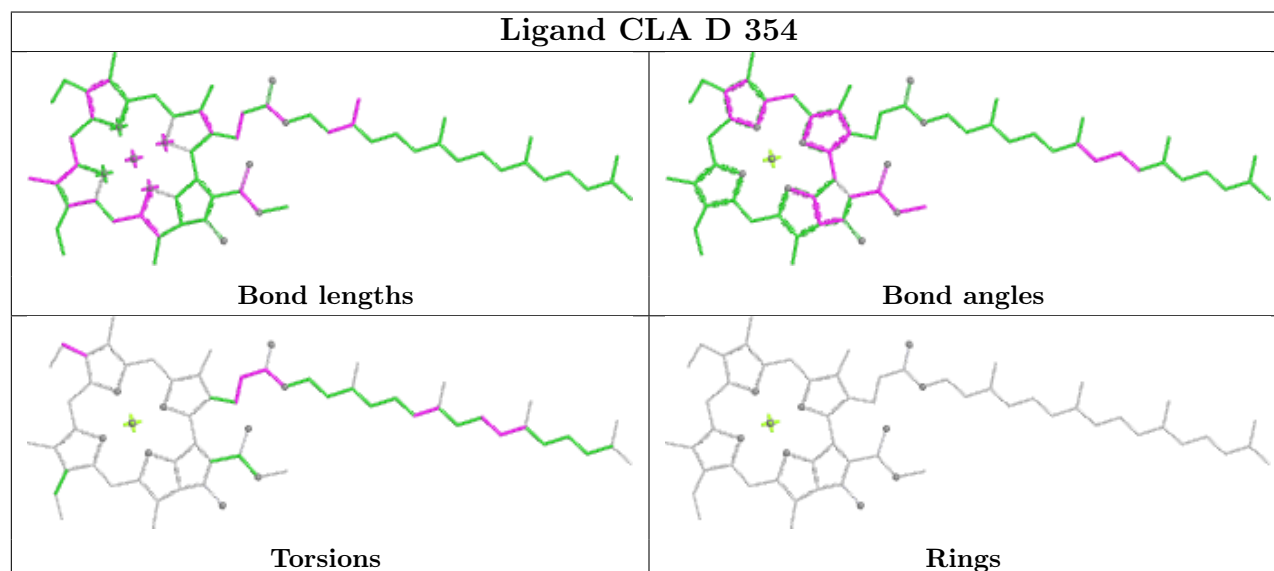
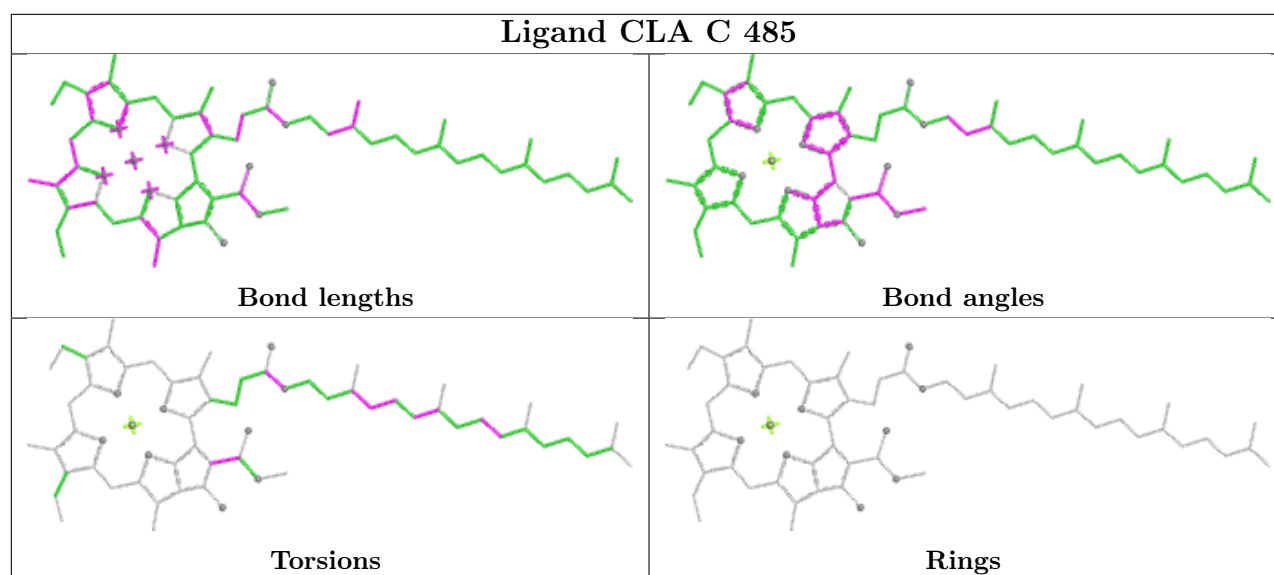
## Ligand HEM F 85



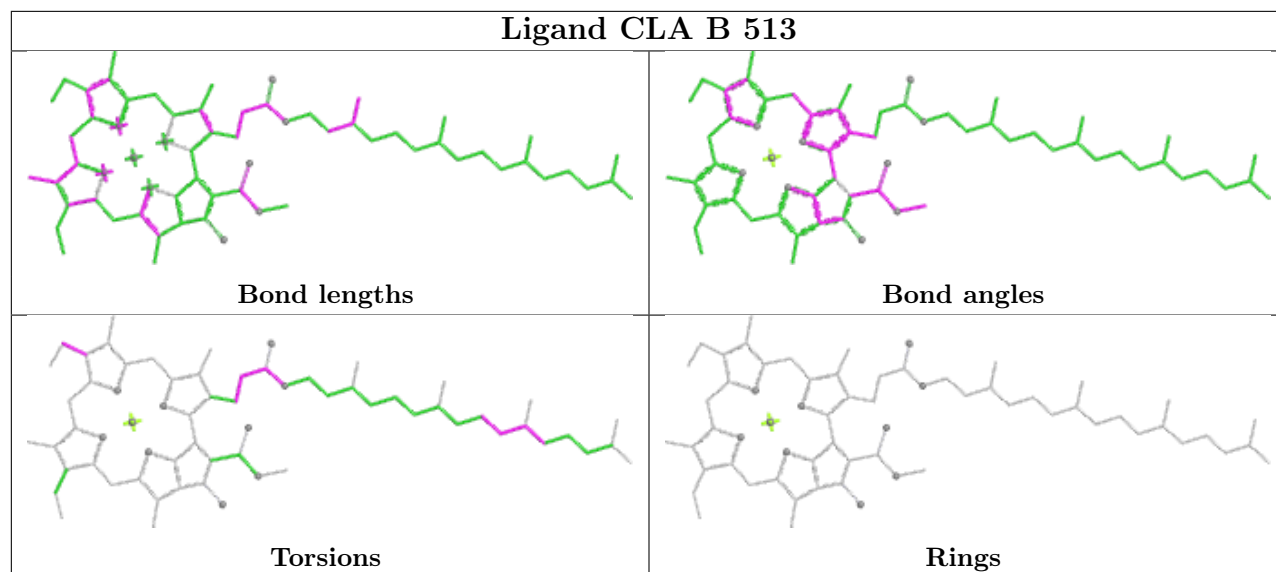
## Ligand DGD D 362



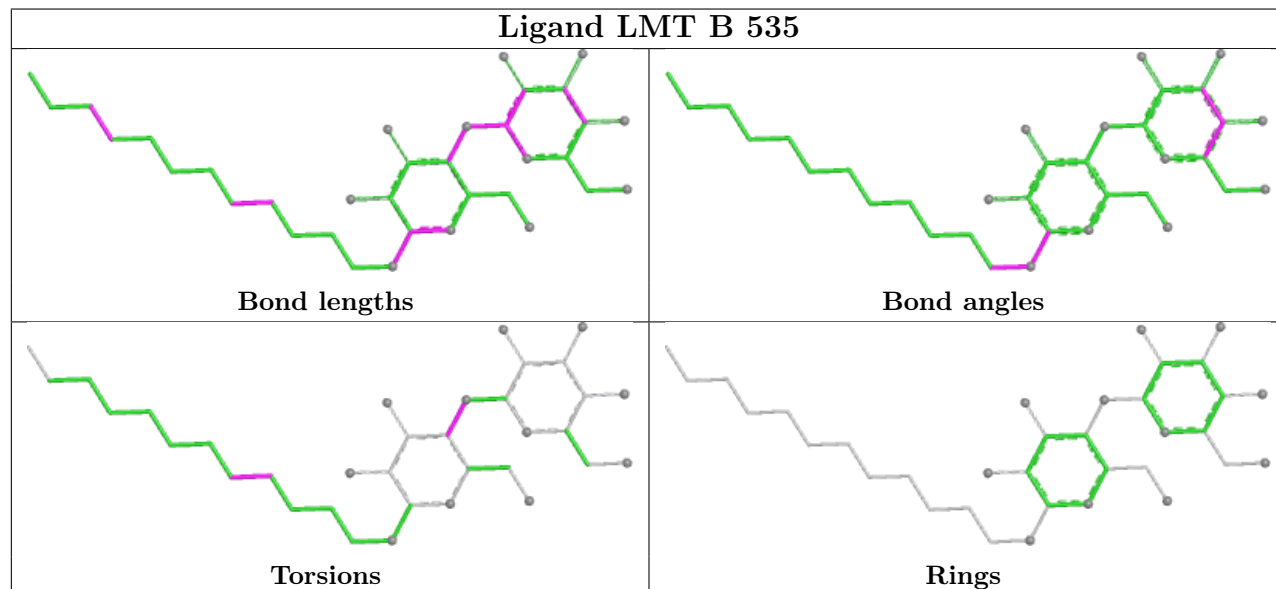




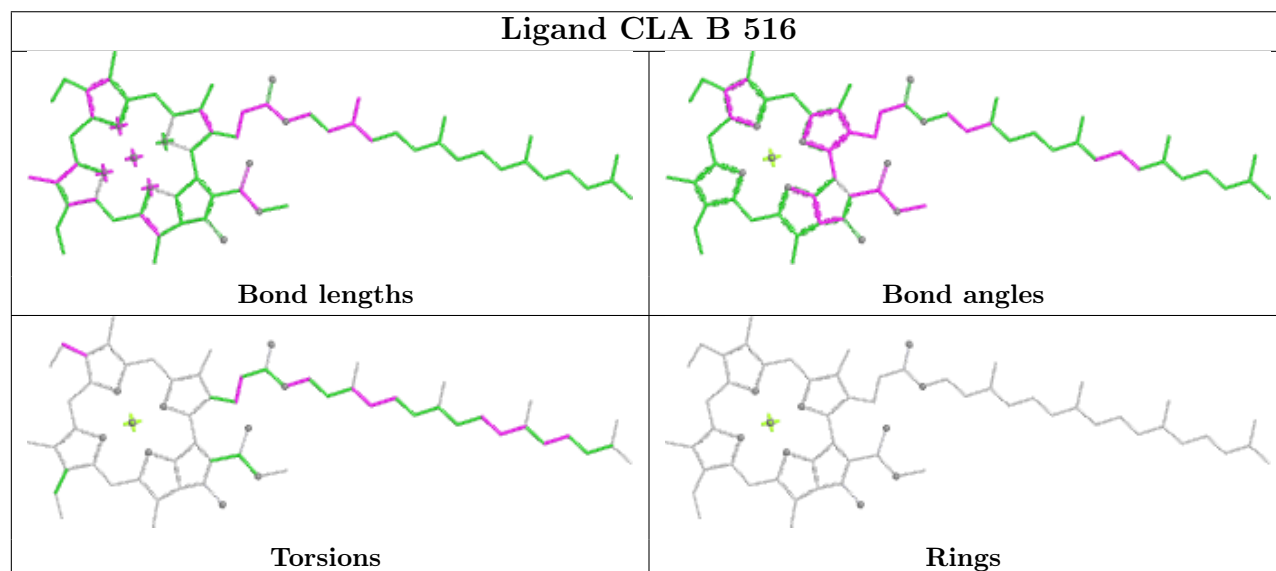
## Ligand CLA B 513

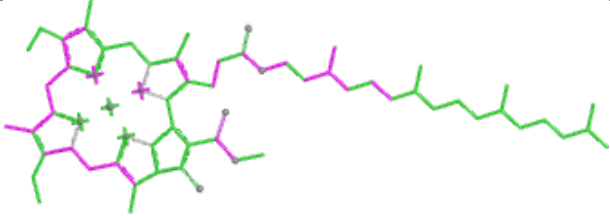
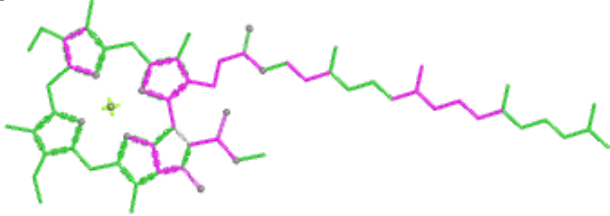
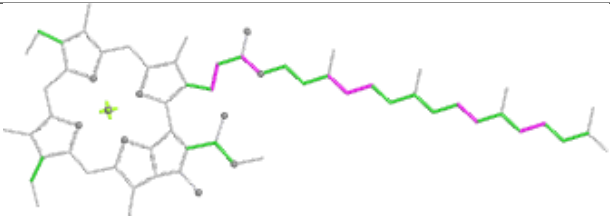
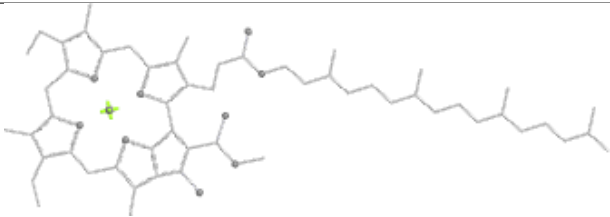
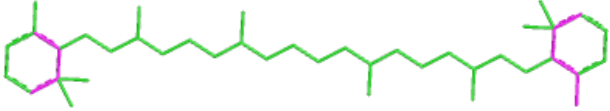
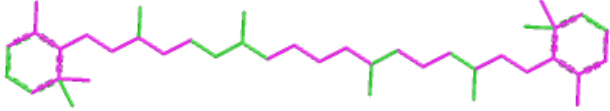
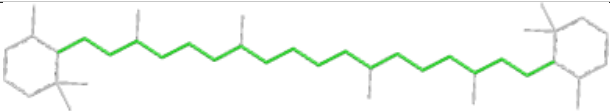
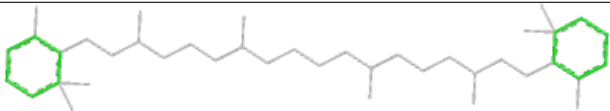
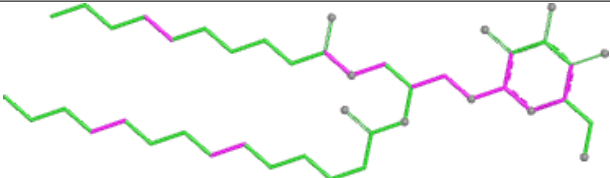
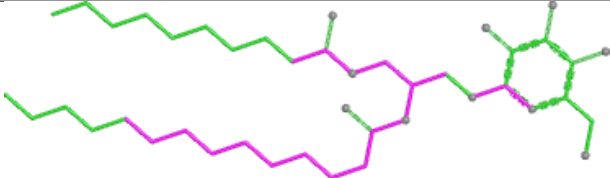
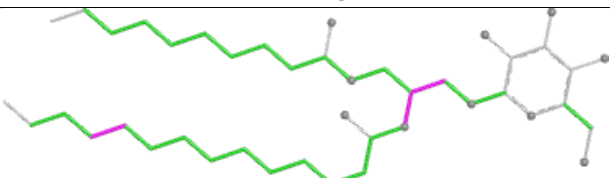
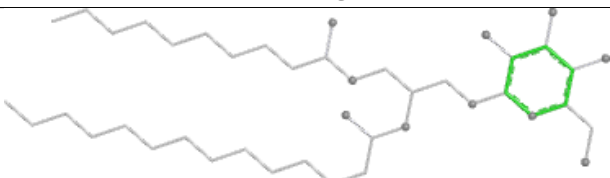


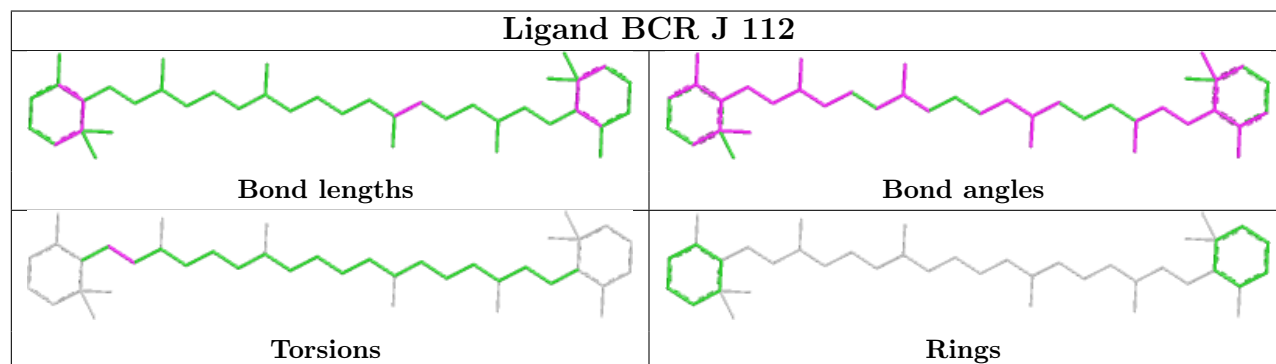
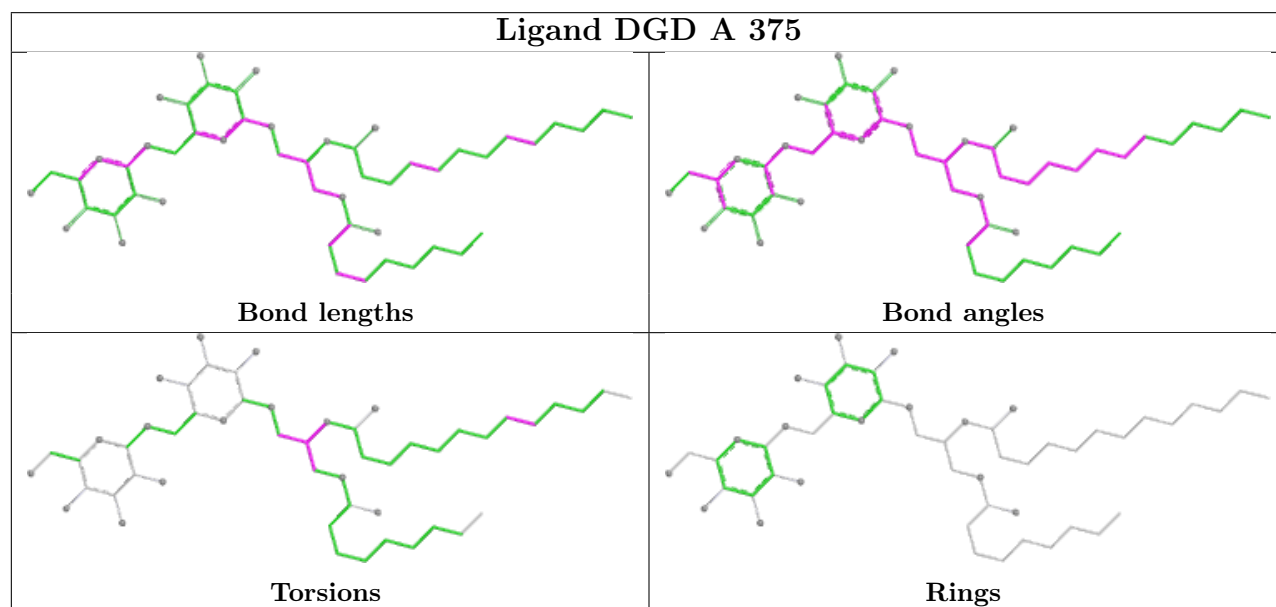
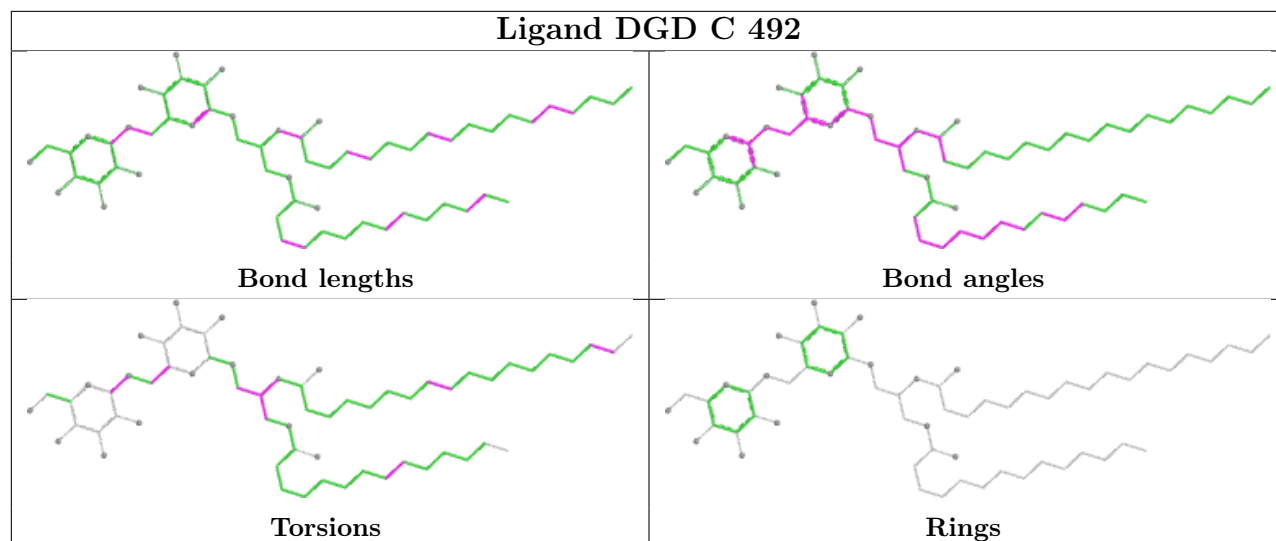
## Ligand LMT B 535

