



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:00 PM UTC

PDB ID : 1W5C / pdb\_00001w5c  
Title : Photosystem II from Thermosynechococcus elongatus  
Authors : Biesiadka, J.; Loll, B.; Kern, J.; Irrgang, K.-D.; Saenger, W.  
Deposited on : 2004-08-06  
Resolution : 3.20 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)               | : | NOT EXECUTED                                                     |
| EDS                            | : | NOT EXECUTED                                                     |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

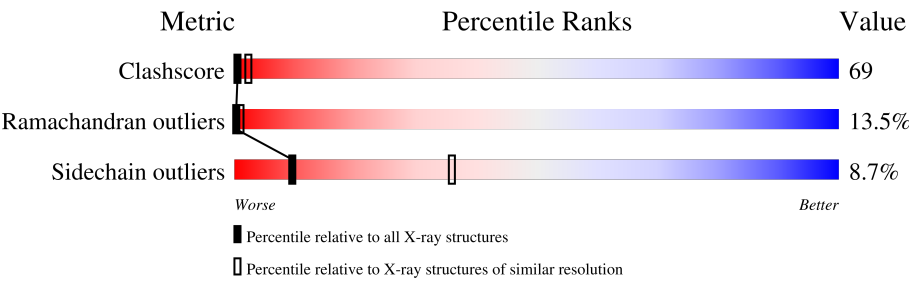
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| Clashscore            | 190562                      | 1573 (3.20-3.20)                                      |
| Ramachandran outliers | 187476                      | 1548 (3.20-3.20)                                      |
| Sidechain outliers    | 187428                      | 1547 (3.20-3.20)                                      |

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  $\leq 5\%$

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain                  |
|-----|-------|--------|-----------------------------------|
| 1   | A     | 360    | <div><div>21%52%17%8%</div></div> |
| 1   | G     | 360    | <div><div>22%51%16%8%</div></div> |
| 2   | B     | 510    | <div><div>29%47%15%6%</div></div> |
| 2   | H     | 510    | <div><div>29%47%14%6%</div></div> |
| 3   | C     | 473    | <div><div>25%47%18%7%</div></div> |
| 3   | I     | 473    | <div><div>26%46%18%7%</div></div> |
| 4   | D     | 352    | <div><div>21%56%20%..</div></div> |
| 4   | J     | 352    | <div><div>23%53%21%..</div></div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 5   | E     | 84     |                  |
| 5   | K     | 84     |                  |
| 6   | F     | 44     |                  |
| 6   | L     | 44     |                  |
| 7   | O     | 179    |                  |
| 7   | P     | 179    |                  |
| 8   | S     | 100    |                  |
| 8   | U     | 100    |                  |
| 9   | T     | 163    |                  |
| 9   | V     | 163    |                  |
| 10  | X     | 359    |                  |
| 10  | Y     | 359    |                  |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 11  | CLA  | A     | 1342 | X         | -        | -       | -                |
| 11  | CLA  | A     | 1343 | X         | -        | -       | -                |
| 11  | CLA  | A     | 1344 | X         | -        | -       | -                |
| 11  | CLA  | A     | 1346 | X         | -        | -       | -                |
| 11  | CLA  | B     | 1482 | X         | -        | -       | -                |
| 11  | CLA  | B     | 1483 | X         | -        | -       | -                |
| 11  | CLA  | B     | 1484 | X         | -        | -       | -                |
| 11  | CLA  | B     | 1485 | X         | -        | -       | -                |
| 11  | CLA  | B     | 1486 | X         | -        | -       | -                |
| 11  | CLA  | B     | 1487 | X         | -        | -       | -                |
| 11  | CLA  | B     | 1488 | X         | -        | -       | -                |
| 11  | CLA  | B     | 1489 | X         | -        | -       | -                |
| 11  | CLA  | B     | 1490 | X         | -        | -       | -                |
| 11  | CLA  | B     | 1491 | X         | -        | -       | -                |
| 11  | CLA  | B     | 1492 | X         | -        | -       | -                |
| 11  | CLA  | B     | 1493 | X         | -        | -       | -                |
| 11  | CLA  | B     | 1494 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 11  | CLA  | B     | 1495 | X         | -        | -       | -                |
| 11  | CLA  | B     | 1496 | X         | -        | -       | -                |
| 11  | CLA  | B     | 1497 | X         | -        | -       | -                |
| 11  | CLA  | C     | 1459 | X         | -        | -       | -                |
| 11  | CLA  | C     | 1460 | X         | -        | -       | -                |
| 11  | CLA  | C     | 1461 | X         | -        | -       | -                |
| 11  | CLA  | C     | 1462 | X         | -        | -       | -                |
| 11  | CLA  | C     | 1463 | X         | -        | -       | -                |
| 11  | CLA  | C     | 1464 | X         | -        | -       | -                |
| 11  | CLA  | C     | 1465 | X         | -        | -       | -                |
| 11  | CLA  | C     | 1466 | X         | -        | -       | -                |
| 11  | CLA  | C     | 1467 | X         | -        | -       | -                |
| 11  | CLA  | C     | 1468 | X         | -        | -       | -                |
| 11  | CLA  | C     | 1469 | X         | -        | -       | -                |
| 11  | CLA  | C     | 1470 | X         | -        | -       | -                |
| 11  | CLA  | C     | 1471 | X         | -        | -       | -                |
| 11  | CLA  | D     | 1351 | X         | -        | -       | -                |
| 11  | CLA  | D     | 1353 | X         | -        | -       | -                |
| 11  | CLA  | G     | 1342 | X         | -        | -       | -                |
| 11  | CLA  | G     | 1343 | X         | -        | -       | -                |
| 11  | CLA  | G     | 1344 | X         | -        | -       | -                |
| 11  | CLA  | G     | 1346 | X         | -        | -       | -                |
| 11  | CLA  | H     | 1482 | X         | -        | -       | -                |
| 11  | CLA  | H     | 1483 | X         | -        | -       | -                |
| 11  | CLA  | H     | 1484 | X         | -        | -       | -                |
| 11  | CLA  | H     | 1485 | X         | -        | -       | -                |
| 11  | CLA  | H     | 1486 | X         | -        | -       | -                |
| 11  | CLA  | H     | 1487 | X         | -        | -       | -                |
| 11  | CLA  | H     | 1488 | X         | -        | -       | -                |
| 11  | CLA  | H     | 1489 | X         | -        | -       | -                |
| 11  | CLA  | H     | 1490 | X         | -        | -       | -                |
| 11  | CLA  | H     | 1491 | X         | -        | -       | -                |
| 11  | CLA  | H     | 1492 | X         | -        | -       | -                |
| 11  | CLA  | H     | 1493 | X         | -        | -       | -                |
| 11  | CLA  | H     | 1494 | X         | -        | -       | -                |
| 11  | CLA  | H     | 1495 | X         | -        | -       | -                |
| 11  | CLA  | H     | 1496 | X         | -        | -       | -                |
| 11  | CLA  | H     | 1497 | X         | -        | -       | -                |
| 11  | CLA  | I     | 1459 | X         | -        | -       | -                |
| 11  | CLA  | I     | 1460 | X         | -        | -       | -                |
| 11  | CLA  | I     | 1461 | X         | -        | -       | -                |
| 11  | CLA  | I     | 1462 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 11  | CLA  | I     | 1463 | X         | -        | -       | -                |
| 11  | CLA  | I     | 1464 | X         | -        | -       | -                |
| 11  | CLA  | I     | 1465 | X         | -        | -       | -                |
| 11  | CLA  | I     | 1466 | X         | -        | -       | -                |
| 11  | CLA  | I     | 1467 | X         | -        | -       | -                |
| 11  | CLA  | I     | 1468 | X         | -        | -       | -                |
| 11  | CLA  | I     | 1469 | X         | -        | -       | -                |
| 11  | CLA  | I     | 1470 | X         | -        | -       | -                |
| 11  | CLA  | I     | 1471 | X         | -        | -       | -                |
| 11  | CLA  | J     | 1351 | X         | -        | -       | -                |
| 11  | CLA  | J     | 1353 | X         | -        | -       | -                |

## 2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 35614 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     | 332      | Total | C    | N   | O   | S  | 0       | 0       | 31    |
|     |       |          | 2279  | 1505 | 370 | 390 | 14 |         |         |       |
| 1   | G     | 332      | Total | C    | N   | O   | S  | 0       | 0       | 31    |
|     |       |          | 2279  | 1505 | 370 | 390 | 14 |         |         |       |

- Molecule 2 is a protein called PHOTOSYSTEM II CORE LIGHT HARVESTING PROTEIN.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | B     | 479      | Total | C    | N   | O   | S  | 0       | 0       | 66    |
|     |       |          | 3053  | 2027 | 504 | 510 | 12 |         |         |       |
| 2   | H     | 479      | Total | C    | N   | O   | S  | 0       | 0       | 66    |
|     |       |          | 3053  | 2027 | 504 | 510 | 12 |         |         |       |

- Molecule 3 is a protein called PHOTOSYSTEM II CP43 PROTEIN.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3   | C     | 438      | Total | C    | N   | O   | S  | 0       | 0       | 73    |
|     |       |          | 2791  | 1861 | 467 | 452 | 11 |         |         |       |
| 3   | I     | 438      | Total | C    | N   | O   | S  | 0       | 0       | 73    |
|     |       |          | 2791  | 1861 | 467 | 452 | 11 |         |         |       |

- Molecule 4 is a protein called PHOTOSYSTEM II REACTION CENTER D2 PROTEIN.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 4   | D     | 350      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2602  | 1719 | 421 | 450 | 12 |         |         |       |
| 4   | J     | 350      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2602  | 1719 | 421 | 450 | 12 |         |         |       |

- Molecule 5 is a protein called CYTOCHROME B559 ALPHA SUBUNIT.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 5   | E     | 76       | Total | C   | N  | O  | 0       | 0       | 5     |
|     |       |          | 536   | 354 | 89 | 93 |         |         |       |
| 5   | K     | 76       | Total | C   | N  | O  | 0       | 0       | 5     |
|     |       |          | 536   | 354 | 89 | 93 |         |         |       |

- Molecule 6 is a protein called CYTOCHROME B559 BETA SUBUNIT.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 6   | F     | 37       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 297   | 202 | 48 | 46 | 1 |         |         |       |
| 6   | L     | 37       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 297   | 202 | 48 | 46 | 1 |         |         |       |

- Molecule 7 is a protein called PHOTOSYSTEM II MANGANESE-STABILIZING POLYPEPTIDE.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 7   | O     | 179      | Total | C   | N   | O   | 0       | 0       | 3     |
|     |       |          | 883   | 531 | 176 | 176 |         |         |       |
| 7   | P     | 179      | Total | C   | N   | O   | 0       | 0       | 3     |
|     |       |          | 883   | 531 | 176 | 176 |         |         |       |

- Molecule 8 is a protein called PHOTOSYSTEM II 12 KDA EXTRINSIC PROTEIN.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 8   | S     | 100      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 499   | 299 | 100 | 100 |         |         |       |
| 8   | U     | 100      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 499   | 299 | 100 | 100 |         |         |       |

- Molecule 9 is a protein called CYTOCHROME C-550.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9   | T     | 136      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1058  | 672 | 176 | 206 | 4 |         |         |       |
| 9   | V     | 136      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1058  | 672 | 176 | 206 | 4 |         |         |       |

- Molecule 10 is a protein called UNASSIGNED SUBUNITS.

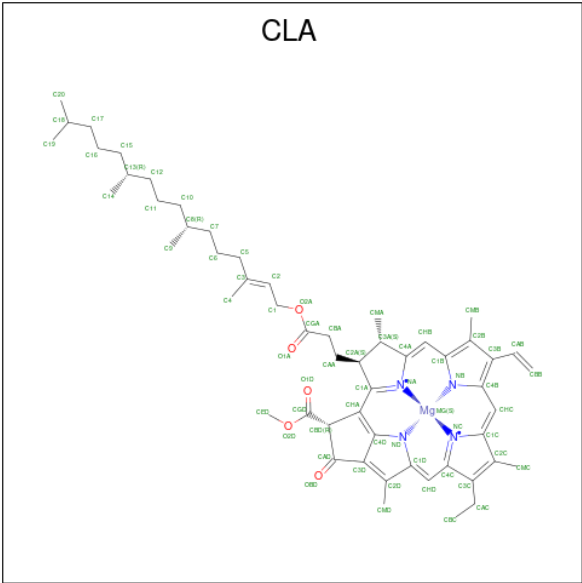
| Mol | Chain | Residues | Atoms |      |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|---------|-------|
| 10  | X     | 359      | Total | C    | N   | O   | 0       | 0       | 0     |
|     |       |          | 1791  | 1073 | 359 | 359 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|---------|-------|
| 10  | Y     | 359      | Total | C    | N   | O   | 0       | 0       | 0     |
|     |       |          | 1791  | 1073 | 359 | 359 |         |         |       |

- Molecule 11 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 11  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 11  | A     | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 11  | A     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 11  | A     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 11  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 11  | B     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 11  | B     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 11  | B     | 1        | Total<br>47 | C<br>37 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |
| 11  | B     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       | 0       |
| 11  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       | 0       |

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| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 11  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 11  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |         |
| 11  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 11  | B     | 1        | Total | C  | Mg | N |   | 0       | 0       |
|     |       |          | 27    | 22 | 1  | 4 |   |         |         |
| 11  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 11  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 11  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 11  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |         |
| 11  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 11  | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 41    | 33 | 1  | 4 | 3 |         |         |
| 11  | C     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 11  | C     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 47    | 37 | 1  | 4 | 5 |         |         |
| 11  | C     | 1        | Total | C  | Mg | N |   | 0       | 0       |
|     |       |          | 27    | 22 | 1  | 4 |   |         |         |
| 11  | C     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 56    | 46 | 1  | 4 | 5 |         |         |
| 11  | C     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |         |
| 11  | C     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 56    | 46 | 1  | 4 | 5 |         |         |
| 11  | C     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 11  | C     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |         |
| 11  | C     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 47    | 37 | 1  | 4 | 5 |         |         |
| 11  | C     | 1        | Total | C  | Mg | N |   | 0       | 0       |
|     |       |          | 27    | 22 | 1  | 4 |   |         |         |
| 11  | C     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 41    | 33 | 1  | 4 | 3 |         |         |

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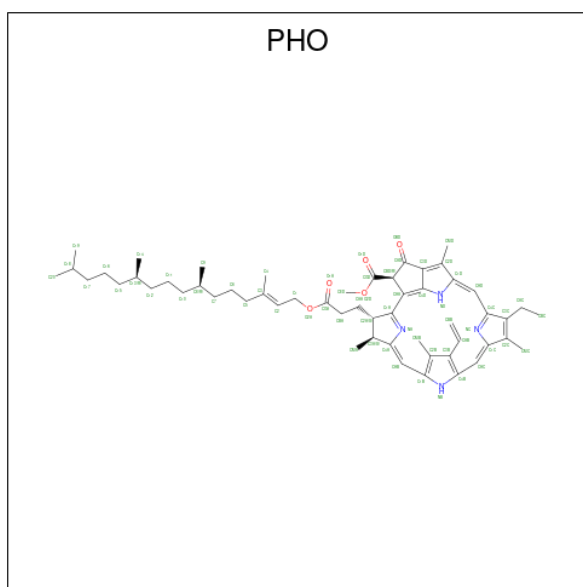
| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 11  | C     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 41    | 33 | 1  | 4 | 3 |         |         |
| 11  | C     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 41    | 33 | 1  | 4 | 3 |         |         |
| 11  | D     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 11  | D     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |         |
| 11  | G     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 11  | G     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 61    | 51 | 1  | 4 | 5 |         |         |
| 11  | G     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 11  | G     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |         |
| 11  | H     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 11  | H     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |         |
| 11  | H     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 11  | H     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 47    | 37 | 1  | 4 | 5 |         |         |
| 11  | H     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 41    | 33 | 1  | 4 | 3 |         |         |
| 11  | H     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 11  | H     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 11  | H     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |         |
| 11  | H     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 11  | H     | 1        | Total | C  | Mg | N |   | 0       | 0       |
|     |       |          | 27    | 22 | 1  | 4 |   |         |         |
| 11  | H     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 11  | H     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 11  | H     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 11  | H     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |         |
| 11  | H     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 11  | H     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 41    | 33 | 1  | 4 | 3 |         |         |
| 11  | I     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |         |
| 11  | I     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 47    | 37 | 1  | 4 | 5 |         |         |
| 11  | I     | 1        | Total | C  | Mg | N |   | 0       | 0       |
|     |       |          | 27    | 22 | 1  | 4 |   |         |         |
| 11  | I     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 56    | 46 | 1  | 4 | 5 |         |         |
| 11  | I     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |         |
| 11  | I     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 56    | 46 | 1  | 4 | 5 |         |         |
| 11  | I     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 11  | I     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |         |
| 11  | I     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 47    | 37 | 1  | 4 | 5 |         |         |
| 11  | I     | 1        | Total | C  | Mg | N |   | 0       | 0       |
|     |       |          | 27    | 22 | 1  | 4 |   |         |         |
| 11  | I     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 41    | 33 | 1  | 4 | 3 |         |         |
| 11  | I     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 41    | 33 | 1  | 4 | 3 |         |         |
| 11  | I     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 41    | 33 | 1  | 4 | 3 |         |         |
| 11  | J     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |         |
| 11  | J     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |         |

- Molecule 12 is PHEOPHYTIN A (CCD ID: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ).



| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 12  | A     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |         |
| 12  | D     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 54    | 45 | 4 | 5 |         |         |
| 12  | G     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |         |
| 12  | J     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 54    | 45 | 4 | 5 |         |         |

- Molecule 13 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

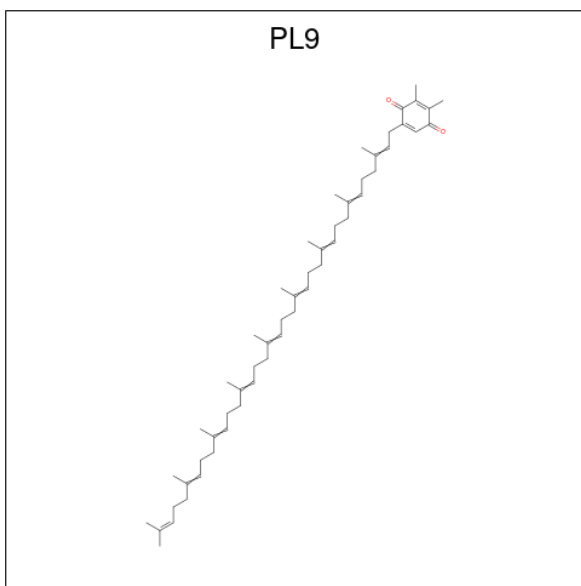
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 13  | A     | 4        | Total | Mn | 0       | 0       |
|     |       |          | 4     | 4  |         |         |
| 13  | G     | 4        | Total | Mn | 0       | 0       |
|     |       |          | 4     | 4  |         |         |

- Molecule 14 is FE (II) ION (CCD ID: FE2) (formula: Fe).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 14  | A     | 1        | Total | Fe | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 14  | G     | 1        | Total | Fe | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

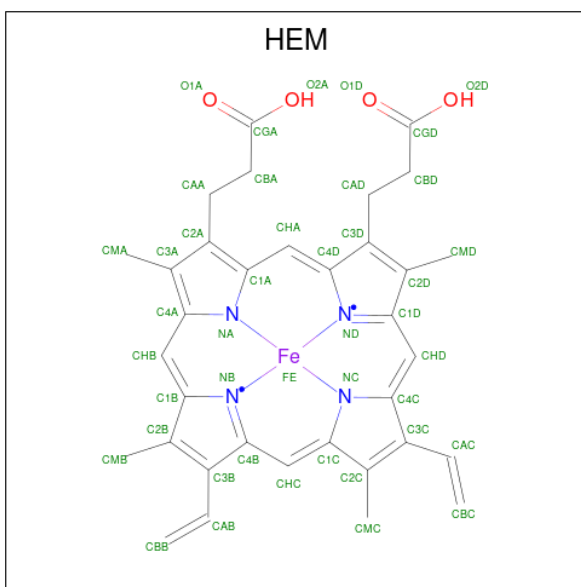
- Molecule 15 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DI

METHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula:  $C_{53}H_{80}O_2$ ).



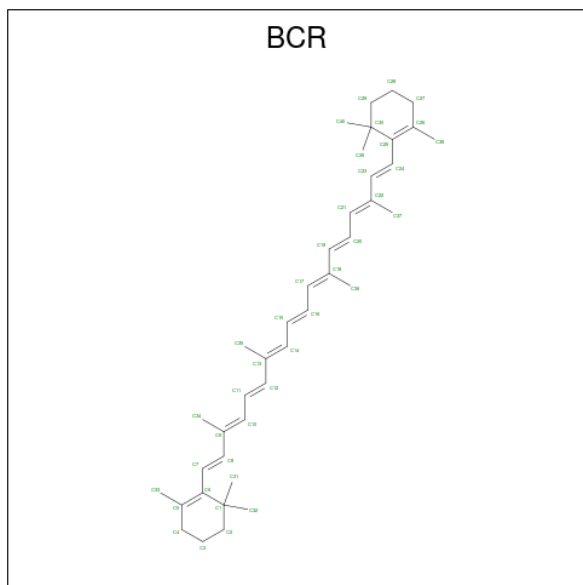
| Mol | Chain | Residues | Atoms          | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 15  | D     | 1        | Total C<br>6 6 | 0       | 0       |
| 15  | J     | 1        | Total C<br>6 6 | 0       | 0       |

- Molecule 16 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



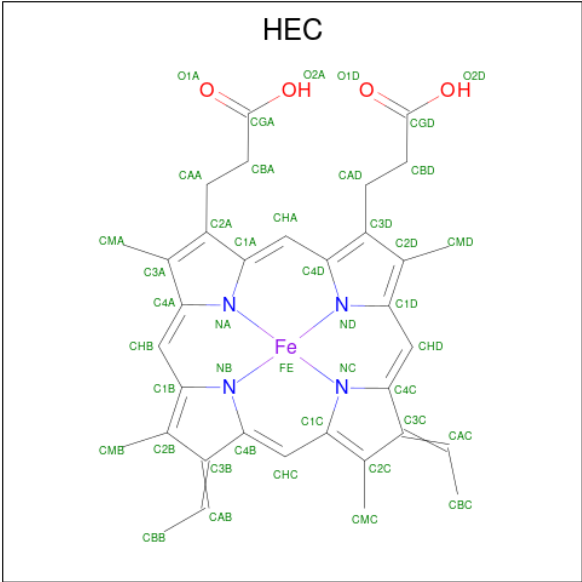
| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 16  | E     | 1        | Total | C  | Fe | N | 0       | 0       |
|     |       |          | 25    | 20 | 1  | 4 |         |         |
| 16  | L     | 1        | Total | C  | Fe | N | 0       | 0       |
|     |       |          | 25    | 20 | 1  | 4 |         |         |

- Molecule 17 is BETA-CAROTENE (CCD ID: BCR) (formula:  $C_{40}H_{56}$ ).



| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 17  | F     | 1        | Total | C  | 0       | 0       |
|     |       |          | 40    | 40 |         |         |
| 17  | L     | 1        | Total | C  | 0       | 0       |
|     |       |          | 40    | 40 |         |         |

- Molecule 18 is HEME C (CCD ID: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



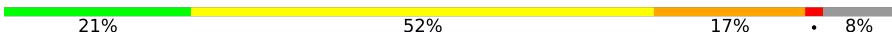
| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 18  | T     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 18  | V     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |

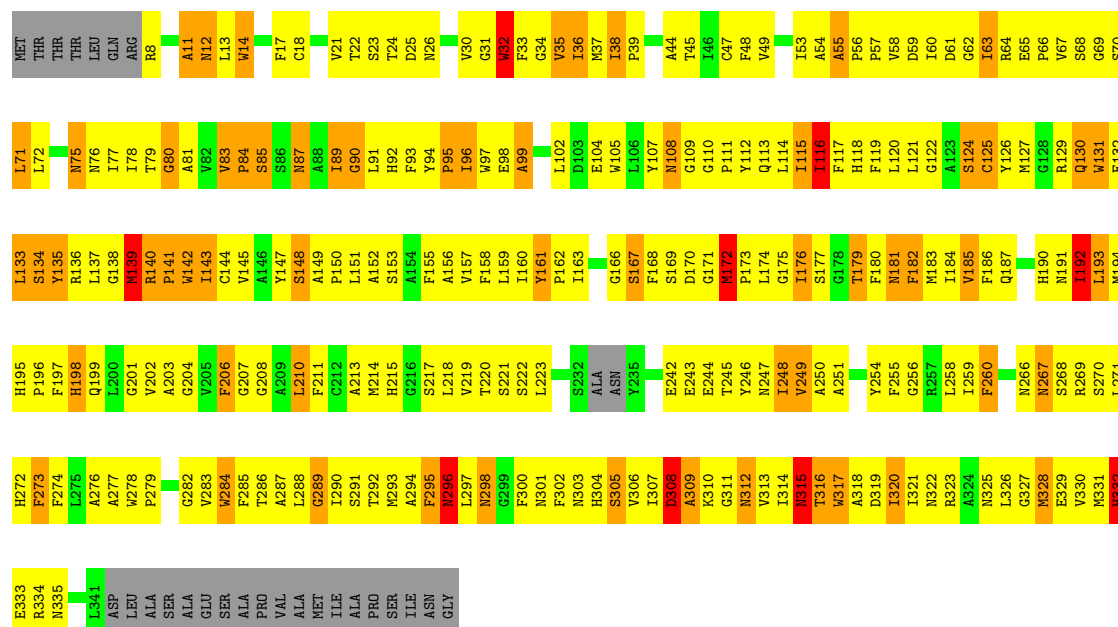
### 3 Residue-property plots

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

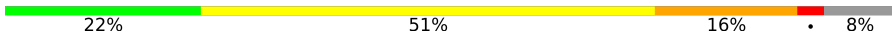
Note EDS was not executed.