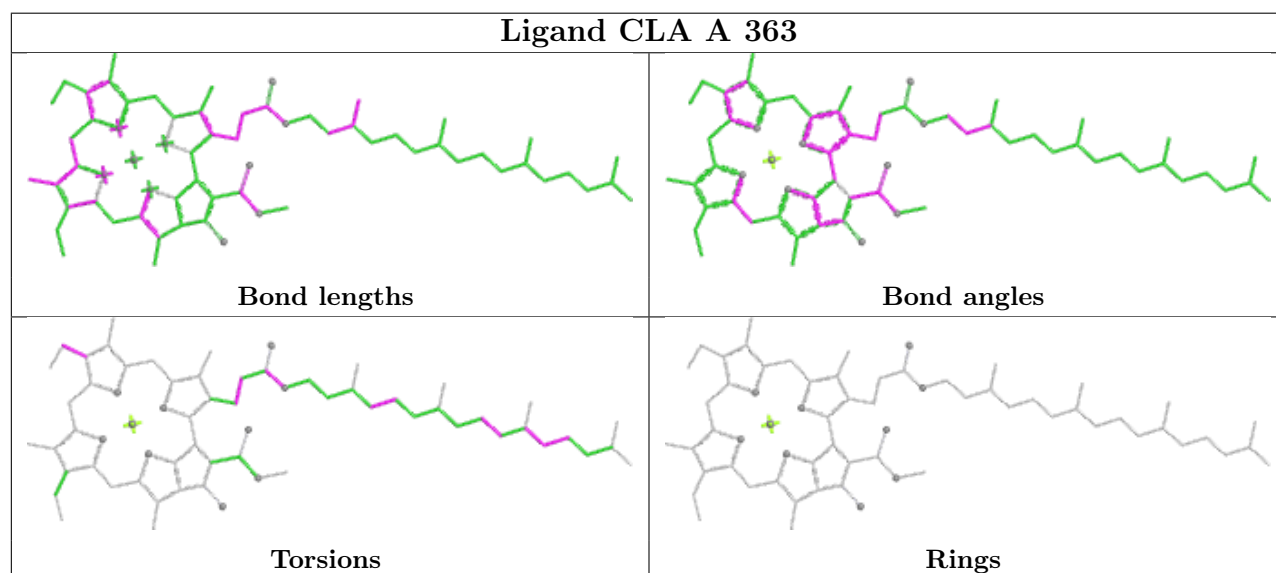
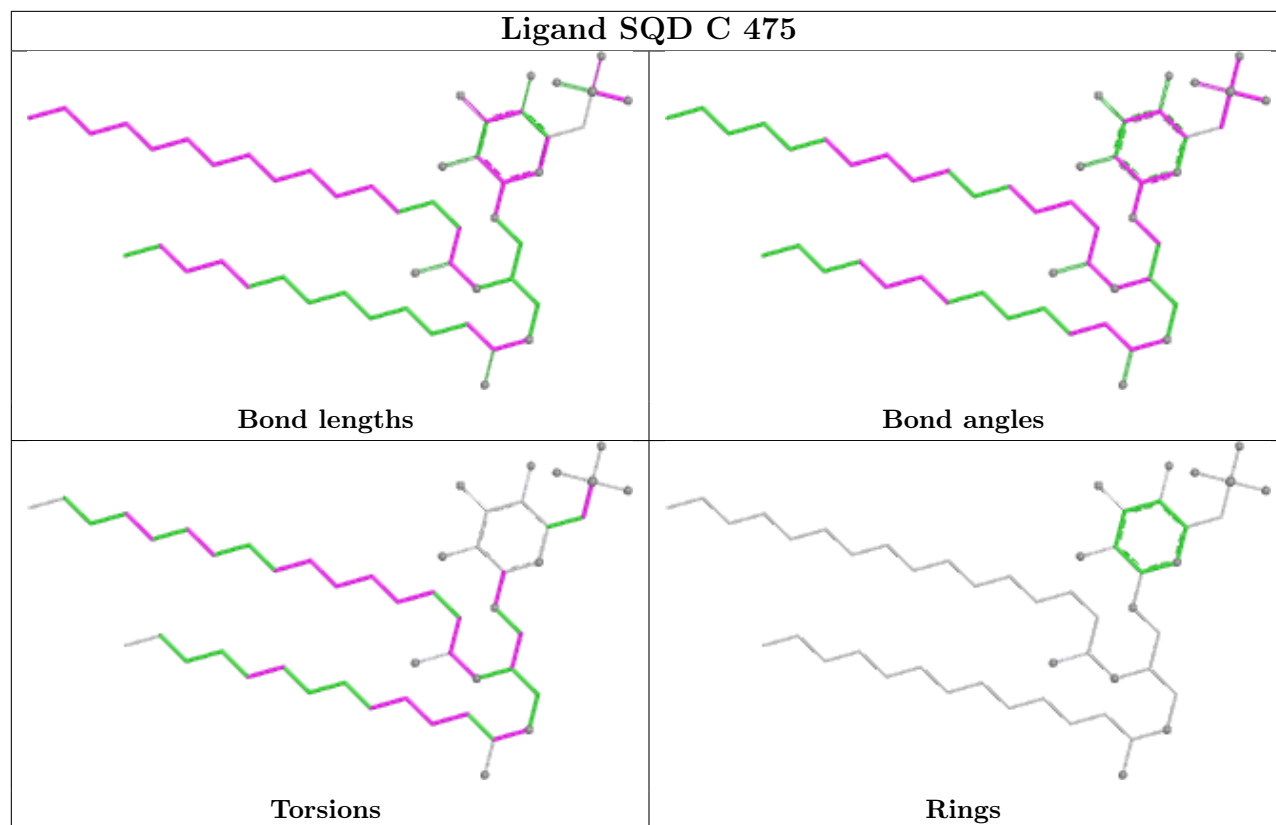


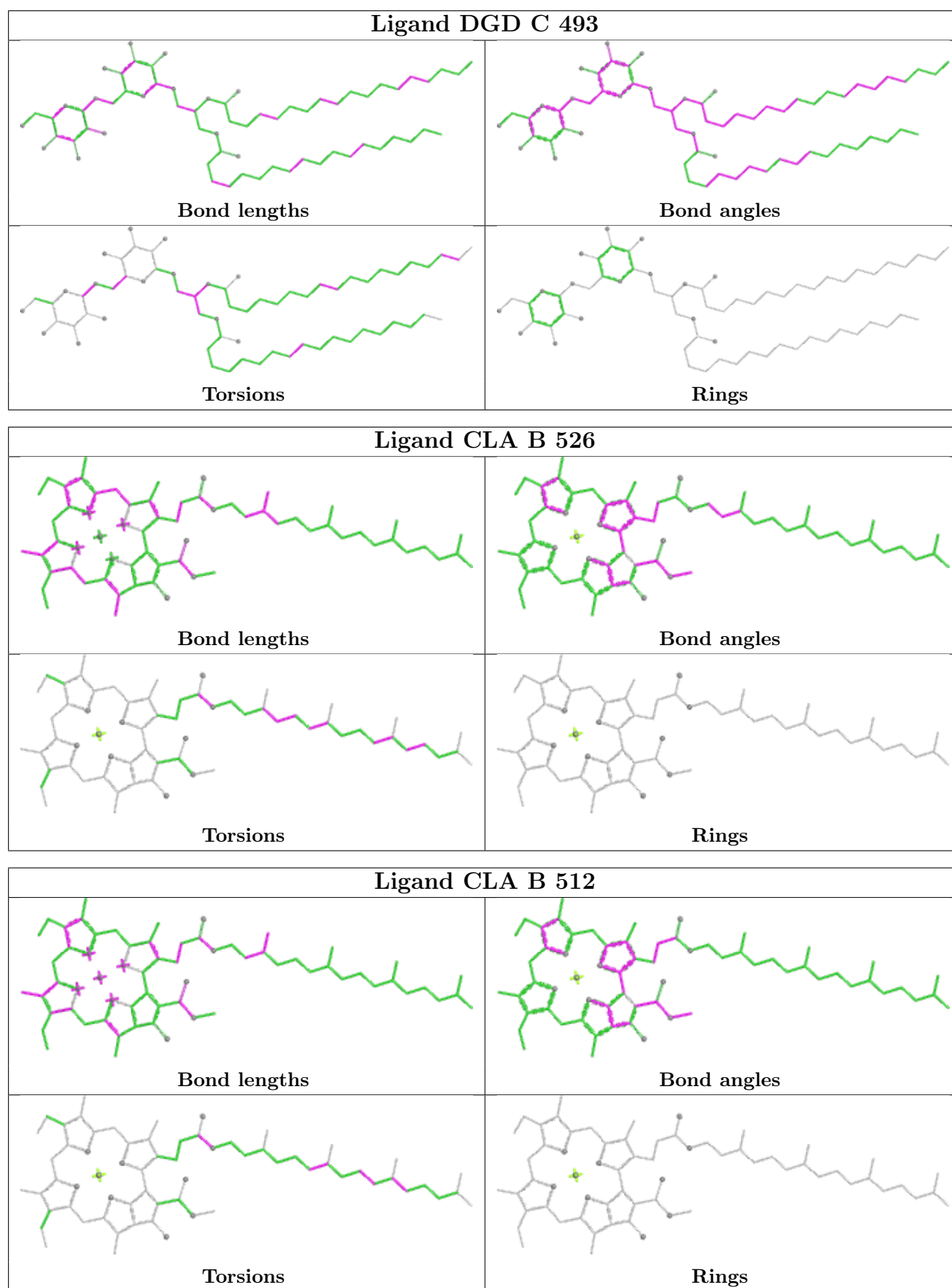
## Ligand CLA B 516



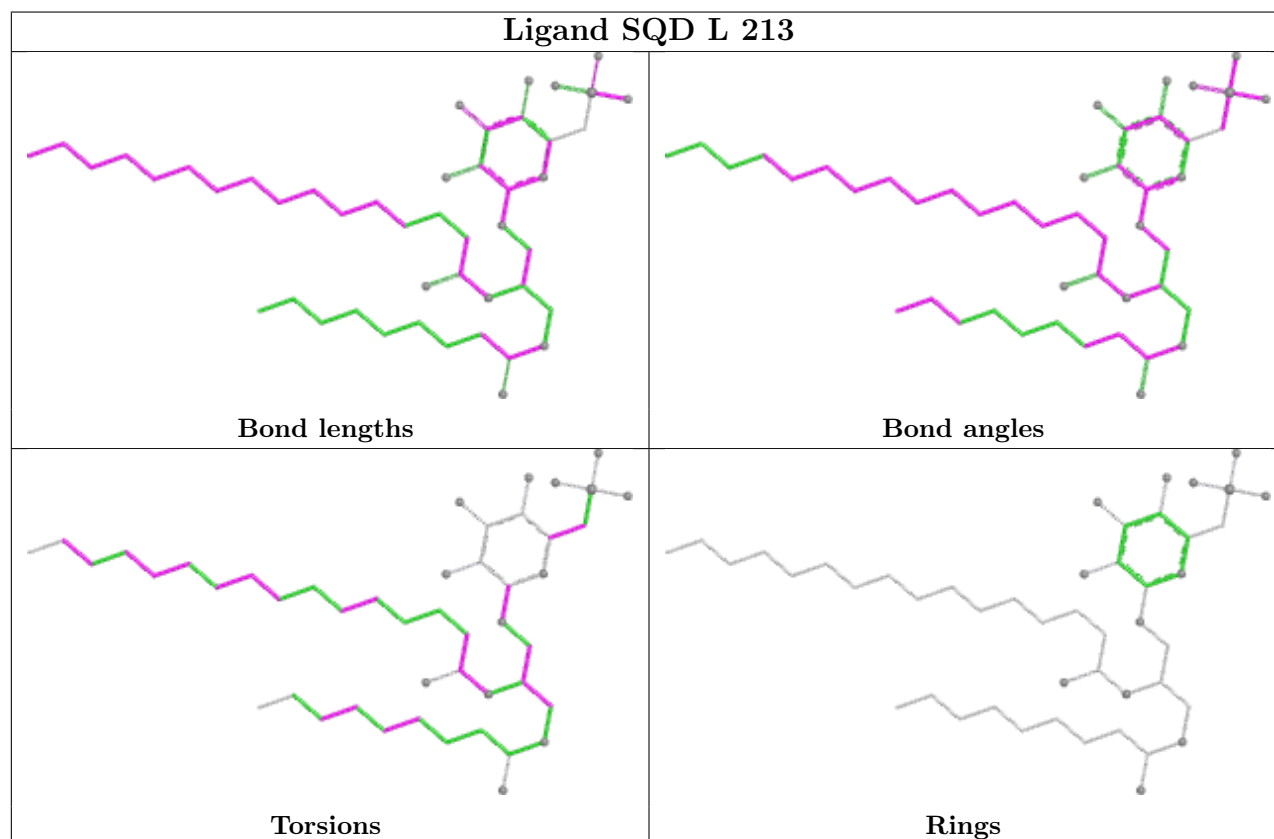
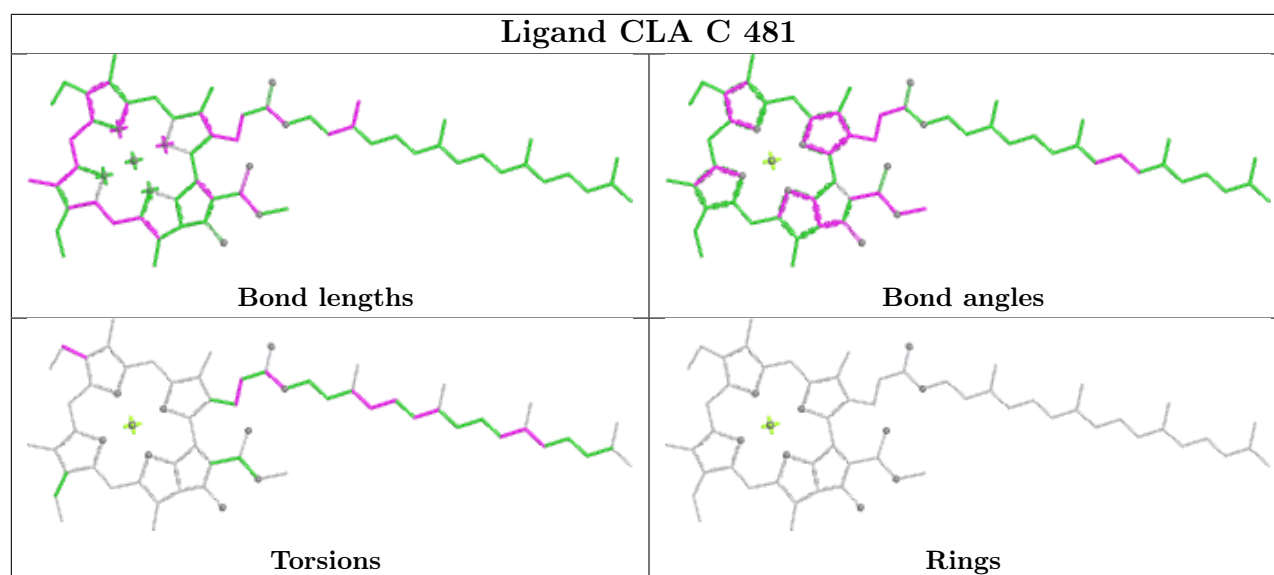
| Ligand CLA B 517                                                                                        |                                                                                                         |
|---------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------|
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>       |  <p>Rings</p>         |
| Ligand BCR B 529                                                                                        |                                                                                                         |
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>      |  <p>Rings</p>        |
| Ligand LMG I 220                                                                                        |                                                                                                         |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>     |  <p>Rings</p>       |

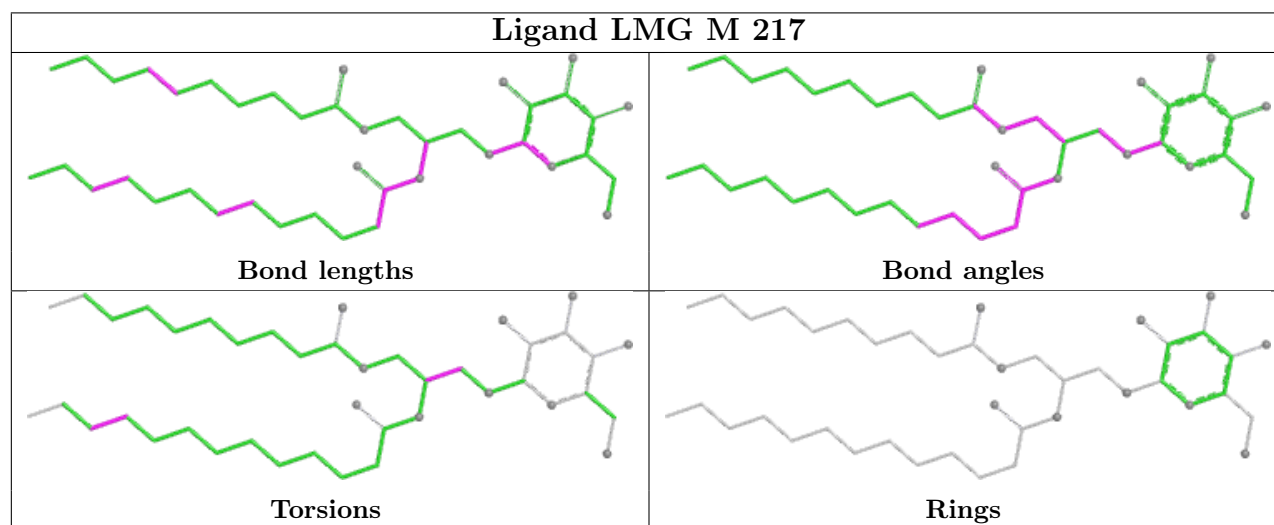
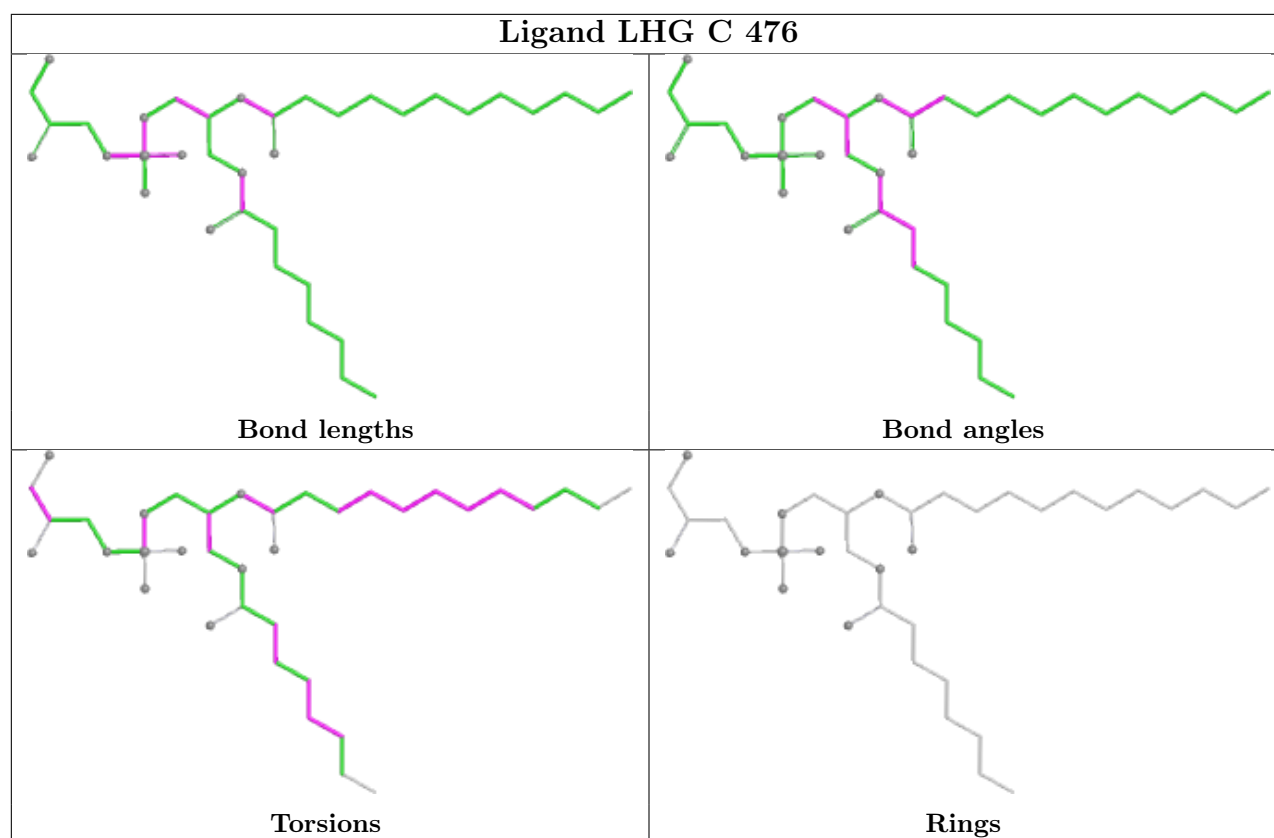




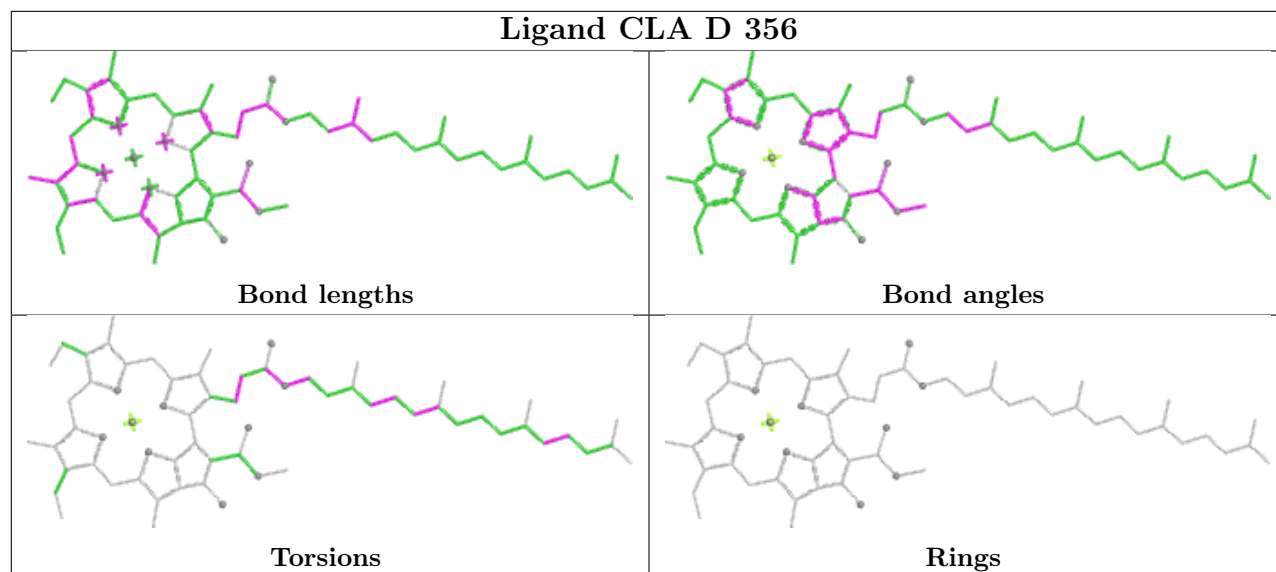




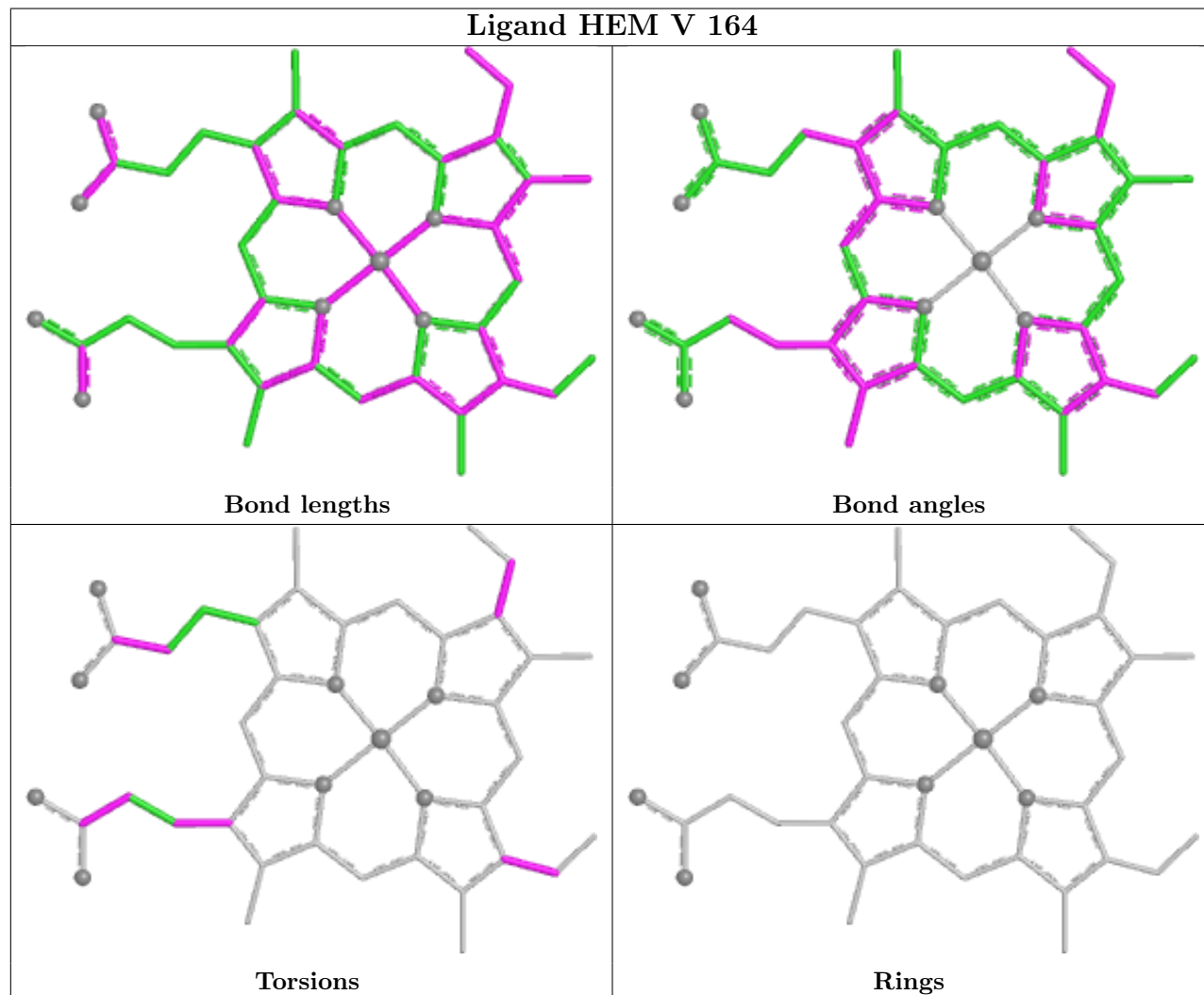




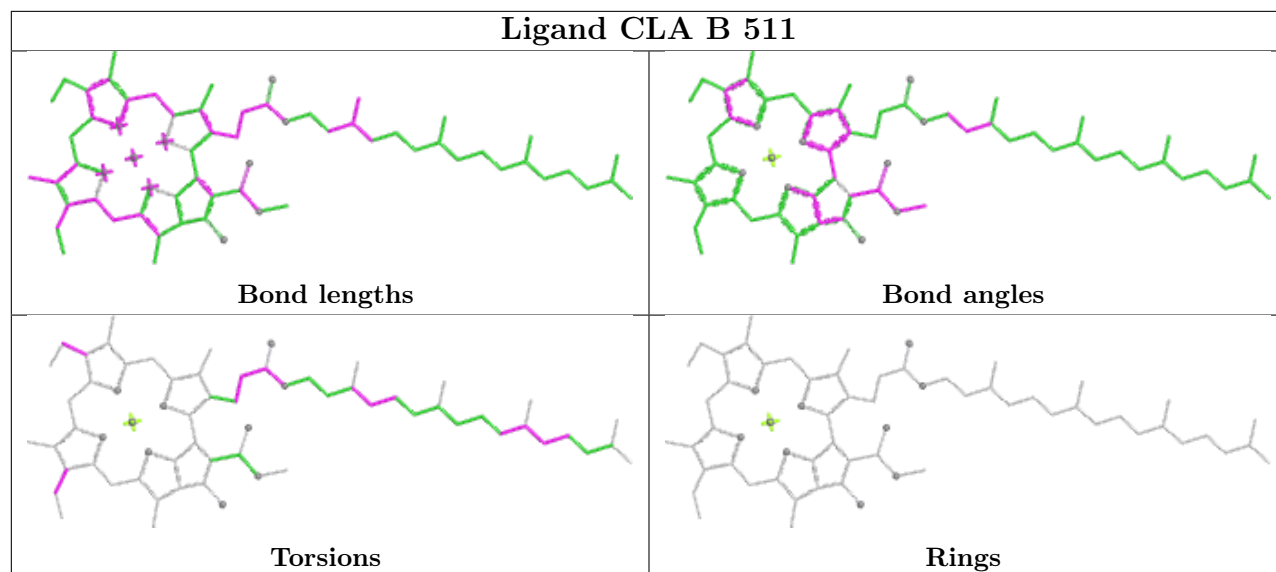
## Ligand CLA D 356



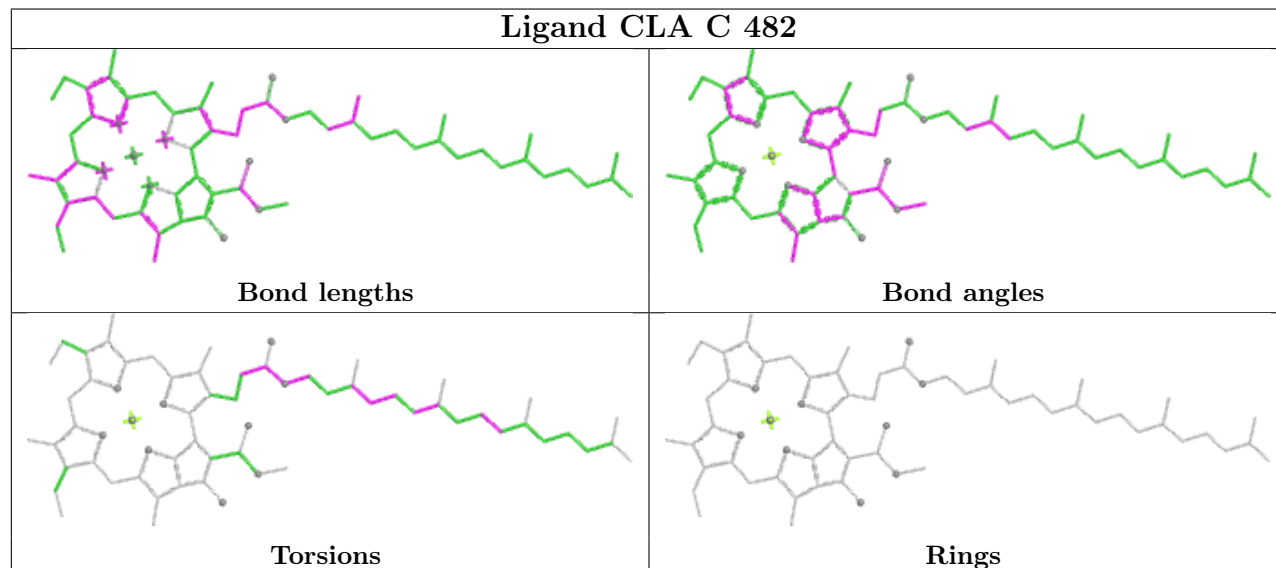
## Ligand HEM V 164



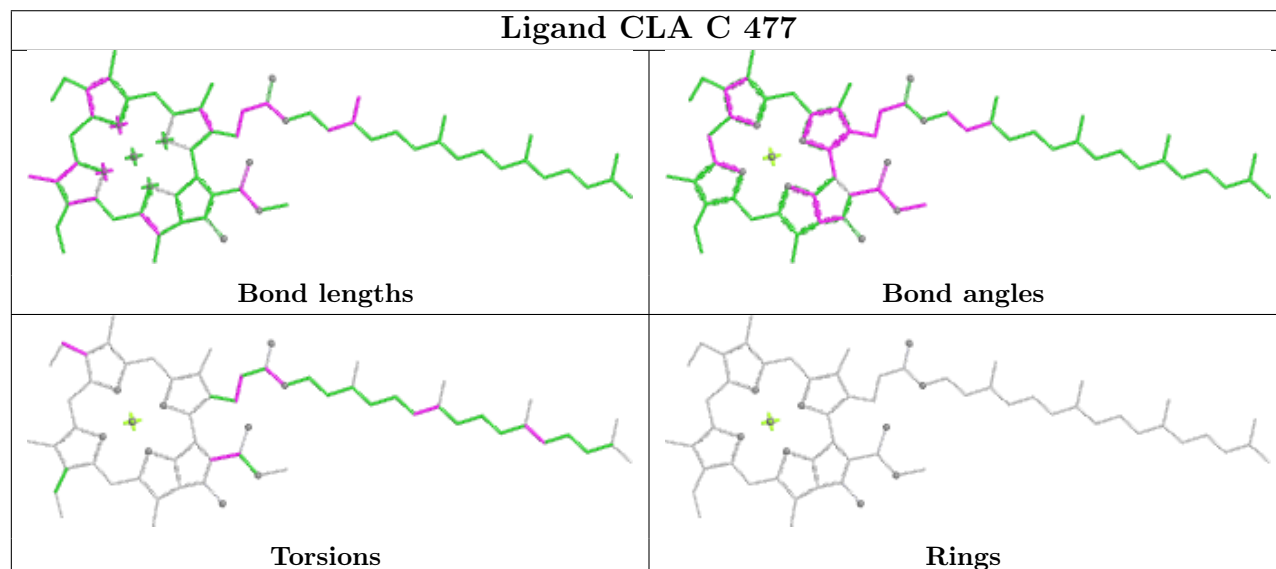
## Ligand CLA B 511

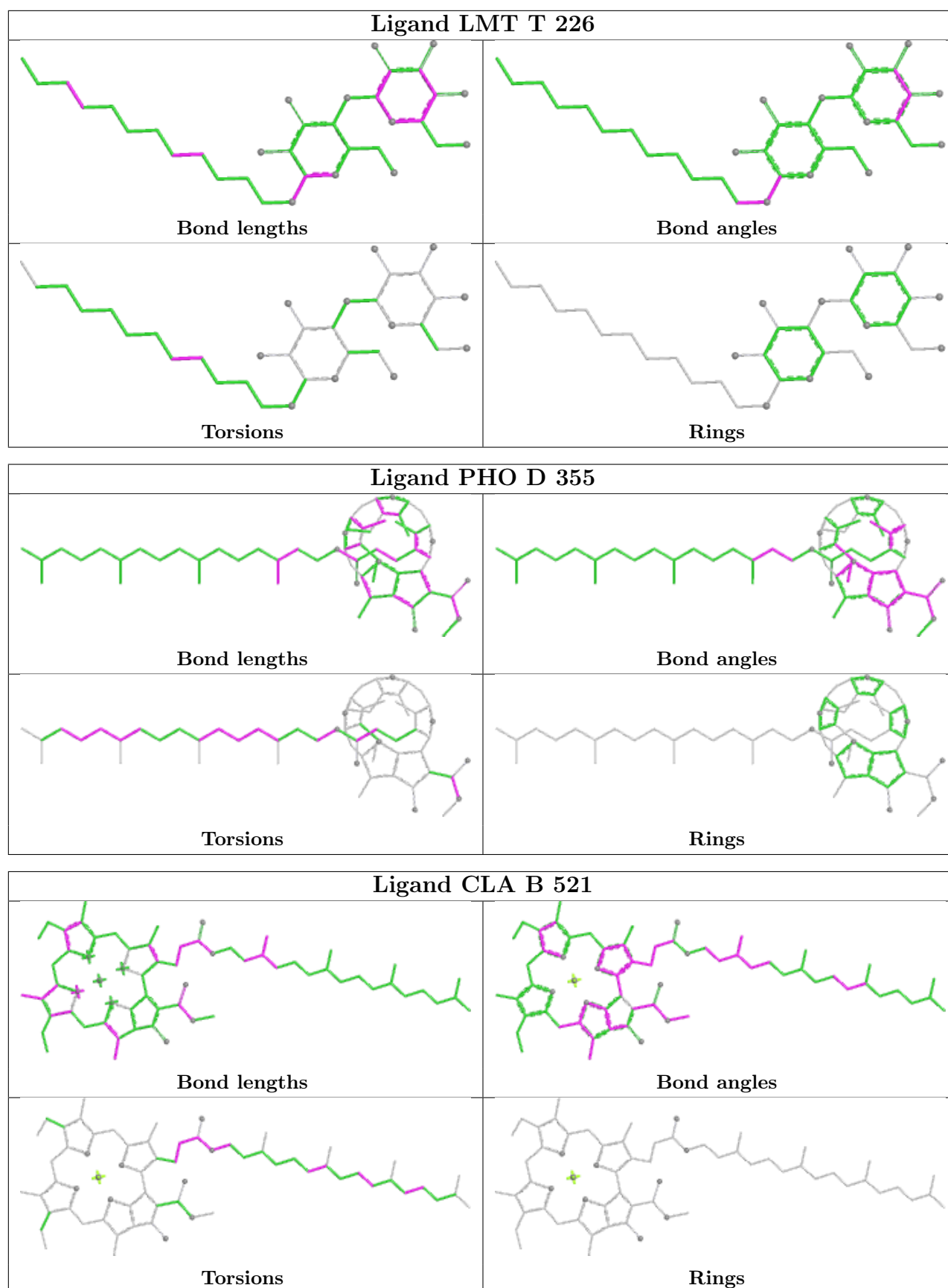


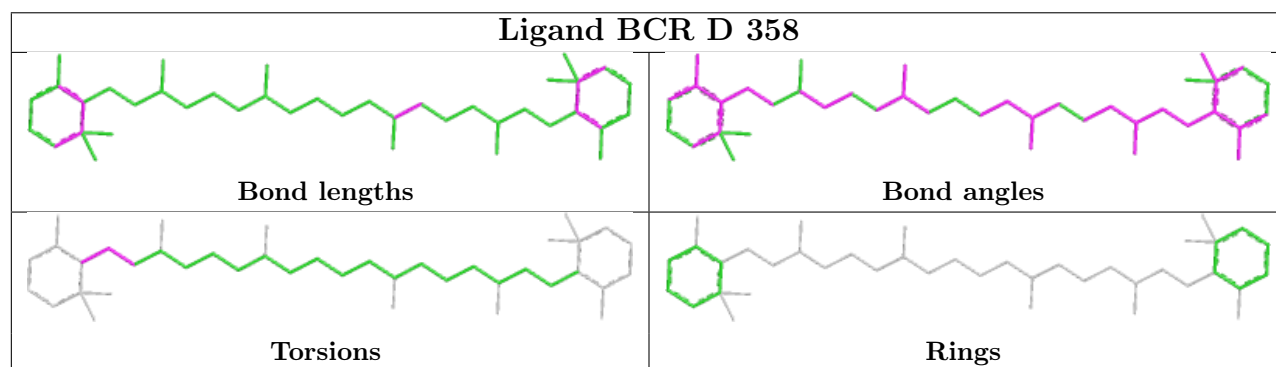
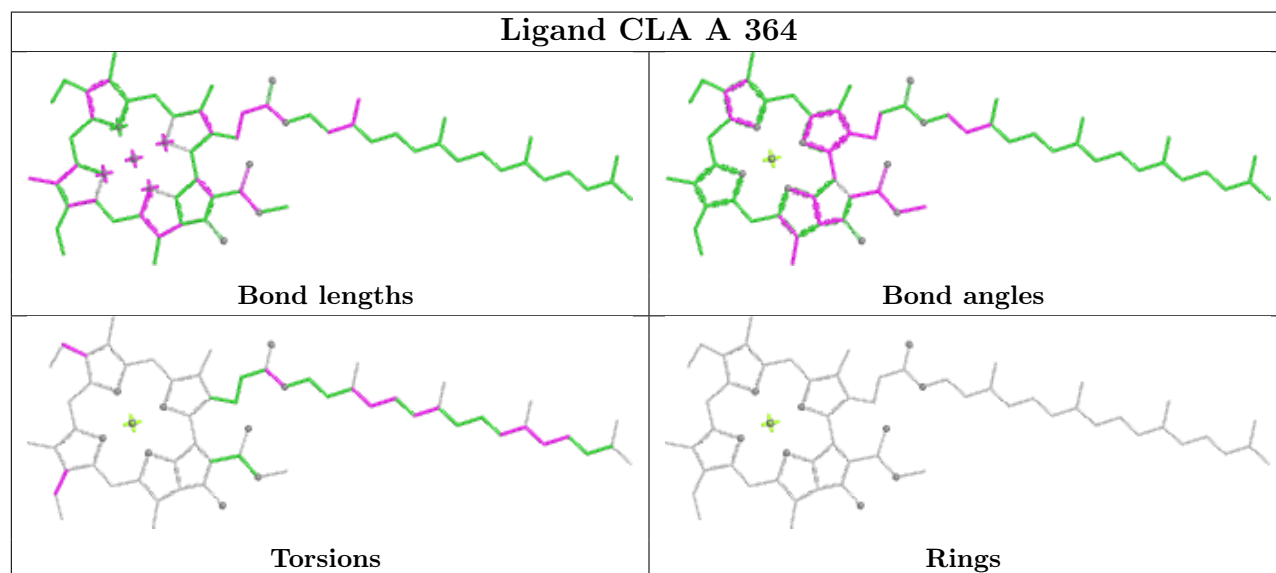
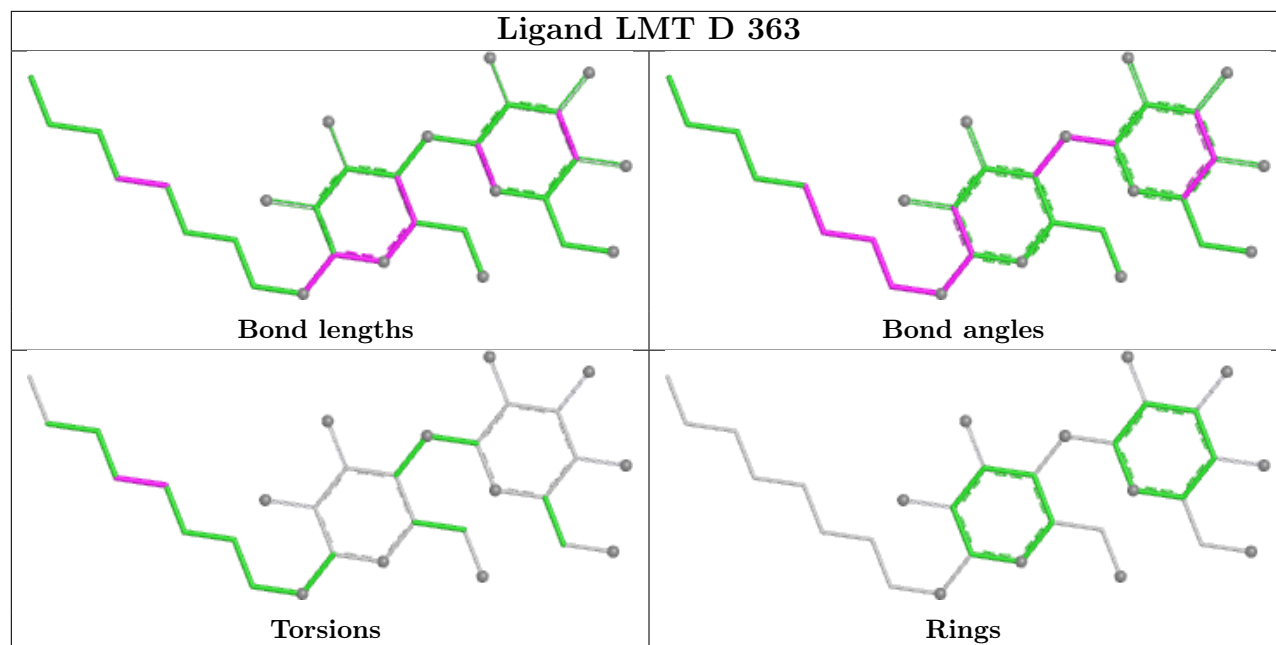
## Ligand CLA C 482

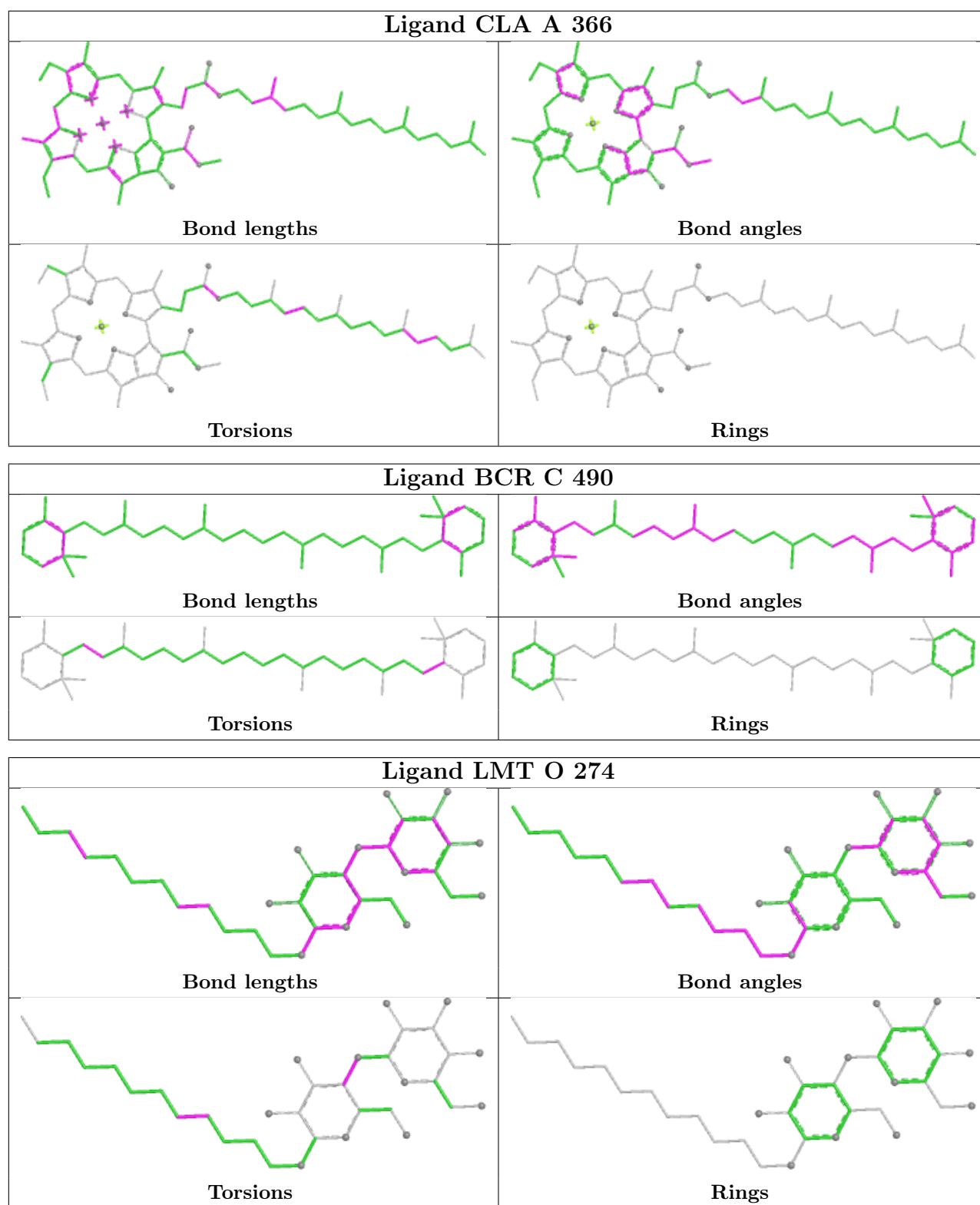


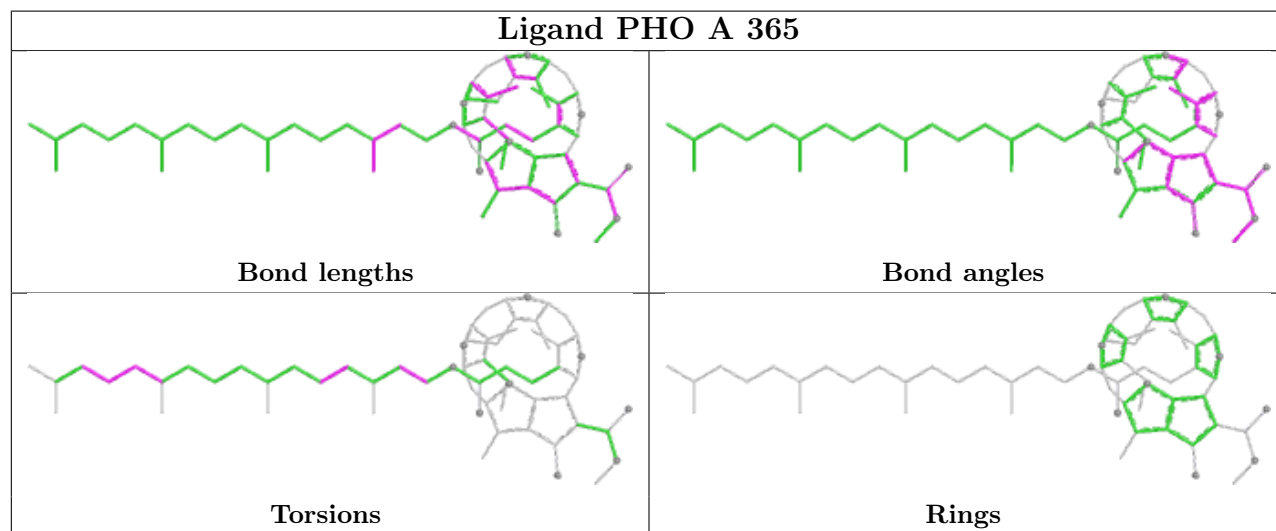
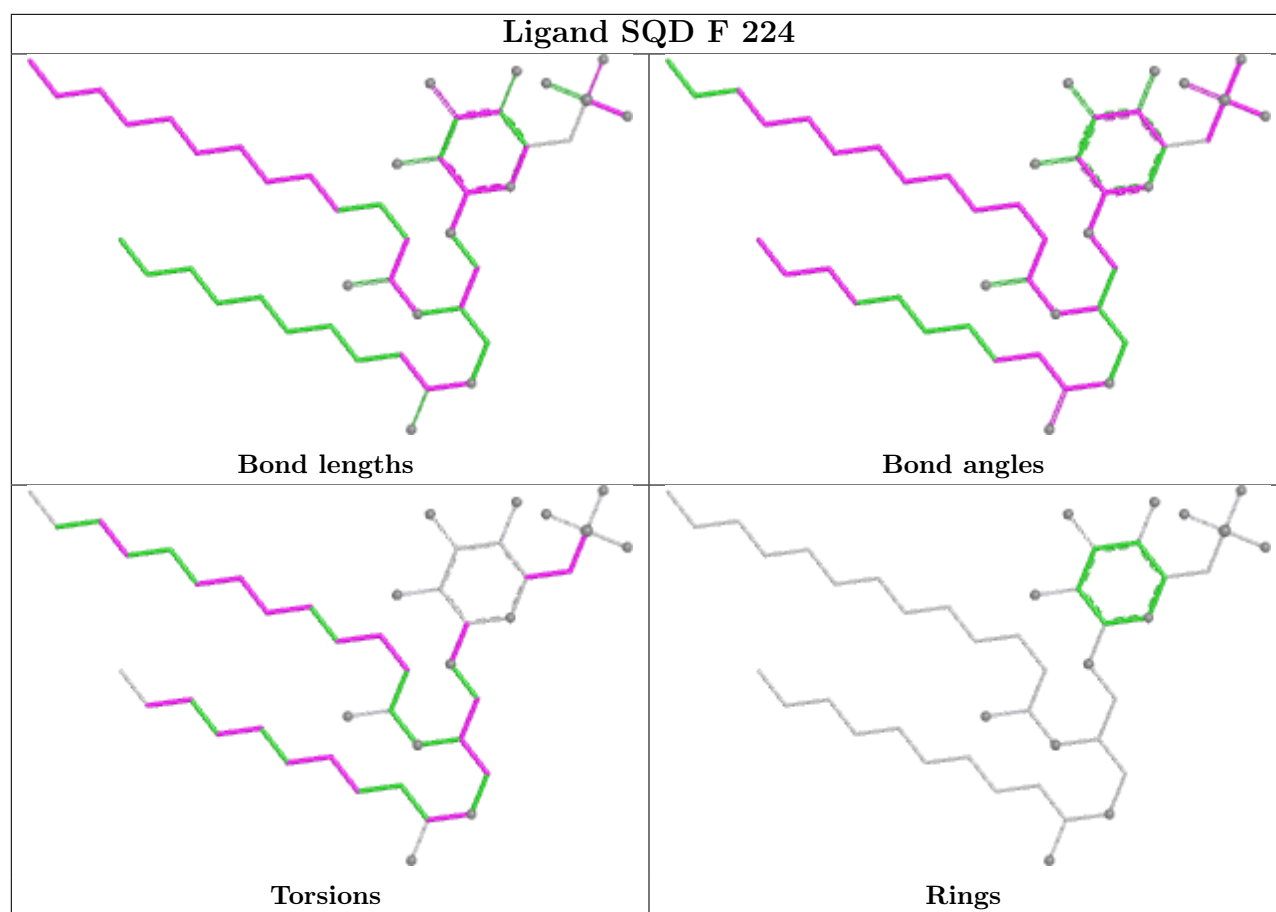
## Ligand CLA C 477