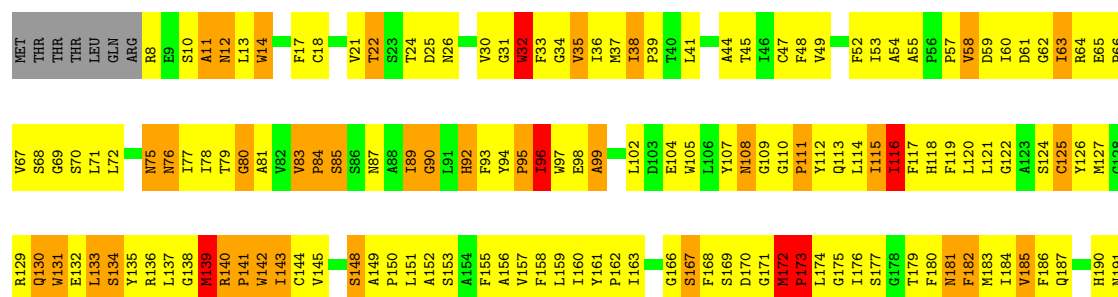
#### • Molecule 1: PHOTOSYSTEM Q(B) PROTEIN 1

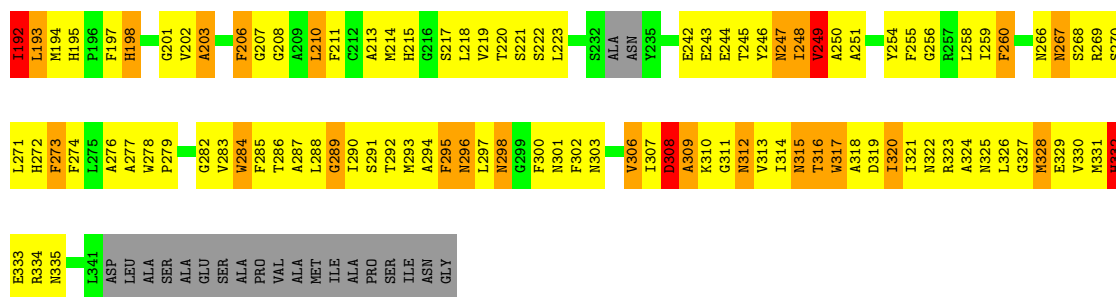
Chain A: 



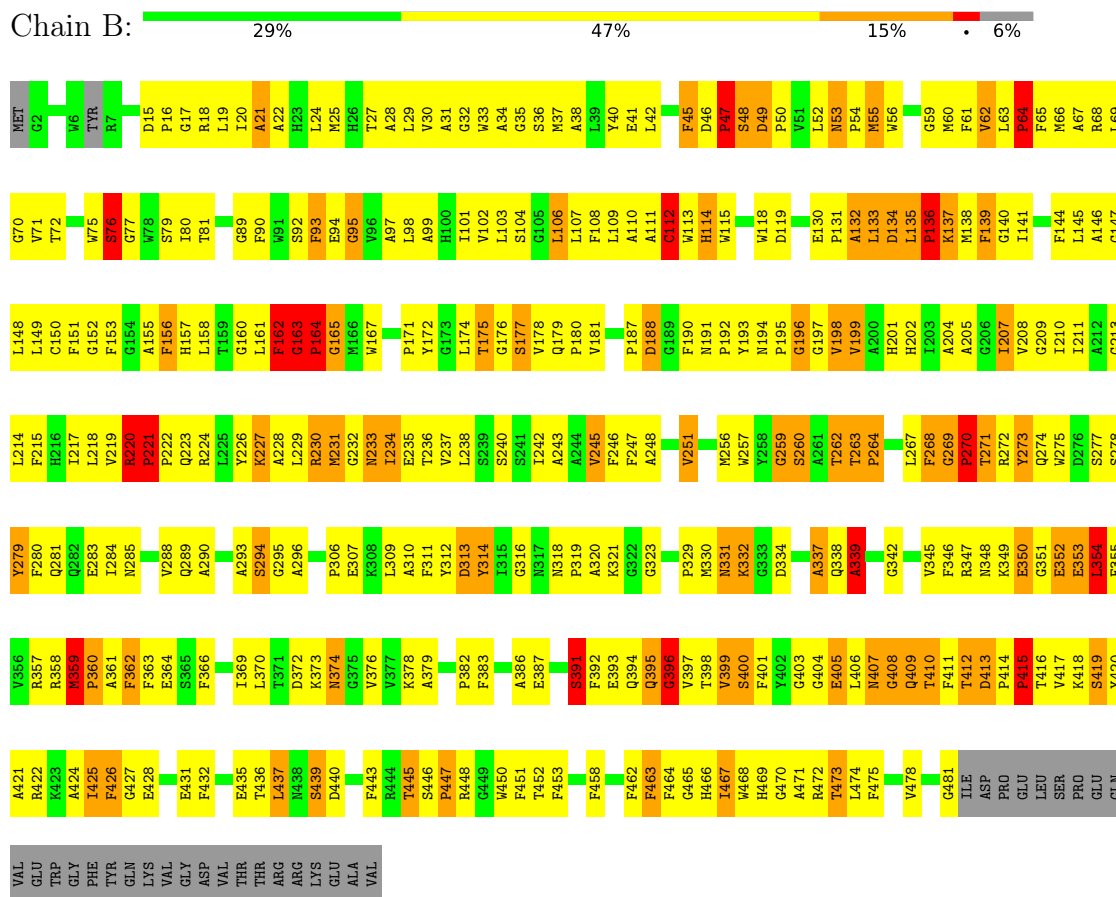
#### • Molecule 1: PHOTOSYSTEM Q(B) PROTEIN 1

Chain G: 

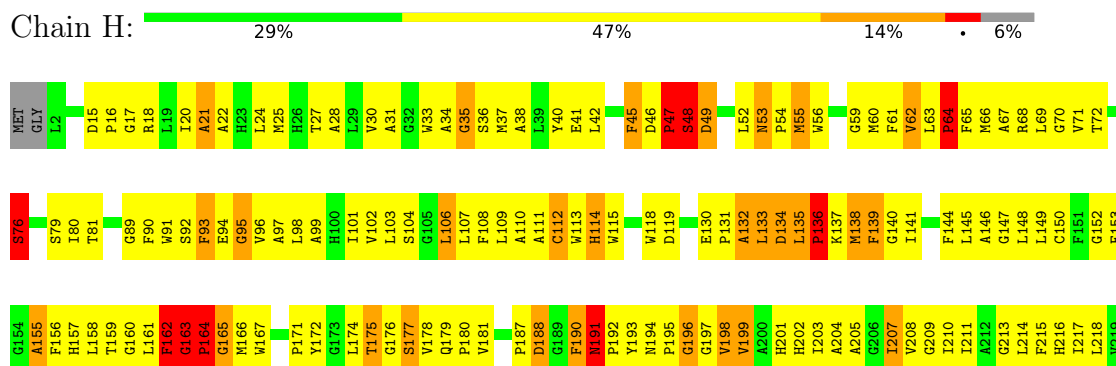


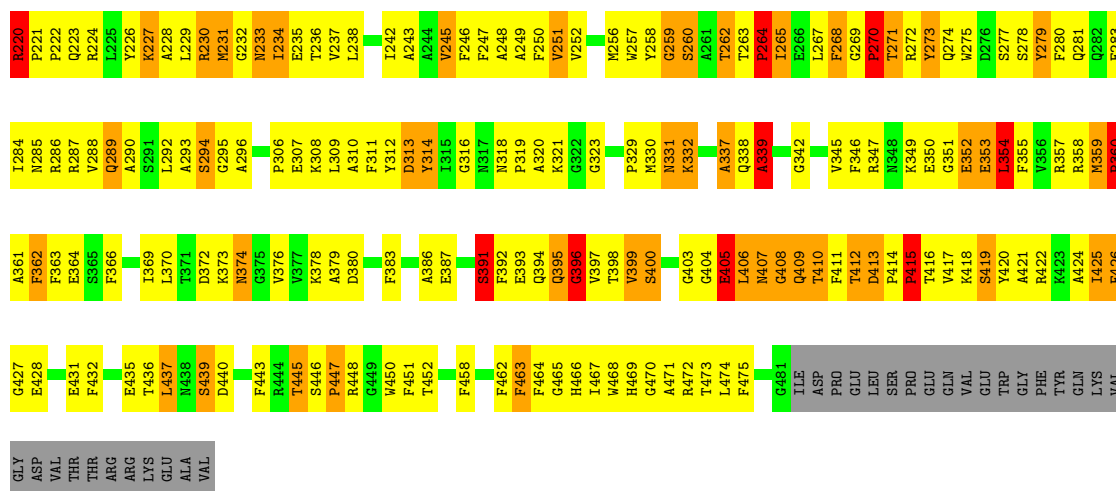


• Molecule 2: PHOTOSYSTEM II CORE LIGHT HARVESTING PROTEIN



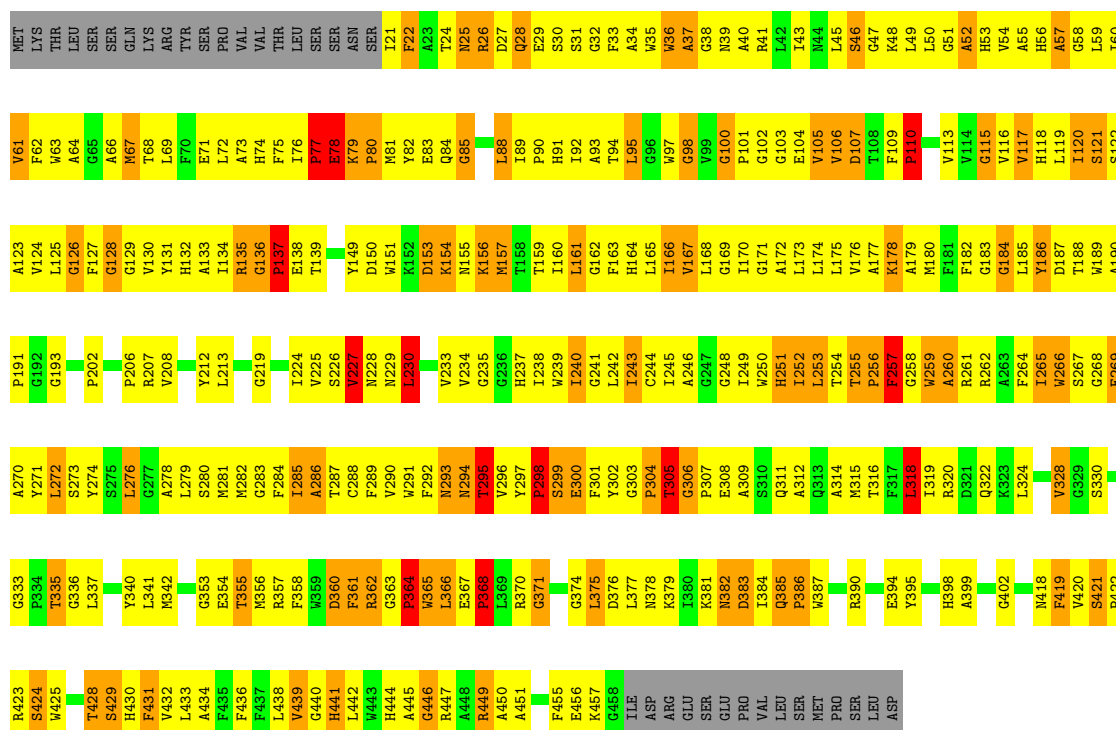
• Molecule 2: PHOTOSYSTEM II CORE LIGHT HARVESTING PROTEIN





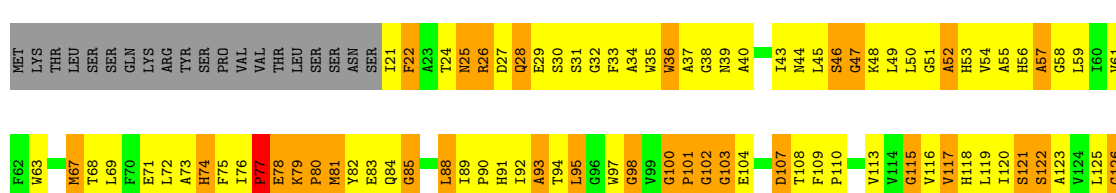
### • Molecule 3: PHOTOSYSTEM II CP43 PROTEIN

Chain C: 25% 47% 18% 7%

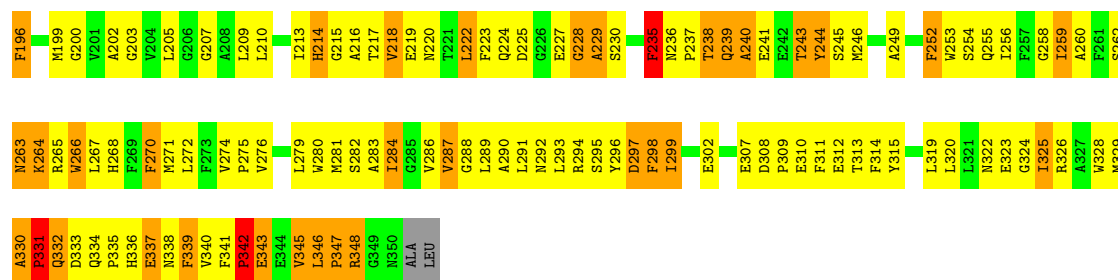


### • Molecule 3: PHOTOSYSTEM II CP43 PROTEIN

Chain I: 26% 46% 18% 7%

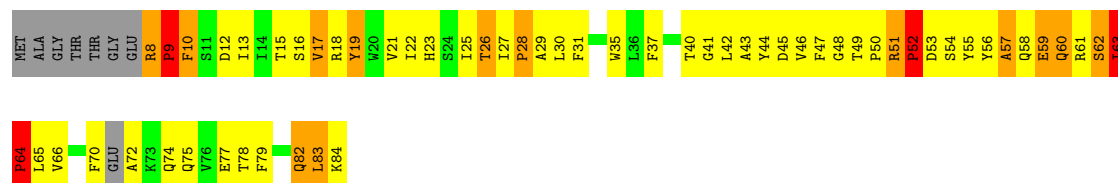






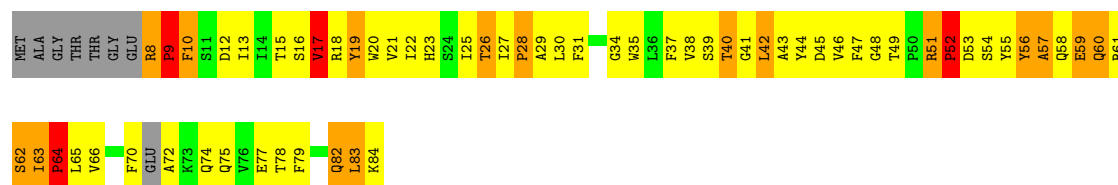
• Molecule 5: CYTOCHROME B559 ALPHA SUBUNIT

Chain E: 20% 50% 15% 5% 10%



• Molecule 5: CYTOCHROME B559 ALPHA SUBUNIT

Chain K: 17% 50% 19% 5% 10%



• Molecule 6: CYTOCHROME B559 BETA SUBUNIT

Chain F: 11% 43% 25% 5% 16%



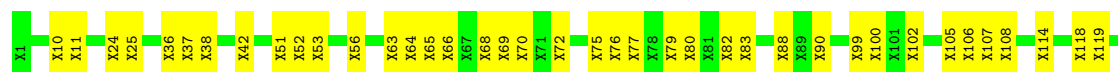
• Molecule 6: CYTOCHROME B559 BETA SUBUNIT

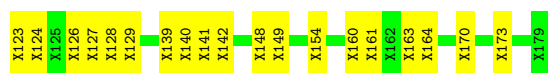
Chain L: 14% 43% 20% 7% 16%



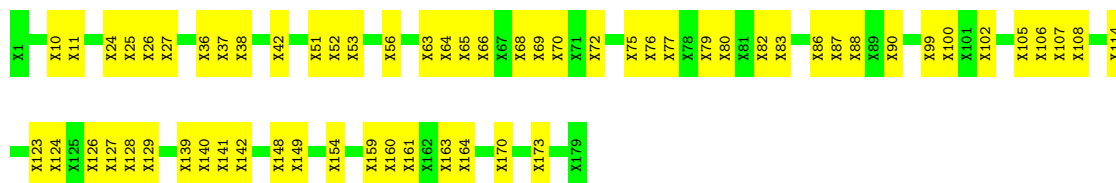
• Molecule 7: PHOTOSYSTEM II MANGANESE-STABILIZING POLYPEPTIDE

Chain O: 68% 32%

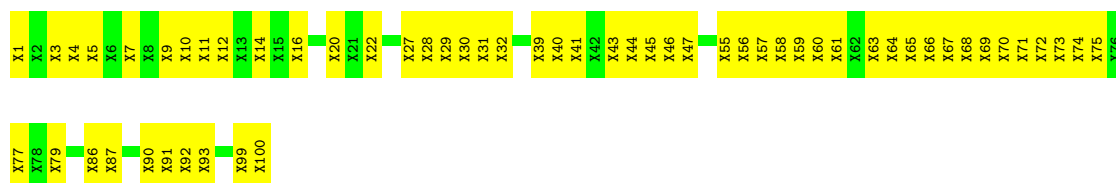




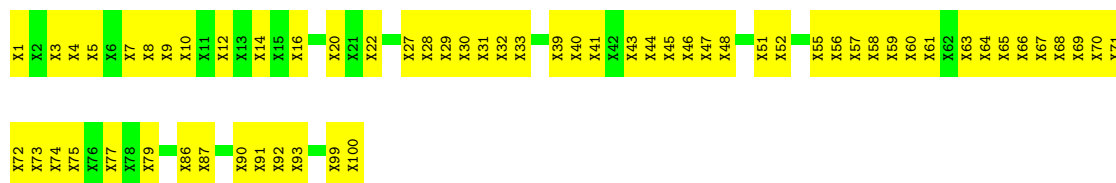
• Molecule 7: PHOTOSYSTEM II MANGANESE-STABILIZING POLYPEPTIDE



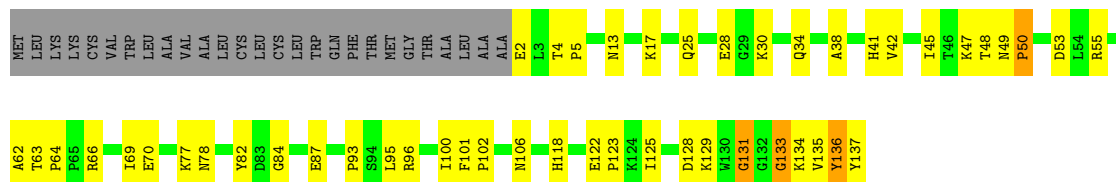
• Molecule 8: PHOTOSYSTEM II 12 KDA EXTRINSIC PROTEIN



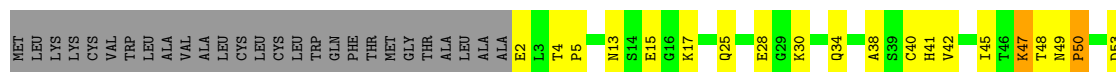
• Molecule 8: PHOTOSYSTEM II 12 KDA EXTRINSIC PROTEIN

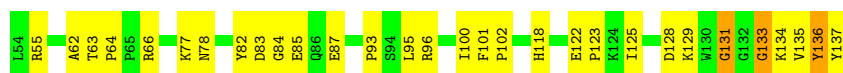


• Molecule 9: CYTOCHROME C-550



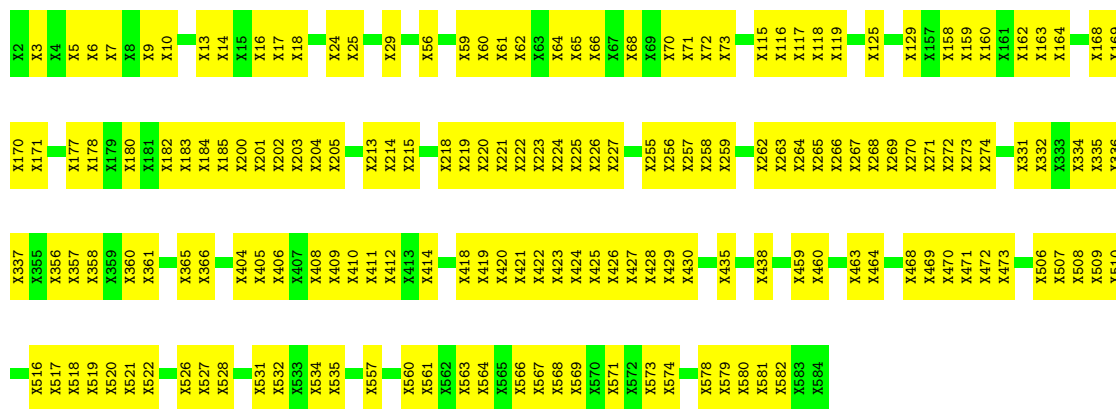
• Molecule 9: CYTOCHROME C-550





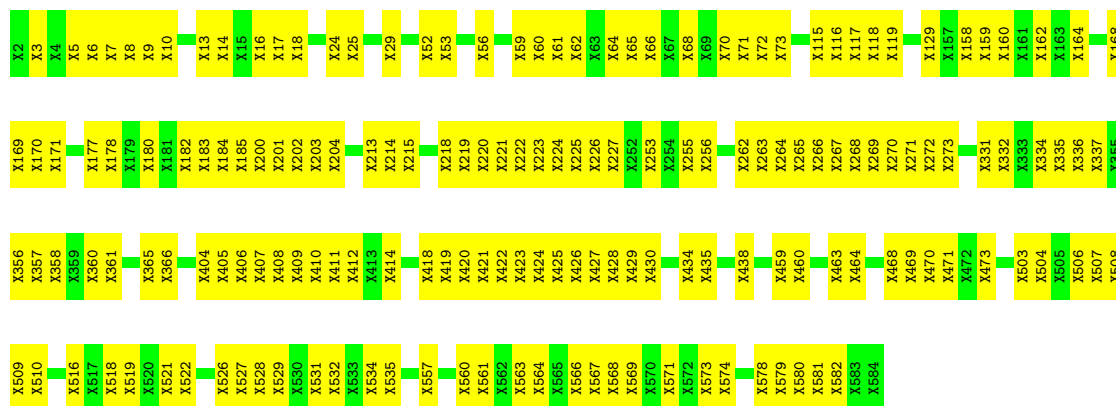
### • Molecule 10: UNASSIGNED SUBUNITS

Chain X: 52% 48%



### • Molecule 10: UNASSIGNED SUBUNITS

Chain Y: 53% 47%



## 4 Data and refinement statistics

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

| Property                                                 | Value                                           | Source    |
|----------------------------------------------------------|-------------------------------------------------|-----------|
| Space group                                              | P 21 21 21                                      | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 127.52Å 224.61Å 305.63Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å)                                           | 10.00 – 3.20                                    | Depositor |
| % Data completeness<br>(in resolution range)             | 75.6 (10.00-3.20)                               | Depositor |
| $R_{merge}$                                              | 0.11                                            | Depositor |
| $R_{sym}$                                                | (Not available)                                 | Depositor |
| Refinement program                                       | CNS 1.0                                         | Depositor |
| R, $R_{free}$                                            | (Not available) , (Not available)               | Depositor |
| Estimated twinning fraction                              | No twinning to report.                          | Xtriage   |
| Total number of atoms                                    | 35614                                           | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 45.0                                            | wwPDB-VP  |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE2, CLA, PL9, PHO, BCR, MN, HEM, HEC