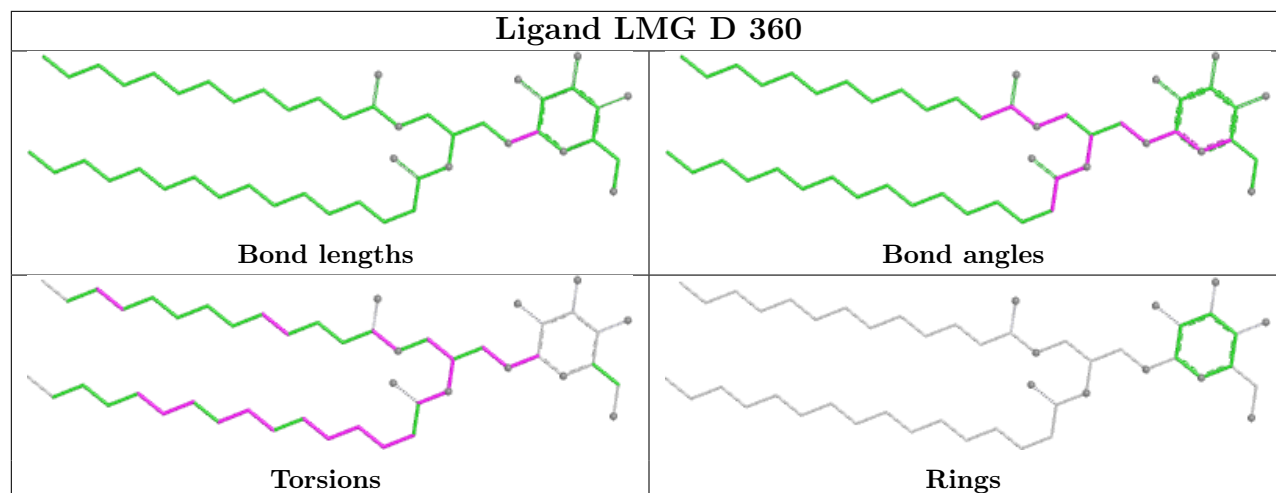












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | A     | 335/344 (97%)   | 0.00   | 7 (2%) 63 37  | 134, 163, 180, 180    | 0     |
| 2   | B     | 485/510 (95%)   | -0.03  | 8 (1%) 70 43  | 129, 158, 178, 180    | 0     |
| 3   | C     | 448/461 (97%)   | -0.03  | 4 (0%) 81 56  | 136, 168, 180, 180    | 0     |
| 4   | D     | 340/352 (96%)   | 0.09   | 9 (2%) 57 33  | 126, 154, 179, 180    | 0     |
| 5   | E     | 77/83 (92%)     | -0.16  | 0 100 100     | 138, 157, 179, 180    | 0     |
| 6   | F     | 38/44 (86%)     | -0.29  | 0 100 100     | 138, 157, 169, 177    | 0     |
| 7   | H     | 65/65 (100%)    | 0.06   | 3 (4%) 37 21  | 139, 164, 177, 180    | 0     |
| 8   | I     | 35/38 (92%)     | -0.34  | 0 100 100     | 163, 172, 180, 180    | 0     |
| 9   | J     | 34/40 (85%)     | -0.28  | 0 100 100     | 141, 155, 169, 171    | 0     |
| 10  | K     | 37/37 (100%)    | 0.07   | 1 (2%) 56 32  | 156, 166, 179, 180    | 0     |
| 11  | L     | 37/37 (100%)    | -0.34  | 0 100 100     | 152, 168, 180, 180    | 0     |
| 12  | M     | 34/36 (94%)     | 0.03   | 0 100 100     | 153, 165, 180, 180    | 0     |
| 13  | O     | 243/246 (98%)   | -0.06  | 2 (0%) 82 58  | 143, 174, 180, 180    | 0     |
| 14  | T     | 30/32 (93%)     | -0.27  | 0 100 100     | 152, 169, 180, 180    | 0     |
| 15  | U     | 97/104 (93%)    | -0.08  | 0 100 100     | 141, 160, 171, 179    | 0     |
| 16  | V     | 137/137 (100%)  | 0.02   | 2 (1%) 72 44  | 136, 160, 171, 174    | 0     |
| 17  | y     | 28/46 (60%)     | -0.22  | 0 100 100     | 158, 175, 180, 180    | 0     |
| 18  | X     | 35/40 (87%)     | -0.15  | 1 (2%) 53 30  | 144, 156, 174, 178    | 0     |
| 19  | Z     | 62/62 (100%)    | -0.05  | 0 100 100     | 166, 178, 180, 180    | 0     |
| All | All   | 2597/2714 (95%) | -0.03  | 37 (1%) 73 46 | 126, 164, 180, 180    | 0     |

All (37) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3   | C     | 341 | LEU  | 4.4  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 7   | H     | 56  | ASP  | 3.8  |
| 4   | D     | 130 | PHE  | 3.7  |
| 1   | A     | 30  | VAL  | 3.5  |
| 4   | D     | 35  | ILE  | 3.4  |
| 1   | A     | 188 | ALA  | 3.2  |
| 2   | B     | 198 | VAL  | 3.0  |
| 1   | A     | 336 | ALA  | 3.0  |
| 2   | B     | 21  | ALA  | 3.0  |
| 16  | V     | 103 | LYS  | 2.9  |
| 1   | A     | 61  | ASP  | 2.7  |
| 1   | A     | 18  | CYS  | 2.7  |
| 3   | C     | 204 | LEU  | 2.7  |
| 7   | H     | 2   | ALA  | 2.7  |
| 4   | D     | 140 | PRO  | 2.6  |
| 4   | D     | 264 | LYS  | 2.4  |
| 2   | B     | 187 | PRO  | 2.4  |
| 16  | V     | 62  | ALA  | 2.4  |
| 4   | D     | 314 | PHE  | 2.4  |
| 18  | X     | 21  | ILE  | 2.3  |
| 13  | O     | 166 | THR  | 2.3  |
| 7   | H     | 24  | GLY  | 2.3  |
| 1   | A     | 248 | ILE  | 2.3  |
| 10  | K     | 27  | VAL  | 2.3  |
| 2   | B     | 116 | VAL  | 2.2  |
| 4   | D     | 78  | VAL  | 2.2  |
| 3   | C     | 375 | LEU  | 2.2  |
| 2   | B     | 386 | ALA  | 2.2  |
| 2   | B     | 336 | ILE  | 2.1  |
| 1   | A     | 171 | GLY  | 2.1  |
| 4   | D     | 165 | SER  | 2.1  |
| 2   | B     | 473 | THR  | 2.1  |
| 13  | O     | 162 | ILE  | 2.1  |
| 2   | B     | 476 | ARG  | 2.0  |
| 4   | D     | 306 | ALA  | 2.0  |
| 3   | C     | 460 | ASP  | 2.0  |
| 4   | D     | 346 | 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 oligosaccharides 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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 26  | LHG  | C     | 476 | 37/49 | 0.39 | 0.12 | 143,176,180,180            | 0     |
| 27  | LMG  | M     | 217 | 42/55 | 0.43 | 0.13 | 166,180,180,180            | 0     |
| 30  | SQD  | F     | 224 | 45/54 | 0.65 | 0.15 | 152,179,180,180            | 0     |
| 25  | BCR  | J     | 115 | 40/40 | 0.67 | 0.14 | 171,180,180,180            | 0     |
| 29  | LMT  | T     | 226 | 35/35 | 0.68 | 0.11 | 156,180,180,180            | 0     |
| 29  | LMT  | O     | 274 | 35/35 | 0.68 | 0.08 | 180,180,180,180            | 0     |
| 27  | LMG  | I     | 220 | 43/55 | 0.69 | 0.10 | 158,180,180,180            | 0     |
| 30  | SQD  | L     | 213 | 47/54 | 0.69 | 0.10 | 155,178,180,180            | 0     |
| 28  | DGD  | D     | 362 | 63/66 | 0.71 | 0.12 | 177,180,180,180            | 0     |
| 28  | DGD  | A     | 375 | 52/66 | 0.72 | 0.09 | 164,180,180,180            | 0     |
| 29  | LMT  | A     | 376 | 35/35 | 0.72 | 0.12 | 162,180,180,180            | 0     |
| 27  | LMG  | C     | 494 | 45/55 | 0.73 | 0.10 | 168,180,180,180            | 0     |
| 34  | CA   | K     | 56  | 1/1   | 0.73 | 0.08 | 180,180,180,180            | 0     |
| 29  | LMT  | B     | 535 | 35/35 | 0.74 | 0.11 | 163,180,180,180            | 0     |
| 29  | LMT  | D     | 536 | 35/35 | 0.75 | 0.17 | 168,173,180,180            | 0     |
| 27  | LMG  | D     | 360 | 48/55 | 0.76 | 0.17 | 140,169,176,177            | 0     |
| 30  | SQD  | C     | 475 | 51/54 | 0.77 | 0.10 | 156,172,180,180            | 0     |
| 29  | LMT  | D     | 363 | 31/35 | 0.77 | 0.13 | 170,180,180,180            | 0     |
| 34  | CA   | O     | 273 | 1/1   | 0.77 | 0.17 | 180,180,180,180            | 0     |
| 21  | CLA  | B     | 526 | 65/65 | 0.78 | 0.12 | 167,177,180,180            | 0     |
| 21  | CLA  | B     | 511 | 65/65 | 0.78 | 0.15 | 148,179,180,180            | 0     |
| 28  | DGD  | C     | 492 | 62/66 | 0.78 | 0.12 | 153,171,180,180            | 0     |
| 28  | DGD  | C     | 474 | 56/66 | 0.79 | 0.13 | 158,180,180,180            | 0     |
| 28  | DGD  | C     | 493 | 66/66 | 0.80 | 0.13 | 159,174,180,180            | 0     |
| 29  | LMT  | I     | 274 | 35/35 | 0.82 | 0.11 | 170,180,180,180            | 0     |
| 28  | DGD  | B     | 533 | 66/66 | 0.82 | 0.12 | 166,179,180,180            | 0     |
| 25  | BCR  | B     | 530 | 40/40 | 0.83 | 0.13 | 173,180,180,180            | 0     |
| 21  | CLA  | C     | 482 | 65/65 | 0.83 | 0.15 | 148,179,180,180            | 0     |
| 27  | LMG  | D     | 359 | 46/55 | 0.83 | 0.13 | 142,163,180,180            | 0     |
| 25  | BCR  | C     | 490 | 40/40 | 0.84 | 0.16 | 164,169,180,180            | 0     |
| 25  | BCR  | B     | 527 | 40/40 | 0.85 | 0.13 | 161,169,176,178            | 0     |
| 27  | LMG  | A     | 373 | 51/55 | 0.85 | 0.18 | 169,174,180,180            | 0     |

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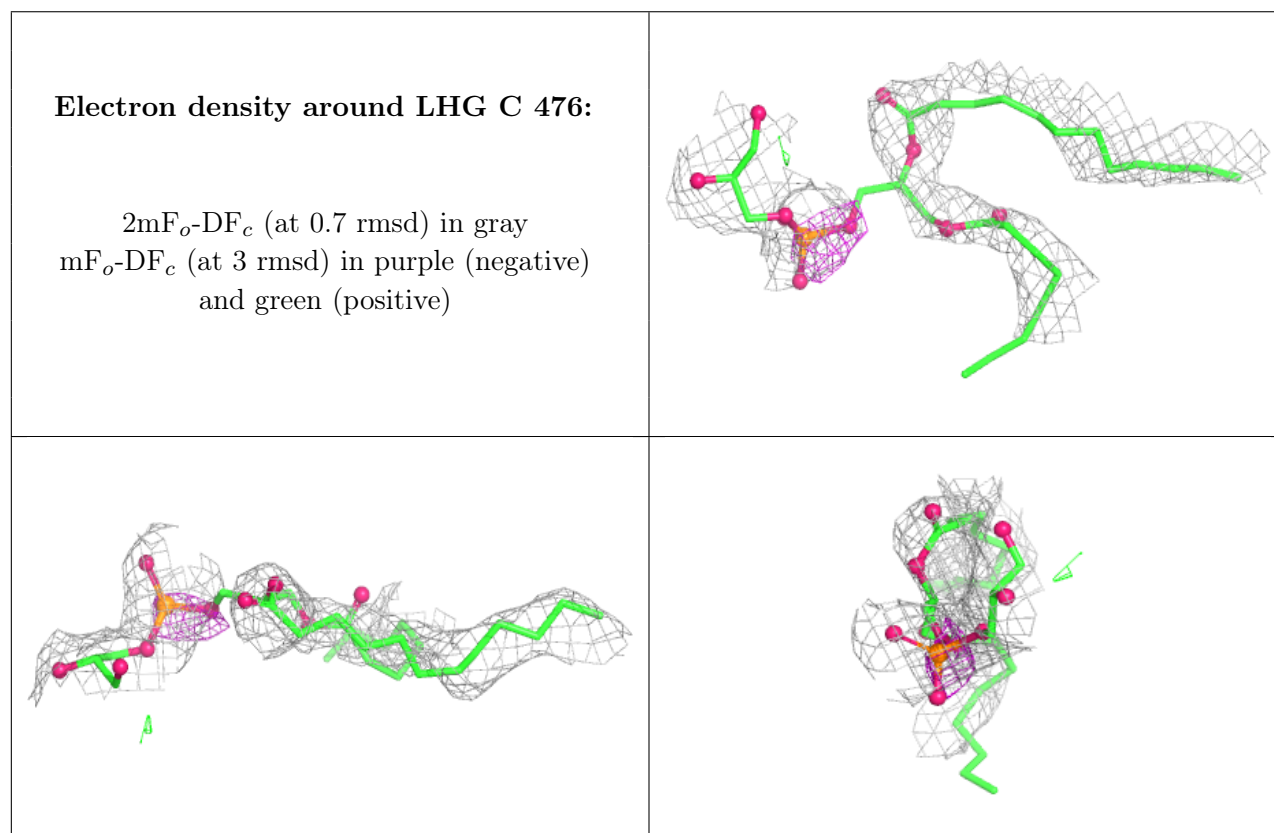
| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 27  | LMG  | J     | 492 | 48/55 | 0.85 | 0.15 | 155,175,180,180             | 0     |
| 28  | DGD  | B     | 528 | 58/66 | 0.85 | 0.16 | 126,136,172,173             | 0     |
| 25  | BCR  | B     | 529 | 40/40 | 0.86 | 0.15 | 166,169,173,174             | 0     |
| 21  | CLA  | C     | 488 | 65/65 | 0.87 | 0.10 | 169,176,179,180             | 0     |
| 21  | CLA  | A     | 363 | 65/65 | 0.87 | 0.13 | 154,161,175,177             | 0     |
| 27  | LMG  | B     | 531 | 49/55 | 0.87 | 0.16 | 160,167,175,176             | 0     |
| 21  | CLA  | B     | 524 | 65/65 | 0.87 | 0.11 | 157,180,180,180             | 0     |
| 25  | BCR  | Z     | 116 | 40/40 | 0.88 | 0.16 | 163,165,170,171             | 0     |
| 30  | SQD  | D     | 361 | 43/54 | 0.88 | 0.11 | 160,173,180,180             | 0     |
| 21  | CLA  | C     | 486 | 65/65 | 0.88 | 0.15 | 143,180,180,180             | 0     |
| 25  | BCR  | J     | 112 | 40/40 | 0.89 | 0.18 | 157,160,172,173             | 0     |
| 21  | CLA  | A     | 364 | 65/65 | 0.90 | 0.12 | 126,141,175,177             | 0     |
| 21  | CLA  | C     | 477 | 65/65 | 0.90 | 0.14 | 163,169,179,180             | 0     |
| 21  | CLA  | C     | 481 | 65/65 | 0.90 | 0.12 | 152,180,180,180             | 0     |
| 21  | CLA  | B     | 525 | 65/65 | 0.91 | 0.12 | 148,167,180,180             | 0     |
| 21  | CLA  | C     | 487 | 65/65 | 0.91 | 0.13 | 176,180,180,180             | 0     |
| 21  | CLA  | C     | 479 | 65/65 | 0.91 | 0.13 | 162,180,180,180             | 0     |
| 24  | OEC  | A     | 368 | 5/9   | 0.91 | 0.11 | 118,138,151,154             | 0     |
| 21  | CLA  | C     | 484 | 65/65 | 0.91 | 0.12 | 168,177,180,180             | 0     |
| 25  | BCR  | X     | 107 | 40/40 | 0.91 | 0.14 | 154,158,161,163             | 0     |
| 21  | CLA  | D     | 356 | 65/65 | 0.92 | 0.13 | 149,154,162,164             | 0     |
| 28  | DGD  | C     | 491 | 53/66 | 0.92 | 0.14 | 155,160,166,168             | 0     |
| 23  | MES  | A     | 367 | 12/12 | 0.92 | 0.11 | 136,144,152,153             | 0     |
| 21  | CLA  | C     | 480 | 65/65 | 0.92 | 0.10 | 151,159,180,180             | 0     |
| 25  | BCR  | A     | 369 | 40/40 | 0.92 | 0.14 | 164,171,178,178             | 0     |
| 21  | CLA  | C     | 485 | 65/65 | 0.92 | 0.14 | 170,176,178,180             | 0     |
| 21  | CLA  | B     | 516 | 65/65 | 0.92 | 0.10 | 152,155,180,180             | 0     |
| 31  | BCT  | D     | 353 | 4/4   | 0.92 | 0.07 | 169,170,170,171             | 0     |
| 21  | CLA  | A     | 366 | 65/65 | 0.92 | 0.09 | 152,162,164,166             | 0     |
| 21  | CLA  | C     | 483 | 65/65 | 0.92 | 0.12 | 164,180,180,180             | 0     |
| 21  | CLA  | K     | 483 | 65/65 | 0.93 | 0.10 | 155,160,174,176             | 0     |
| 25  | BCR  | C     | 489 | 40/40 | 0.93 | 0.16 | 152,169,171,171             | 0     |
| 21  | CLA  | C     | 478 | 65/65 | 0.93 | 0.11 | 153,155,166,170             | 0     |
| 32  | PL9  | D     | 357 | 55/55 | 0.93 | 0.13 | 146,153,161,162             | 0     |
| 26  | LHG  | A     | 371 | 39/49 | 0.93 | 0.11 | 156,175,179,180             | 0     |
| 21  | CLA  | B     | 518 | 65/65 | 0.93 | 0.12 | 150,164,167,169             | 0     |
| 22  | PHO  | A     | 365 | 64/64 | 0.94 | 0.10 | 143,154,162,164             | 0     |
| 22  | PHO  | D     | 355 | 64/64 | 0.94 | 0.11 | 140,162,169,171             | 0     |
| 21  | CLA  | B     | 521 | 65/65 | 0.94 | 0.11 | 149,169,175,179             | 0     |
| 21  | CLA  | D     | 354 | 65/65 | 0.94 | 0.14 | 135,154,164,168             | 0     |
| 25  | BCR  | D     | 358 | 40/40 | 0.94 | 0.11 | 135,151,162,162             | 0     |
| 33  | HEM  | F     | 85  | 43/43 | 0.94 | 0.11 | 154,159,162,163             | 0     |

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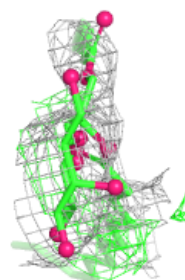
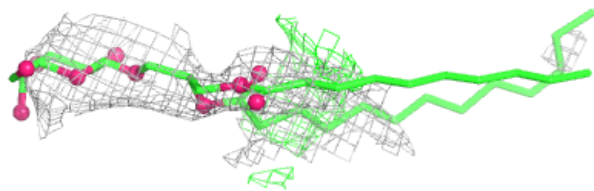
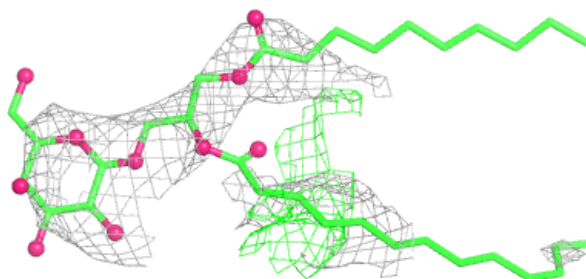
| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 21  | CLA  | B     | 517 | 65/65 | 0.94 | 0.11 | 144,160,164,167             | 0     |
| 21  | CLA  | B     | 512 | 65/65 | 0.94 | 0.14 | 142,165,172,173             | 0     |
| 21  | CLA  | B     | 514 | 65/65 | 0.95 | 0.13 | 139,146,168,169             | 0     |
| 21  | CLA  | B     | 519 | 65/65 | 0.95 | 0.11 | 152,157,158,159             | 0     |
| 21  | CLA  | A     | 362 | 65/65 | 0.95 | 0.12 | 149,154,159,163             | 0     |
| 21  | CLA  | B     | 522 | 65/65 | 0.95 | 0.12 | 134,144,163,165             | 0     |
| 21  | CLA  | B     | 523 | 65/65 | 0.95 | 0.10 | 134,142,169,170             | 0     |
| 21  | CLA  | B     | 513 | 65/65 | 0.95 | 0.12 | 133,170,171,172             | 0     |
| 21  | CLA  | B     | 515 | 65/65 | 0.96 | 0.12 | 142,162,168,170             | 0     |
| 34  | CA   | F     | 225 | 1/1   | 0.97 | 0.07 | 142,142,142,142             | 0     |
| 21  | CLA  | B     | 520 | 65/65 | 0.97 | 0.14 | 150,162,165,167             | 0     |
| 33  | HEM  | V     | 164 | 43/43 | 0.97 | 0.11 | 89,102,122,129              | 0     |
| 20  | FE2  | A     | 361 | 1/1   | 0.99 | 0.03 | 160,160,160,160             | 0     |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

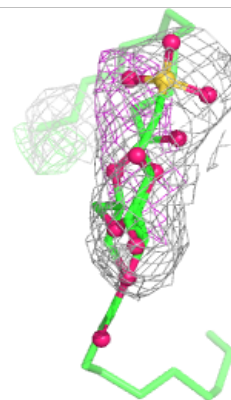
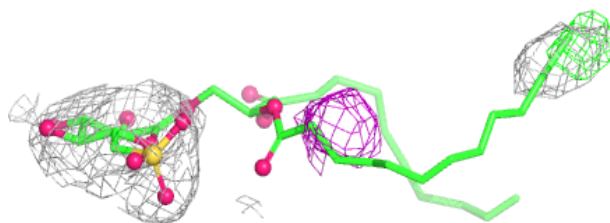
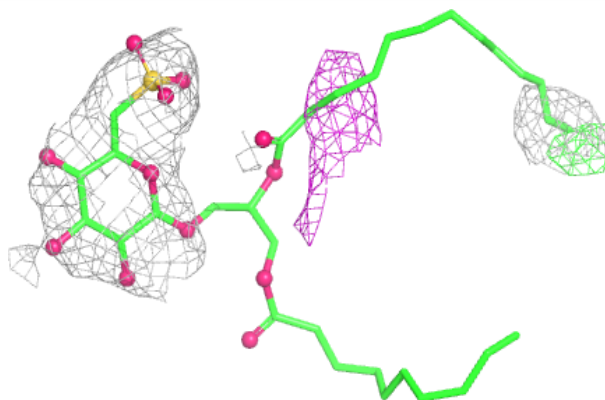