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     | 0.93         | 1/2315 (0.0%)  | 1.40        | 39/3161 (1.2%)   |
| 1   | G     | 0.89         | 1/2315 (0.0%)  | 1.38        | 33/3161 (1.0%)   |
| 2   | B     | 0.91         | 0/3081         | 1.46        | 55/4202 (1.3%)   |
| 2   | H     | 0.86         | 0/3081         | 1.48        | 50/4202 (1.2%)   |
| 3   | C     | 0.79         | 0/2806         | 1.41        | 53/3822 (1.4%)   |
| 3   | I     | 0.77         | 0/2806         | 1.38        | 43/3822 (1.1%)   |
| 4   | D     | 0.95         | 0/2688         | 1.42        | 43/3678 (1.2%)   |
| 4   | J     | 0.91         | 1/2688 (0.0%)  | 1.43        | 48/3678 (1.3%)   |
| 5   | E     | 0.83         | 0/547          | 1.39        | 6/751 (0.8%)     |
| 5   | K     | 0.87         | 1/547 (0.2%)   | 1.36        | 7/751 (0.9%)     |
| 6   | F     | 1.02         | 0/307          | 1.75        | 12/421 (2.9%)    |
| 6   | L     | 1.00         | 0/307          | 1.56        | 7/421 (1.7%)     |
| 9   | T     | 0.85         | 0/1079         | 1.14        | 5/1466 (0.3%)    |
| 9   | V     | 0.90         | 0/1079         | 1.15        | 5/1466 (0.3%)    |
| All | All   | 0.88         | 4/25646 (0.0%) | 1.41        | 406/35002 (1.2%) |

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                   |
| 1   | G     | 0                   | 1                   |
| 2   | B     | 0                   | 1                   |
| 2   | H     | 0                   | 1                   |
| All | All   | 0                   | 4                   |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 320 | ILE  | CA-CB | -5.45 | 1.48        | 1.54     |
| 1   | G     | 320 | ILE  | CA-CB | -5.14 | 1.48        | 1.54     |
| 4   | J     | 339 | PHE  | CA-C  | -5.02 | 1.46        | 1.52     |
| 5   | K     | 17  | VAL  | CA-CB | 5.02  | 1.61        | 1.54     |

All (406) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 2   | H     | 270 | PRO  | CA-N-CD    | -15.33 | 90.54       | 112.00   |
| 2   | B     | 270 | PRO  | CA-N-CD    | -13.84 | 92.62       | 112.00   |
| 2   | B     | 76  | SER  | N-CA-C     | -13.04 | 83.02       | 110.80   |
| 2   | H     | 76  | SER  | N-CA-C     | -12.99 | 83.12       | 110.80   |
| 1   | G     | 83  | VAL  | CA-C-N     | 12.20  | 132.33      | 119.89   |
| 1   | G     | 83  | VAL  | C-N-CA     | 12.20  | 132.33      | 119.89   |
| 4   | J     | 171 | PRO  | CA-N-CD    | -12.05 | 95.12       | 112.00   |
| 2   | B     | 47  | PRO  | CA-N-CD    | -11.56 | 95.81       | 112.00   |
| 2   | B     | 396 | GLY  | N-CA-C     | -11.52 | 85.88       | 113.18   |
| 2   | H     | 396 | GLY  | N-CA-C     | -11.41 | 86.13       | 113.18   |
| 1   | A     | 83  | VAL  | CA-C-N     | 11.40  | 131.52      | 119.89   |
| 1   | A     | 83  | VAL  | C-N-CA     | 11.40  | 131.52      | 119.89   |
| 2   | H     | 53  | ASN  | CA-C-N     | 11.26  | 131.18      | 120.03   |
| 2   | H     | 53  | ASN  | C-N-CA     | 11.26  | 131.18      | 120.03   |
| 3   | C     | 110 | PRO  | CA-N-CD    | -11.14 | 96.40       | 112.00   |
| 2   | B     | 53  | ASN  | CA-C-N     | 10.93  | 130.85      | 120.03   |
| 2   | B     | 53  | ASN  | C-N-CA     | 10.93  | 130.85      | 120.03   |
| 4   | J     | 342 | PRO  | CA-N-CD    | -10.89 | 96.75       | 112.00   |
| 5   | E     | 63  | ILE  | CA-C-N     | 10.83  | 133.38      | 119.84   |
| 5   | E     | 63  | ILE  | C-N-CA     | 10.83  | 133.38      | 119.84   |
| 4   | D     | 342 | PRO  | CA-N-CD    | -10.63 | 97.12       | 112.00   |
| 2   | H     | 264 | PRO  | CA-N-CD    | -10.59 | 97.17       | 112.00   |
| 3   | C     | 318 | LEU  | N-CA-C     | -10.49 | 99.93       | 111.36   |
| 3   | C     | 300 | GLU  | N-CA-C     | -10.47 | 99.76       | 112.54   |
| 4   | D     | 332 | GLN  | OE1-CD-NE2 | -10.33 | 112.27      | 122.60   |
| 1   | G     | 173 | PRO  | CA-N-CD    | -10.29 | 97.59       | 112.00   |
| 2   | B     | 359 | MET  | CA-C-N     | 10.20  | 132.59      | 119.84   |
| 2   | B     | 359 | MET  | C-N-CA     | 10.20  | 132.59      | 119.84   |
| 4   | J     | 101 | PHE  | N-CA-C     | -10.20 | 99.15       | 111.69   |
| 4   | D     | 335 | PRO  | CA-N-CD    | -10.15 | 97.78       | 112.00   |
| 6   | L     | 14  | PRO  | CA-N-CD    | -10.13 | 97.82       | 112.00   |
| 2   | B     | 220 | ARG  | CA-C-N     | 10.06  | 130.74      | 120.38   |
| 2   | B     | 220 | ARG  | C-N-CA     | 10.06  | 130.74      | 120.38   |
| 4   | J     | 332 | GLN  | OE1-CD-NE2 | -10.02 | 112.58      | 122.60   |
| 2   | H     | 359 | MET  | CA-C-N     | 9.98   | 132.31      | 119.84   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | H     | 359 | MET  | C-N-CA     | 9.98  | 132.31      | 119.84   |
| 4   | D     | 101 | PHE  | N-CA-C     | -9.97 | 99.42       | 111.69   |
| 2   | H     | 289 | GLN  | OE1-CD-NE2 | -9.95 | 112.65      | 122.60   |
| 3   | I     | 259 | TRP  | N-CA-C     | -9.94 | 99.70       | 112.93   |
| 3   | I     | 318 | LEU  | N-CA-C     | -9.91 | 100.48      | 111.28   |
| 6   | L     | 10  | PRO  | CA-N-CD    | -9.89 | 98.15       | 112.00   |
| 1   | A     | 36  | ILE  | N-CA-C     | -9.84 | 103.85      | 111.62   |
| 6   | F     | 44  | GLN  | OE1-CD-NE2 | -9.75 | 112.85      | 122.60   |
| 2   | H     | 362 | PHE  | N-CA-C     | -9.74 | 100.23      | 113.18   |
| 4   | D     | 167 | TRP  | N-CA-C     | -9.71 | 97.61       | 110.24   |
| 2   | H     | 47  | PRO  | CA-N-CD    | -9.64 | 98.50       | 112.00   |
| 3   | I     | 333 | GLY  | CA-C-N     | 9.62  | 129.24      | 119.24   |
| 3   | I     | 333 | GLY  | C-N-CA     | 9.62  | 129.24      | 119.24   |
| 9   | V     | 47  | LYS  | N-CA-C     | 9.61  | 121.70      | 111.03   |
| 1   | A     | 172 | MET  | CA-C-N     | 9.60  | 131.12      | 120.66   |
| 1   | A     | 172 | MET  | C-N-CA     | 9.60  | 131.12      | 120.66   |
| 2   | B     | 362 | PHE  | N-CA-C     | -9.57 | 100.46      | 113.18   |
| 3   | I     | 439 | VAL  | N-CA-C     | -9.56 | 100.28      | 110.23   |
| 4   | D     | 345 | VAL  | N-CA-C     | 9.56  | 121.71      | 111.77   |
| 3   | I     | 300 | GLU  | N-CA-C     | -9.48 | 100.97      | 112.54   |
| 2   | H     | 162 | PHE  | CA-C-N     | 9.46  | 136.72      | 121.87   |
| 2   | H     | 162 | PHE  | C-N-CA     | 9.46  | 136.72      | 121.87   |
| 2   | H     | 220 | ARG  | CA-C-N     | 9.30  | 129.97      | 120.38   |
| 2   | H     | 220 | ARG  | C-N-CA     | 9.30  | 129.97      | 120.38   |
| 3   | C     | 355 | THR  | N-CA-C     | -9.29 | 102.09      | 113.15   |
| 3   | C     | 385 | GLN  | CA-C-N     | 9.24  | 131.39      | 119.84   |
| 3   | C     | 385 | GLN  | C-N-CA     | 9.24  | 131.39      | 119.84   |
| 6   | F     | 14  | PRO  | CA-N-CD    | -9.23 | 99.08       | 112.00   |
| 3   | C     | 357 | ARG  | N-CA-C     | 9.22  | 121.10      | 111.14   |
| 3   | C     | 259 | TRP  | N-CA-C     | -9.17 | 100.73      | 112.93   |
| 1   | G     | 328 | MET  | N-CA-C     | -9.14 | 102.26      | 113.41   |
| 9   | T     | 47  | LYS  | N-CA-C     | 9.13  | 120.92      | 110.97   |
| 3   | C     | 52  | ALA  | N-CA-C     | -9.12 | 100.17      | 111.11   |
| 3   | C     | 333 | GLY  | CA-C-N     | 9.05  | 128.66      | 119.24   |
| 3   | C     | 333 | GLY  | C-N-CA     | 9.05  | 128.66      | 119.24   |
| 3   | I     | 357 | ARG  | N-CA-C     | 8.98  | 120.84      | 111.14   |
| 3   | C     | 137 | PRO  | CA-N-CD    | -8.98 | 99.43       | 112.00   |
| 4   | J     | 345 | VAL  | N-CA-C     | 8.97  | 121.10      | 111.77   |
| 3   | I     | 107 | ASP  | CB-CA-C    | -8.95 | 99.47       | 111.82   |
| 3   | C     | 439 | VAL  | N-CA-C     | -8.92 | 100.95      | 110.23   |
| 1   | G     | 55  | ALA  | CA-C-N     | 8.65  | 129.29      | 120.38   |
| 1   | G     | 55  | ALA  | C-N-CA     | 8.65  | 129.29      | 120.38   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | B     | 162 | PHE  | CA-C-N  | 8.64  | 135.44      | 121.87   |
| 2   | B     | 162 | PHE  | C-N-CA  | 8.64  | 135.44      | 121.87   |
| 6   | F     | 9   | GLU  | CA-C-N  | -8.64 | 111.73      | 120.98   |
| 6   | F     | 9   | GLU  | C-N-CA  | -8.64 | 111.73      | 120.98   |
| 2   | H     | 156 | PHE  | N-CA-C  | 8.60  | 122.75      | 111.75   |
| 5   | K     | 64  | PRO  | CA-N-CD | -8.51 | 100.09      | 112.00   |
| 3   | I     | 355 | THR  | N-CA-C  | -8.51 | 103.03      | 113.15   |
| 4   | J     | 167 | TRP  | N-CA-C  | -8.50 | 99.19       | 110.24   |
| 4   | D     | 298 | PHE  | N-CA-C  | -8.50 | 102.10      | 111.36   |
| 3   | I     | 137 | PRO  | CA-N-CD | -8.47 | 100.13      | 112.00   |
| 3   | I     | 260 | ALA  | N-CA-C  | -8.46 | 100.96      | 111.11   |
| 2   | H     | 245 | VAL  | N-CA-C  | -8.38 | 101.86      | 111.00   |
| 1   | G     | 306 | VAL  | N-CA-C  | 8.31  | 120.76      | 108.96   |
| 3   | I     | 385 | GLN  | CA-C-N  | 8.25  | 130.15      | 119.84   |
| 3   | I     | 385 | GLN  | C-N-CA  | 8.25  | 130.15      | 119.84   |
| 4   | J     | 129 | GLN  | N-CA-C  | -8.16 | 103.84      | 113.88   |
| 1   | A     | 309 | ALA  | N-CA-C  | -8.12 | 102.83      | 112.89   |
| 3   | I     | 360 | ASP  | N-CA-C  | -8.10 | 102.96      | 113.17   |
| 3   | I     | 421 | SER  | N-CA-C  | 8.10  | 121.41      | 109.50   |
| 1   | A     | 140 | ARG  | CA-C-N  | 8.08  | 129.94      | 119.84   |
| 1   | A     | 140 | ARG  | C-N-CA  | 8.08  | 129.94      | 119.84   |
| 3   | C     | 360 | ASP  | N-CA-C  | -8.08 | 102.99      | 113.17   |
| 4   | J     | 298 | PHE  | N-CA-C  | -8.05 | 102.58      | 111.36   |
| 4   | D     | 5   | ILE  | N-CA-C  | 8.03  | 126.04      | 109.34   |
| 2   | H     | 199 | VAL  | N-CA-C  | 8.00  | 118.80      | 110.72   |
| 4   | J     | 123 | ILE  | N-CA-C  | -7.99 | 103.02      | 110.53   |
| 2   | B     | 245 | VAL  | N-CA-C  | -7.98 | 102.30      | 111.00   |
| 3   | C     | 336 | GLY  | N-CA-C  | -7.97 | 103.69      | 115.72   |
| 4   | D     | 129 | GLN  | N-CA-C  | -7.95 | 104.10      | 113.88   |
| 3   | C     | 260 | ALA  | N-CA-C  | -7.94 | 101.58      | 111.11   |
| 4   | J     | 284 | ILE  | N-CA-C  | -7.92 | 102.82      | 110.42   |
| 2   | H     | 260 | SER  | N-CA-C  | 7.88  | 118.66      | 108.34   |
| 4   | J     | 5   | ILE  | N-CA-C  | 7.74  | 125.44      | 109.34   |
| 1   | A     | 328 | MET  | N-CA-C  | -7.69 | 103.50      | 113.12   |
| 6   | F     | 45  | ARG  | N-CA-C  | -7.68 | 89.49       | 111.00   |
| 4   | D     | 194 | ASN  | CA-C-N  | 7.68  | 128.38      | 119.47   |
| 4   | D     | 194 | ASN  | C-N-CA  | 7.68  | 128.38      | 119.47   |
| 3   | C     | 37  | ALA  | N-CA-C  | -7.67 | 101.98      | 112.03   |
| 6   | F     | 13  | TYR  | N-CA-C  | 7.65  | 126.71      | 109.81   |
| 3   | C     | 79  | LYS  | CA-C-N  | 7.65  | 129.40      | 119.84   |
| 3   | C     | 79  | LYS  | C-N-CA  | 7.65  | 129.40      | 119.84   |
| 5   | K     | 54  | SER  | N-CA-C  | 7.62  | 122.42      | 113.20   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 3   | C     | 451 | ALA  | N-CA-C    | -7.61 | 102.12      | 111.40   |
| 3   | I     | 28  | GLN  | N-CA-C    | 7.60  | 119.97      | 109.18   |
| 6   | L     | 13  | TYR  | N-CA-C    | 7.56  | 126.52      | 109.81   |
| 3   | C     | 421 | SER  | N-CA-C    | 7.52  | 120.55      | 109.50   |
| 1   | G     | 140 | ARG  | CA-C-N    | 7.51  | 129.22      | 119.84   |
| 1   | G     | 140 | ARG  | C-N-CA    | 7.51  | 129.22      | 119.84   |
| 2   | B     | 391 | SER  | N-CA-C    | 7.50  | 126.77      | 110.80   |
| 3   | I     | 208 | VAL  | N-CA-C    | -7.49 | 102.98      | 110.62   |
| 2   | B     | 350 | GLU  | N-CA-C    | -7.48 | 104.77      | 114.04   |
| 3   | I     | 336 | GLY  | N-CA-C    | -7.46 | 103.80      | 115.67   |
| 2   | H     | 391 | SER  | N-CA-C    | 7.46  | 126.68      | 110.80   |
| 3   | C     | 28  | GLN  | N-CA-C    | 7.40  | 119.69      | 109.18   |
| 3   | C     | 208 | VAL  | N-CA-C    | -7.40 | 103.07      | 110.62   |
| 3   | I     | 79  | LYS  | CA-C-N    | 7.37  | 129.05      | 119.84   |
| 3   | I     | 79  | LYS  | C-N-CA    | 7.37  | 129.05      | 119.84   |
| 1   | G     | 287 | ALA  | N-CA-C    | -7.32 | 103.38      | 111.36   |
| 1   | A     | 305 | SER  | N-CA-C    | -7.32 | 98.31       | 109.95   |
| 4   | D     | 104 | TRP  | N-CA-C    | -7.31 | 102.34      | 111.11   |
| 2   | B     | 199 | VAL  | N-CA-C    | 7.31  | 118.10      | 110.72   |
| 3   | C     | 324 | LEU  | N-CA-C    | -7.27 | 104.54      | 113.41   |
| 5   | E     | 54  | SER  | N-CA-C    | 7.27  | 121.99      | 113.20   |
| 3   | C     | 77  | PRO  | N-CA-C    | 7.25  | 122.29      | 111.41   |
| 2   | H     | 463 | PHE  | N-CA-C    | -7.24 | 103.00      | 111.03   |
| 4   | J     | 332 | GLN  | CG-CD-NE2 | 7.15  | 127.12      | 116.40   |
| 3   | I     | 77  | PRO  | N-CA-C    | 7.12  | 122.70      | 111.38   |
| 1   | G     | 18  | CYS  | N-CA-C    | -7.10 | 103.23      | 110.97   |
| 2   | H     | 289 | GLN  | CG-CD-NE2 | 7.10  | 127.06      | 116.40   |
| 2   | B     | 132 | ALA  | N-CA-C    | -7.07 | 103.58      | 111.71   |
| 1   | A     | 303 | ASN  | N-CA-C    | 7.03  | 118.94      | 111.28   |
| 4   | D     | 123 | ILE  | N-CA-C    | -7.02 | 103.63      | 110.72   |
| 3   | I     | 324 | LEU  | N-CA-C    | -6.98 | 104.89      | 113.41   |
| 2   | B     | 260 | SER  | N-CA-C    | 6.97  | 117.68      | 108.07   |
| 4   | J     | 194 | ASN  | CA-C-N    | 6.97  | 127.55      | 119.47   |
| 4   | J     | 194 | ASN  | C-N-CA    | 6.97  | 127.55      | 119.47   |
| 4   | D     | 169 | PHE  | N-CA-C    | -6.96 | 104.36      | 112.92   |
| 2   | H     | 191 | ASN  | CA-C-N    | 6.96  | 128.54      | 119.84   |
| 2   | H     | 191 | ASN  | C-N-CA    | 6.96  | 128.54      | 119.84   |
| 1   | A     | 287 | ALA  | N-CA-C    | -6.94 | 103.64      | 111.14   |
| 4   | D     | 332 | GLN  | CG-CD-NE2 | 6.92  | 126.78      | 116.40   |
| 3   | C     | 100 | GLY  | N-CA-C    | -6.92 | 98.23       | 112.34   |
| 1   | A     | 55  | ALA  | CA-C-N    | 6.87  | 127.46      | 120.38   |
| 1   | A     | 55  | ALA  | C-N-CA    | 6.87  | 127.46      | 120.38   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 9   | V     | 136 | TYR  | N-CA-C    | -6.87 | 104.93      | 113.38   |
| 6   | F     | 44  | GLN  | CG-CD-NE2 | 6.86  | 126.68      | 116.40   |
| 2   | B     | 432 | PHE  | N-CA-C    | 6.84  | 120.67      | 109.72   |
| 3   | C     | 88  | LEU  | N-CA-C    | 6.83  | 121.63      | 111.04   |
| 2   | H     | 132 | ALA  | N-CA-C    | -6.83 | 103.85      | 111.71   |
| 3   | I     | 230 | LEU  | N-CA-C    | -6.83 | 103.90      | 111.82   |
| 9   | T     | 136 | TYR  | N-CA-C    | -6.82 | 104.95      | 113.28   |
| 1   | A     | 134 | SER  | N-CA-C    | -6.82 | 100.47      | 111.04   |
| 2   | H     | 350 | GLU  | N-CA-C    | -6.79 | 105.52      | 113.88   |
| 3   | I     | 451 | ALA  | N-CA-C    | -6.79 | 103.34      | 111.69   |
| 4   | J     | 169 | PHE  | N-CA-C    | -6.78 | 104.99      | 112.72   |
| 2   | B     | 191 | ASN  | CA-C-N    | 6.76  | 128.29      | 119.84   |
| 2   | B     | 191 | ASN  | C-N-CA    | 6.76  | 128.29      | 119.84   |
| 3   | I     | 100 | GLY  | N-CA-C    | -6.73 | 98.61       | 112.34   |
| 3   | C     | 265 | ILE  | N-CA-C    | -6.71 | 100.20      | 109.46   |
| 5   | E     | 51  | ARG  | N-CA-C    | -6.71 | 101.61      | 109.93   |
| 2   | B     | 163 | GLY  | N-CA-C    | 6.69  | 125.99      | 112.34   |
| 2   | B     | 463 | PHE  | N-CA-C    | -6.69 | 103.61      | 111.03   |
| 2   | B     | 156 | PHE  | N-CA-C    | 6.69  | 120.54      | 112.38   |
| 4   | J     | 104 | TRP  | N-CA-C    | -6.66 | 103.27      | 111.33   |
| 4   | J     | 14  | TRP  | N-CA-C    | 6.65  | 118.42      | 111.03   |
| 3   | I     | 88  | LEU  | N-CA-C    | 6.65  | 121.34      | 111.04   |
| 3   | C     | 166 | ILE  | N-CA-C    | -6.64 | 104.38      | 110.82   |
| 1   | A     | 304 | HIS  | N-CA-C    | 6.59  | 119.75      | 108.02   |
| 6   | F     | 44  | GLN  | CA-C-N    | 6.56  | 133.51      | 121.70   |
| 6   | F     | 44  | GLN  | C-N-CA    | 6.56  | 133.51      | 121.70   |
| 5   | K     | 26  | THR  | N-CA-C    | 6.55  | 119.40      | 111.40   |
| 3   | C     | 120 | ILE  | N-CA-C    | -6.54 | 104.78      | 110.74   |
| 4   | J     | 9   | PRO  | N-CA-CB   | 6.50  | 109.37      | 103.33   |
| 2   | B     | 21  | ALA  | N-CA-C    | -6.49 | 103.83      | 111.03   |
| 1   | G     | 172 | MET  | N-CA-C    | 6.47  | 124.10      | 109.81   |
| 4   | D     | 15  | PHE  | N-CA-C    | 6.45  | 124.55      | 110.80   |
| 4   | J     | 54  | PHE  | N-CA-C    | 6.45  | 121.81      | 113.88   |
| 4   | J     | 238 | THR  | N-CA-C    | -6.44 | 104.34      | 111.36   |
| 3   | C     | 431 | PHE  | N-CA-C    | -6.44 | 103.95      | 110.97   |
| 2   | B     | 164 | PRO  | CA-N-CD   | -6.40 | 103.04      | 112.00   |
| 3   | I     | 156 | LYS  | N-CA-C    | -6.40 | 104.38      | 111.36   |
| 3   | I     | 61  | VAL  | N-CA-C    | -6.39 | 103.64      | 110.36   |
| 2   | H     | 163 | GLY  | N-CA-C    | 6.38  | 125.36      | 112.34   |
| 4   | D     | 54  | PHE  | N-CA-C    | 6.37  | 121.71      | 113.88   |
| 2   | B     | 227 | LYS  | N-CA-C    | -6.34 | 103.89      | 111.69   |
| 2   | H     | 432 | PHE  | N-CA-C    | 6.33  | 119.84      | 109.72   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | G     | 134 | SER  | N-CA-C   | -6.32 | 101.24      | 111.04   |
| 5   | E     | 26  | THR  | N-CA-C   | 6.32  | 119.11      | 111.40   |
| 2   | H     | 227 | LYS  | N-CA-C   | -6.30 | 103.94      | 111.69   |
| 3   | I     | 377 | LEU  | N-CA-C   | -6.29 | 104.16      | 112.34   |
| 2   | H     | 164 | PRO  | CB-CA-C  | 6.27  | 121.91      | 111.56   |
| 5   | K     | 51  | ARG  | N-CA-C   | -6.26 | 102.17      | 109.93   |
| 1   | A     | 198 | HIS  | N-CA-C   | -6.25 | 103.03      | 112.04   |
| 2   | H     | 21  | ALA  | N-CA-C   | -6.25 | 104.09      | 111.03   |
| 1   | G     | 198 | HIS  | N-CA-C   | -6.24 | 103.05      | 112.04   |
| 3   | I     | 256 | PRO  | CA-N-CD  | -6.24 | 103.26      | 112.00   |
| 1   | G     | 203 | ALA  | N-CA-C   | -6.24 | 103.63      | 111.11   |
| 2   | B     | 45  | PHE  | CA-CB-CG | -6.22 | 107.58      | 113.80   |
| 3   | C     | 255 | THR  | N-CA-C   | -6.21 | 101.18      | 110.24   |
| 3   | C     | 328 | VAL  | N-CA-C   | 6.20  | 116.38      | 110.42   |
| 1   | A     | 179 | THR  | N-CA-C   | -6.20 | 104.44      | 111.14   |
| 1   | G     | 89  | ILE  | N-CA-C   | -6.19 | 103.31      | 111.05   |
| 4   | J     | 139 | ARG  | N-CA-C   | 6.17  | 117.48      | 109.64   |
| 6   | F     | 12  | SER  | N-CA-C   | 6.17  | 119.58      | 108.17   |
| 4   | J     | 15  | PHE  | N-CA-C   | 6.17  | 123.93      | 110.80   |
| 1   | A     | 89  | ILE  | N-CA-C   | -6.15 | 103.36      | 111.05   |
| 6   | L     | 43  | ILE  | N-CA-C   | 6.12  | 116.95      | 109.30   |
| 3   | I     | 52  | ALA  | N-CA-C   | -6.12 | 103.77      | 111.11   |
| 1   | A     | 71  | LEU  | N-CA-C   | 6.11  | 117.74      | 111.14   |
| 9   | T     | 25  | GLN  | N-CA-C   | -6.11 | 104.54      | 112.23   |
| 1   | A     | 18  | CYS  | N-CA-C   | -6.09 | 103.59      | 111.02   |
| 4   | J     | 266 | TRP  | N-CA-C   | -6.08 | 105.77      | 113.43   |
| 3   | C     | 371 | GLY  | CA-C-N   | 6.08  | 125.29      | 118.97   |
| 3   | C     | 371 | GLY  | C-N-CA   | 6.08  | 125.29      | 118.97   |
| 1   | A     | 203 | ALA  | N-CA-C   | -6.08 | 104.57      | 111.07   |
| 3   | C     | 335 | THR  | CB-CA-C  | -6.08 | 100.71      | 110.79   |
| 4   | J     | 144 | ILE  | N-CA-C   | -6.05 | 104.84      | 110.53   |
| 4   | D     | 284 | ILE  | N-CA-C   | -6.04 | 104.62      | 110.42   |
| 1   | A     | 312 | ASN  | N-CA-C   | -6.03 | 102.40      | 110.24   |
| 2   | H     | 164 | PRO  | CA-N-CD  | -6.03 | 103.56      | 112.00   |
| 4   | J     | 4   | ALA  | N-CA-C   | 6.03  | 118.12      | 109.14   |
| 3   | I     | 67  | MET  | N-CA-C   | 6.03  | 117.65      | 111.14   |
| 3   | C     | 230 | LEU  | N-CA-C   | -6.02 | 104.83      | 111.82   |
| 4   | D     | 4   | ALA  | N-CA-C   | 6.02  | 118.11      | 109.14   |
| 1   | G     | 303 | ASN  | N-CA-C   | 6.00  | 117.49      | 111.07   |
| 3   | I     | 328 | VAL  | N-CA-C   | 6.00  | 116.12      | 110.30   |
| 1   | G     | 58  | VAL  | N-CA-C   | 5.99  | 117.21      | 108.53   |
| 3   | C     | 254 | THR  | N-CA-C   | 5.97  | 118.28      | 109.69   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | B     | 339 | ALA  | N-CA-C   | 5.96  | 123.48      | 110.80   |
| 2   | B     | 95  | GLY  | N-CA-C   | 5.95  | 119.40      | 112.50   |
| 4   | D     | 29  | PHE  | N-CA-C   | 5.95  | 123.46      | 110.80   |
| 1   | A     | 148 | SER  | N-CA-C   | -5.94 | 105.99      | 113.18   |
| 2   | H     | 339 | ALA  | N-CA-C   | 5.94  | 123.46      | 110.80   |
| 4   | J     | 29  | PHE  | N-CA-C   | 5.94  | 123.45      | 110.80   |
| 5   | E     | 45  | ASP  | N-CA-C   | 5.93  | 119.62      | 112.38   |
| 2   | B     | 263 | THR  | CA-C-N   | 5.92  | 125.68      | 119.76   |
| 2   | B     | 263 | THR  | C-N-CA   | 5.92  | 125.68      | 119.76   |
| 2   | H     | 72  | THR  | N-CA-C   | 5.90  | 120.41      | 109.56   |
| 3   | I     | 240 | ILE  | N-CA-C   | 5.90  | 116.08      | 110.42   |
| 2   | H     | 284 | ILE  | N-CA-C   | -5.89 | 104.99      | 110.53   |
| 4   | J     | 270 | PHE  | N-CA-C   | -5.88 | 104.95      | 111.71   |
| 3   | I     | 136 | GLY  | N-CA-C   | -5.87 | 100.37      | 112.34   |
| 3   | C     | 240 | ILE  | N-CA-C   | 5.86  | 116.05      | 110.42   |
| 3   | I     | 265 | ILE  | N-CA-C   | -5.85 | 100.16      | 109.17   |
| 2   | B     | 162 | PHE  | N-CA-C   | -5.85 | 98.35       | 110.80   |
| 1   | A     | 172 | MET  | N-CA-C   | 5.84  | 122.72      | 109.81   |
| 2   | B     | 400 | SER  | N-CA-C   | 5.83  | 119.05      | 110.30   |
| 2   | H     | 220 | ARG  | N-CA-C   | 5.82  | 122.66      | 109.81   |
| 1   | A     | 14  | TRP  | N-CA-C   | -5.81 | 103.93      | 111.02   |
| 9   | V     | 25  | GLN  | N-CA-C   | -5.78 | 104.94      | 112.23   |
| 2   | B     | 190 | PHE  | N-CA-C   | -5.78 | 106.39      | 113.50   |
| 2   | H     | 419 | SER  | N-CA-C   | -5.78 | 103.97      | 111.02   |
| 4   | J     | 170 | ALA  | N-CA-C   | -5.78 | 102.32      | 110.29   |
| 4   | J     | 45  | LEU  | N-CA-C   | -5.77 | 104.59      | 111.69   |
| 4   | J     | 332 | GLN  | N-CA-C   | -5.77 | 104.43      | 112.45   |
| 2   | H     | 190 | PHE  | N-CA-C   | -5.77 | 106.41      | 113.50   |
| 3   | C     | 123 | ALA  | N-CA-C   | -5.76 | 104.20      | 111.11   |
| 4   | D     | 9   | PRO  | N-CA-CB  | 5.76  | 108.74      | 103.15   |
| 4   | D     | 87  | HIS  | N-CA-C   | 5.75  | 119.85      | 112.26   |
| 4   | D     | 331 | PRO  | CB-CA-C  | 5.74  | 121.03      | 111.56   |
| 2   | B     | 164 | PRO  | CB-CA-C  | 5.71  | 120.98      | 111.56   |
| 3   | C     | 67  | MET  | N-CA-C   | 5.70  | 117.30      | 111.14   |
| 3   | C     | 61  | VAL  | N-CA-C   | -5.70 | 104.38      | 110.36   |
| 3   | C     | 137 | PRO  | N-CA-C   | 5.69  | 121.32      | 113.98   |
| 1   | G     | 309 | ALA  | N-CA-C   | -5.68 | 104.45      | 111.33   |
| 2   | H     | 91  | TRP  | CA-CB-CG | -5.67 | 102.84      | 113.60   |
| 1   | G     | 312 | ASN  | CA-C-N   | -5.66 | 115.80      | 122.93   |
| 1   | G     | 312 | ASN  | C-N-CA   | -5.66 | 115.80      | 122.93   |
| 1   | A     | 315 | ASN  | N-CA-C   | 5.66  | 122.85      | 110.80   |
| 2   | B     | 220 | ARG  | N-CA-C   | 5.66  | 122.31      | 109.81   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | A     | 125 | CYS  | N-CA-C   | -5.65 | 105.12      | 111.28   |
| 2   | B     | 221 | PRO  | N-CA-C   | 5.64  | 117.59      | 110.70   |
| 2   | H     | 95  | GLY  | N-CA-C   | 5.63  | 119.03      | 112.50   |
| 4   | D     | 330 | ALA  | CA-C-N   | 5.63  | 126.87      | 119.84   |
| 4   | D     | 330 | ALA  | C-N-CA   | 5.63  | 126.87      | 119.84   |
| 5   | K     | 45  | ASP  | N-CA-C   | 5.62  | 119.24      | 112.38   |
| 4   | J     | 9   | PRO  | N-CA-C   | 5.62  | 120.31      | 111.38   |
| 4   | J     | 287 | VAL  | N-CA-C   | -5.61 | 104.04      | 111.05   |
| 4   | J     | 180 | ARG  | N-CA-C   | -5.60 | 105.18      | 111.28   |
| 2   | H     | 42  | LEU  | N-CA-C   | 5.59  | 118.14      | 111.71   |
| 4   | D     | 332 | GLN  | N-CA-C   | -5.59 | 104.82      | 111.69   |
| 3   | C     | 156 | LYS  | N-CA-C   | -5.58 | 105.27      | 111.36   |
| 2   | B     | 332 | LYS  | N-CA-C   | -5.58 | 105.34      | 111.82   |
| 2   | H     | 400 | SER  | N-CA-C   | 5.58  | 118.67      | 110.30   |
| 3   | I     | 154 | LYS  | N-CA-C   | -5.57 | 106.44      | 113.18   |
| 3   | C     | 136 | GLY  | N-CA-C   | -5.57 | 100.98      | 112.34   |
| 2   | B     | 419 | SER  | N-CA-C   | -5.57 | 104.23      | 111.02   |
| 4   | J     | 131 | GLU  | N-CA-C   | -5.56 | 104.91      | 110.97   |
| 1   | G     | 22  | THR  | N-CA-C   | -5.55 | 104.45      | 111.11   |
| 3   | C     | 446 | GLY  | N-CA-C   | -5.54 | 107.02      | 115.66   |
| 4   | J     | 188 | PHE  | N-CA-C   | 5.52  | 119.99      | 112.04   |
| 4   | D     | 45  | LEU  | N-CA-C   | -5.52 | 104.90      | 111.69   |
| 2   | H     | 313 | ASP  | N-CA-C   | -5.52 | 99.05       | 110.80   |
| 5   | K     | 42  | LEU  | N-CA-C   | -5.52 | 104.49      | 111.11   |
| 4   | J     | 331 | PRO  | CA-N-CD  | -5.51 | 104.29      | 112.00   |
| 4   | D     | 139 | ARG  | N-CA-C   | 5.50  | 116.62      | 109.64   |
| 1   | G     | 71  | LEU  | N-CA-C   | 5.50  | 117.08      | 111.14   |
| 3   | C     | 100 | GLY  | CA-C-N   | -5.49 | 112.98      | 119.84   |
| 3   | C     | 100 | GLY  | C-N-CA   | -5.49 | 112.98      | 119.84   |
| 2   | B     | 106 | LEU  | N-CA-C   | -5.48 | 105.21      | 111.07   |
| 4   | D     | 131 | GLU  | N-CA-C   | -5.47 | 105.01      | 110.97   |
| 4   | J     | 196 | PHE  | N-CA-C   | 5.47  | 117.33      | 111.36   |
| 3   | I     | 254 | THR  | N-CA-C   | 5.47  | 117.57      | 109.69   |
| 1   | G     | 273 | PHE  | N-CA-C   | -5.46 | 105.25      | 111.14   |
| 1   | A     | 308 | ASP  | CA-CB-CG | -5.45 | 107.15      | 112.60   |
| 4   | D     | 273 | PHE  | N-CA-C   | 5.45  | 117.65      | 111.11   |
| 4   | D     | 235 | PHE  | N-CA-C   | -5.44 | 100.03      | 108.90   |
| 4   | J     | 240 | ALA  | N-CA-C   | 5.43  | 122.36      | 110.80   |
| 6   | L     | 26  | LEU  | N-CA-C   | -5.42 | 104.23      | 112.04   |
| 3   | I     | 431 | PHE  | N-CA-C   | -5.42 | 104.40      | 111.02   |
| 1   | A     | 312 | ASN  | CA-C-N   | -5.41 | 115.17      | 122.91   |
| 1   | A     | 312 | ASN  | C-N-CA   | -5.41 | 115.17      | 122.91   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 273 | PHE  | N-CA-C  | -5.41 | 105.47      | 111.36   |
| 4   | D     | 57  | SER  | N-CA-C  | -5.40 | 105.81      | 112.72   |
| 4   | D     | 226 | GLY  | N-CA-C  | -5.40 | 103.37      | 114.16   |
| 4   | D     | 287 | VAL  | N-CA-C  | -5.39 | 104.32      | 111.05   |
| 2   | B     | 268 | PHE  | CB-CA-C | -5.38 | 99.03       | 109.68   |
| 2   | B     | 382 | PRO  | N-CA-CB | 5.37  | 108.89      | 103.25   |
| 4   | J     | 77  | ALA  | N-CA-C  | 5.35  | 116.65      | 108.42   |
| 6   | F     | 26  | LEU  | N-CA-C  | -5.34 | 104.35      | 112.04   |
| 1   | G     | 312 | ASN  | N-CA-C  | -5.33 | 102.73      | 110.24   |
| 4   | D     | 85  | MET  | N-CA-C  | 5.32  | 119.41      | 113.02   |
| 1   | A     | 124 | SER  | N-CA-C  | -5.29 | 105.18      | 111.69   |
| 1   | A     | 161 | TYR  | CA-C-N  | -5.29 | 113.47      | 118.97   |
| 1   | A     | 161 | TYR  | C-N-CA  | -5.29 | 113.47      | 118.97   |
| 1   | G     | 179 | THR  | N-CA-C  | -5.28 | 105.44      | 111.14   |
| 5   | K     | 64  | PRO  | N-CA-C  | 5.27  | 119.49      | 111.11   |
| 4   | J     | 235 | PHE  | N-CA-C  | -5.27 | 100.31      | 108.90   |
| 2   | H     | 332 | LYS  | N-CA-C  | -5.26 | 105.72      | 111.82   |
| 2   | B     | 72  | THR  | N-CA-C  | 5.25  | 119.22      | 109.56   |
| 2   | B     | 221 | PRO  | CA-C-N  | 5.25  | 125.25      | 119.90   |
| 2   | B     | 221 | PRO  | C-N-CA  | 5.25  | 125.25      | 119.90   |
| 3   | I     | 270 | ALA  | N-CA-C  | -5.24 | 105.25      | 110.97   |
| 4   | D     | 196 | PHE  | N-CA-C  | 5.24  | 117.07      | 111.36   |
| 2   | B     | 137 | LYS  | N-CA-C  | -5.21 | 105.04      | 111.40   |
| 2   | B     | 264 | PRO  | N-CA-C  | 5.21  | 119.36      | 111.19   |
| 1   | G     | 10  | SER  | N-CA-C  | -5.20 | 105.61      | 111.28   |
| 4   | D     | 314 | PHE  | N-CA-C  | -5.18 | 106.65      | 112.87   |
| 4   | J     | 325 | ILE  | CB-CA-C | -5.18 | 105.07      | 112.22   |
| 4   | D     | 94  | GLY  | CA-C-N  | 5.18  | 126.31      | 119.84   |
| 4   | D     | 94  | GLY  | C-N-CA  | 5.18  | 126.31      | 119.84   |
| 3   | C     | 295 | THR  | N-CA-C  | -5.18 | 99.78       | 110.80   |
| 1   | A     | 296 | ASN  | CA-C-N  | 5.17  | 128.57      | 121.33   |
| 1   | A     | 296 | ASN  | C-N-CA  | 5.17  | 128.57      | 121.33   |
| 1   | G     | 76  | ASN  | N-CA-C  | -5.17 | 101.43      | 109.24   |
| 2   | H     | 35  | GLY  | N-CA-C  | -5.17 | 106.15      | 112.77   |
| 9   | T     | 38  | ALA  | N-CA-C  | 5.17  | 117.65      | 111.71   |
| 4   | J     | 38  | PHE  | CA-C-N  | -5.16 | 113.39      | 119.84   |
| 4   | J     | 38  | PHE  | C-N-CA  | -5.16 | 113.39      | 119.84   |
| 2   | B     | 313 | ASP  | N-CA-C  | -5.15 | 99.82       | 110.80   |
| 4   | J     | 243 | THR  | N-CA-C  | -5.15 | 104.62      | 112.04   |
| 1   | G     | 14  | TRP  | N-CA-C  | -5.14 | 104.75      | 111.02   |
| 3   | C     | 154 | LYS  | N-CA-C  | -5.13 | 106.97      | 113.18   |
| 6   | F     | 18  | VAL  | N-CA-C  | -5.13 | 105.39      | 110.62   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 6   | L     | 12  | SER  | N-CA-C   | 5.13  | 117.66      | 108.17   |
| 2   | B     | 32  | GLY  | N-CA-C   | -5.12 | 101.04      | 113.18   |
| 2   | B     | 284 | ILE  | N-CA-C   | -5.12 | 105.72      | 110.53   |
| 1   | G     | 148 | SER  | N-CA-C   | -5.12 | 106.98      | 113.18   |
| 1   | G     | 125 | CYS  | N-CA-C   | -5.11 | 105.79      | 111.36   |
| 4   | J     | 8   | ALA  | N-CA-C   | 5.11  | 121.11      | 109.81   |
| 2   | H     | 268 | PHE  | CA-CB-CG | 5.10  | 118.90      | 113.80   |
| 1   | A     | 192 | ILE  | CB-CA-C  | -5.09 | 102.94      | 111.29   |
| 4   | J     | 87  | HIS  | N-CA-C   | 5.09  | 119.65      | 111.81   |
| 2   | H     | 45  | PHE  | CA-CB-CG | -5.08 | 108.72      | 113.80   |
| 4   | D     | 77  | ALA  | N-CA-C   | 5.07  | 116.23      | 108.42   |
| 9   | T     | 50  | PRO  | N-CA-C   | 5.07  | 122.92      | 112.47   |
| 9   | V     | 38  | ALA  | N-CA-C   | 5.06  | 117.53      | 111.71   |
| 4   | D     | 8   | ALA  | N-CA-C   | 5.06  | 120.98      | 109.81   |
| 1   | G     | 192 | ILE  | CB-CA-C  | -5.06 | 103.00      | 111.29   |
| 3   | C     | 227 | VAL  | N-CA-C   | 5.05  | 119.84      | 109.34   |
| 2   | H     | 380 | ASP  | N-CA-C   | 5.04  | 117.18      | 107.44   |
| 2   | H     | 162 | PHE  | N-CA-C   | -5.03 | 100.08      | 110.80   |
| 3   | I     | 135 | ARG  | CA-C-N   | -5.03 | 113.98      | 121.87   |
| 3   | I     | 135 | ARG  | C-N-CA   | -5.03 | 113.98      | 121.87   |
| 4   | J     | 331 | PRO  | N-CA-C   | 5.03  | 122.83      | 112.47   |
| 3   | I     | 295 | THR  | N-CA-C   | -5.02 | 100.10      | 110.80   |
| 4   | D     | 178 | ILE  | N-CA-C   | -5.02 | 105.27      | 112.35   |
| 4   | J     | 331 | PRO  | CB-CA-C  | 5.02  | 119.84      | 111.56   |
| 1   | A     | 77  | ILE  | N-CA-C   | 5.02  | 115.45      | 110.23   |
| 9   | V     | 50  | PRO  | N-CA-C   | 5.01  | 122.80      | 112.47   |
| 2   | B     | 112 | CYS  | N-CA-C   | 5.01  | 116.59      | 111.03   |
| 6   | L     | 18  | VAL  | N-CA-C   | -5.01 | 105.61      | 110.42   |
| 4   | D     | 331 | PRO  | N-CA-CB  | -5.01 | 97.99       | 103.25   |
| 2   | B     | 268 | PHE  | CA-CB-CG | 5.01  | 118.81      | 113.80   |
| 2   | B     | 42  | LEU  | N-CA-C   | 5.00  | 116.73      | 111.28   |
| 3   | C     | 76  | ILE  | CA-C-N   | -5.00 | 115.08      | 120.03   |
| 3   | C     | 76  | ILE  | C-N-CA   | -5.00 | 115.08      | 120.03   |
| 2   | H     | 106 | LEU  | N-CA-C   | -5.00 | 105.72      | 111.07   |
| 1   | G     | 249 | VAL  | N-CA-C   | 5.00  | 119.74      | 109.34   |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 332 | HIS  | Sidechain |
| 2   | B     | 273 | TYR  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | G     | 332 | HIS  | Sidechain |
| 2   | H     | 273 | 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     | 2279  | 0        | 2113     | 471     | 0            |
| 1   | G     | 2279  | 0        | 2113     | 479     | 0            |
| 2   | B     | 3053  | 0        | 2666     | 463     | 0            |
| 2   | H     | 3053  | 0        | 2666     | 479     | 0            |
| 3   | C     | 2791  | 0        | 2530     | 480     | 0            |
| 3   | I     | 2791  | 0        | 2530     | 477     | 0            |
| 4   | D     | 2602  | 0        | 2383     | 490     | 0            |
| 4   | J     | 2602  | 0        | 2383     | 501     | 0            |
| 5   | E     | 536   | 0        | 480      | 89      | 0            |
| 5   | K     | 536   | 0        | 480      | 94      | 0            |
| 6   | F     | 297   | 0        | 304      | 60      | 0            |
| 6   | L     | 297   | 0        | 304      | 62      | 0            |
| 7   | O     | 883   | 0        | 221      | 43      | 0            |
| 7   | P     | 883   | 0        | 219      | 45      | 0            |
| 8   | S     | 499   | 0        | 116      | 50      | 0            |
| 8   | U     | 499   | 0        | 115      | 52      | 0            |
| 9   | T     | 1058  | 0        | 1066     | 61      | 0            |
| 9   | V     | 1058  | 0        | 1066     | 63      | 0            |
| 10  | X     | 1791  | 0        | 396      | 137     | 0            |
| 10  | Y     | 1791  | 0        | 393      | 135     | 0            |
| 11  | A     | 222   | 0        | 207      | 38      | 0            |
| 11  | B     | 846   | 0        | 774      | 74      | 0            |
| 11  | C     | 598   | 0        | 458      | 65      | 0            |
| 11  | D     | 115   | 0        | 111      | 18      | 0            |
| 11  | G     | 222   | 0        | 207      | 33      | 0            |
| 11  | H     | 846   | 0        | 774      | 78      | 0            |
| 11  | I     | 598   | 0        | 458      | 65      | 0            |
| 11  | J     | 115   | 0        | 111      | 16      | 0            |
| 12  | A     | 64    | 0        | 74       | 13      | 0            |
| 12  | D     | 54    | 0        | 51       | 4       | 0            |
| 12  | G     | 64    | 0        | 74       | 16      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 12  | J     | 54    | 0        | 51       | 9       | 0            |
| 13  | A     | 4     | 0        | 0        | 0       | 0            |
| 13  | G     | 4     | 0        | 0        | 0       | 0            |
| 14  | A     | 1     | 0        | 0        | 0       | 0            |
| 14  | G     | 1     | 0        | 0        | 0       | 0            |
| 15  | D     | 6     | 0        | 1        | 1       | 0            |
| 15  | J     | 6     | 0        | 1        | 1       | 0            |
| 16  | E     | 25    | 0        | 4        | 2       | 0            |
| 16  | L     | 25    | 0        | 4        | 2       | 0            |
| 17  | F     | 40    | 0        | 56       | 4       | 0            |
| 17  | L     | 40    | 0        | 56       | 3       | 0            |
| 18  | T     | 43    | 0        | 31       | 2       | 0            |
| 18  | V     | 43    | 0        | 31       | 2       | 0            |
| All | All   | 35614 | 0        | 28078    | 4407    | 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 69.