**Electron density around LMG M 217:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

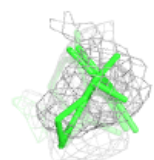
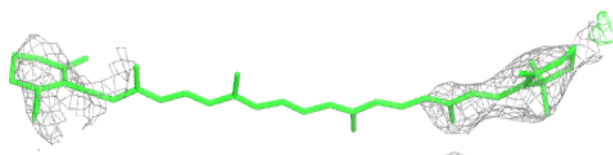
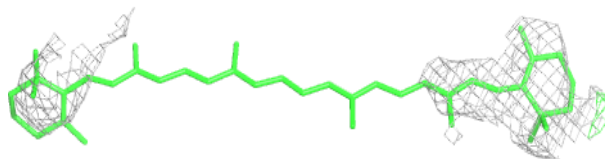
**Electron density around SQD F 224:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

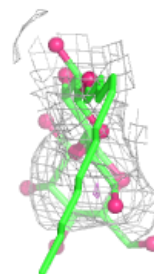
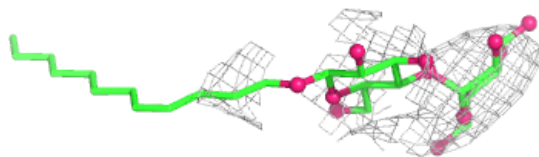
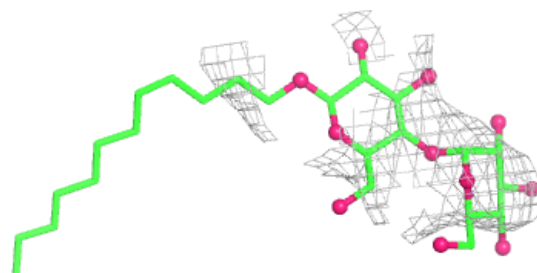


**Electron density around BCR J 115:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around LMT T 226:**

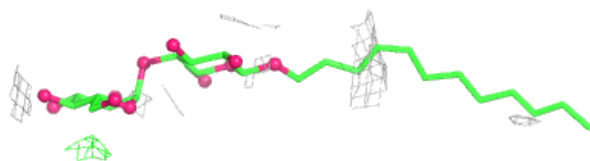
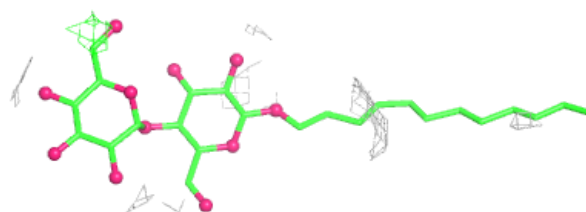
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



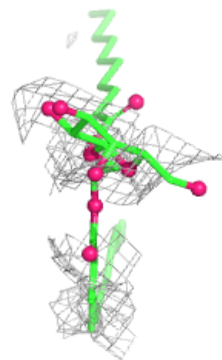
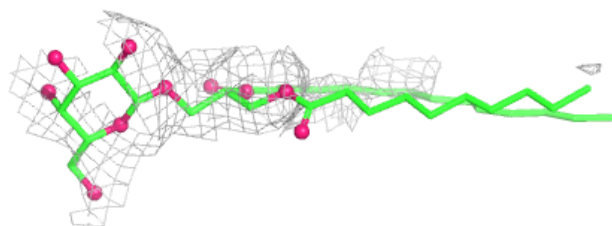


**Electron density around LMT O 274:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

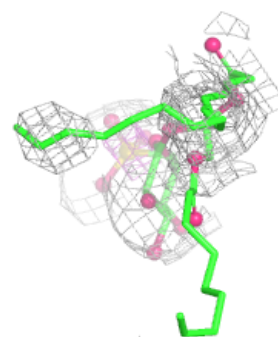
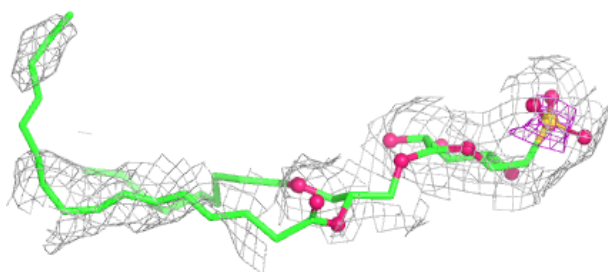
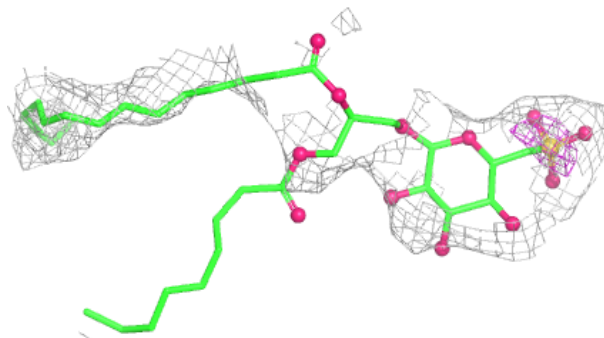
**Electron density around LMG I 220:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

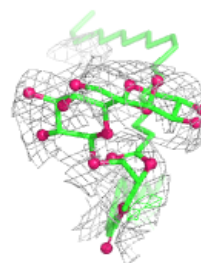
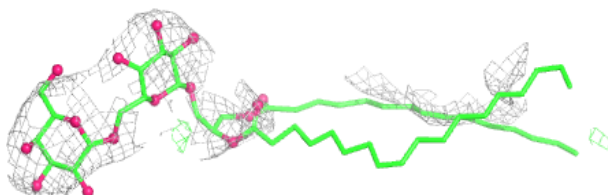
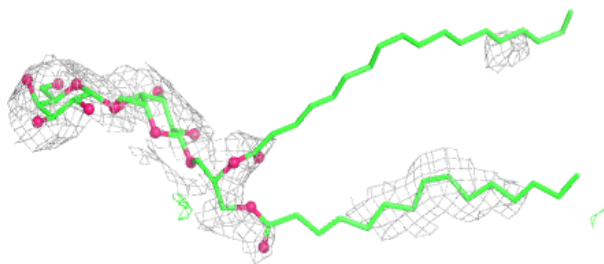


**Electron density around SQD L 213:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

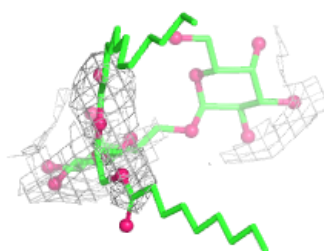
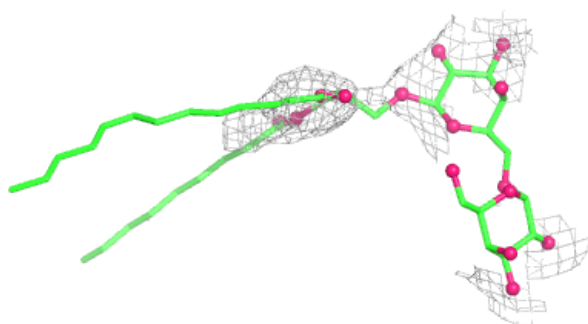
**Electron density around DGD D 362:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

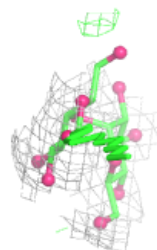
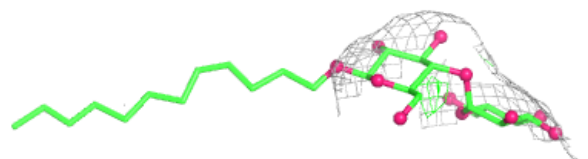
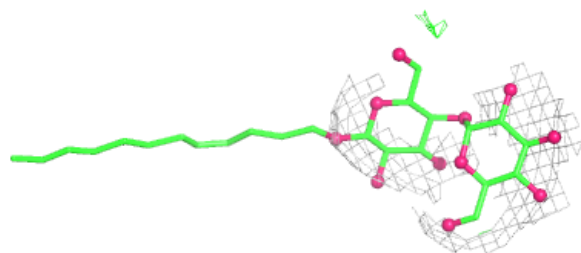


**Electron density around DGD A 375:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

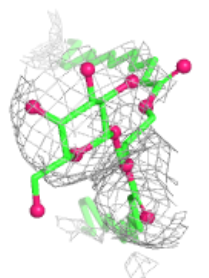
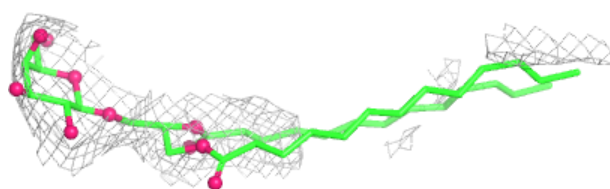
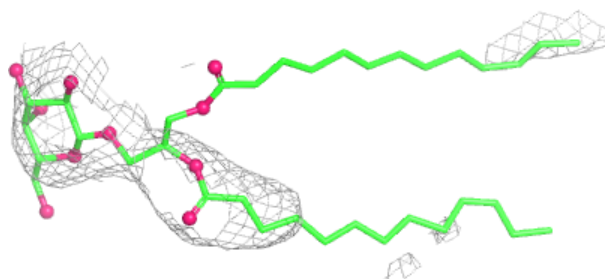
**Electron density around LMT A 376:**

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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

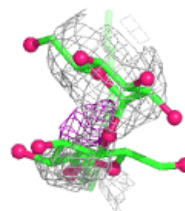
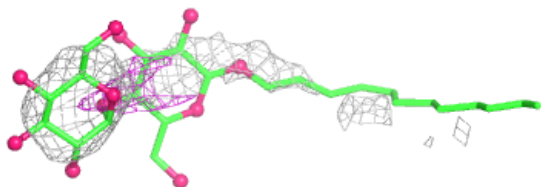
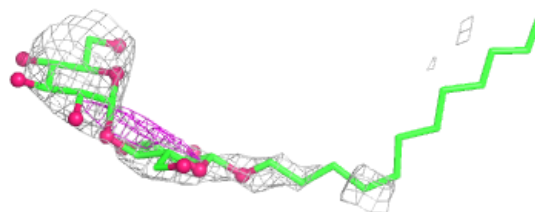


**Electron density around LMG C 494:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

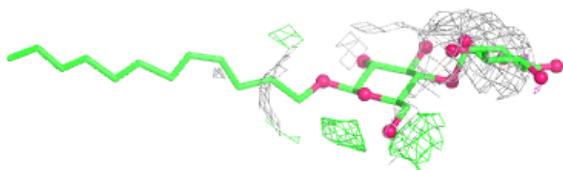
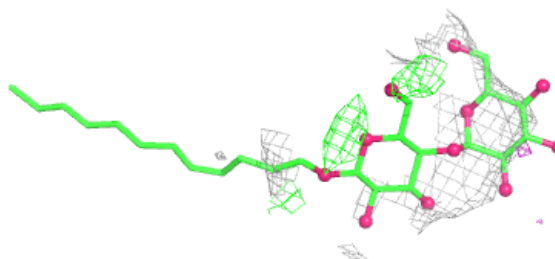
**Electron density around LMT B 535:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

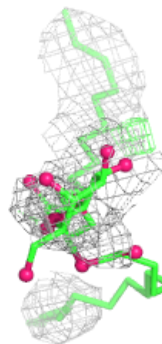
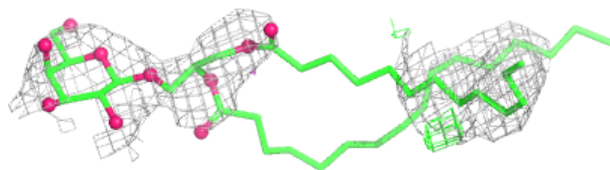
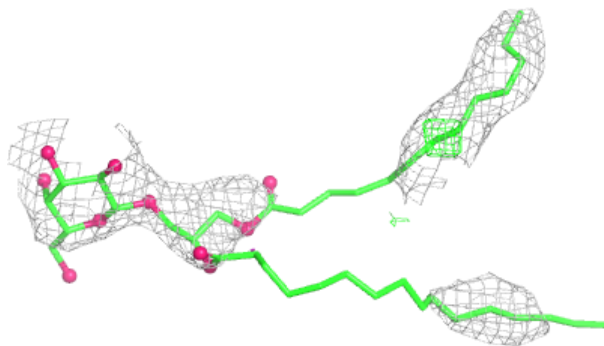


**Electron density around LMT D 536:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

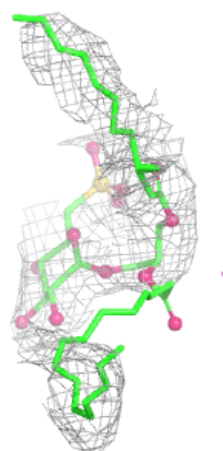
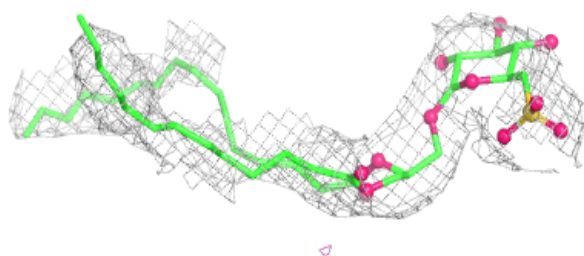
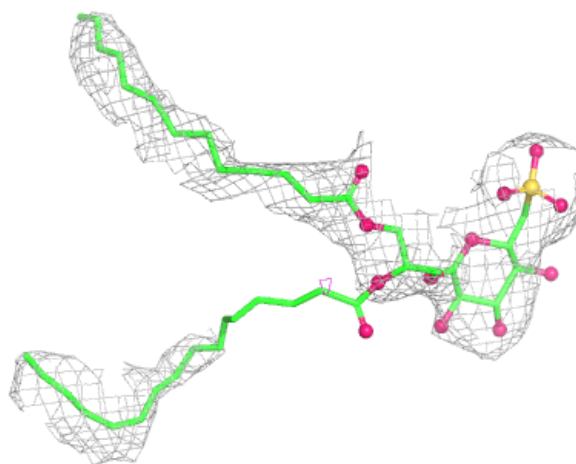
**Electron density around LMG D 360:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



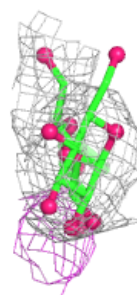
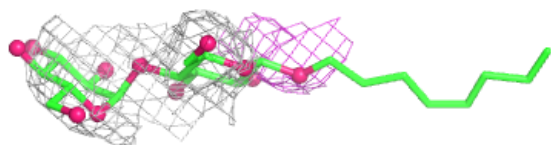
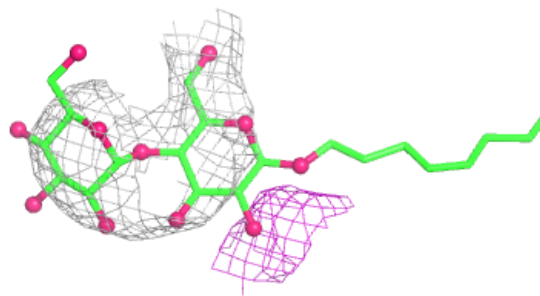
**Electron density around SQD C 475:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



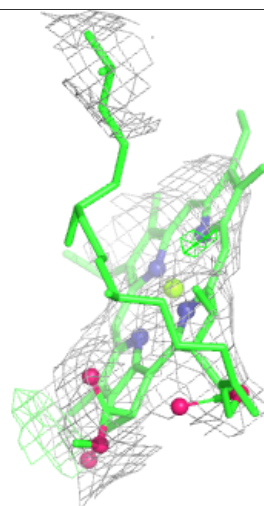
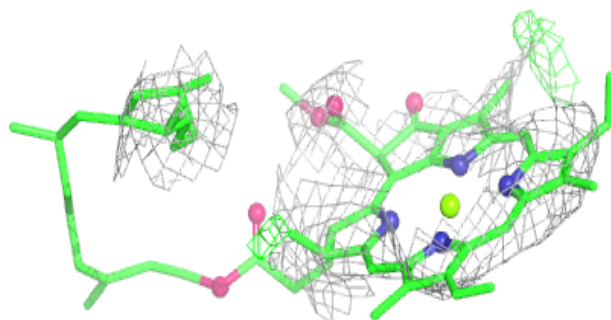
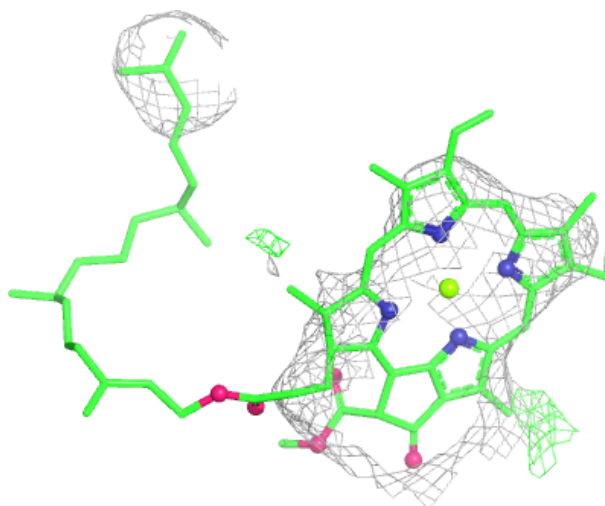
**Electron density around LMT D 363:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA B 526:**

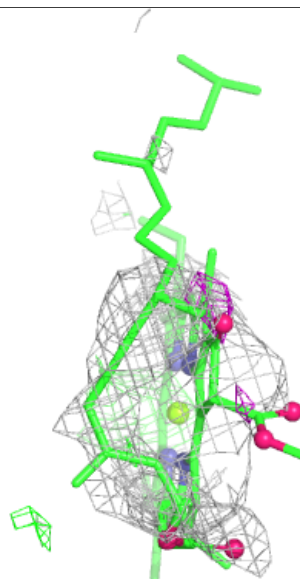
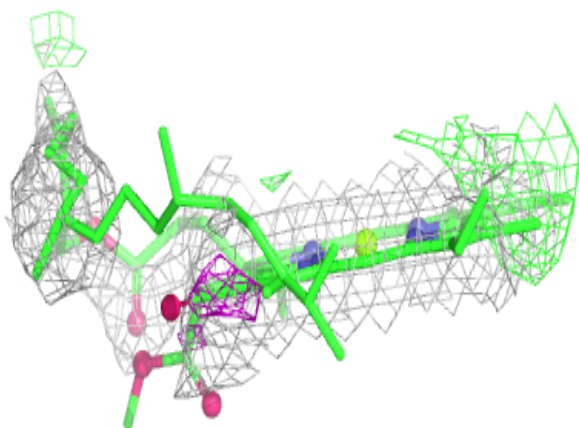
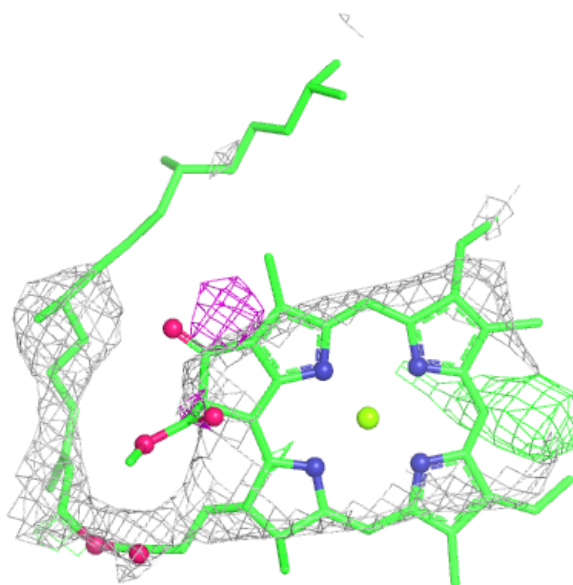
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





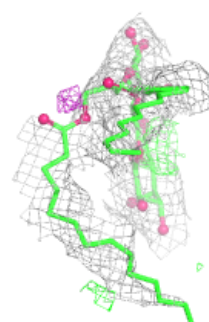
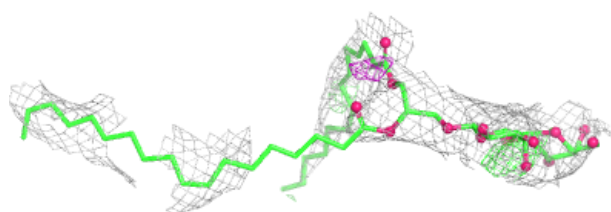
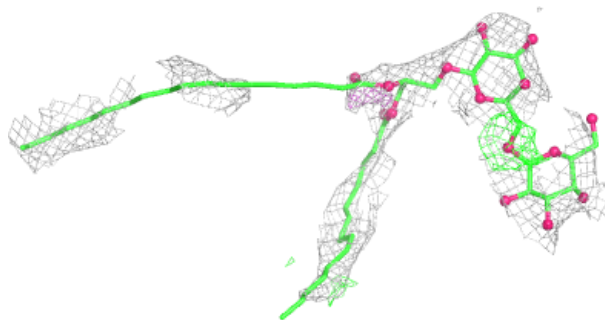
**Electron density around CLA B 511:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

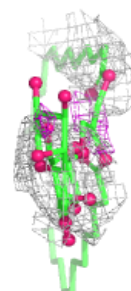
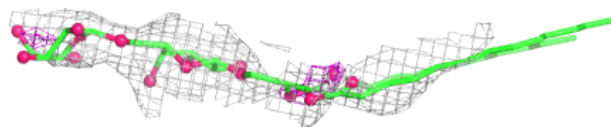
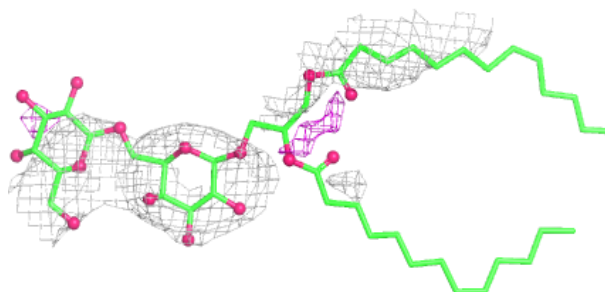


**Electron density around DGD C 492:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

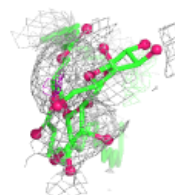
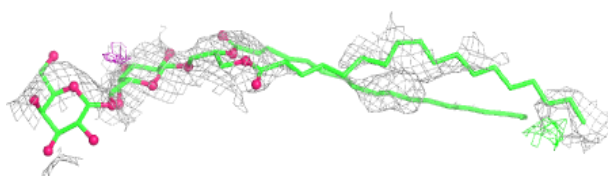
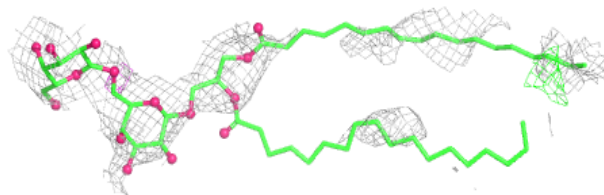
**Electron density around DGD C 474:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

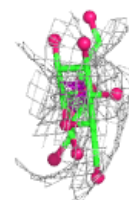
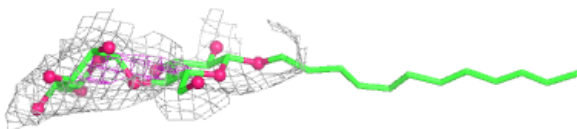
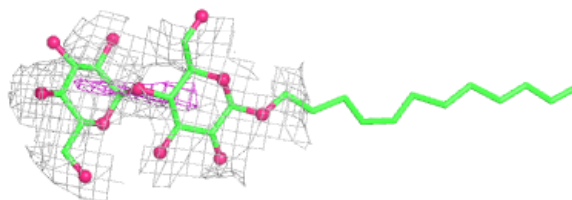