All (4407) 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) |
|------------------|--------------------|--------------------------|-------------------|
| 4:D:330:ALA:HB1  | 4:D:331:PRO:CD     | 1.48                     | 1.42              |
| 4:J:330:ALA:HB1  | 4:J:331:PRO:CD     | 1.54                     | 1.36              |
| 1:G:84:PRO:CG    | 1:G:173:PRO:HG3    | 1.56                     | 1.35              |
| 4:D:330:ALA:CB   | 4:D:331:PRO:CD     | 1.99                     | 1.33              |
| 4:J:330:ALA:CB   | 4:J:331:PRO:CD     | 2.07                     | 1.28              |
| 1:G:84:PRO:CD    | 1:G:173:PRO:HG3    | 1.64                     | 1.26              |
| 1:A:309:ALA:O    | 9:V:2:GLU:HA       | 1.27                     | 1.23              |
| 4:J:171:PRO:HD3  | 4:J:181:PHE:CE2    | 1.75                     | 1.21              |
| 2:H:45:PHE:CD2   | 2:H:47:PRO:HD3     | 1.75                     | 1.21              |
| 5:K:62:SER:C     | 5:K:64:PRO:HD3     | 1.67                     | 1.19              |
| 1:A:309:ALA:O    | 9:V:2:GLU:CA       | 1.91                     | 1.17              |
| 6:L:12:SER:O     | 6:L:14:PRO:HD2     | 1.43                     | 1.17              |
| 4:J:331:PRO:CG   | 4:J:339:PHE:HB3    | 1.74                     | 1.17              |
| 2:B:45:PHE:CD2   | 2:B:47:PRO:HD3     | 1.80                     | 1.15              |
| 2:H:61:PHE:O     | 2:H:64:PRO:HD2     | 1.44                     | 1.15              |
| 3:I:296:VAL:CG1  | 11:I:1459:CLA:HAA1 | 1.77                     | 1.14              |
| 6:F:12:SER:O     | 6:F:14:PRO:HD2     | 1.48                     | 1.13              |
| 3:I:449:ARG:HH11 | 3:I:449:ARG:HG3    | 1.08                     | 1.13              |
| 4:D:331:PRO:CG   | 4:D:339:PHE:HB3    | 1.78                     | 1.13              |
| 4:J:330:ALA:HB3  | 4:J:331:PRO:HD2    | 1.28                     | 1.13              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 4:D:52:THR:HG22  | 4:D:67:TYR:HE1     | 1.09                     | 1.12              |
| 4:J:171:PRO:HD3  | 4:J:181:PHE:CD2    | 1.83                     | 1.12              |
| 4:D:126:MET:HA   | 4:D:129:GLN:HE21   | 1.11                     | 1.12              |
| 1:A:142:TRP:HB3  | 4:D:220:ASN:OD1    | 1.49                     | 1.10              |
| 4:J:330:ALA:CB   | 4:J:331:PRO:HD2    | 1.74                     | 1.10              |
| 4:J:331:PRO:HG3  | 4:J:339:PHE:CB     | 1.79                     | 1.10              |
| 4:J:126:MET:HA   | 4:J:129:GLN:HE21   | 1.03                     | 1.10              |
| 1:G:186:PHE:HD2  | 1:G:192:ILE:HD11   | 1.16                     | 1.09              |
| 4:J:331:PRO:CG   | 4:J:339:PHE:CB     | 2.29                     | 1.09              |
| 3:I:228:ASN:HA   | 3:I:295:THR:HG21   | 1.34                     | 1.09              |
| 4:J:113:PHE:HA   | 11:J:1353:CLA:HED1 | 1.34                     | 1.09              |
| 1:A:47:CYS:SG    | 1:A:114:LEU:HD23   | 1.93                     | 1.08              |
| 1:A:143:ILE:HG13 | 4:D:220:ASN:HD22   | 1.12                     | 1.08              |
| 3:C:296:VAL:CG1  | 11:C:1459:CLA:HAA1 | 1.81                     | 1.08              |
| 1:G:142:TRP:HB3  | 4:J:220:ASN:OD1    | 1.51                     | 1.08              |
| 4:D:330:ALA:CB   | 4:D:331:PRO:HD2    | 1.73                     | 1.08              |
| 1:A:186:PHE:HD2  | 1:A:192:ILE:HD11   | 1.13                     | 1.08              |
| 3:C:449:ARG:HH11 | 3:C:449:ARG:HG3    | 1.07                     | 1.08              |
| 3:C:228:ASN:HA   | 3:C:295:THR:HG21   | 1.37                     | 1.07              |
| 1:G:84:PRO:HG2   | 1:G:173:PRO:HG3    | 1.26                     | 1.07              |
| 4:J:52:THR:HG22  | 4:J:67:TYR:HE1     | 1.12                     | 1.07              |
| 2:B:330:MET:HE2  | 2:B:446:SER:HB3    | 1.30                     | 1.07              |
| 4:D:113:PHE:HA   | 11:D:1353:CLA:HED1 | 1.35                     | 1.07              |
| 5:K:62:SER:O     | 5:K:64:PRO:HD3     | 1.50                     | 1.07              |
| 4:D:331:PRO:HG3  | 4:D:339:PHE:CB     | 1.84                     | 1.07              |
| 2:H:330:MET:HE2  | 2:H:446:SER:HB3    | 1.27                     | 1.06              |
| 3:I:296:VAL:HG11 | 11:I:1459:CLA:CAA  | 1.85                     | 1.06              |
| 2:B:61:PHE:O     | 2:B:64:PRO:HD2     | 1.52                     | 1.06              |
| 3:C:296:VAL:HG11 | 11:C:1459:CLA:CAA  | 1.86                     | 1.06              |
| 1:G:114:LEU:HA   | 11:G:1346:CLA:HED1 | 1.35                     | 1.06              |
| 2:H:45:PHE:CE2   | 2:H:47:PRO:HD3     | 1.90                     | 1.05              |
| 4:J:126:MET:O    | 4:J:129:GLN:HG2    | 1.55                     | 1.05              |
| 4:J:331:PRO:HG2  | 4:J:339:PHE:HB3    | 1.24                     | 1.05              |
| 4:D:330:ALA:HB3  | 4:D:331:PRO:HD2    | 1.21                     | 1.05              |
| 3:C:187:ASP:HB3  | 3:C:230:LEU:HD23   | 1.37                     | 1.04              |
| 1:G:47:CYS:SG    | 1:G:114:LEU:HD23   | 1.97                     | 1.04              |
| 3:I:296:VAL:HG11 | 11:I:1459:CLA:HAA1 | 1.04                     | 1.04              |
| 4:D:330:ALA:CB   | 4:D:331:PRO:HD3    | 1.75                     | 1.04              |
| 2:B:400:SER:HB3  | 2:B:410:THR:HB     | 1.38                     | 1.03              |
| 3:C:106:VAL:O    | 3:C:107:ASP:CB     | 1.98                     | 1.03              |
| 1:A:138:GLY:HA2  | 3:C:455:PHE:CE1    | 1.93                     | 1.03              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 4:D:126:MET:O    | 4:D:129:GLN:HG2    | 1.58                     | 1.03              |
| 1:A:63:ILE:HG12  | 1:A:64:ARG:H       | 1.20                     | 1.02              |
| 1:G:63:ILE:HG12  | 1:G:64:ARG:H       | 1.23                     | 1.02              |
| 1:A:127:MET:HE2  | 1:A:151:LEU:HD22   | 1.37                     | 1.01              |
| 4:D:331:PRO:HG2  | 4:D:339:PHE:HB3    | 1.39                     | 1.01              |
| 1:G:84:PRO:HG2   | 1:G:173:PRO:CG     | 1.89                     | 1.01              |
| 4:D:122:LEU:HD21 | 11:D:1351:CLA:H92  | 1.39                     | 1.01              |
| 5:K:65:LEU:C     | 5:K:66:VAL:CA      | 2.33                     | 1.01              |
| 1:A:309:ALA:O    | 9:V:2:GLU:CB       | 2.09                     | 1.01              |
| 3:I:187:ASP:HB3  | 3:I:230:LEU:HD23   | 1.43                     | 1.01              |
| 1:G:138:GLY:HA2  | 3:I:455:PHE:CE1    | 1.96                     | 1.00              |
| 2:H:30:VAL:HG12  | 11:H:1486:CLA:HAC1 | 1.39                     | 1.00              |
| 2:H:400:SER:HB3  | 2:H:410:THR:HB     | 1.38                     | 1.00              |
| 1:G:143:ILE:HG13 | 4:J:220:ASN:HD22   | 1.26                     | 1.00              |
| 4:J:330:ALA:HB1  | 4:J:331:PRO:HD3    | 1.01                     | 1.00              |
| 1:A:63:ILE:HG13  | 3:C:335:THR:CG2    | 1.91                     | 1.00              |
| 5:E:22:ILE:HG23  | 10:X:568:UNK:CB    | 1.92                     | 0.99              |
| 4:J:171:PRO:CD   | 4:J:181:PHE:CE2    | 2.44                     | 0.99              |
| 3:C:296:VAL:HG11 | 11:C:1459:CLA:HAA1 | 1.00                     | 0.99              |
| 1:G:310:LYS:HA   | 9:T:2:GLU:HA       | 1.43                     | 0.99              |
| 3:I:398:HIS:C    | 3:I:399:ALA:CA     | 2.36                     | 0.99              |
| 4:J:122:LEU:HD21 | 11:J:1351:CLA:H92  | 1.41                     | 0.99              |
| 2:B:347:ARG:HB3  | 2:B:351:GLY:HA2    | 1.41                     | 0.98              |
| 4:J:86:GLY:HA2   | 4:J:166:SER:HB3    | 1.44                     | 0.98              |
| 3:C:37:ALA:HA    | 11:C:1466:CLA:HBA2 | 1.45                     | 0.98              |
| 4:D:86:GLY:HA2   | 4:D:166:SER:HB3    | 1.44                     | 0.98              |
| 2:H:347:ARG:HB3  | 2:H:351:GLY:HA2    | 1.46                     | 0.98              |
| 3:I:311:GLN:HG2  | 3:I:355:THR:CG2    | 1.94                     | 0.98              |
| 1:G:63:ILE:HG13  | 3:I:335:THR:CG2    | 1.93                     | 0.97              |
| 3:C:311:GLN:HG2  | 3:C:355:THR:CG2    | 1.94                     | 0.97              |
| 4:D:160:TYR:HB3  | 4:D:161:PRO:HD3    | 1.47                     | 0.97              |
| 5:K:22:ILE:HG23  | 10:Y:568:UNK:CB    | 1.94                     | 0.97              |
| 3:C:398:HIS:C    | 3:C:399:ALA:CA     | 2.37                     | 0.97              |
| 1:A:114:LEU:HA   | 11:A:1346:CLA:HED1 | 1.43                     | 0.97              |
| 1:G:278:TRP:HB3  | 1:G:279:PRO:HD3    | 1.42                     | 0.97              |
| 1:G:310:LYS:HB2  | 9:T:2:GLU:N        | 1.78                     | 0.97              |
| 4:D:331:PRO:CG   | 4:D:339:PHE:CB     | 2.43                     | 0.97              |
| 2:H:30:VAL:CG1   | 11:H:1486:CLA:HAC1 | 1.93                     | 0.97              |
| 4:J:340:VAL:O    | 4:J:342:PRO:CD     | 2.13                     | 0.97              |
| 3:I:311:GLN:HG2  | 3:I:355:THR:HG21   | 1.44                     | 0.97              |
| 4:D:52:THR:HG22  | 4:D:67:TYR:CE1     | 2.00                     | 0.96              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 3:I:37:ALA:HA    | 11:I:1466:CLA:HBA2 | 1.45                     | 0.96              |
| 6:L:37:ILE:HA    | 6:L:40:MET:HE2     | 1.47                     | 0.96              |
| 7:P:65:UNK:C     | 7:P:66:UNK:CA      | 2.42                     | 0.96              |
| 2:H:135:LEU:HB2  | 2:H:136:PRO:HD3    | 1.44                     | 0.96              |
| 3:I:107:ASP:O    | 3:I:110:PRO:HD2    | 1.63                     | 0.96              |
| 3:I:363:GLY:O    | 3:I:367:GLU:HG2    | 1.65                     | 0.96              |
| 4:J:340:VAL:O    | 4:J:342:PRO:HD2    | 1.64                     | 0.96              |
| 9:T:129:LYS:HE3  | 9:T:135:VAL:HG21   | 1.45                     | 0.96              |
| 1:A:310:LYS:HB2  | 9:V:2:GLU:N        | 1.81                     | 0.96              |
| 7:O:65:UNK:C     | 7:O:66:UNK:CA      | 2.44                     | 0.96              |
| 2:B:149:LEU:HG   | 11:B:1484:CLA:HBC1 | 1.47                     | 0.96              |
| 1:A:186:PHE:CD2  | 1:A:192:ILE:HD11   | 2.00                     | 0.95              |
| 2:B:135:LEU:HB2  | 2:B:136:PRO:HD3    | 1.49                     | 0.95              |
| 4:D:345:VAL:O    | 4:D:345:VAL:HG12   | 1.63                     | 0.95              |
| 6:F:41:GLN:HB3   | 10:X:331:UNK:CB    | 1.96                     | 0.95              |
| 1:G:221:SER:HA   | 4:J:139:ARG:HB2    | 1.49                     | 0.95              |
| 4:J:52:THR:HG22  | 4:J:67:TYR:CE1     | 2.01                     | 0.95              |
| 6:L:41:GLN:HB3   | 10:Y:331:UNK:CB    | 1.96                     | 0.94              |
| 4:J:160:TYR:HB3  | 4:J:161:PRO:HD3    | 1.47                     | 0.94              |
| 9:V:133:GLY:O    | 9:V:137:TYR:HB2    | 1.67                     | 0.94              |
| 2:B:45:PHE:CE2   | 2:B:47:PRO:HD3     | 2.01                     | 0.94              |
| 1:G:272:HIS:CD2  | 4:J:218:VAL:HG21   | 2.02                     | 0.94              |
| 1:A:221:SER:HA   | 4:D:139:ARG:HB2    | 1.48                     | 0.94              |
| 3:I:173:LEU:O    | 3:I:176:VAL:HG12   | 1.67                     | 0.94              |
| 1:A:222:SER:C    | 1:A:223:LEU:CA     | 2.40                     | 0.94              |
| 2:H:180:PRO:C    | 2:H:181:VAL:CA     | 2.41                     | 0.94              |
| 4:J:253:TRP:HB2  | 4:J:260:ALA:HB2    | 1.50                     | 0.94              |
| 1:G:186:PHE:CD2  | 1:G:192:ILE:HD11   | 2.03                     | 0.93              |
| 2:H:31:ALA:H     | 11:H:1486:CLA:HBC3 | 1.31                     | 0.93              |
| 2:H:149:LEU:HG   | 11:H:1484:CLA:HBC1 | 1.51                     | 0.93              |
| 1:A:272:HIS:CD2  | 4:D:218:VAL:HG21   | 2.04                     | 0.93              |
| 3:C:363:GLY:O    | 3:C:367:GLU:HG2    | 1.68                     | 0.93              |
| 4:J:345:VAL:O    | 4:J:345:VAL:HG12   | 1.68                     | 0.93              |
| 4:J:148:ALA:HB3  | 4:J:149:PRO:HD3    | 1.51                     | 0.93              |
| 2:B:180:PRO:C    | 2:B:181:VAL:CA     | 2.41                     | 0.93              |
| 3:C:106:VAL:O    | 3:C:107:ASP:HB2    | 1.13                     | 0.93              |
| 4:D:307:GLU:O    | 4:D:309:PRO:HD3    | 1.67                     | 0.93              |
| 5:E:26:THR:HG21  | 16:E:1085:HEM:C2C  | 2.03                     | 0.93              |
| 3:C:224:ILE:CA   | 3:C:225:VAL:N      | 2.32                     | 0.92              |
| 6:L:10:PRO:HB2   | 6:L:19:ARG:HH11    | 1.34                     | 0.92              |
| 4:D:164:GLN:HE22 | 4:D:189:HIS:HE1    | 1.13                     | 0.92              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:G:24:THR:C     | 1:G:25:ASP:CA      | 2.42                     | 0.92              |
| 1:G:84:PRO:CG    | 1:G:173:PRO:CG     | 2.44                     | 0.92              |
| 3:I:224:ILE:CA   | 3:I:225:VAL:N      | 2.32                     | 0.92              |
| 3:I:449:ARG:HH11 | 3:I:449:ARG:CG     | 1.82                     | 0.92              |
| 3:C:311:GLN:HG2  | 3:C:355:THR:HG21   | 1.51                     | 0.92              |
| 2:B:59:GLY:CA    | 11:B:1488:CLA:HED1 | 1.98                     | 0.92              |
| 5:K:62:SER:C     | 5:K:64:PRO:CD      | 2.43                     | 0.92              |
| 2:B:263:THR:HG22 | 2:B:263:THR:O      | 1.69                     | 0.92              |
| 3:C:173:LEU:O    | 3:C:176:VAL:HG12   | 1.70                     | 0.92              |
| 1:A:24:THR:C     | 1:A:25:ASP:CA      | 2.43                     | 0.91              |
| 3:C:190:ALA:C    | 3:C:191:PRO:CA     | 2.43                     | 0.91              |
| 3:I:155:ASN:O    | 3:I:159:THR:HG23   | 1.70                     | 0.91              |
| 5:K:62:SER:O     | 5:K:64:PRO:CD      | 2.18                     | 0.91              |
| 2:H:53:ASN:N     | 2:H:54:PRO:HD3     | 1.83                     | 0.91              |
| 2:H:80:ILE:C     | 2:H:81:THR:CA      | 2.43                     | 0.91              |
| 2:B:60:MET:CA    | 2:B:61:PHE:N       | 2.33                     | 0.91              |
| 3:C:155:ASN:HB2  | 3:C:255:THR:HG22   | 1.53                     | 0.91              |
| 3:C:341:LEU:C    | 3:C:342:MET:CA     | 2.43                     | 0.91              |
| 1:A:330:VAL:HG12 | 4:D:347:PRO:HA     | 1.53                     | 0.91              |
| 2:B:53:ASN:N     | 2:B:54:PRO:HD3     | 1.83                     | 0.91              |
| 2:B:80:ILE:C     | 2:B:81:THR:CA      | 2.43                     | 0.91              |
| 9:V:129:LYS:HE3  | 9:V:135:VAL:HG21   | 1.50                     | 0.91              |
| 1:A:175:GLY:H    | 12:A:1345:PHO:H192 | 1.35                     | 0.91              |
| 3:C:294:ASN:O    | 3:C:295:THR:HG23   | 1.70                     | 0.91              |
| 6:F:37:ILE:HA    | 6:F:40:MET:HE2     | 1.50                     | 0.91              |
| 1:A:310:LYS:HA   | 9:V:2:GLU:HA       | 1.51                     | 0.91              |
| 4:J:307:GLU:O    | 4:J:309:PRO:HD3    | 1.71                     | 0.91              |
| 3:C:212:TYR:C    | 3:C:213:LEU:CA     | 2.43                     | 0.91              |
| 1:A:81:ALA:HB3   | 1:A:174:LEU:O      | 1.70                     | 0.90              |
| 5:E:65:LEU:C     | 5:E:66:VAL:CA      | 2.44                     | 0.90              |
| 1:A:129:ARG:HH21 | 4:D:256:ILE:HG23   | 1.33                     | 0.90              |
| 1:A:334:ARG:C    | 1:A:335:ASN:CA     | 2.44                     | 0.90              |
| 1:G:129:ARG:HH21 | 4:J:256:ILE:HG23   | 1.32                     | 0.90              |
| 1:G:222:SER:C    | 1:G:223:LEU:CA     | 2.44                     | 0.90              |
| 5:K:26:THR:HG21  | 16:L:1046:HEM:C2C  | 2.06                     | 0.90              |
| 9:T:133:GLY:O    | 9:T:137:TYR:HB2    | 1.71                     | 0.90              |
| 3:I:190:ALA:C    | 3:I:191:PRO:CA     | 2.44                     | 0.90              |
| 3:I:95:LEU:O     | 3:I:185:LEU:HA     | 1.71                     | 0.90              |
| 2:H:60:MET:CA    | 2:H:61:PHE:N       | 2.35                     | 0.90              |
| 4:D:148:ALA:HB3  | 4:D:149:PRO:HD3    | 1.54                     | 0.90              |
| 1:A:278:TRP:HB3  | 1:A:279:PRO:HD3    | 1.53                     | 0.90              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:G:286:THR:HG22 | 11:G:1342:CLA:O1D  | 1.72                     | 0.90              |
| 2:H:263:THR:O    | 2:H:263:THR:HG22   | 1.71                     | 0.90              |
| 3:I:212:TYR:C    | 3:I:213:LEU:CA     | 2.45                     | 0.90              |
| 4:J:331:PRO:HG3  | 4:J:339:PHE:CG     | 2.07                     | 0.90              |
| 1:A:57:PRO:HG3   | 1:A:68:SER:HB3     | 1.52                     | 0.89              |
| 3:I:341:LEU:C    | 3:I:342:MET:CA     | 2.45                     | 0.89              |
| 1:G:334:ARG:C    | 1:G:335:ASN:CA     | 2.45                     | 0.89              |
| 1:G:92:HIS:HA    | 3:I:219:GLY:CA     | 2.02                     | 0.89              |
| 2:H:397:VAL:HA   | 2:H:417:VAL:HG21   | 1.54                     | 0.89              |
| 4:J:126:MET:HA   | 4:J:129:GLN:NE2    | 1.86                     | 0.89              |
| 4:D:253:TRP:HB2  | 4:D:260:ALA:HB2    | 1.54                     | 0.89              |
| 4:J:323:GLU:HG2  | 4:J:326:ARG:HH21   | 1.36                     | 0.89              |
| 4:D:102:THR:HG22 | 5:E:46:VAL:O       | 1.71                     | 0.89              |
| 1:G:63:ILE:HG13  | 3:I:335:THR:HG21   | 1.54                     | 0.89              |
| 3:I:155:ASN:HB2  | 3:I:255:THR:HG22   | 1.54                     | 0.89              |
| 2:B:320:ALA:C    | 2:B:321:LYS:CA     | 2.46                     | 0.89              |
| 1:G:81:ALA:HB3   | 1:G:174:LEU:O      | 1.74                     | 0.88              |
| 1:G:137:LEU:HD12 | 1:G:139:MET:HE1    | 1.54                     | 0.88              |
| 1:G:175:GLY:H    | 12:G:1345:PHO:H192 | 1.39                     | 0.88              |
| 5:E:59:GLU:O     | 5:E:60:GLN:HB3     | 1.72                     | 0.88              |
| 2:H:55:MET:C     | 2:H:56:TRP:CA      | 2.47                     | 0.88              |
| 2:H:320:ALA:C    | 2:H:321:LYS:CA     | 2.47                     | 0.87              |
| 3:I:242:LEU:O    | 3:I:245:ILE:HG13   | 1.74                     | 0.87              |
| 3:I:456:GLU:C    | 3:I:457:LYS:CA     | 2.48                     | 0.87              |
| 2:H:59:GLY:CA    | 11:H:1488:CLA:HED1 | 2.04                     | 0.87              |
| 1:A:286:THR:HG22 | 11:A:1342:CLA:O1D  | 1.73                     | 0.87              |
| 3:C:95:LEU:O     | 3:C:185:LEU:HA     | 1.75                     | 0.87              |
| 4:J:323:GLU:HG2  | 4:J:326:ARG:NH2    | 1.90                     | 0.87              |
| 1:G:57:PRO:HG3   | 1:G:68:SER:HB3     | 1.54                     | 0.87              |
| 1:G:309:ALA:O    | 9:T:2:GLU:HA       | 1.75                     | 0.87              |
| 1:G:330:VAL:HG12 | 4:J:347:PRO:HA     | 1.53                     | 0.87              |
| 3:C:242:LEU:O    | 3:C:245:ILE:HG13   | 1.75                     | 0.86              |
| 3:I:273:SER:HB2  | 3:I:445:ALA:HB2    | 1.57                     | 0.86              |
| 4:J:102:THR:HG22 | 5:K:46:VAL:O       | 1.74                     | 0.86              |
| 1:A:92:HIS:HA    | 3:C:219:GLY:CA     | 2.05                     | 0.86              |
| 3:C:149:TYR:CA   | 3:C:150:ASP:N      | 2.39                     | 0.86              |
| 2:H:329:PRO:CA   | 2:H:330:MET:N      | 2.39                     | 0.86              |
| 3:C:245:ILE:HD12 | 3:C:246:ALA:N      | 1.90                     | 0.86              |
| 3:C:456:GLU:C    | 3:C:457:LYS:CA     | 2.48                     | 0.86              |
| 4:D:330:ALA:HB1  | 4:D:331:PRO:HD3    | 0.87                     | 0.86              |