**Electron density around DGD C 493:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

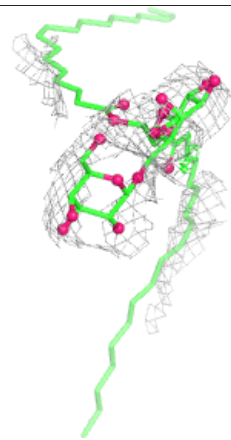
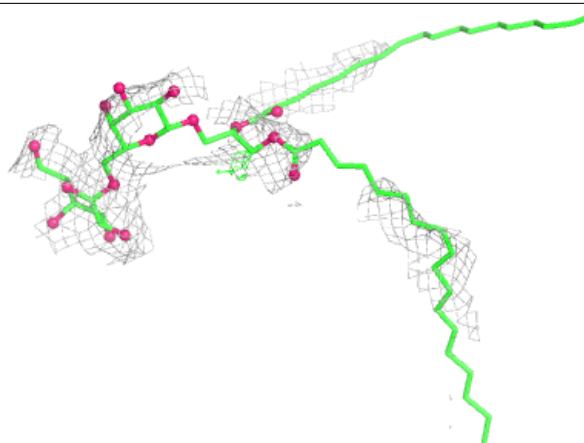
**Electron density around LMT I 274:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

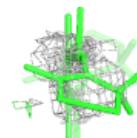
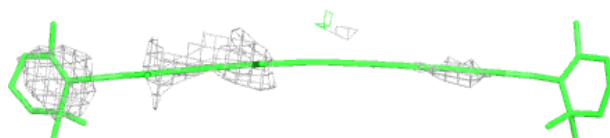
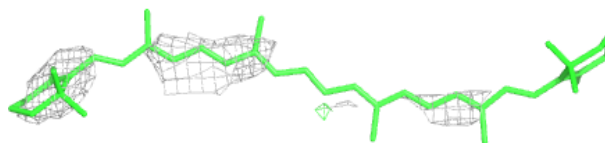


**Electron density around DGD B 533:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

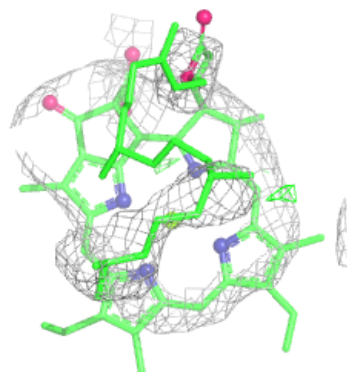
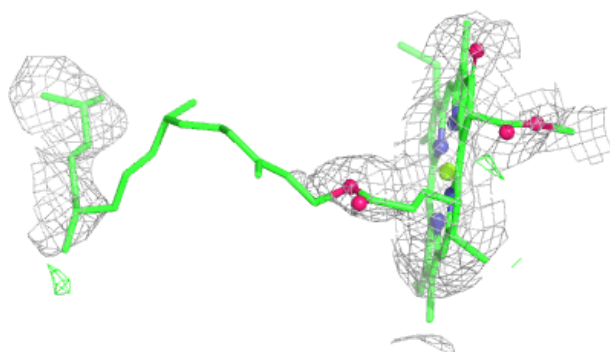
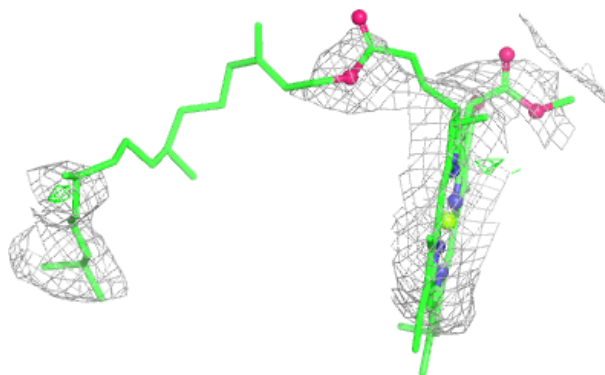
**Electron density around BCR B 530:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

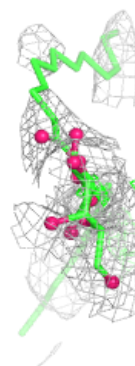
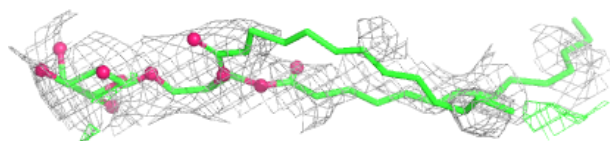
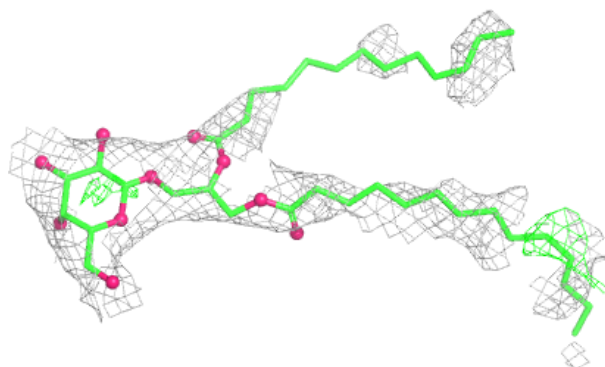


**Electron density around CLA C 482:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

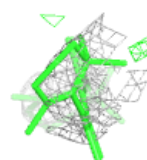
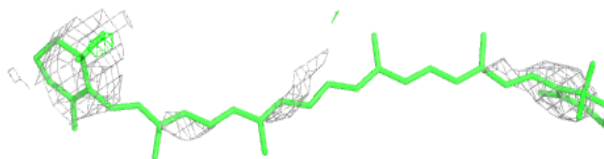
**Electron density around LMG D 359:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

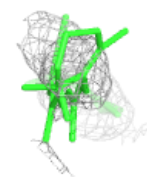
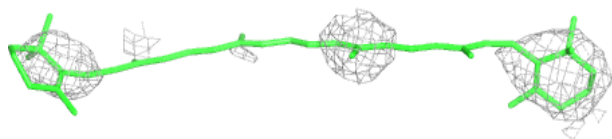
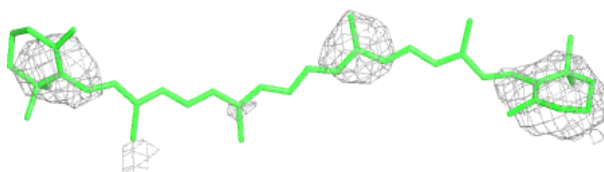


**Electron density around BCR C 490:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

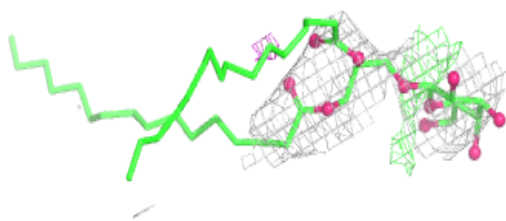
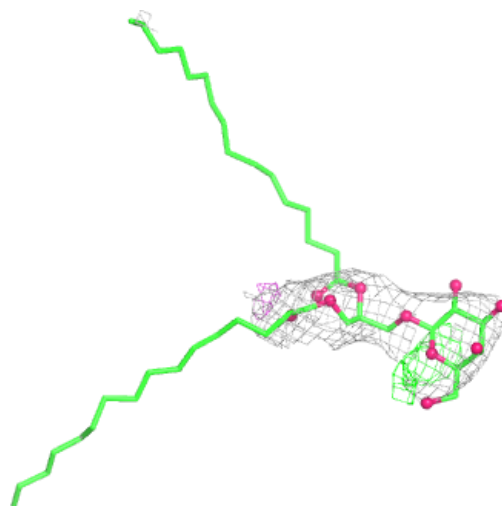
**Electron density around BCR B 527:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



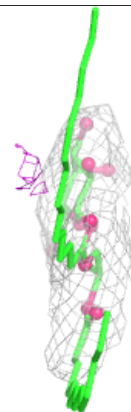
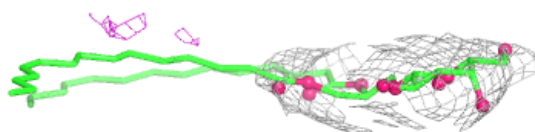
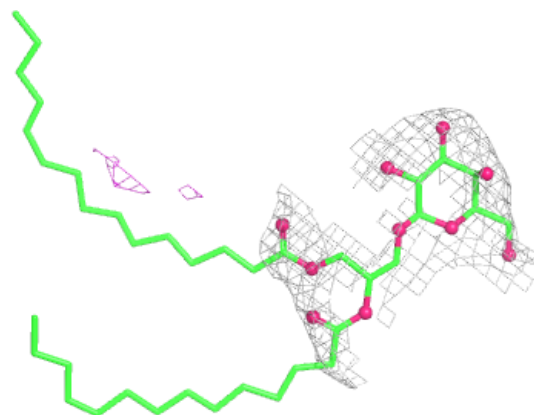
**Electron density around LMG A 373:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

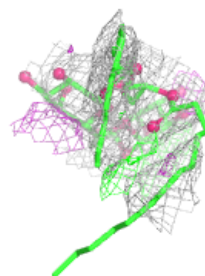
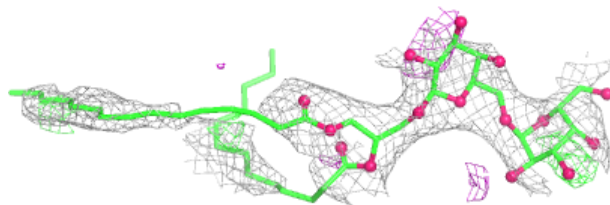
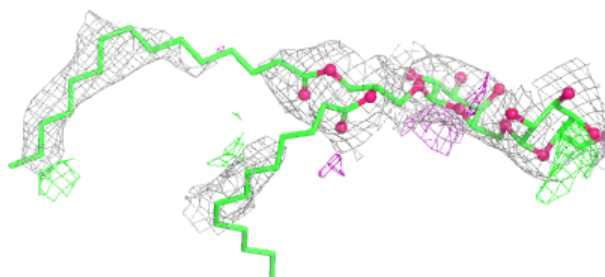


**Electron density around LMG J 492:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around DGD B 528:**

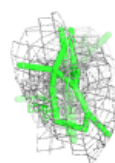
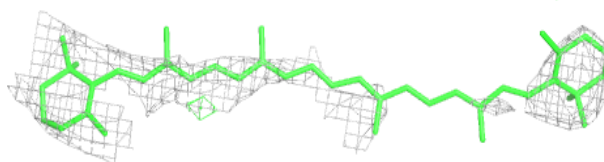
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



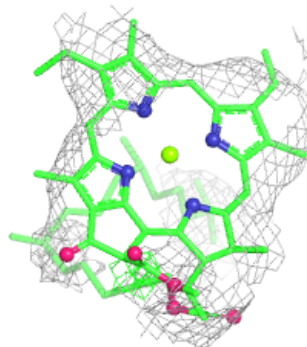
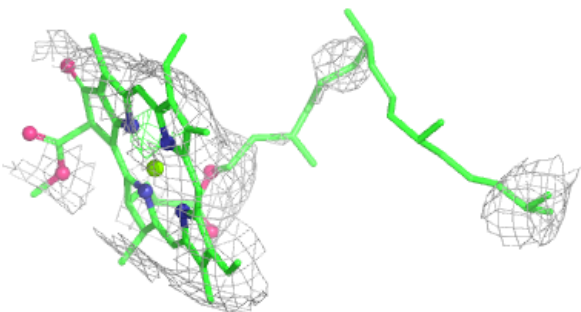
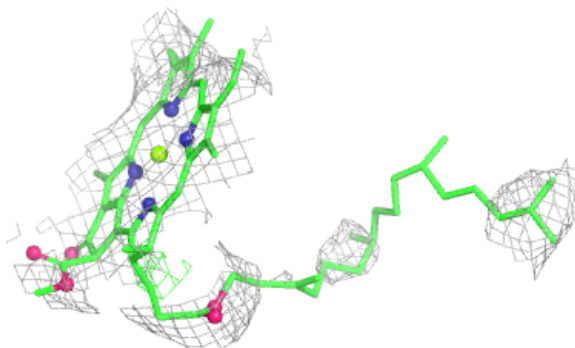


**Electron density around BCR B 529:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

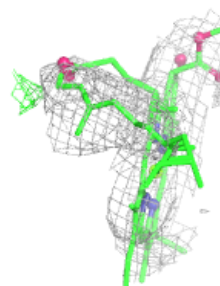
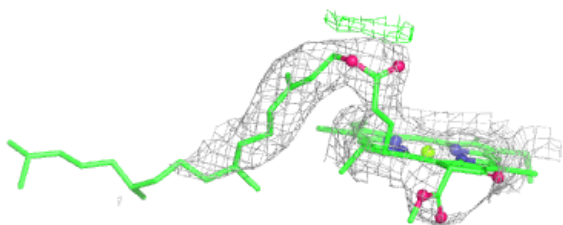
**Electron density around CLA C 488:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

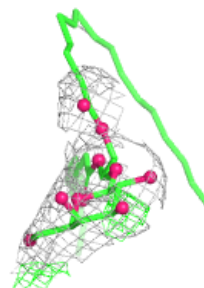
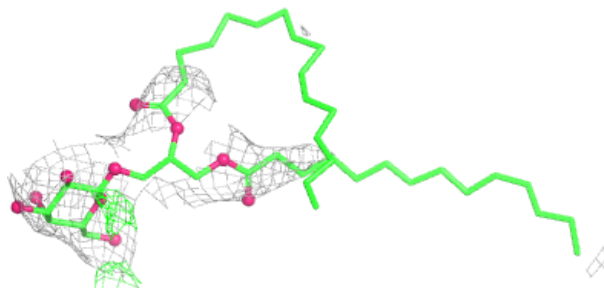


**Electron density around CLA A 363:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

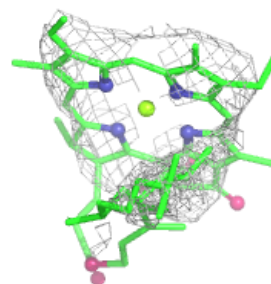
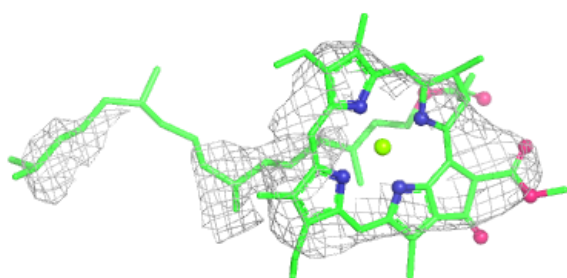
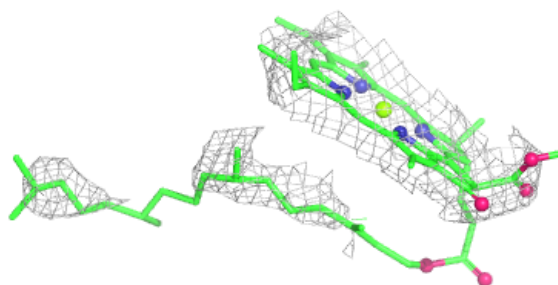
**Electron density around LMG B 531:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

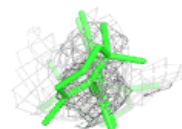
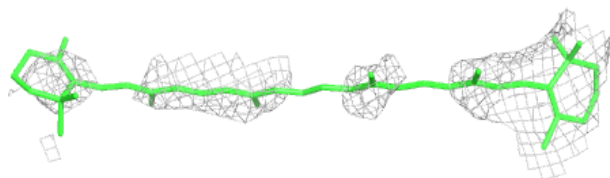
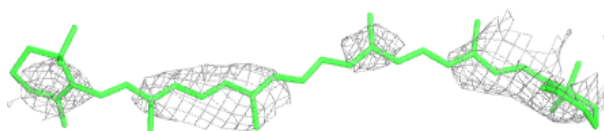


**Electron density around CLA B 524:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

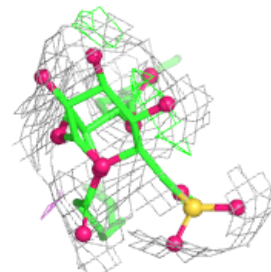
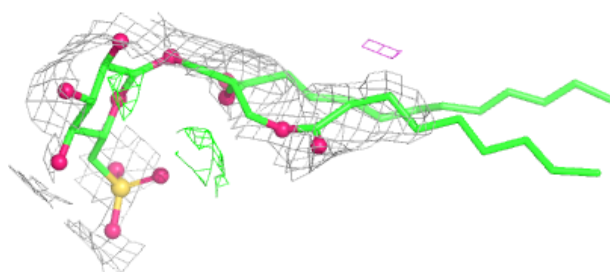
**Electron density around BCR Z 116:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

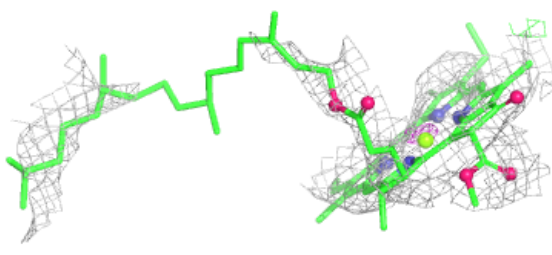
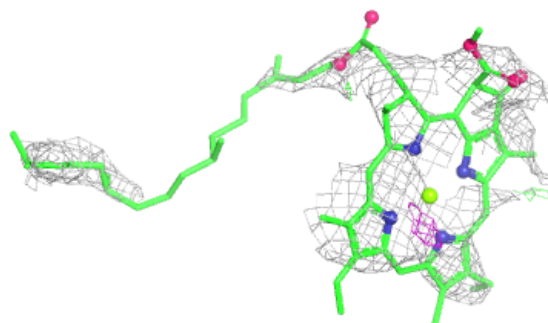


**Electron density around SQD D 361:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

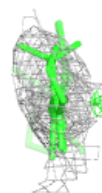
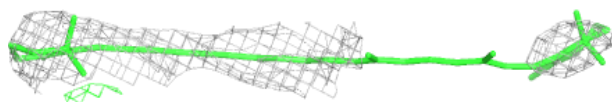
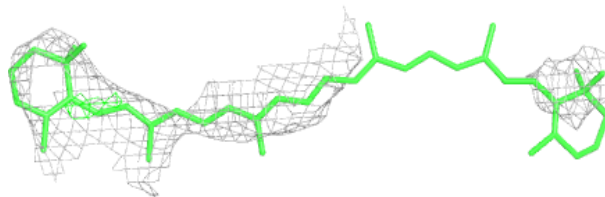
**Electron density around CLA C 486:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

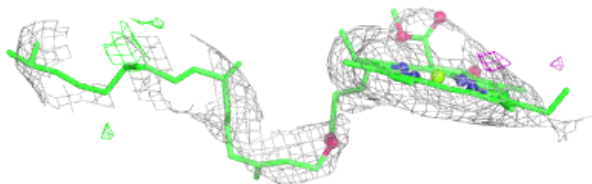
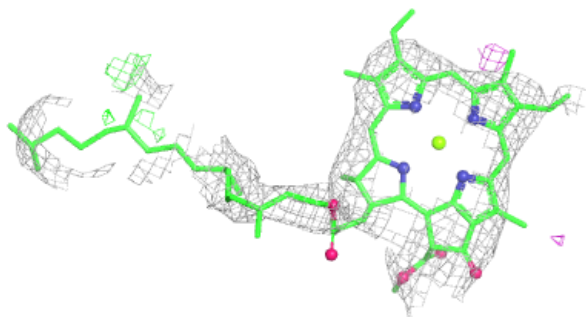


**Electron density around BCR J 112:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

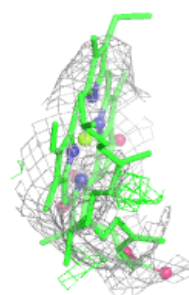
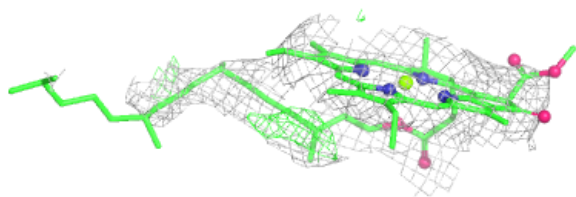
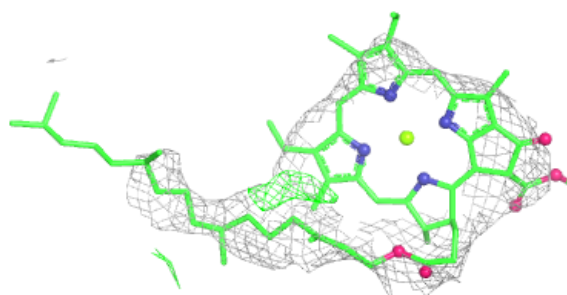
**Electron density around CLA A 364:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

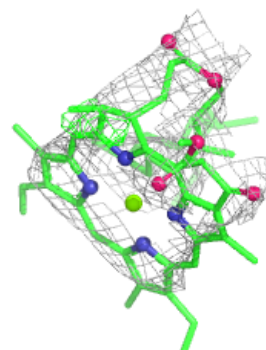
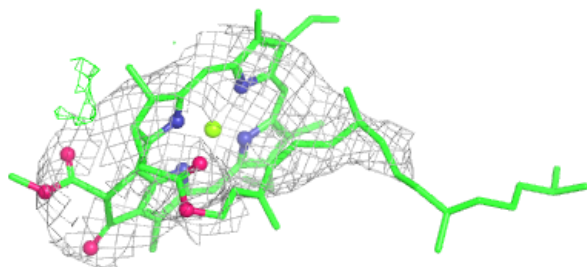


**Electron density around CLA C 477:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

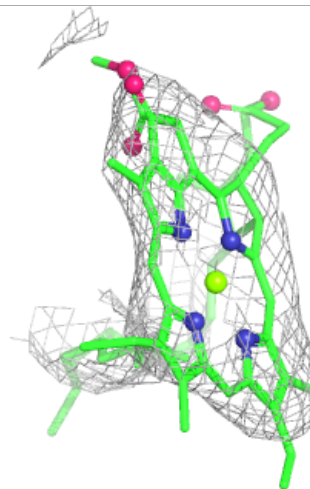
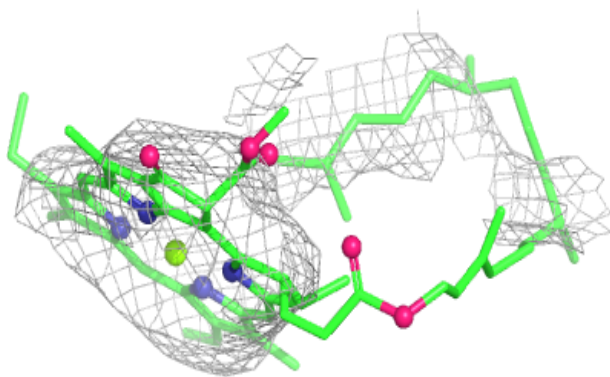
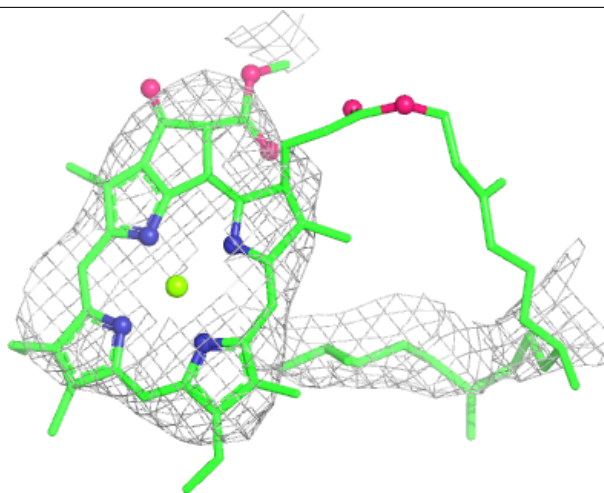
**Electron density around CLA C 481:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA B 525:**

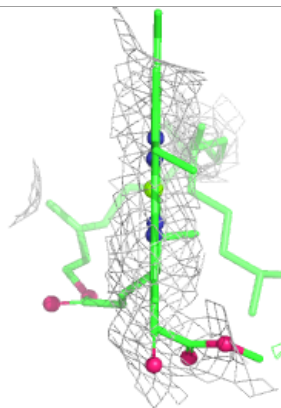
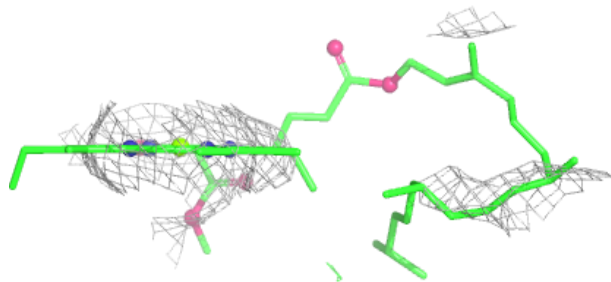
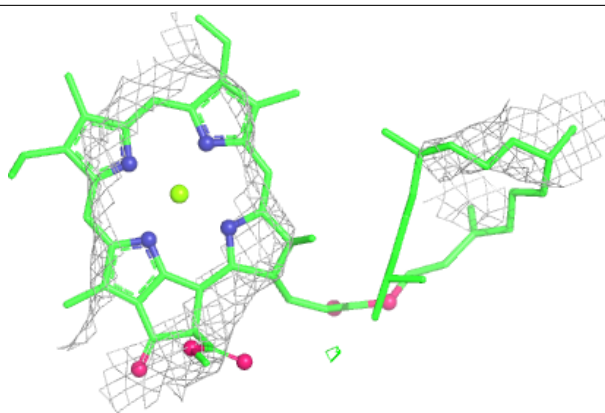
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA C 487:**