| 3:C:449:ARG:HH11 | 3:C:449:ARG:CG     | 1.86                     | 0.85              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 4:D:323:GLU:HG2    | 4:D:326:ARG:HH21  | 1.41                     | 0.85              |
| 4:D:258:GLY:O      | 4:D:259:ILE:HG13  | 1.76                     | 0.85              |
| 2:B:55:MET:C       | 2:B:56:TRP:CA     | 2.49                     | 0.85              |
| 2:B:329:PRO:CA     | 2:B:330:MET:N     | 2.39                     | 0.85              |
| 2:H:31:ALA:HA      | 2:H:34:ALA:HB3    | 1.56                     | 0.85              |
| 2:H:135:LEU:HB2    | 2:H:136:PRO:CD    | 2.06                     | 0.85              |
| 4:J:331:PRO:HG3    | 4:J:339:PHE:HB2   | 1.59                     | 0.85              |
| 2:H:354:LEU:HD11   | 2:H:378:LYS:CB    | 2.06                     | 0.85              |
| 3:C:82:TYR:HA      | 3:C:422:PRO:HG2   | 1.57                     | 0.85              |
| 2:H:414:PRO:HB2    | 2:H:415:PRO:HD3   | 1.59                     | 0.85              |
| 1:A:254:TYR:OH     | 4:D:129:GLN:HB2   | 1.77                     | 0.85              |
| 2:H:295:GLY:C      | 2:H:296:ALA:CA    | 2.50                     | 0.85              |
| 2:B:295:GLY:C      | 2:B:296:ALA:CA    | 2.50                     | 0.85              |
| 3:I:82:TYR:HA      | 3:I:422:PRO:HG2   | 1.59                     | 0.84              |
| 3:I:353:GLY:CA     | 3:I:354:GLU:N     | 2.40                     | 0.84              |
| 7:P:68:UNK:CA      | 7:P:69:UNK:N      | 2.40                     | 0.84              |
| 6:F:10:PRO:HB2     | 6:F:19:ARG:HH11   | 1.40                     | 0.84              |
| 3:I:376:ASP:HB2    | 3:I:379:LYS:HG3   | 1.57                     | 0.84              |
| 3:I:449:ARG:HG3    | 3:I:449:ARG:NH1   | 1.87                     | 0.84              |
| 4:J:223:PHE:CE2    | 4:J:245:SER:HB3   | 2.13                     | 0.84              |
| 3:C:353:GLY:CA     | 3:C:354:GLU:N     | 2.40                     | 0.84              |
| 3:C:376:ASP:HB2    | 3:C:379:LYS:HG3   | 1.56                     | 0.84              |
| 1:G:254:TYR:OH     | 4:J:129:GLN:HB2   | 1.78                     | 0.84              |
| 2:H:263:THR:H      | 2:H:264:PRO:CD    | 1.91                     | 0.84              |
| 11:H:1488:CLA:H171 | 4:J:281:MET:HE1   | 1.58                     | 0.84              |
| 5:E:70:PHE:CA      | 5:E:72:ALA:N      | 2.41                     | 0.84              |
| 4:D:103:ARG:HG2    | 4:D:106:GLN:OE1   | 1.78                     | 0.84              |
| 4:D:164:GLN:HE22   | 4:D:189:HIS:CE1   | 1.96                     | 0.84              |
| 4:D:274:VAL:HB     | 4:D:275:PRO:HD3   | 1.57                     | 0.84              |
| 2:H:271:THR:HG1    | 2:H:274:GLN:HG3   | 1.43                     | 0.84              |
| 3:I:228:ASN:CA     | 3:I:295:THR:HG21  | 2.07                     | 0.84              |
| 7:O:68:UNK:CA      | 7:O:69:UNK:N      | 2.41                     | 0.84              |
| 3:I:100:GLY:O      | 3:I:101:PRO:C     | 2.17                     | 0.83              |
| 4:J:343:GLU:OE1    | 4:J:343:GLU:N     | 2.11                     | 0.83              |
| 1:G:34:GLY:HA2     | 1:G:37:MET:HB3    | 1.61                     | 0.83              |
| 3:I:53:HIS:HB3     | 11:I:1470:CLA:OBD | 1.78                     | 0.83              |
| 1:A:137:LEU:HD12   | 1:A:139:MET:HE1   | 1.58                     | 0.83              |
| 1:G:248:ILE:HD12   | 4:J:235:PHE:HZ    | 1.43                     | 0.83              |
| 5:K:70:PHE:CA      | 5:K:72:ALA:N      | 2.41                     | 0.83              |
| 10:Y:334:UNK:C     | 10:Y:335:UNK:O    | 2.22                     | 0.83              |
| 2:B:425:ILE:HG23   | 2:B:425:ILE:O     | 1.78                     | 0.83              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 4:J:164:GLN:HE22 | 4:J:189:HIS:HE1    | 1.23                     | 0.83              |
| 1:A:63:ILE:HG13  | 3:C:335:THR:HG21   | 1.59                     | 0.83              |
| 3:C:155:ASN:O    | 3:C:159:THR:HG23   | 1.78                     | 0.83              |
| 3:I:128:GLY:HA3  | 11:I:1471:CLA:HMC1 | 1.60                     | 0.83              |
| 3:I:149:TYR:CA   | 3:I:150:ASP:N      | 2.41                     | 0.83              |
| 5:K:59:GLU:O     | 5:K:60:GLN:HB3     | 1.75                     | 0.83              |
| 3:I:40:ALA:O     | 3:I:43:ILE:HG12    | 1.78                     | 0.83              |
| 1:G:176:ILE:HG12 | 11:G:1343:CLA:HED3 | 1.61                     | 0.83              |
| 2:H:271:THR:OG1  | 2:H:274:GLN:HG3    | 1.78                     | 0.83              |
| 2:H:316:GLY:HA2  | 2:H:443:PHE:CD1    | 2.13                     | 0.83              |
| 2:B:316:GLY:HA2  | 2:B:443:PHE:CD1    | 2.14                     | 0.82              |
| 2:B:397:VAL:HA   | 2:B:417:VAL:HG21   | 1.61                     | 0.82              |
| 2:H:130:GLU:CA   | 2:H:131:PRO:N      | 2.42                     | 0.82              |
| 3:I:280:SER:HB2  | 3:I:434:ALA:O      | 1.79                     | 0.82              |
| 3:C:128:GLY:HA3  | 11:C:1471:CLA:HMC1 | 1.60                     | 0.82              |
| 1:A:307:ILE:O    | 1:A:309:ALA:N      | 2.09                     | 0.82              |
| 2:H:31:ALA:N     | 11:H:1486:CLA:HBC3 | 1.94                     | 0.82              |
| 4:J:126:MET:HE3  | 4:J:146:PHE:HD2    | 1.42                     | 0.82              |
| 1:G:217:SER:OG   | 4:J:142:ASN:HA     | 1.79                     | 0.82              |
| 2:H:355:PHE:O    | 2:H:370:LEU:HA     | 1.80                     | 0.82              |
| 2:B:161:LEU:O    | 2:B:162:PHE:HB2    | 1.80                     | 0.82              |
| 2:H:236:THR:HB   | 2:H:473:THR:CG2    | 2.09                     | 0.82              |
| 4:J:274:VAL:HB   | 4:J:275:PRO:HD3    | 1.61                     | 0.82              |
| 2:H:141:ILE:HB   | 2:H:217:ILE:HD12   | 1.62                     | 0.82              |
| 3:I:294:ASN:O    | 3:I:295:THR:HG23   | 1.80                     | 0.82              |
| 6:F:12:SER:C     | 6:F:14:PRO:HD2     | 2.03                     | 0.82              |
| 2:H:89:GLY:CA    | 2:H:90:PHE:N       | 2.43                     | 0.82              |
| 1:A:290:ILE:HD11 | 11:A:1342:CLA:OBD  | 1.80                     | 0.81              |
| 6:F:12:SER:O     | 6:F:14:PRO:CD      | 2.26                     | 0.81              |
| 2:H:24:LEU:HD23  | 2:H:111:ALA:N      | 1.96                     | 0.81              |
| 2:H:229:LEU:C    | 2:H:231:MET:H      | 1.86                     | 0.81              |
| 4:J:61:HIS:HB3   | 4:J:63:LEU:HD13    | 1.61                     | 0.81              |
| 4:J:171:PRO:HG3  | 4:J:181:PHE:CG     | 2.15                     | 0.81              |
| 2:B:130:GLU:CA   | 2:B:131:PRO:N      | 2.43                     | 0.81              |
| 2:B:236:THR:HB   | 2:B:473:THR:CG2    | 2.11                     | 0.81              |
| 2:H:45:PHE:CD2   | 2:H:47:PRO:CD      | 2.60                     | 0.81              |
| 3:I:266:TRP:HB3  | 3:I:271:TYR:OH     | 1.81                     | 0.81              |
| 1:G:294:ALA:C    | 1:G:296:ASN:H      | 1.88                     | 0.81              |
| 3:I:89:ILE:HB    | 3:I:90:PRO:HD3     | 1.62                     | 0.81              |
| 4:J:258:GLY:O    | 4:J:259:ILE:HG13   | 1.80                     | 0.81              |
| 3:C:445:ALA:HB1  | 11:C:1463:CLA:HED1 | 1.61                     | 0.81              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 2:H:306:PRO:CA   | 2:H:307:GLU:N      | 2.43                     | 0.81              |
| 1:A:242:GLU:CA   | 1:A:243:GLU:N      | 2.43                     | 0.81              |
| 3:I:260:ALA:HB1  | 11:I:1464:CLA:HAA2 | 1.60                     | 0.81              |
| 8:U:5:UNK:C      | 8:U:7:UNK:N        | 2.40                     | 0.81              |
| 2:B:15:ASP:CA    | 2:B:16:PRO:N       | 2.43                     | 0.81              |
| 2:B:89:GLY:CA    | 2:B:90:PHE:N       | 2.43                     | 0.81              |
| 2:B:163:GLY:O    | 2:B:165:GLY:N      | 2.13                     | 0.81              |
| 2:B:354:LEU:HD11 | 2:B:378:LYS:CB     | 2.09                     | 0.81              |
| 4:D:86:GLY:HA2   | 4:D:166:SER:CB     | 2.10                     | 0.81              |
| 3:I:95:LEU:HD23  | 3:I:97:TRP:HZ3     | 1.45                     | 0.81              |
| 2:B:414:PRO:HB2  | 2:B:415:PRO:HD3    | 1.63                     | 0.81              |
| 2:H:15:ASP:CA    | 2:H:16:PRO:N       | 2.44                     | 0.81              |
| 1:A:34:GLY:HA2   | 1:A:37:MET:HB3     | 1.61                     | 0.80              |
| 1:A:63:ILE:HG12  | 1:A:64:ARG:N       | 1.96                     | 0.80              |
| 3:C:228:ASN:CA   | 3:C:295:THR:HG21   | 2.11                     | 0.80              |
| 4:D:126:MET:HE3  | 4:D:146:PHE:HD2    | 1.45                     | 0.80              |
| 4:D:223:PHE:CE2  | 4:D:245:SER:HB3    | 2.15                     | 0.80              |
| 2:H:118:TRP:C    | 2:H:119:ASP:CA     | 2.54                     | 0.80              |
| 2:B:306:PRO:CA   | 2:B:307:GLU:N      | 2.43                     | 0.80              |
| 2:H:330:MET:HE2  | 2:H:446:SER:CB     | 2.11                     | 0.80              |
| 1:A:39:PRO:HB2   | 11:A:1346:CLA:HAB  | 1.63                     | 0.80              |
| 2:B:229:LEU:C    | 2:B:231:MET:H      | 1.89                     | 0.80              |
| 2:H:187:PRO:CA   | 2:H:188:ASP:N      | 2.44                     | 0.80              |
| 1:A:202:VAL:O    | 1:A:206:PHE:HB2    | 1.82                     | 0.80              |
| 2:B:236:THR:HB   | 2:B:473:THR:HG23   | 1.64                     | 0.80              |
| 3:C:53:HIS:HB3   | 11:C:1470:CLA:OBD  | 1.80                     | 0.80              |
| 4:D:53:THR:HG22  | 4:D:67:TYR:CD1     | 2.16                     | 0.80              |
| 4:J:122:LEU:HD21 | 11:J:1351:CLA:C9   | 2.11                     | 0.80              |
| 1:A:217:SER:OG   | 4:D:142:ASN:HA     | 1.80                     | 0.80              |
| 3:C:185:LEU:O    | 3:C:230:LEU:HD21   | 1.82                     | 0.80              |
| 3:C:449:ARG:HG3  | 3:C:449:ARG:NH1    | 1.88                     | 0.80              |
| 6:F:19:ARG:O     | 6:F:23:VAL:HG23    | 1.80                     | 0.80              |
| 1:G:30:VAL:CA    | 1:G:31:GLY:N       | 2.45                     | 0.80              |
| 3:I:154:LYS:NZ   | 3:I:261:ARG:HD3    | 1.97                     | 0.80              |
| 10:X:334:UNK:C   | 10:X:335:UNK:O     | 2.26                     | 0.80              |
| 4:D:126:MET:HA   | 4:D:129:GLN:NE2    | 1.95                     | 0.80              |
| 1:G:141:PRO:HG2  | 3:I:446:GLY:O      | 1.81                     | 0.80              |
| 1:A:141:PRO:HG2  | 3:C:446:GLY:O      | 1.82                     | 0.80              |
| 1:A:30:VAL:CA    | 1:A:31:GLY:N       | 2.45                     | 0.79              |
| 2:B:118:TRP:C    | 2:B:119:ASP:CA     | 2.55                     | 0.79              |
| 1:G:63:ILE:HG12  | 1:G:64:ARG:N       | 1.97                     | 0.79              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:A:294:ALA:C    | 1:A:296:ASN:H      | 1.87                     | 0.79              |
| 2:B:27:THR:HG22  | 2:B:107:LEU:HD13   | 1.63                     | 0.79              |
| 1:G:39:PRO:HB2   | 11:G:1346:CLA:HAB  | 1.64                     | 0.79              |
| 1:G:84:PRO:CD    | 1:G:173:PRO:CG     | 2.55                     | 0.79              |
| 1:G:193:LEU:HB3  | 4:J:179:PHE:CD1    | 2.18                     | 0.79              |
| 4:J:103:ARG:HG2  | 4:J:106:GLN:OE1    | 1.82                     | 0.79              |
| 1:A:142:TRP:CB   | 4:D:220:ASN:OD1    | 2.31                     | 0.79              |
| 2:B:187:PRO:CA   | 2:B:188:ASP:N      | 2.46                     | 0.79              |
| 2:H:61:PHE:O     | 2:H:64:PRO:CD      | 2.29                     | 0.79              |
| 3:C:260:ALA:HB1  | 11:C:1464:CLA:HAA2 | 1.63                     | 0.79              |
| 1:G:219:VAL:HG21 | 4:J:268:HIS:CD2    | 2.16                     | 0.79              |
| 2:H:161:LEU:O    | 2:H:162:PHE:HB2    | 1.81                     | 0.79              |
| 3:C:266:TRP:HB3  | 3:C:271:TYR:OH     | 1.81                     | 0.79              |
| 1:G:222:SER:O    | 1:G:246:TYR:HA     | 1.83                     | 0.79              |
| 2:H:270:PRO:O    | 2:H:271:THR:HG23   | 1.82                     | 0.79              |
| 2:B:135:LEU:HB2  | 2:B:136:PRO:CD     | 2.11                     | 0.79              |
| 4:J:196:PHE:CE1  | 4:J:284:ILE:HB     | 2.18                     | 0.79              |
| 6:L:12:SER:O     | 6:L:14:PRO:CD      | 2.30                     | 0.79              |
| 1:A:176:ILE:HG12 | 11:A:1343:CLA:HED3 | 1.65                     | 0.79              |
| 2:B:474:LEU:HD11 | 11:B:1489:CLA:HAA2 | 1.65                     | 0.79              |
| 2:H:45:PHE:O     | 2:H:47:PRO:HD2     | 1.84                     | 0.78              |
| 4:J:74:LEU:HD23  | 4:J:175:VAL:HG11   | 1.62                     | 0.78              |
| 4:J:164:GLN:HE22 | 4:J:189:HIS:CE1    | 2.00                     | 0.78              |
| 5:K:62:SER:O     | 5:K:63:ILE:C       | 2.26                     | 0.78              |
| 1:A:107:TYR:C    | 1:A:109:GLY:H      | 1.91                     | 0.78              |
| 2:H:52:LEU:C     | 2:H:54:PRO:HD3     | 2.08                     | 0.78              |
| 4:J:86:GLY:HA2   | 4:J:166:SER:CB     | 2.12                     | 0.78              |
| 1:G:81:ALA:HB3   | 1:G:174:LEU:C      | 2.08                     | 0.78              |
| 3:C:206:PRO:CA   | 3:C:207:ARG:N      | 2.46                     | 0.78              |
| 1:G:258:LEU:HA   | 4:J:128:ARG:HH12   | 1.49                     | 0.78              |
| 4:D:69:GLU:HG2   | 5:E:55:TYR:OH      | 1.83                     | 0.78              |
| 10:X:59:UNK:O    | 10:X:60:UNK:C      | 2.31                     | 0.78              |
| 3:I:245:ILE:HD12 | 3:I:246:ALA:N      | 1.99                     | 0.78              |
| 3:C:100:GLY:O    | 3:C:101:PRO:C      | 2.23                     | 0.78              |
| 5:E:62:SER:O     | 5:E:63:ILE:C       | 2.26                     | 0.78              |
| 9:T:129:LYS:HE3  | 9:T:135:VAL:CG2    | 2.14                     | 0.78              |
| 1:A:143:ILE:HG13 | 4:D:220:ASN:ND2    | 1.96                     | 0.78              |
| 4:D:196:PHE:CE1  | 4:D:284:ILE:HB     | 2.18                     | 0.78              |
| 2:H:383:PHE:O    | 7:P:107:UNK:HA     | 1.82                     | 0.78              |
| 3:I:206:PRO:CA   | 3:I:207:ARG:N      | 2.46                     | 0.78              |
| 3:I:304:PRO:HG2  | 3:I:398:HIS:O      | 1.83                     | 0.78              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 3:I:305:THR:OG1  | 3:I:307:PRO:HD2    | 1.84                     | 0.78              |
| 1:G:161:TYR:CE2  | 1:G:186:PHE:HE1    | 2.00                     | 0.78              |
| 6:L:19:ARG:O     | 6:L:23:VAL:HG23    | 1.84                     | 0.78              |
| 3:C:261:ARG:HA   | 3:C:266:TRP:HZ2    | 1.49                     | 0.77              |
| 4:D:37:LEU:HD23  | 4:D:37:LEU:C       | 2.10                     | 0.77              |
| 1:A:297:LEU:CD2  | 3:C:428:THR:HG21   | 2.14                     | 0.77              |
| 1:A:193:LEU:HB3  | 4:D:179:PHE:CD1    | 2.19                     | 0.77              |
| 3:C:273:SER:HB2  | 3:C:445:ALA:HB2    | 1.65                     | 0.77              |
| 4:D:331:PRO:HG3  | 4:D:339:PHE:CG     | 2.19                     | 0.77              |
| 1:G:183:MET:HG2  | 11:G:1342:CLA:HBC2 | 1.65                     | 0.77              |
| 1:G:187:GLN:HB2  | 11:G:1342:CLA:HAC2 | 1.66                     | 0.77              |
| 2:B:52:LEU:C     | 2:B:54:PRO:HD3     | 2.08                     | 0.77              |
| 3:C:305:THR:OG1  | 3:C:307:PRO:HD2    | 1.84                     | 0.77              |
| 6:F:28:VAL:HB    | 6:F:29:PRO:HD3     | 1.66                     | 0.77              |
| 2:H:248:ALA:O    | 2:H:251:VAL:HG23   | 1.85                     | 0.77              |
| 1:A:248:ILE:HD12 | 4:D:235:PHE:HZ     | 1.49                     | 0.77              |
| 4:D:323:GLU:HG2  | 4:D:326:ARG:NH2    | 1.99                     | 0.77              |
| 6:L:28:VAL:HB    | 6:L:29:PRO:HD3     | 1.66                     | 0.77              |
| 4:D:122:LEU:HD21 | 11:D:1351:CLA:C9   | 2.14                     | 0.77              |
| 4:D:290:ALA:C    | 4:D:291:LEU:HD12   | 2.09                     | 0.77              |
| 2:H:474:LEU:HD11 | 11:H:1489:CLA:HAA2 | 1.67                     | 0.77              |
| 4:J:87:HIS:CE1   | 4:J:162:LEU:HA     | 2.19                     | 0.77              |
| 1:A:81:ALA:HB3   | 1:A:174:LEU:C      | 2.09                     | 0.77              |
| 3:C:167:VAL:O    | 3:C:170:ILE:HG22   | 1.85                     | 0.77              |
| 3:I:261:ARG:HA   | 3:I:266:TRP:HZ2    | 1.50                     | 0.77              |
| 1:A:330:VAL:CG1  | 4:D:347:PRO:HA     | 2.14                     | 0.77              |
| 7:P:11:UNK:HA    | 7:P:173:UNK:CB     | 2.14                     | 0.77              |
| 4:D:343:GLU:OE1  | 4:D:343:GLU:N      | 2.16                     | 0.76              |
| 1:G:242:GLU:CA   | 1:G:243:GLU:N      | 2.48                     | 0.76              |
| 4:J:267:LEU:O    | 4:J:271:MET:HG3    | 1.84                     | 0.76              |
| 4:D:83:ASN:CG    | 4:D:336:HIS:HD2    | 1.92                     | 0.76              |
| 1:A:127:MET:CE   | 1:A:151:LEU:HD22   | 2.16                     | 0.76              |
| 1:A:149:ALA:HB3  | 1:A:150:PRO:HD3    | 1.66                     | 0.76              |
| 2:B:24:LEU:HD23  | 2:B:111:ALA:N      | 2.00                     | 0.76              |
| 2:H:24:LEU:HD11  | 11:H:1497:CLA:HBC2 | 1.64                     | 0.76              |
| 2:H:236:THR:HB   | 2:H:473:THR:HG23   | 1.66                     | 0.76              |
| 4:J:83:ASN:CG    | 4:J:336:HIS:HD2    | 1.92                     | 0.76              |
| 2:B:355:PHE:O    | 2:B:370:LEU:HA     | 1.84                     | 0.76              |
| 4:D:340:VAL:O    | 4:D:342:PRO:HD2    | 1.86                     | 0.76              |
| 4:J:176:ALA:HA   | 4:J:179:PHE:HD2    | 1.49                     | 0.76              |
| 4:D:87:HIS:CE1   | 4:D:162:LEU:HA     | 2.21                     | 0.76              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:H:134:ASP:O      | 2:H:136:PRO:HD2    | 1.85                     | 0.76              |
| 4:J:53:THR:HG22    | 4:J:67:TYR:CD1     | 2.20                     | 0.76              |
| 7:O:11:UNK:HA      | 7:O:173:UNK:CB     | 2.16                     | 0.76              |
| 2:B:45:PHE:CD2     | 2:B:47:PRO:CD      | 2.65                     | 0.76              |
| 2:B:271:THR:OG1    | 2:B:274:GLN:HG3    | 1.84                     | 0.76              |
| 2:B:383:PHE:O      | 7:O:107:UNK:HA     | 1.85                     | 0.76              |
| 4:J:290:ALA:C      | 4:J:291:LEU:HD12   | 2.10                     | 0.76              |
| 1:G:62:GLY:CA      | 1:G:87:ASN:HB3     | 2.16                     | 0.76              |
| 4:J:345:VAL:O      | 4:J:346:LEU:CB     | 2.32                     | 0.76              |
| 5:K:27:ILE:HB      | 5:K:28:PRO:HD3     | 1.67                     | 0.76              |
| 6:L:10:PRO:HB2     | 6:L:19:ARG:NH1     | 2.00                     | 0.76              |
| 2:B:160:GLY:HA2    | 2:B:163:GLY:HA2    | 1.66                     | 0.76              |
| 2:B:163:GLY:O      | 2:B:164:PRO:C      | 2.25                     | 0.76              |
| 10:X:470:UNK:O     | 10:X:473:UNK:N     | 2.19                     | 0.76              |
| 2:B:141:ILE:HB     | 2:B:217:ILE:HD12   | 1.66                     | 0.76              |
| 11:B:1496:CLA:H171 | 11:B:1497:CLA:HMD2 | 1.67                     | 0.75              |
| 1:G:206:PHE:CE1    | 11:G:1342:CLA:HMB1 | 2.21                     | 0.75              |
| 1:G:290:ILE:HD11   | 11:G:1342:CLA:OBD  | 1.85                     | 0.75              |
| 2:H:233:ASN:CG     | 2:H:233:ASN:O      | 2.28                     | 0.75              |
| 8:U:59:UNK:O       | 8:U:61:UNK:N       | 2.20                     | 0.75              |
| 1:A:64:ARG:O       | 1:A:66:PRO:HD3     | 1.86                     | 0.75              |
| 2:B:31:ALA:HA      | 2:B:34:ALA:HB3     | 1.66                     | 0.75              |
| 1:G:143:ILE:HD11   | 4:J:217:THR:HA     | 1.68                     | 0.75              |
| 2:H:52:LEU:HD22    | 2:H:337:ALA:HB1    | 1.68                     | 0.75              |
| 2:H:246:PHE:HE1    | 2:H:463:PHE:HB2    | 1.51                     | 0.75              |
| 3:I:169:GLY:HA2    | 3:I:244:CYS:SG     | 2.26                     | 0.75              |
| 4:J:88:SER:C       | 4:J:90:LEU:H       | 1.91                     | 0.75              |
| 1:A:62:GLY:CA      | 1:A:87:ASN:HB3     | 2.16                     | 0.75              |
| 4:J:37:LEU:C       | 4:J:37:LEU:HD23    | 2.11                     | 0.75              |
| 6:L:37:ILE:HA      | 6:L:40:MET:CE      | 2.16                     | 0.75              |
| 8:S:59:UNK:O       | 8:S:61:UNK:N       | 2.18                     | 0.75              |
| 4:D:340:VAL:O      | 4:D:342:PRO:CD     | 2.34                     | 0.75              |
| 1:G:330:VAL:CG1    | 4:J:347:PRO:HA     | 2.16                     | 0.75              |
| 2:H:138:MET:SD     | 11:H:1496:CLA:HBC2 | 2.26                     | 0.75              |
| 2:B:233:ASN:CG     | 2:B:233:ASN:O      | 2.30                     | 0.75              |
| 2:B:263:THR:N      | 2:B:264:PRO:HD3    | 2.02                     | 0.75              |
| 3:I:185:LEU:O      | 3:I:230:LEU:HD21   | 1.86                     | 0.75              |
| 4:J:38:PHE:O       | 4:J:39:PRO:C       | 2.27                     | 0.75              |
| 5:K:13:ILE:HG22    | 5:K:19:TYR:CD2     | 2.21                     | 0.75              |
| 2:B:248:ALA:O      | 2:B:251:VAL:HG23   | 1.86                     | 0.75              |
| 2:B:270:PRO:O      | 2:B:271:THR:HG23   | 1.86                     | 0.75              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:C:35:TRP:CE2     | 3:C:36:TRP:HD1     | 2.05                     | 0.75              |
| 3:C:225:VAL:HG13   | 3:C:289:PHE:HA     | 1.67                     | 0.75              |
| 2:H:229:LEU:O      | 2:H:231:MET:N      | 2.20                     | 0.75              |
| 7:O:83:UNK:HA      | 7:O:90:UNK:CB      | 2.16                     | 0.75              |
| 1:A:143:ILE:N      | 4:D:220:ASN:ND2    | 2.35                     | 0.75              |
| 4:D:167:TRP:O      | 4:D:168:PHE:HB2    | 1.86                     | 0.75              |
| 5:E:13:ILE:HG22    | 5:E:19:TYR:CD2     | 2.21                     | 0.75              |
| 5:E:62:SER:O       | 5:E:64:PRO:N       | 2.20                     | 0.75              |
| 2:H:31:ALA:H       | 11:H:1486:CLA:CBC  | 1.99                     | 0.75              |
| 1:A:222:SER:O      | 1:A:246:TYR:HA     | 1.86                     | 0.74              |
| 3:C:315:MET:HG3    | 3:C:365:TRP:HZ3    | 1.52                     | 0.74              |
| 2:H:398:THR:C      | 2:H:400:SER:H      | 1.93                     | 0.74              |
| 11:H:1496:CLA:H171 | 11:H:1497:CLA:HMD2 | 1.67                     | 0.74              |
| 4:J:69:GLU:HG2     | 5:K:55:TYR:OH      | 1.86                     | 0.74              |
| 8:S:5:UNK:C        | 8:S:7:UNK:N        | 2.42                     | 0.74              |
| 2:B:268:PHE:HB2    | 2:B:448:ARG:HH11   | 1.52                     | 0.74              |
| 3:C:189:TRP:HE1    | 3:C:295:THR:HG22   | 1.50                     | 0.74              |
| 4:D:61:HIS:HB3     | 4:D:63:LEU:HD13    | 1.68                     | 0.74              |
| 2:B:246:PHE:HE1    | 2:B:463:PHE:HB2    | 1.53                     | 0.74              |
| 4:D:74:LEU:HD23    | 4:D:175:VAL:HG11   | 1.67                     | 0.74              |
| 1:G:84:PRO:HG2     | 1:G:173:PRO:CD     | 2.16                     | 0.74              |
| 1:G:142:TRP:CB     | 4:J:220:ASN:OD1    | 2.32                     | 0.74              |
| 2:B:271:THR:HG1    | 2:B:274:GLN:HG3    | 1.50                     | 0.74              |
| 3:I:178:LYS:C      | 3:I:178:LYS:HD3    | 2.13                     | 0.74              |
| 9:V:129:LYS:HE3    | 9:V:135:VAL:CG2    | 2.17                     | 0.74              |
| 1:A:258:LEU:HD12   | 4:D:128:ARG:NH1    | 2.02                     | 0.74              |
| 2:B:79:SER:C       | 2:B:80:ILE:HG13    | 2.13                     | 0.74              |
| 2:B:138:MET:SD     | 11:B:1496:CLA:HBC2 | 2.27                     | 0.74              |
| 4:D:308:ASP:HB3    | 4:D:311:PHE:HB2    | 1.68                     | 0.74              |
| 1:G:107:TYR:C      | 1:G:109:GLY:H      | 1.94                     | 0.74              |
| 2:B:257:TRP:HB2    | 2:B:452:THR:HG21   | 1.69                     | 0.74              |
| 4:D:329:MET:O      | 4:D:330:ALA:O      | 2.06                     | 0.74              |
| 1:A:247:ASN:O      | 1:A:247:ASN:ND2    | 2.20                     | 0.74              |
| 4:D:88:SER:C       | 4:D:90:LEU:H       | 1.94                     | 0.74              |
| 2:H:263:THR:N      | 2:H:264:PRO:HD2    | 2.03                     | 0.74              |
| 3:C:304:PRO:HG2    | 3:C:398:HIS:O      | 1.87                     | 0.74              |
| 1:G:258:LEU:HD12   | 4:J:128:ARG:NH1    | 2.03                     | 0.74              |
| 3:I:116:VAL:HG23   | 3:I:117:VAL:N      | 2.01                     | 0.74              |
| 3:C:78:GLU:OE2     | 3:C:104:GLU:HA     | 1.88                     | 0.74              |
| 3:C:278:ALA:O      | 3:C:282:MET:HG3    | 1.87                     | 0.74              |
| 1:G:310:LYS:NZ     | 5:K:58:GLN:HG2     | 2.03                     | 0.74              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 2:H:62:VAL:HG12  | 2:H:66:MET:HE2     | 1.69                     | 0.74              |
| 10:Y:507:UNK:O   | 10:Y:509:UNK:N     | 2.21                     | 0.74              |
| 1:A:309:ALA:C    | 9:V:2:GLU:HA       | 2.11                     | 0.73              |
| 2:B:134:ASP:O    | 2:B:136:PRO:HD2    | 1.88                     | 0.73              |
| 3:C:370:ARG:HE   | 3:C:371:GLY:H      | 1.34                     | 0.73              |
| 1:A:63:ILE:HG13  | 3:C:335:THR:HG23   | 1.68                     | 0.73              |
| 1:A:258:LEU:HD12 | 4:D:128:ARG:CZ     | 2.18                     | 0.73              |
| 1:A:309:ALA:O    | 9:V:2:GLU:CG       | 2.36                     | 0.73              |
| 2:B:229:LEU:O    | 2:B:231:MET:N      | 2.21                     | 0.73              |
| 4:D:209:LEU:HD23 | 4:D:209:LEU:C      | 2.12                     | 0.73              |
| 1:A:62:GLY:HA2   | 1:A:87:ASN:HB3     | 1.70                     | 0.73              |
| 1:G:206:PHE:HE1  | 11:G:1342:CLA:HMB1 | 1.53                     | 0.73              |
| 1:G:306:VAL:HG12 | 1:G:313:VAL:HG22   | 1.69                     | 0.73              |
| 4:J:308:ASP:HB3  | 4:J:311:PHE:HB2    | 1.69                     | 0.73              |
| 2:B:167:TRP:CG   | 2:B:267:LEU:HD11   | 2.23                     | 0.73              |
| 3:C:120:ILE:O    | 3:C:122:SER:N      | 2.21                     | 0.73              |
| 1:G:149:ALA:HB3  | 1:G:150:PRO:HD3    | 1.71                     | 0.73              |
| 2:H:330:MET:O    | 2:H:331:ASN:CG     | 2.32                     | 0.73              |
| 4:J:196:PHE:HE1  | 4:J:284:ILE:HB     | 1.52                     | 0.73              |
| 4:J:292:ASN:O    | 4:J:294:ARG:HG2    | 1.88                     | 0.73              |
| 1:A:309:ALA:O    | 9:V:2:GLU:HG2      | 1.88                     | 0.73              |
| 2:B:24:LEU:HD11  | 11:B:1497:CLA:HBC2 | 1.69                     | 0.73              |
| 1:G:62:GLY:HA2   | 1:G:87:ASN:HB3     | 1.69                     | 0.73              |
| 3:I:315:MET:HG3  | 3:I:365:TRP:HZ3    | 1.54                     | 0.73              |
| 4:J:15:PHE:O     | 4:J:18:LEU:N       | 2.21                     | 0.73              |
| 1:A:332:HIS:CD2  | 1:A:333:GLU:H      | 2.06                     | 0.73              |
| 1:G:258:LEU:HD12 | 4:J:128:ARG:CZ     | 2.17                     | 0.73              |
| 3:I:113:VAL:O    | 3:I:117:VAL:HG23   | 1.89                     | 0.73              |
| 6:F:43:ILE:CG2   | 6:F:45:ARG:O       | 2.36                     | 0.73              |
| 2:H:347:ARG:HB2  | 2:H:398:THR:CB     | 2.19                     | 0.73              |
| 2:B:234:ILE:O    | 2:B:235:GLU:C      | 2.30                     | 0.73              |
| 1:G:202:VAL:O    | 1:G:206:PHE:HB2    | 1.89                     | 0.73              |
| 1:G:248:ILE:HD12 | 4:J:235:PHE:CZ     | 2.24                     | 0.73              |
| 3:I:445:ALA:HB1  | 11:I:1463:CLA:HED1 | 1.71                     | 0.73              |
| 4:J:340:VAL:O    | 4:J:342:PRO:HD3    | 1.87                     | 0.73              |
| 9:V:133:GLY:O    | 9:V:137:TYR:CB     | 2.37                     | 0.73              |
| 1:G:222:SER:O    | 1:G:246:TYR:CA     | 2.37                     | 0.73              |
| 1:G:219:VAL:HG11 | 4:J:268:HIS:CG     | 2.24                     | 0.72              |
| 2:H:234:ILE:O    | 2:H:235:GLU:C      | 2.32                     | 0.72              |
| 2:H:247:PHE:O    | 2:H:251:VAL:HG22   | 1.89                     | 0.72              |
| 3:C:423:ARG:HG3  | 3:C:423:ARG:O      | 1.89                     | 0.72              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:J:171:PRO:CD    | 4:J:181:PHE:CD2    | 2.67                     | 0.72              |
| 4:J:343:GLU:OE2   | 9:T:134:LYS:NZ     | 2.22                     | 0.72              |
| 3:C:187:ASP:CB    | 3:C:230:LEU:HD23   | 2.19                     | 0.72              |
| 1:G:64:ARG:O      | 1:G:66:PRO:HD3     | 1.89                     | 0.72              |
| 7:O:42:UNK:CB     | 7:O:53:UNK:HA      | 2.18                     | 0.72              |
| 2:H:263:THR:N     | 2:H:264:PRO:CD     | 2.52                     | 0.72              |
| 3:C:89:ILE:HB     | 3:C:90:PRO:HD3     | 1.69                     | 0.72              |
| 3:C:178:LYS:HD3   | 3:C:178:LYS:C      | 2.14                     | 0.72              |
| 2:H:395:GLN:CB    | 2:H:397:VAL:H      | 2.02                     | 0.72              |
| 3:I:315:MET:O     | 3:I:319:ILE:HG13   | 1.88                     | 0.72              |
| 7:O:68:UNK:CA     | 7:O:69:UNK:H       | 2.03                     | 0.72              |
| 7:P:83:UNK:HA     | 7:P:90:UNK:CB      | 2.20                     | 0.72              |
| 3:C:287:THR:HG22  | 3:C:430:HIS:CB     | 2.19                     | 0.72              |
| 1:G:38:ILE:HB     | 1:G:39:PRO:HD3     | 1.70                     | 0.72              |
| 2:H:172:TYR:HA    | 2:H:280:PHE:HE1    | 1.55                     | 0.72              |
| 3:I:287:THR:HG22  | 3:I:430:HIS:CB     | 2.20                     | 0.72              |
| 2:B:31:ALA:HB2    | 11:B:1486:CLA:HBC3 | 1.70                     | 0.72              |
| 2:B:330:MET:HE2   | 2:B:446:SER:CB     | 2.15                     | 0.72              |
| 1:G:214:MET:HE1   | 12:J:1352:PHO:HED1 | 1.71                     | 0.72              |
| 2:B:172:TYR:HA    | 2:B:280:PHE:HE1    | 1.55                     | 0.72              |
| 3:C:95:LEU:HD23   | 3:C:97:TRP:HZ3     | 1.55                     | 0.72              |
| 2:H:257:TRP:HB2   | 2:H:452:THR:HG21   | 1.71                     | 0.72              |
| 3:I:154:LYS:HZ1   | 3:I:261:ARG:HD3    | 1.54                     | 0.72              |
| 3:C:154:LYS:HZ1   | 3:C:261:ARG:HD3    | 1.54                     | 0.72              |
| 4:D:145:ALA:HA    | 4:D:276:VAL:HG22   | 1.70                     | 0.72              |
| 11:G:1344:CLA:HAB | 11:J:1351:CLA:H62  | 1.70                     | 0.72              |
| 2:H:349:LYS:HD2   | 2:H:394:GLN:HA     | 1.71                     | 0.72              |
| 1:A:258:LEU:HA    | 4:D:128:ARG:HH12   | 1.54                     | 0.72              |
| 2:B:61:PHE:O      | 2:B:64:PRO:CD      | 2.33                     | 0.72              |
| 1:G:94:TYR:OH     | 1:G:108:ASN:ND2    | 2.22                     | 0.72              |
| 1:G:129:ARG:NH2   | 4:J:256:ILE:HG23   | 2.04                     | 0.72              |
| 3:I:102:GLY:H     | 3:I:193:GLY:CA     | 2.03                     | 0.72              |
| 4:J:152:VAL:HG13  | 11:J:1351:CLA:HED3 | 1.72                     | 0.72              |
| 10:Y:509:UNK:O    | 10:Y:510:UNK:C     | 2.35                     | 0.72              |
| 3:C:169:GLY:HA2   | 3:C:244:CYS:SG     | 2.29                     | 0.71              |
| 4:D:331:PRO:HG3   | 4:D:339:PHE:HB2    | 1.72                     | 0.71              |
| 3:I:167:VAL:O     | 3:I:170:ILE:HG22   | 1.90                     | 0.71              |
| 4:J:329:MET:O     | 4:J:330:ALA:O      | 2.08                     | 0.71              |
| 1:A:112:TYR:CZ    | 1:A:116:ILE:HD11   | 2.25                     | 0.71              |
| 1:G:247:ASN:ND2   | 1:G:247:ASN:O      | 2.22                     | 0.71              |
| 10:X:177:UNK:O    | 10:X:178:UNK:C     | 2.38                     | 0.71              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:A:143:ILE:HD11 | 4:D:217:THR:HA     | 1.72                     | 0.71              |
| 3:C:354:GLU:C    | 3:C:356:MET:H      | 1.97                     | 0.71              |
| 1:A:127:MET:HE2  | 1:A:151:LEU:CD2    | 2.15                     | 0.71              |
| 1:A:133:LEU:HA   | 1:A:136:ARG:HB2    | 1.70                     | 0.71              |
| 2:H:61:PHE:O     | 2:H:62:VAL:C       | 2.33                     | 0.71              |
| 4:J:209:LEU:C    | 4:J:209:LEU:HD23   | 2.14                     | 0.71              |
| 1:A:143:ILE:H    | 4:D:220:ASN:ND2    | 1.89                     | 0.71              |
| 3:C:113:VAL:O    | 3:C:117:VAL:HG23   | 1.90                     | 0.71              |
| 5:E:26:THR:O     | 5:E:29:ALA:HB3     | 1.90                     | 0.71              |
| 1:G:297:LEU:CD2  | 3:I:428:THR:HG21   | 2.21                     | 0.71              |
| 3:I:423:ARG:O    | 3:I:423:ARG:HG3    | 1.90                     | 0.71              |
| 5:K:10:PHE:HE2   | 6:L:19:ARG:NE      | 1.88                     | 0.71              |
| 4:D:38:PHE:O     | 4:D:39:PRO:C       | 2.32                     | 0.71              |
| 2:H:106:LEU:HB3  | 11:H:1496:CLA:H121 | 1.72                     | 0.71              |
| 3:I:304:PRO:O    | 3:I:305:THR:HG23   | 1.90                     | 0.71              |
| 1:A:129:ARG:NH2  | 4:D:256:ILE:HG23   | 2.05                     | 0.71              |
| 4:D:196:PHE:HE1  | 4:D:284:ILE:HB     | 1.53                     | 0.71              |
| 5:E:56:TYR:O     | 5:E:57:ALA:HB2     | 1.90                     | 0.71              |
| 1:G:63:ILE:O     | 1:G:64:ARG:HD2     | 1.89                     | 0.71              |
| 2:B:31:ALA:H     | 11:B:1486:CLA:HBC3 | 1.56                     | 0.71              |
| 3:C:116:VAL:HG23 | 3:C:117:VAL:N      | 2.04                     | 0.71              |
| 3:C:154:LYS:NZ   | 3:C:261:ARG:HD3    | 2.05                     | 0.71              |
| 2:H:425:ILE:HG23 | 2:H:425:ILE:O      | 1.90                     | 0.71              |
| 4:D:176:ALA:HA   | 4:D:179:PHE:HD2    | 1.55                     | 0.71              |
| 1:G:295:PHE:O    | 3:I:291:TRP:CZ3    | 2.44                     | 0.71              |
| 6:L:12:SER:C     | 6:L:14:PRO:HD2     | 2.14                     | 0.71              |
| 3:I:50:LEU:HD23  | 3:I:132:HIS:CD2    | 2.26                     | 0.71              |
| 7:P:42:UNK:CB    | 7:P:53:UNK:HA      | 2.21                     | 0.71              |
| 1:G:310:LYS:CA   | 9:T:2:GLU:HA       | 2.20                     | 0.70              |
| 2:H:391:SER:O    | 2:H:392:PHE:CB     | 2.38                     | 0.70              |
| 4:J:72:ASN:O     | 4:J:74:LEU:N       | 2.23                     | 0.70              |
| 4:J:253:TRP:O    | 4:J:256:ILE:N      | 2.22                     | 0.70              |
| 2:B:247:PHE:O    | 2:B:251:VAL:HG22   | 1.91                     | 0.70              |
| 5:E:27:ILE:HB    | 5:E:28:PRO:HD3     | 1.72                     | 0.70              |
| 1:G:219:VAL:HG21 | 4:J:268:HIS:HD2    | 1.53                     | 0.70              |
| 3:I:370:ARG:HE   | 3:I:371:GLY:H      | 1.37                     | 0.70              |
| 4:D:15:PHE:O     | 4:D:18:LEU:N       | 2.25                     | 0.70              |
| 1:G:310:LYS:CB   | 9:T:2:GLU:N        | 2.52                     | 0.70              |
| 3:I:225:VAL:HG13 | 3:I:289:PHE:HA     | 1.73                     | 0.70              |
| 3:I:278:ALA:O    | 3:I:282:MET:HG3    | 1.91                     | 0.70              |
| 4:J:235:PHE:CE1  | 4:J:237:PRO:HB3    | 2.26                     | 0.70              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 4:D:113:PHE:CA   | 11:D:1353:CLA:HED1 | 2.19                     | 0.70              |
| 4:D:148:ALA:HA   | 4:D:280:TRP:NE1    | 2.06                     | 0.70              |
| 5:E:10:PHE:HE2   | 6:F:19:ARG:NE      | 1.89                     | 0.70              |
| 2:H:27:THR:HG22  | 2:H:107:LEU:HD13   | 1.74                     | 0.70              |
| 3:I:189:TRP:HE1  | 3:I:295:THR:HG22   | 1.55                     | 0.70              |
| 1:A:84:PRO:HD3   | 1:A:173:PRO:HB3    | 1.72                     | 0.70              |
| 1:A:142:TRP:HB3  | 4:D:220:ASN:CG     | 2.16                     | 0.70              |
| 1:A:219:VAL:HG21 | 4:D:268:HIS:CD2    | 2.26                     | 0.70              |
| 2:B:45:PHE:O     | 2:B:47:PRO:HD2     | 1.91                     | 0.70              |
| 3:C:261:ARG:HA   | 3:C:266:TRP:CZ2    | 2.26                     | 0.70              |
| 1:G:142:TRP:HB3  | 4:J:220:ASN:CG     | 2.17                     | 0.70              |
| 9:V:55:ARG:HH21  | 9:V:128:ASP:HA     | 1.57                     | 0.70              |
| 10:Y:59:UNK:O    | 10:Y:60:UNK:C      | 2.38                     | 0.70              |
| 1:A:187:GLN:HB2  | 11:A:1342:CLA:HAC2 | 1.73                     | 0.70              |
| 1:G:307:ILE:O    | 1:G:309:ALA:N      | 2.24                     | 0.70              |
| 2:H:468:TRP:O    | 2:H:471:ALA:HB3    | 1.92                     | 0.70              |
| 7:P:68:UNK:CA    | 7:P:69:UNK:H       | 2.04                     | 0.70              |
| 3:C:45:LEU:O     | 3:C:46:SER:C       | 2.35                     | 0.70              |
| 1:G:60:ILE:HD12  | 1:G:83:VAL:CG1     | 2.22                     | 0.70              |
| 4:J:111:TRP:O    | 4:J:114:ILE:N      | 2.25                     | 0.70              |
| 4:J:291:LEU:HD12 | 4:J:291:LEU:N      | 2.06                     | 0.70              |
| 2:B:195:PRO:O    | 2:B:196:GLY:C      | 2.35                     | 0.70              |
| 3:I:178:LYS:HA   | 3:I:182:PHE:HB2    | 1.74                     | 0.70              |
| 2:B:263:THR:HG22 | 2:B:448:ARG:CZ     | 2.22                     | 0.69              |
| 4:J:188:PHE:CZ   | 4:J:326:ARG:HG2    | 2.27                     | 0.69              |
| 2:B:330:MET:O    | 2:B:331:ASN:CG     | 2.36                     | 0.69              |
| 1:G:314:ILE:HG23 | 4:J:58:TRP:CZ3     | 2.27                     | 0.69              |
| 3:I:187:ASP:O    | 3:I:187:ASP:OD1    | 2.10                     | 0.69              |
| 5:K:58:GLN:HE22  | 9:T:4:THR:HG23     | 1.57                     | 0.69              |
| 1:A:60:ILE:HB    | 1:A:83:VAL:CG1     | 2.22                     | 0.69              |
| 3:I:390:ARG:HD2  | 9:T:100:ILE:HD12   | 1.73                     | 0.69              |
| 10:Y:71:UNK:C    | 10:Y:73:UNK:N      | 2.54                     | 0.69              |
| 2:B:360:PRO:HB2  | 2:B:363:PHE:HD2    | 1.57                     | 0.69              |
| 1:G:70:SER:O     | 1:G:75:ASN:HB2     | 1.93                     | 0.69              |
| 4:J:145:ALA:HA   | 4:J:276:VAL:HG22   | 1.74                     | 0.69              |
| 9:T:93:PRO:HA    | 9:T:101:PHE:CD2    | 2.27                     | 0.69              |
| 3:C:189:TRP:CH2  | 3:C:363:GLY:HA2    | 2.27                     | 0.69              |
| 1:A:129:ARG:HH22 | 4:D:256:ILE:HA     | 1.58                     | 0.69              |