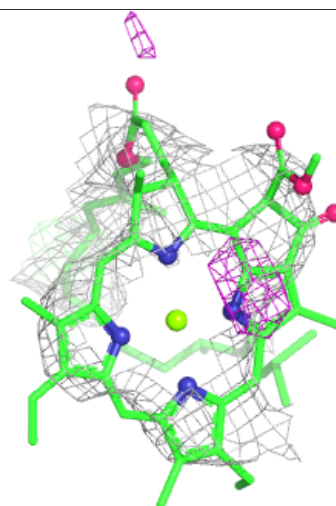
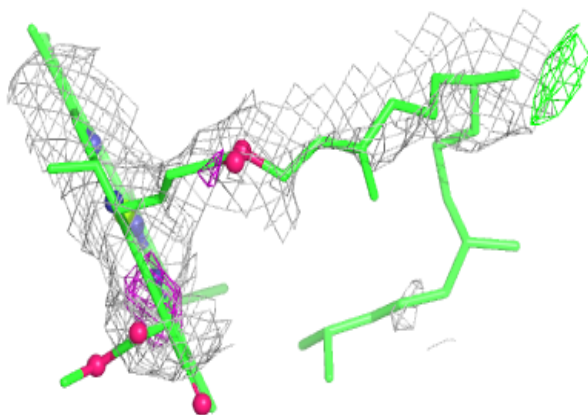
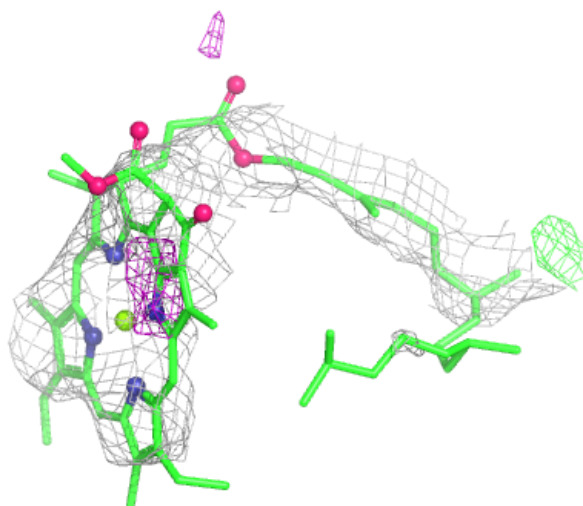
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





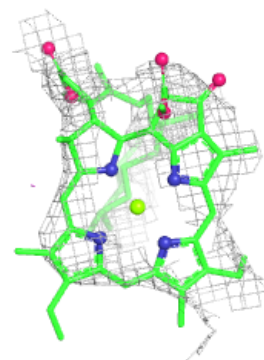
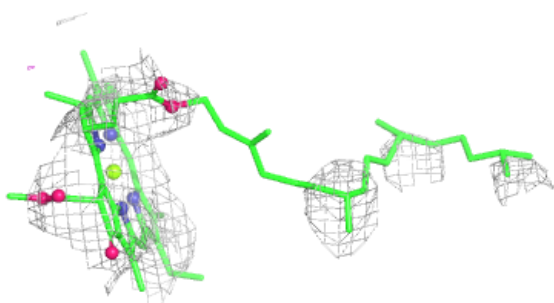
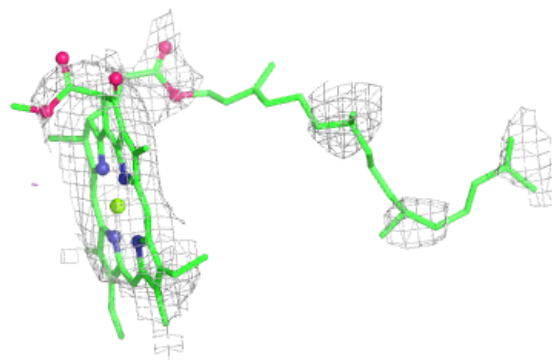
**Electron density around CLA C 479:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

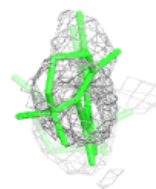
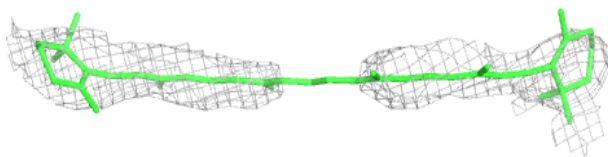
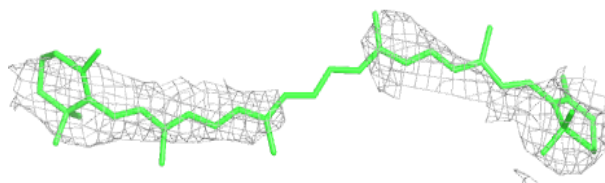


**Electron density around CLA C 484:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

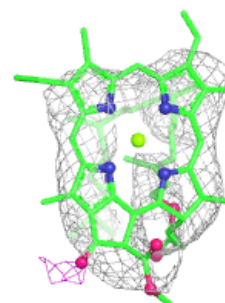
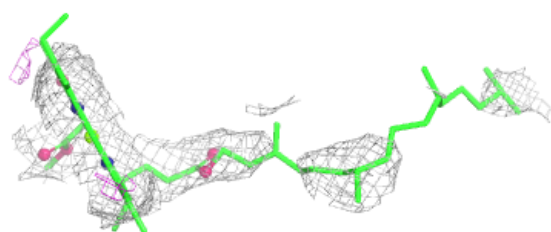
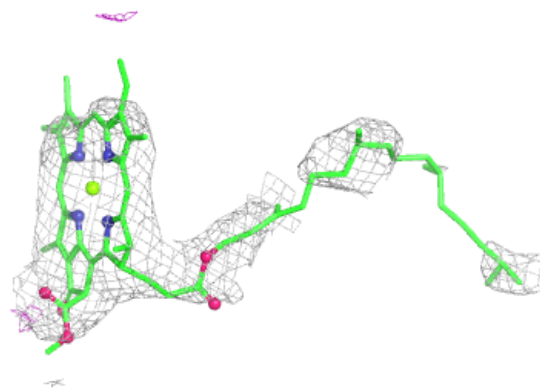
**Electron density around BCR X 107:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

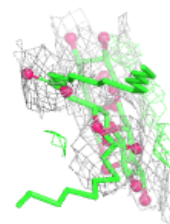
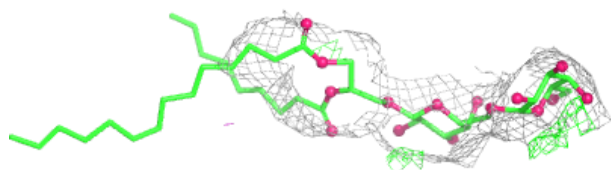
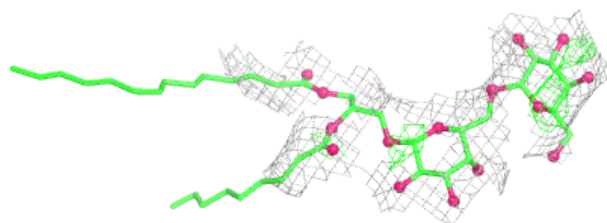


**Electron density around CLA D 356:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

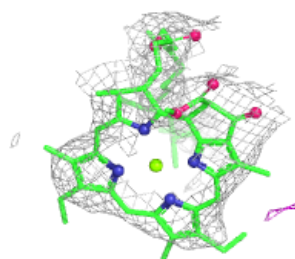
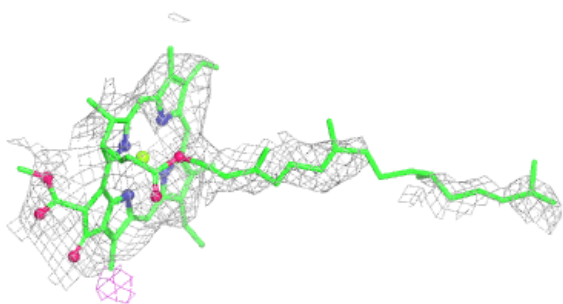
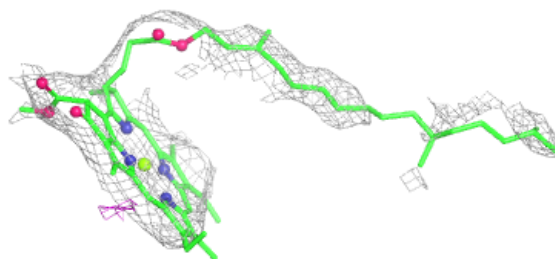
**Electron density around DGD C 491:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

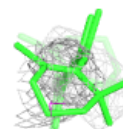
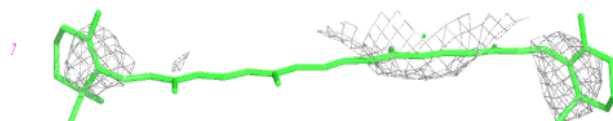
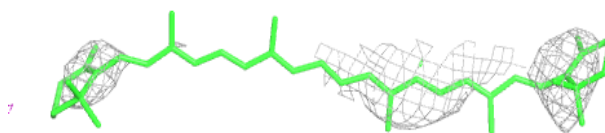


**Electron density around CLA C 480:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

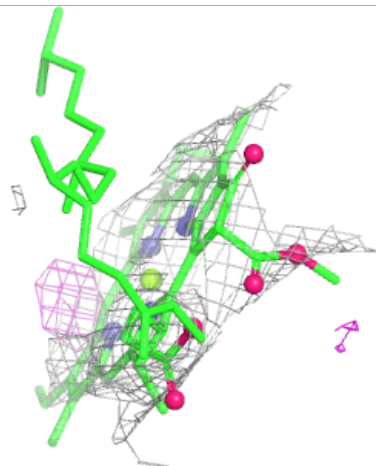
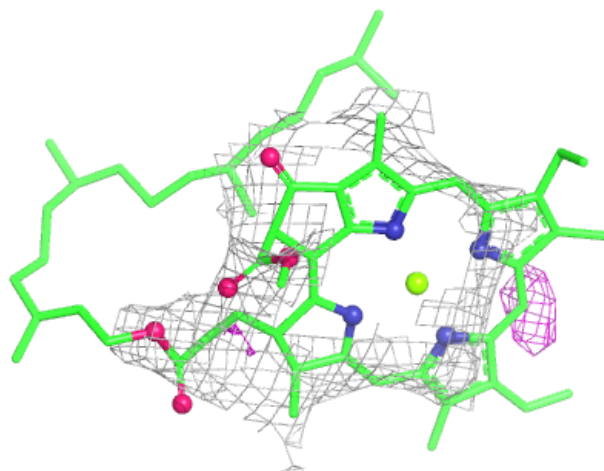
**Electron density around BCR A 369:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



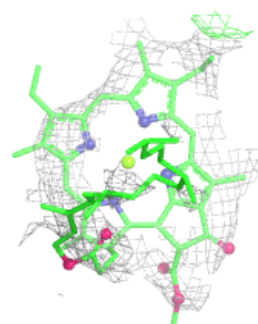
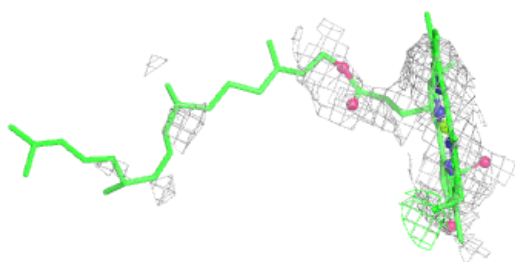
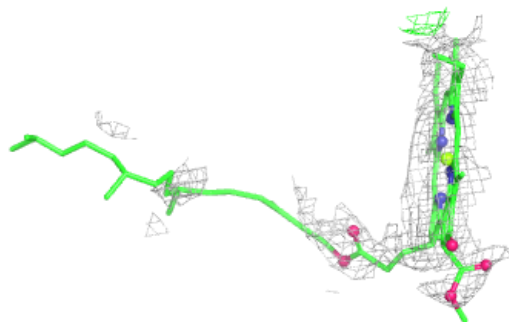
**Electron density around CLA C 485:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

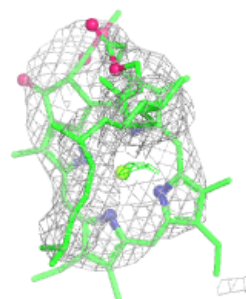
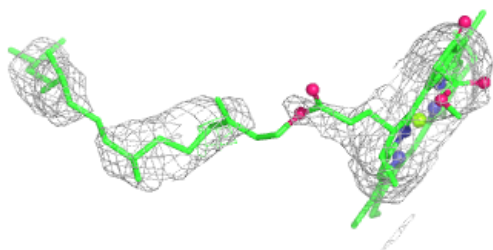
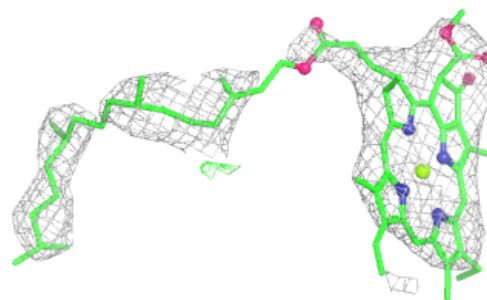


**Electron density around CLA B 516:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

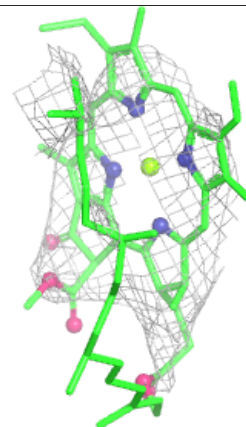
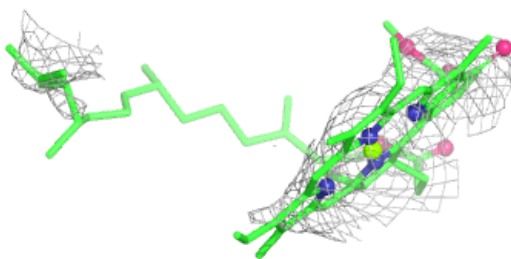
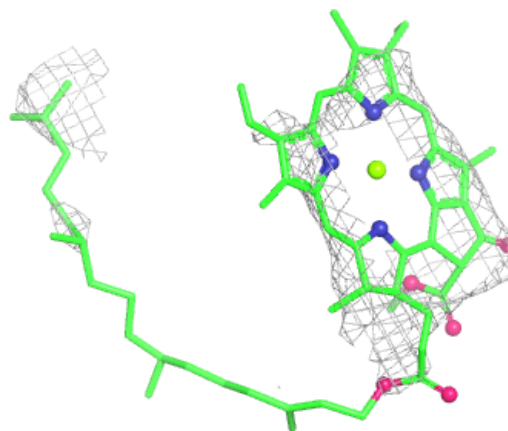
**Electron density around CLA A 366:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA C 483:**

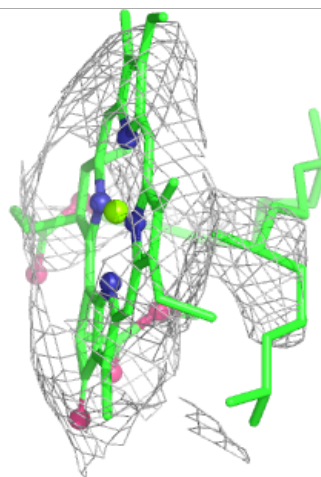
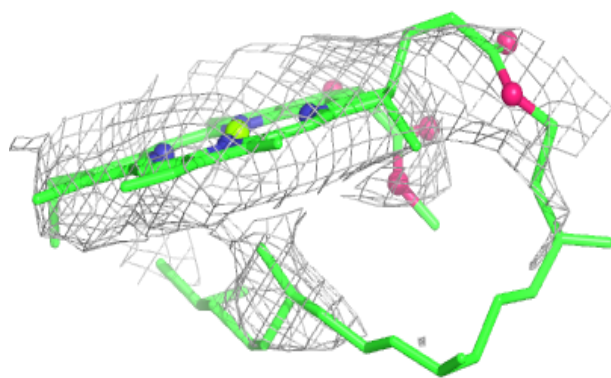
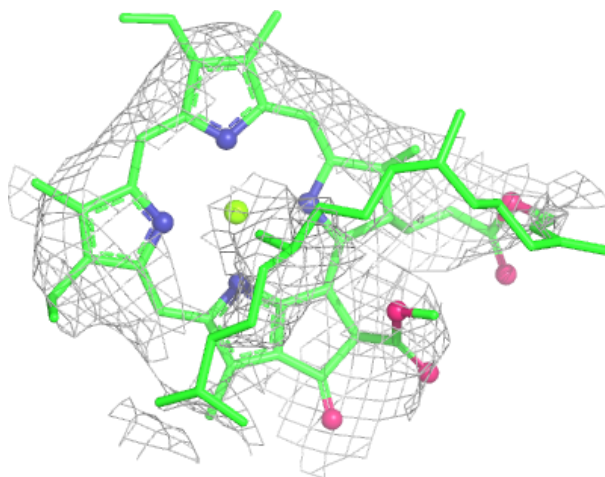
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA K 483:**

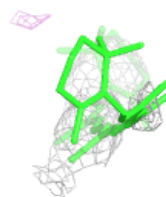
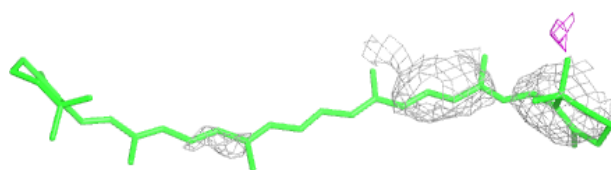
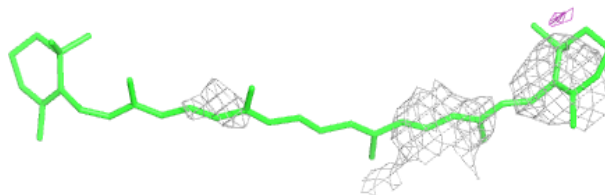
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



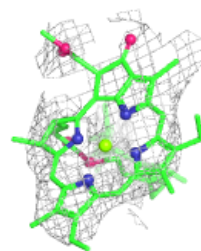
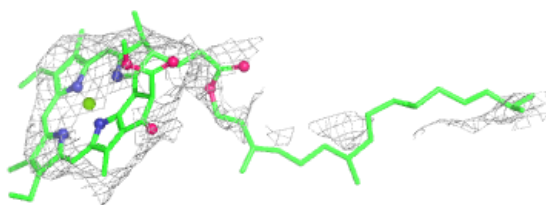


**Electron density around BCR C 489:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

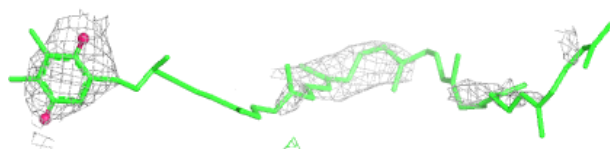
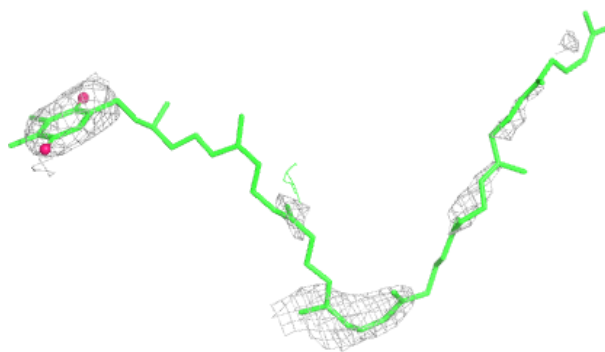
**Electron density around CLA C 478:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

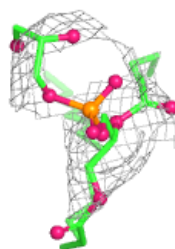
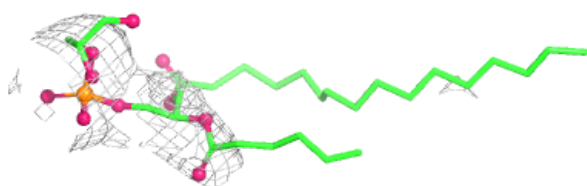
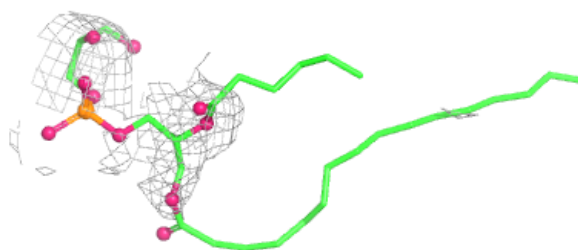


**Electron density around PL9 D 357:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

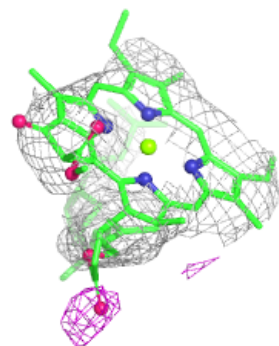
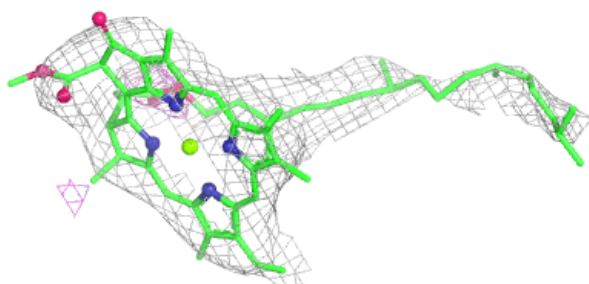
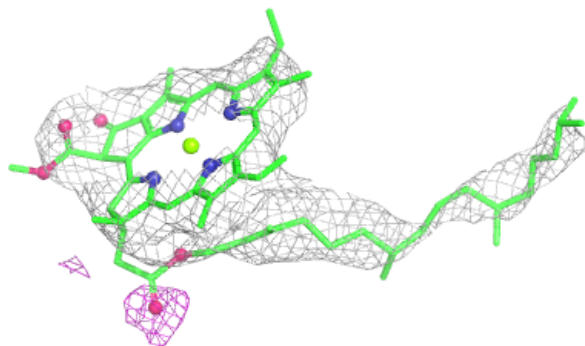
**Electron density around LHG A 371:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

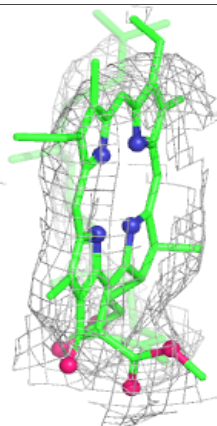
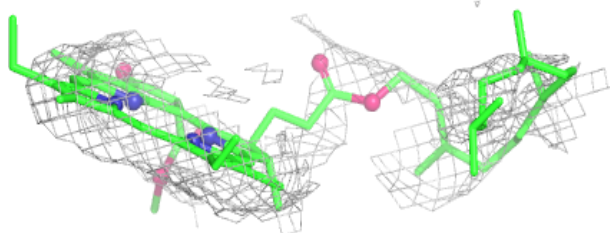
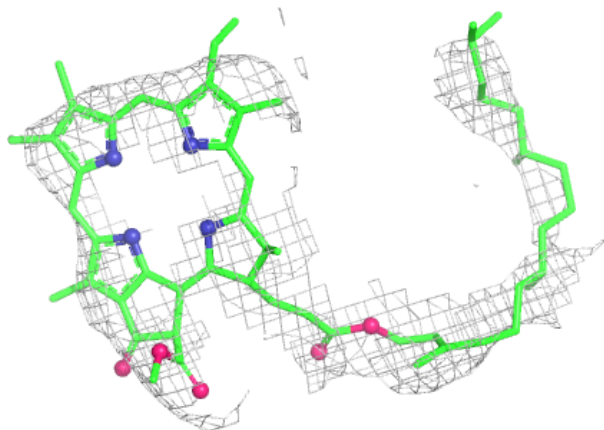


**Electron density around CLA B 518:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

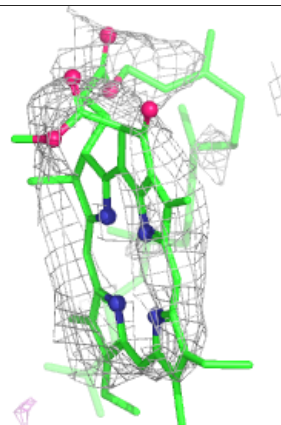
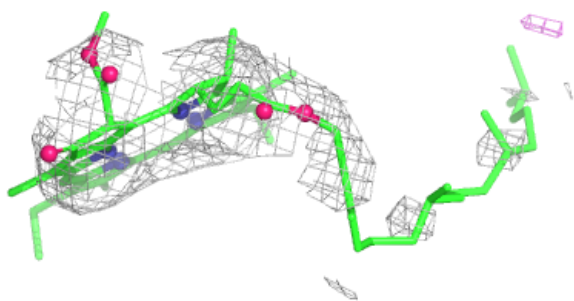
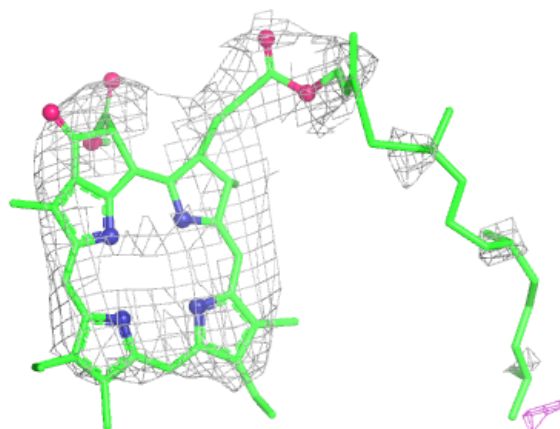
**Electron density around PHO A 365:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



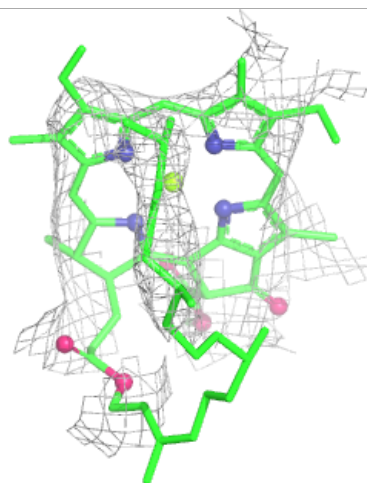
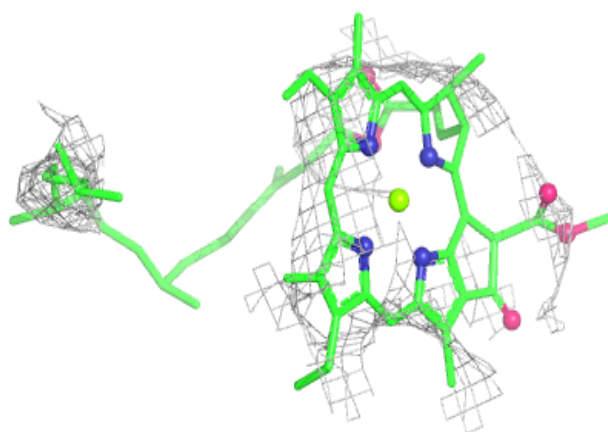
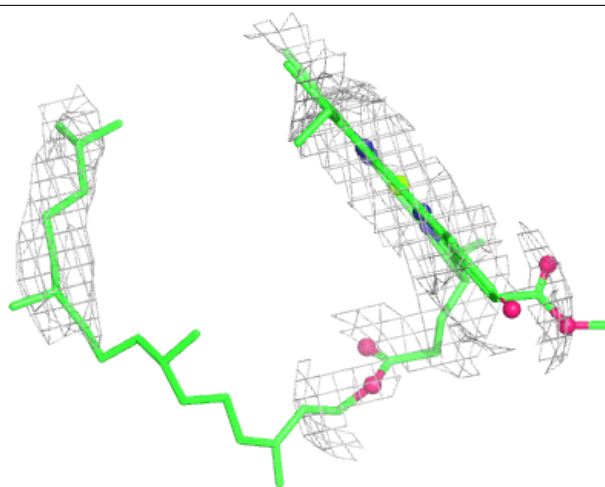
**Electron density around PHO D 355:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



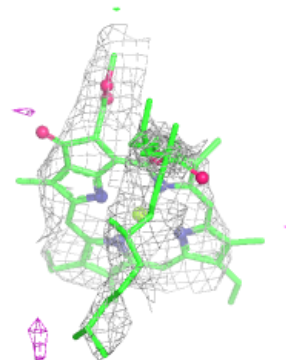
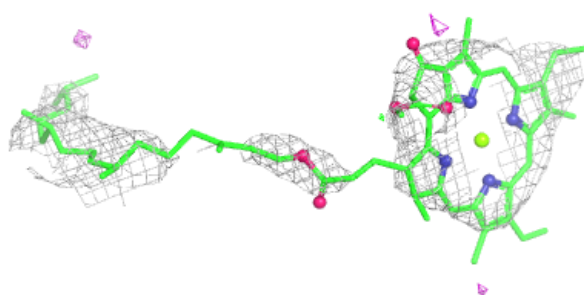
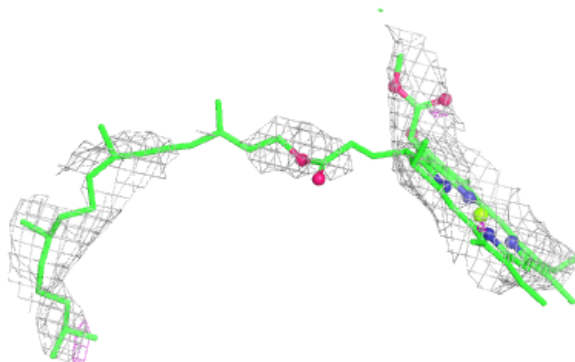
**Electron density around CLA B 521:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

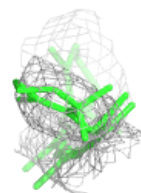
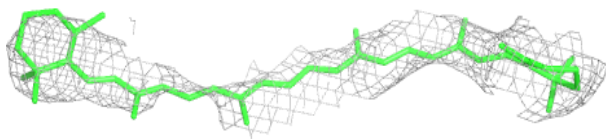
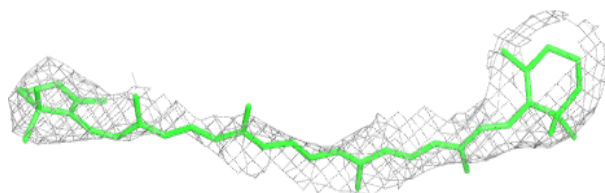


**Electron density around CLA D 354:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

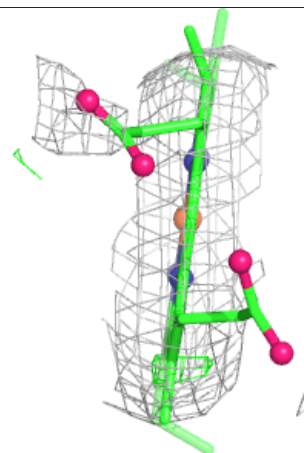
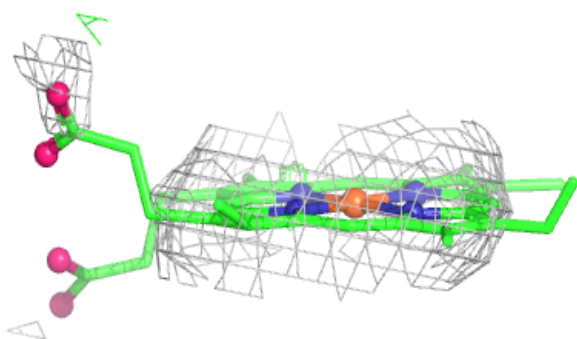
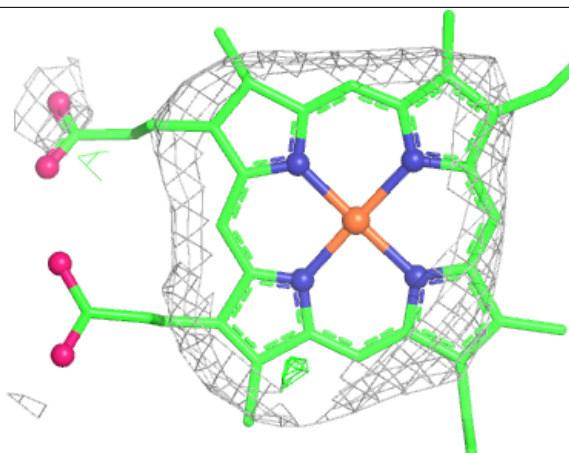
**Electron density around BCR D 358:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM F 85:**

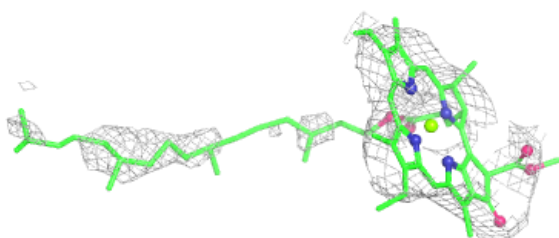
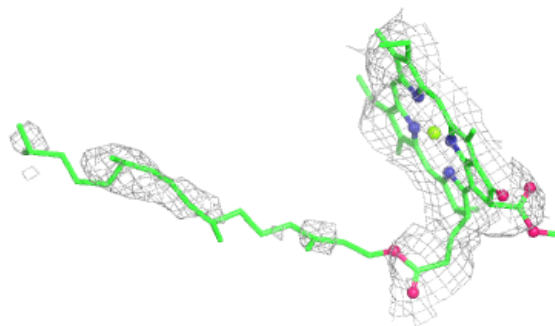
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



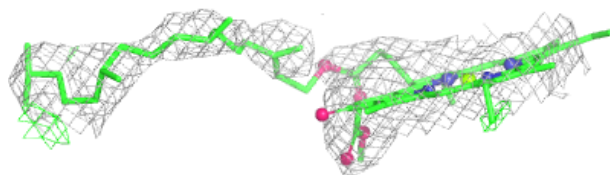
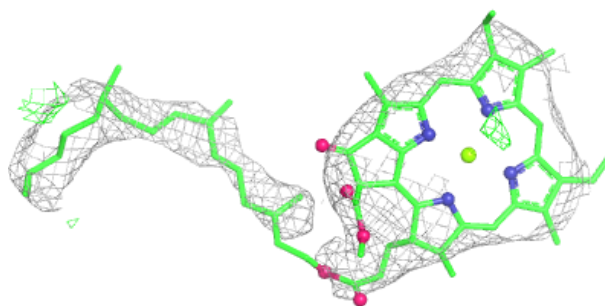


**Electron density around CLA B 517:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CLA B 512:**

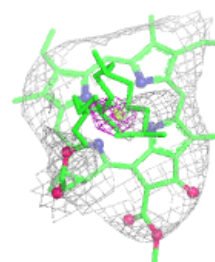
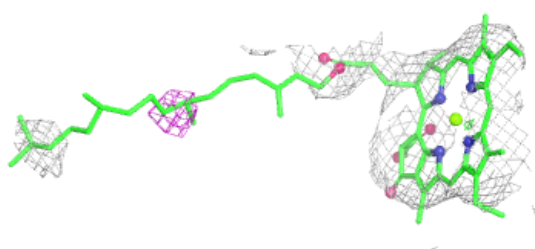
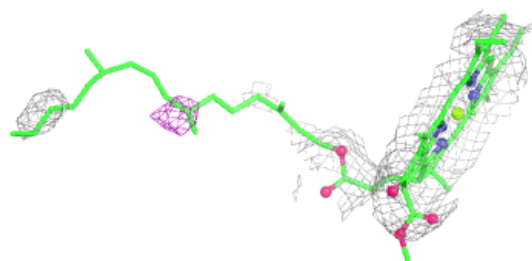
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



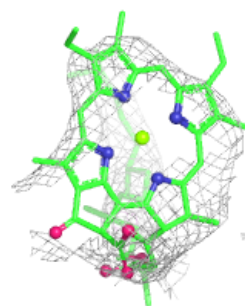
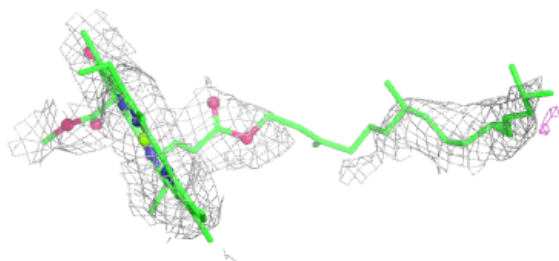
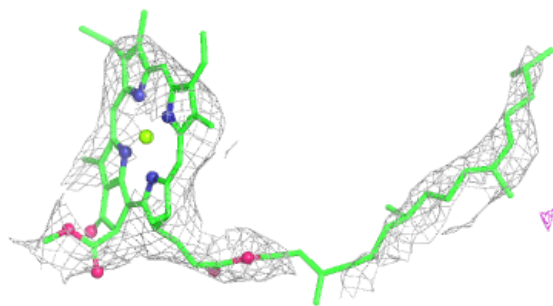


**Electron density around CLA B 514:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

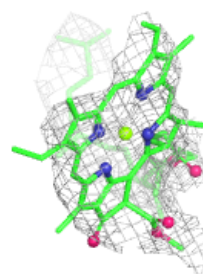
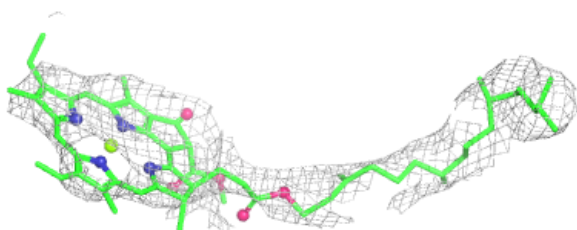
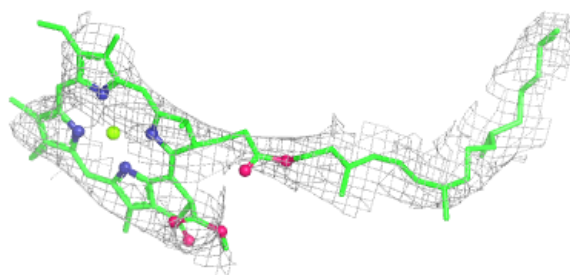
**Electron density around CLA B 519:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

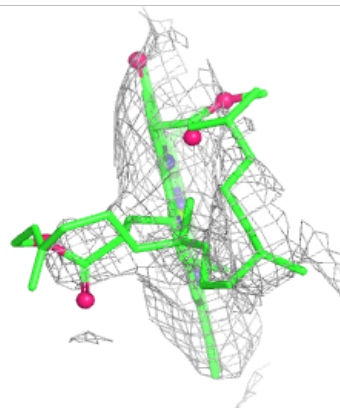
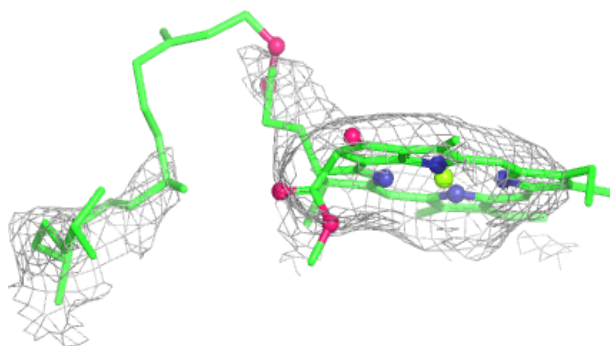
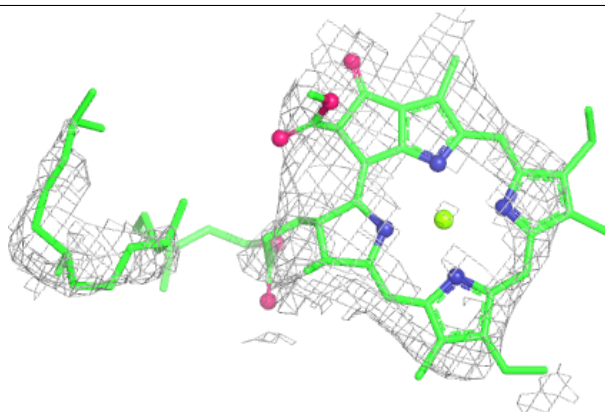


**Electron density around CLA A 362:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

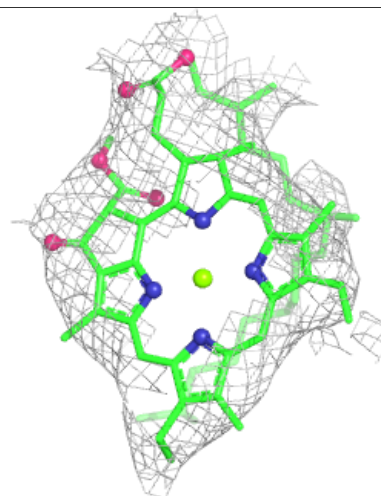
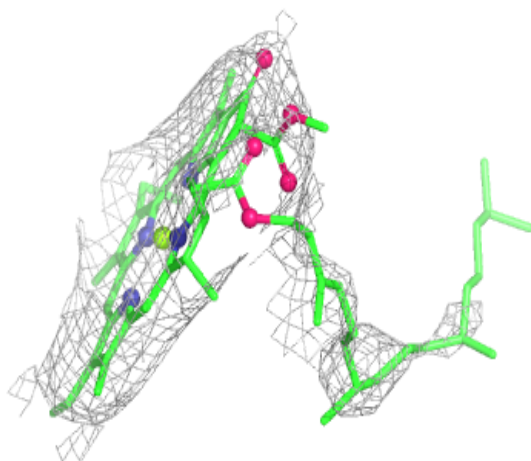
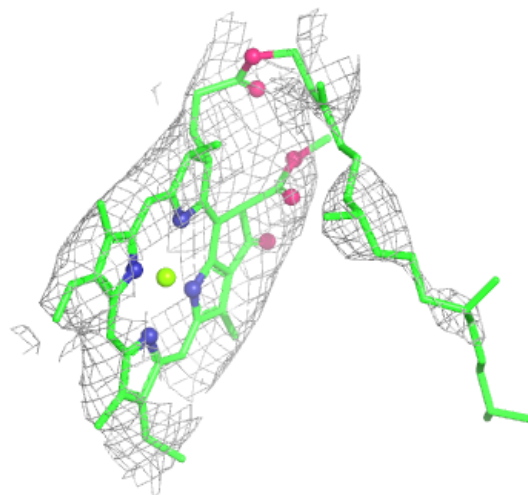
**Electron density around CLA B 522:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



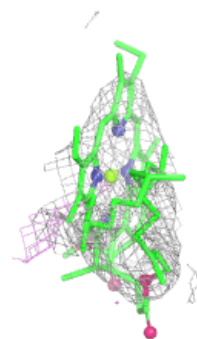
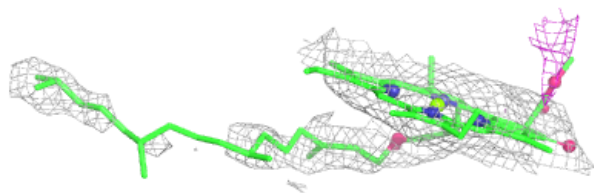
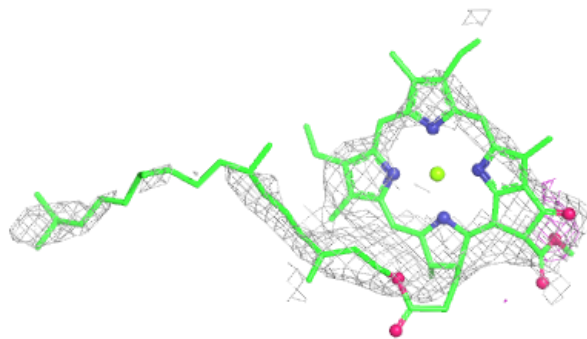
**Electron density around CLA B 523:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

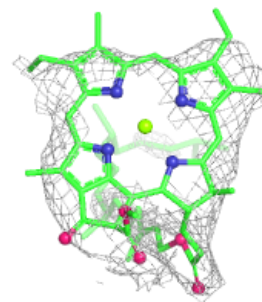
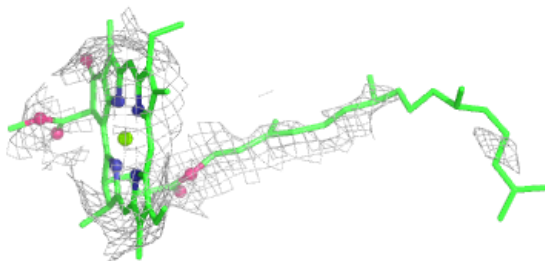
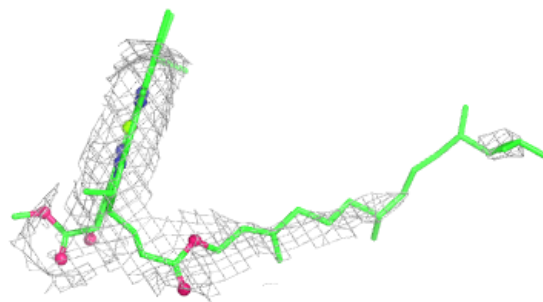


**Electron density around CLA B 513:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

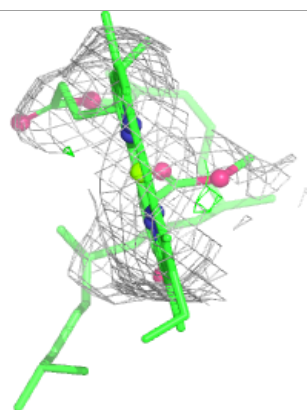
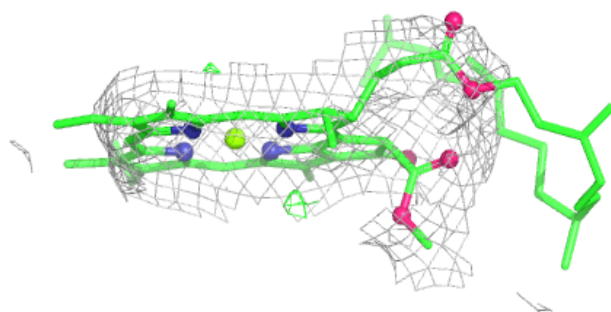
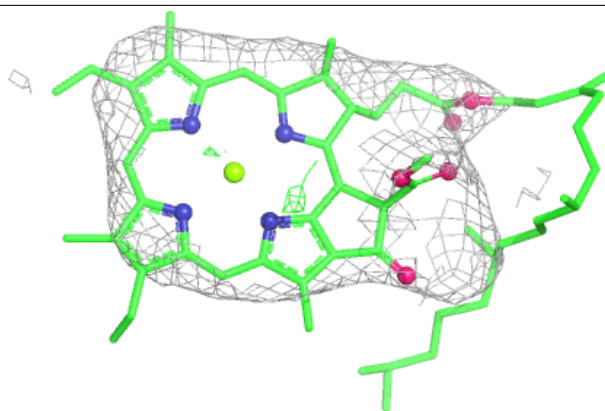
**Electron density around CLA B 515:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

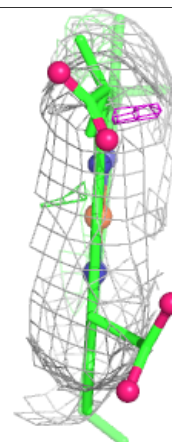
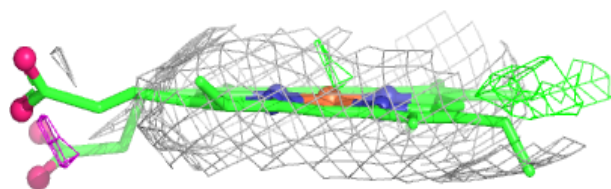
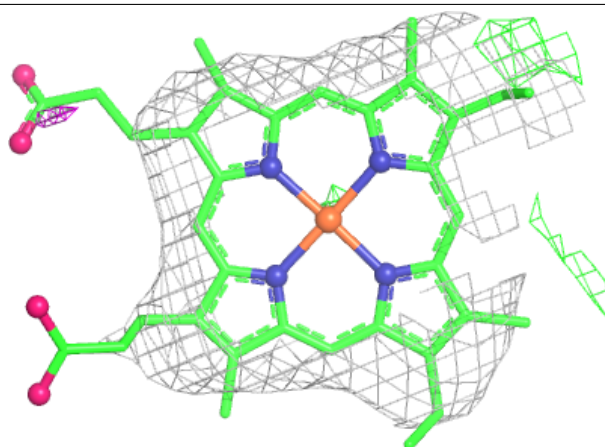


**Electron density around CLA B 520:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around HEM V 164:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.