| 1:G:129:ARG:NH2  | 4:J:256:ILE:HA     | 2.06                     | 0.69              |
| 3:C:120:ILE:C    | 3:C:122:SER:H      | 2.01                     | 0.69              |
| 1:G:307:ILE:C    | 1:G:309:ALA:H      | 2.01                     | 0.69              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 4:J:91:LEU:HA    | 11:J:1353:CLA:O1D  | 1.93                     | 0.69              |
| 7:P:142:UNK:HA   | 7:P:149:UNK:CB     | 2.22                     | 0.69              |
| 3:C:318:LEU:O    | 3:C:318:LEU:HD12   | 1.92                     | 0.69              |
| 4:D:272:LEU:C    | 4:D:272:LEU:HD23   | 2.17                     | 0.69              |
| 1:G:214:MET:O    | 1:G:215:HIS:C      | 2.34                     | 0.69              |
| 1:G:330:VAL:HG11 | 4:J:328:TRP:CZ2    | 2.28                     | 0.69              |
| 2:H:360:PRO:HB2  | 2:H:363:PHE:HD2    | 1.57                     | 0.69              |
| 1:A:38:ILE:HB    | 1:A:39:PRO:HD3     | 1.74                     | 0.69              |
| 2:B:221:PRO:HB3  | 11:B:1490:CLA:HED3 | 1.74                     | 0.69              |
| 2:B:233:ASN:O    | 2:B:235:GLU:N      | 2.26                     | 0.69              |
| 3:C:280:SER:HB2  | 3:C:434:ALA:O      | 1.92                     | 0.69              |
| 1:G:307:ILE:C    | 1:G:309:ALA:N      | 2.46                     | 0.69              |
| 2:H:94:GLU:HG3   | 2:H:95:GLY:N       | 2.07                     | 0.69              |
| 2:H:468:TRP:CD1  | 4:J:144:ILE:HD11   | 2.27                     | 0.69              |
| 3:I:77:PRO:C     | 3:I:79:LYS:H       | 2.01                     | 0.69              |
| 1:A:129:ARG:NH2  | 4:D:256:ILE:HA     | 2.07                     | 0.69              |
| 2:B:332:LYS:O    | 2:B:439:SER:HA     | 1.93                     | 0.69              |
| 2:B:359:MET:HE2  | 2:B:366:PHE:HB2    | 1.74                     | 0.69              |
| 2:B:398:THR:C    | 2:B:400:SER:H      | 1.98                     | 0.69              |
| 3:C:77:PRO:C     | 3:C:79:LYS:H       | 1.99                     | 0.69              |
| 4:D:39:PRO:O     | 4:D:43:LEU:HB2     | 1.93                     | 0.69              |
| 3:I:376:ASP:CB   | 3:I:379:LYS:HG3    | 2.23                     | 0.69              |
| 4:J:235:PHE:O    | 4:J:235:PHE:CD1    | 2.46                     | 0.69              |
| 1:A:141:PRO:O    | 1:A:143:ILE:N      | 2.26                     | 0.68              |
| 1:A:310:LYS:CB   | 9:V:2:GLU:N        | 2.53                     | 0.68              |
| 2:B:468:TRP:O    | 2:B:471:ALA:HB3    | 1.91                     | 0.68              |
| 3:C:178:LYS:HA   | 3:C:182:PHE:HB2    | 1.75                     | 0.68              |
| 4:J:61:HIS:HB3   | 4:J:63:LEU:CD1     | 2.22                     | 0.68              |
| 1:A:113:GLN:O    | 1:A:117:PHE:HD2    | 1.75                     | 0.68              |
| 9:V:93:PRO:HA    | 9:V:101:PHE:CD2    | 2.29                     | 0.68              |
| 3:C:176:VAL:O    | 3:C:180:MET:HG2    | 1.93                     | 0.68              |
| 4:D:169:PHE:O    | 4:D:181:PHE:HE2    | 1.76                     | 0.68              |
| 1:A:307:ILE:C    | 1:A:309:ALA:H      | 2.01                     | 0.68              |
| 1:A:328:MET:HE2  | 4:D:325:ILE:HD11   | 1.75                     | 0.68              |
| 3:C:376:ASP:CB   | 3:C:379:LYS:HG3    | 2.22                     | 0.68              |
| 3:C:377:LEU:O    | 3:C:381:LYS:HD3    | 1.93                     | 0.68              |
| 9:T:78:ASN:OD1   | 9:T:96:ARG:NH2     | 2.26                     | 0.68              |
| 2:B:66:MET:O     | 2:B:71:VAL:HB      | 1.93                     | 0.68              |
| 4:D:343:GLU:OE2  | 9:V:134:LYS:NZ     | 2.26                     | 0.68              |
| 1:G:129:ARG:HH22 | 4:J:256:ILE:HA     | 1.57                     | 0.68              |
| 2:H:256:MET:SD   | 2:H:263:THR:HG23   | 2.34                     | 0.68              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:J:88:SER:C      | 4:J:90:LEU:N       | 2.50                     | 0.68              |
| 4:J:176:ALA:HA    | 4:J:179:PHE:CD2    | 2.27                     | 0.68              |
| 2:B:349:LYS:HD2   | 2:B:394:GLN:HA     | 1.75                     | 0.68              |
| 2:B:468:TRP:CD1   | 4:D:144:ILE:HD11   | 2.29                     | 0.68              |
| 3:C:35:TRP:C      | 3:C:37:ALA:H       | 2.01                     | 0.68              |
| 1:G:133:LEU:HA    | 1:G:136:ARG:HB2    | 1.76                     | 0.68              |
| 3:I:35:TRP:CE2    | 3:I:36:TRP:HD1     | 2.11                     | 0.68              |
| 3:I:37:ALA:HA     | 11:I:1466:CLA:CBA  | 2.21                     | 0.68              |
| 3:I:128:GLY:HA3   | 11:I:1471:CLA:CMC  | 2.24                     | 0.68              |
| 11:A:1344:CLA:HAB | 11:D:1351:CLA:H62  | 1.74                     | 0.68              |
| 1:G:143:ILE:N     | 4:J:220:ASN:ND2    | 2.41                     | 0.68              |
| 2:H:61:PHE:O      | 2:H:63:LEU:N       | 2.26                     | 0.68              |
| 3:I:225:VAL:O     | 3:I:225:VAL:HG12   | 1.94                     | 0.68              |
| 4:J:79:SER:HA     | 4:J:172:SER:HB3    | 1.76                     | 0.68              |
| 7:O:142:UNK:HA    | 7:O:149:UNK:CB     | 2.22                     | 0.68              |
| 1:A:121:LEU:HD23  | 1:A:121:LEU:O      | 1.94                     | 0.68              |
| 1:A:181:ASN:O     | 1:A:182:PHE:C      | 2.36                     | 0.68              |
| 2:B:52:LEU:HD22   | 2:B:337:ALA:HB1    | 1.75                     | 0.68              |
| 1:G:136:ARG:HE    | 10:Y:29:UNK:CB     | 2.07                     | 0.68              |
| 2:H:229:LEU:C     | 2:H:231:MET:N      | 2.49                     | 0.68              |
| 3:I:176:VAL:CG2   | 3:I:180:MET:HE3    | 2.24                     | 0.68              |
| 3:I:261:ARG:HA    | 3:I:266:TRP:CZ2    | 2.28                     | 0.68              |
| 3:C:187:ASP:OD1   | 3:C:187:ASP:O      | 2.11                     | 0.68              |
| 4:D:345:VAL:O     | 4:D:345:VAL:CG1    | 2.36                     | 0.68              |
| 5:K:13:ILE:HG22   | 5:K:19:TYR:HD2     | 1.59                     | 0.68              |
| 3:C:170:ILE:HG23  | 3:C:171:GLY:N      | 2.08                     | 0.68              |
| 1:G:181:ASN:O     | 1:G:182:PHE:C      | 2.37                     | 0.68              |
| 4:J:15:PHE:O      | 4:J:16:ASP:C       | 2.36                     | 0.68              |
| 1:A:175:GLY:N     | 12:A:1345:PHO:H192 | 2.08                     | 0.67              |
| 1:A:330:VAL:HG11  | 4:D:328:TRP:CZ2    | 2.29                     | 0.67              |
| 1:G:96:ILE:HG22   | 11:G:1346:CLA:OBD  | 1.94                     | 0.67              |
| 3:I:354:GLU:C     | 3:I:356:MET:H      | 2.02                     | 0.67              |
| 1:A:94:TYR:OH     | 1:A:108:ASN:ND2    | 2.27                     | 0.67              |
| 1:A:133:LEU:HD12  | 4:D:256:ILE:CG1    | 2.23                     | 0.67              |
| 2:B:64:PRO:O      | 2:B:67:ALA:HB3     | 1.95                     | 0.67              |
| 3:C:43:ILE:HG22   | 11:C:1467:CLA:HMC3 | 1.76                     | 0.67              |
| 3:C:225:VAL:O     | 3:C:225:VAL:HG12   | 1.95                     | 0.67              |
| 3:I:45:LEU:O      | 3:I:46:SER:C       | 2.37                     | 0.67              |
| 6:L:10:PRO:CB     | 6:L:19:ARG:HH11    | 2.07                     | 0.67              |
| 1:A:127:MET:CE    | 1:A:151:LEU:CD2    | 2.72                     | 0.67              |
| 2:B:93:PHE:O      | 2:B:94:GLU:C       | 2.37                     | 0.67              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:C:240:ILE:HD12  | 11:C:1465:CLA:H91  | 1.76                     | 0.67              |
| 5:E:41:GLY:O      | 5:E:44:TYR:N       | 2.27                     | 0.67              |
| 2:H:318:ASN:O     | 2:H:320:ALA:N      | 2.27                     | 0.67              |
| 3:I:260:ALA:O     | 3:I:264:PHE:HD2    | 1.77                     | 0.67              |
| 1:A:222:SER:O     | 1:A:246:TYR:CA     | 2.41                     | 0.67              |
| 4:D:291:LEU:HD12  | 4:D:291:LEU:N      | 2.09                     | 0.67              |
| 3:I:54:VAL:O      | 3:I:57:ALA:HB3     | 1.94                     | 0.67              |
| 2:B:201:HIS:HD2   | 2:B:202:HIS:ND1    | 1.92                     | 0.67              |
| 3:C:186:TYR:HE2   | 3:C:188:THR:HG23   | 1.60                     | 0.67              |
| 1:G:60:ILE:HD12   | 1:G:83:VAL:HG13    | 1.76                     | 0.67              |
| 1:G:315:ASN:O     | 1:G:316:THR:OG1    | 2.13                     | 0.67              |
| 2:H:214:LEU:O     | 2:H:217:ILE:HG22   | 1.95                     | 0.67              |
| 4:J:289:LEU:CD2   | 4:J:294:ARG:HB3    | 2.24                     | 0.67              |
| 4:J:331:PRO:CG    | 4:J:339:PHE:CG     | 2.74                     | 0.67              |
| 8:S:59:UNK:O      | 8:S:60:UNK:C       | 2.42                     | 0.67              |
| 10:X:71:UNK:C     | 10:X:73:UNK:N      | 2.57                     | 0.67              |
| 1:A:294:ALA:C     | 1:A:296:ASN:N      | 2.51                     | 0.67              |
| 1:A:331:MET:CE    | 4:D:346:LEU:O      | 2.42                     | 0.67              |
| 4:D:329:MET:O     | 4:D:330:ALA:C      | 2.36                     | 0.67              |
| 1:G:332:HIS:CD2   | 1:G:333:GLU:H      | 2.12                     | 0.67              |
| 2:H:138:MET:C     | 2:H:140:GLY:H      | 2.02                     | 0.67              |
| 2:H:195:PRO:O     | 2:H:196:GLY:C      | 2.37                     | 0.67              |
| 1:A:219:VAL:HG11  | 4:D:268:HIS:CG     | 2.29                     | 0.67              |
| 1:A:328:MET:HE2   | 4:D:325:ILE:CD1    | 2.24                     | 0.67              |
| 2:B:347:ARG:HB2   | 2:B:398:THR:CB     | 2.24                     | 0.67              |
| 4:J:126:MET:O     | 4:J:129:GLN:CG     | 2.37                     | 0.67              |
| 5:K:58:GLN:CD     | 9:T:2:GLU:N        | 2.53                     | 0.67              |
| 1:A:297:LEU:HD23  | 3:C:428:THR:HG21   | 1.75                     | 0.67              |
| 11:B:1495:CLA:HBD | 11:B:1495:CLA:HBA1 | 1.76                     | 0.67              |
| 3:C:37:ALA:HA     | 11:C:1466:CLA:CBA  | 2.23                     | 0.67              |
| 1:G:99:ALA:CB     | 1:G:104:GLU:OE1    | 2.43                     | 0.67              |
| 1:G:214:MET:HA    | 1:G:217:SER:HB3    | 1.77                     | 0.67              |
| 11:H:1495:CLA:HBD | 11:H:1495:CLA:HBA1 | 1.77                     | 0.67              |
| 10:Y:177:UNK:O    | 10:Y:178:UNK:C     | 2.42                     | 0.67              |
| 1:A:8:ARG:N       | 1:A:11:ALA:HB3     | 2.10                     | 0.67              |
| 1:A:183:MET:CE    | 11:A:1343:CLA:HHD  | 2.25                     | 0.67              |
| 3:C:128:GLY:HA3   | 11:C:1471:CLA:CMC  | 2.23                     | 0.67              |
| 3:C:269:GLU:O     | 3:C:272:LEU:HB3    | 1.93                     | 0.67              |
| 4:D:145:ALA:HA    | 4:D:276:VAL:CG2    | 2.24                     | 0.67              |
| 1:G:84:PRO:HD3    | 1:G:173:PRO:HG3    | 1.73                     | 0.67              |
| 2:H:233:ASN:O     | 2:H:235:GLU:N      | 2.27                     | 0.67              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 4:J:272:LEU:HD23 | 4:J:272:LEU:C      | 2.20                     | 0.67              |
| 1:A:267:ASN:O    | 1:A:270:SER:N      | 2.27                     | 0.67              |
| 2:B:395:GLN:CB   | 2:B:397:VAL:H      | 2.08                     | 0.67              |
| 2:H:288:VAL:O    | 2:H:292:LEU:HB2    | 1.95                     | 0.67              |
| 3:I:82:TYR:CD2   | 3:I:302:TYR:O      | 2.48                     | 0.67              |
| 1:A:70:SER:O     | 1:A:75:ASN:HB2     | 1.93                     | 0.66              |
| 2:B:30:VAL:O     | 2:B:34:ALA:N       | 2.21                     | 0.66              |
| 2:B:106:LEU:HB3  | 11:B:1496:CLA:H121 | 1.77                     | 0.66              |
| 4:D:126:MET:O    | 4:D:129:GLN:CG     | 2.41                     | 0.66              |
| 5:E:8:ARG:HB2    | 5:E:9:PRO:HD2      | 1.76                     | 0.66              |
| 2:H:79:SER:C     | 2:H:80:ILE:HG13    | 2.20                     | 0.66              |
| 4:J:113:PHE:CA   | 11:J:1353:CLA:HED1 | 2.21                     | 0.66              |
| 1:A:63:ILE:CG1   | 3:C:335:THR:HG23   | 2.25                     | 0.66              |
| 2:B:256:MET:SD   | 2:B:263:THR:HG23   | 2.35                     | 0.66              |
| 3:C:79:LYS:HE2   | 3:C:83:GLU:HG2     | 1.75                     | 0.66              |
| 1:G:316:THR:HG22 | 1:G:318:ALA:H      | 1.60                     | 0.66              |
| 2:H:49:ASP:OD2   | 2:H:52:LEU:N       | 2.29                     | 0.66              |
| 3:I:176:VAL:O    | 3:I:180:MET:HG2    | 1.94                     | 0.66              |
| 4:J:126:MET:HE3  | 4:J:146:PHE:CD2    | 2.28                     | 0.66              |
| 1:G:214:MET:CE   | 12:J:1352:PHO:HED1 | 2.25                     | 0.66              |
| 1:G:286:THR:CG2  | 11:G:1342:CLA:O1D  | 2.43                     | 0.66              |
| 2:H:64:PRO:O     | 2:H:67:ALA:HB3     | 1.96                     | 0.66              |
| 3:I:187:ASP:CB   | 3:I:230:LEU:HD23   | 2.21                     | 0.66              |
| 3:I:315:MET:O    | 3:I:319:ILE:CG1    | 2.43                     | 0.66              |
| 2:B:413:ASP:N    | 2:B:413:ASP:OD1    | 2.27                     | 0.66              |
| 3:C:298:PRO:O    | 3:C:299:SER:CB     | 2.44                     | 0.66              |
| 4:D:61:HIS:HB3   | 4:D:63:LEU:CD1     | 2.24                     | 0.66              |
| 2:H:167:TRP:CG   | 2:H:267:LEU:HD11   | 2.30                     | 0.66              |
| 10:X:509:UNK:O   | 10:X:510:UNK:C     | 2.43                     | 0.66              |
| 4:D:72:ASN:O     | 4:D:74:LEU:N       | 2.29                     | 0.66              |
| 4:D:188:PHE:CZ   | 4:D:326:ARG:HG2    | 2.30                     | 0.66              |
| 6:F:9:GLU:N      | 6:F:10:PRO:HD3     | 2.10                     | 0.66              |
| 1:G:218:LEU:HD11 | 1:G:255:PHE:HD2    | 1.60                     | 0.66              |
| 1:A:99:ALA:CB    | 1:A:104:GLU:OE1    | 2.44                     | 0.66              |
| 1:A:131:TRP:CH2  | 11:C:1463:CLA:HAA2 | 2.30                     | 0.66              |
| 1:A:266:ASN:O    | 1:A:267:ASN:C      | 2.37                     | 0.66              |
| 2:B:197:GLY:O    | 2:B:198:VAL:C      | 2.39                     | 0.66              |
| 1:G:8:ARG:N      | 1:G:11:ALA:HB3     | 2.10                     | 0.66              |
| 1:G:326:LEU:C    | 1:G:328:MET:H      | 2.04                     | 0.66              |
| 3:I:318:LEU:HD12 | 3:I:318:LEU:O      | 1.96                     | 0.66              |
| 1:A:63:ILE:O     | 1:A:64:ARG:HD2     | 1.96                     | 0.66              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:143:ILE:CG1   | 4:D:220:ASN:HD22 | 2.00                     | 0.66              |
| 2:H:332:LYS:O     | 2:H:439:SER:HA   | 1.94                     | 0.66              |
| 3:I:135:ARG:C     | 3:I:136:GLY:O    | 2.36                     | 0.66              |
| 6:L:33:PHE:O      | 6:L:36:ALA:N     | 2.29                     | 0.66              |
| 1:A:214:MET:O     | 1:A:215:HIS:C    | 2.38                     | 0.66              |
| 1:G:113:GLN:O     | 1:G:117:PHE:HD2  | 1.79                     | 0.66              |
| 1:G:133:LEU:HD12  | 4:J:256:ILE:CG1  | 2.26                     | 0.66              |
| 2:H:163:GLY:O     | 2:H:164:PRO:C    | 2.38                     | 0.66              |
| 4:J:263:ASN:O     | 4:J:266:TRP:N    | 2.28                     | 0.66              |
| 3:C:50:LEU:O      | 3:C:54:VAL:HG23  | 1.96                     | 0.66              |
| 4:J:235:PHE:HE1   | 4:J:237:PRO:HB3  | 1.61                     | 0.66              |
| 1:A:315:ASN:O     | 1:A:316:THR:CB   | 2.44                     | 0.66              |
| 3:C:40:ALA:O      | 3:C:43:ILE:HG12  | 1.95                     | 0.66              |
| 1:A:266:ASN:O     | 1:A:267:ASN:O    | 2.14                     | 0.65              |
| 3:C:312:ALA:O     | 3:C:316:THR:HG23 | 1.96                     | 0.65              |
| 6:F:10:PRO:HB2    | 6:F:19:ARG:NH1   | 2.10                     | 0.65              |
| 2:H:16:PRO:HG3    | 2:H:132:ALA:O    | 1.96                     | 0.65              |
| 3:I:170:ILE:HG23  | 3:I:171:GLY:N    | 2.11                     | 0.65              |
| 1:A:316:THR:HG22  | 1:A:318:ALA:H    | 1.61                     | 0.65              |
| 2:B:139:PHE:O     | 2:B:139:PHE:CG   | 2.49                     | 0.65              |
| 3:C:367:GLU:O     | 3:C:368:PRO:C    | 2.38                     | 0.65              |
| 2:H:263:THR:H     | 2:H:264:PRO:HD2  | 1.58                     | 0.65              |
| 3:C:81:MET:HE1    | 3:C:301:PHE:CD1  | 2.32                     | 0.65              |
| 3:C:189:TRP:HE1   | 3:C:295:THR:CG2  | 2.09                     | 0.65              |
| 1:G:84:PRO:HD2    | 1:G:173:PRO:HG3  | 1.71                     | 0.65              |
| 1:G:294:ALA:C     | 1:G:296:ASN:N    | 2.50                     | 0.65              |
| 2:H:397:VAL:HA    | 2:H:417:VAL:CG2  | 2.26                     | 0.65              |
| 1:A:310:LYS:CA    | 9:V:2:GLU:HA     | 2.22                     | 0.65              |
| 3:C:50:LEU:HD23   | 3:C:132:HIS:CD2  | 2.31                     | 0.65              |
| 4:D:88:SER:C      | 4:D:90:LEU:N     | 2.52                     | 0.65              |
| 1:G:63:ILE:HG13   | 3:I:335:THR:HG23 | 1.79                     | 0.65              |
| 1:G:315:ASN:O     | 1:G:316:THR:CB   | 2.45                     | 0.65              |
| 2:H:217:ILE:O     | 2:H:217:ILE:HG12 | 1.96                     | 0.65              |
| 5:K:56:TYR:O      | 5:K:57:ALA:HB2   | 1.96                     | 0.65              |
| 1:A:134:SER:HA    | 1:A:139:MET:HB3  | 1.78                     | 0.65              |
| 2:B:94:GLU:HG3    | 2:B:95:GLY:N     | 2.11                     | 0.65              |
| 2:B:352:GLU:O     | 2:B:354:LEU:N    | 2.29                     | 0.65              |
| 3:C:315:MET:O     | 3:C:319:ILE:HG13 | 1.95                     | 0.65              |
| 11:G:1344:CLA:CED | 4:J:175:VAL:HG13 | 2.27                     | 0.65              |
| 2:H:372:ASP:N     | 2:H:376:VAL:O    | 2.24                     | 0.65              |
| 1:A:248:ILE:HD12  | 4:D:235:PHE:CZ   | 2.31                     | 0.65              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:H:93:PHE:O      | 2:H:94:GLU:C       | 2.40                     | 0.65              |
| 3:I:180:MET:HG3   | 3:I:181:PHE:H      | 1.62                     | 0.65              |
| 4:J:253:TRP:HB2   | 4:J:260:ALA:CB     | 2.24                     | 0.65              |
| 1:A:286:THR:CG2   | 11:A:1342:CLA:O1D  | 2.45                     | 0.65              |
| 1:A:315:ASN:O     | 1:A:316:THR:OG1    | 2.14                     | 0.65              |
| 2:B:138:MET:C     | 2:B:140:GLY:H      | 2.04                     | 0.65              |
| 4:D:253:TRP:HB2   | 4:D:260:ALA:CB     | 2.27                     | 0.65              |
| 2:H:194:ASN:OD1   | 2:H:196:GLY:N      | 2.30                     | 0.65              |
| 3:I:289:PHE:O     | 3:I:293:ASN:CB     | 2.45                     | 0.65              |
| 10:Y:470:UNK:O    | 10:Y:473:UNK:N     | 2.29                     | 0.65              |
| 2:B:288:VAL:HG23  | 2:B:289:GLN:N      | 2.12                     | 0.65              |
| 4:D:167:TRP:O     | 4:D:168:PHE:CB     | 2.45                     | 0.65              |
| 1:G:180:PHE:CD2   | 4:J:192:THR:HB     | 2.32                     | 0.65              |
| 2:H:263:THR:HG22  | 2:H:448:ARG:CZ     | 2.26                     | 0.65              |
| 4:J:148:ALA:HA    | 4:J:280:TRP:NE1    | 2.12                     | 0.65              |
| 1:A:60:ILE:HD12   | 1:A:83:VAL:HG13    | 1.79                     | 0.65              |
| 1:A:136:ARG:HE    | 10:X:29:UNK:CB     | 2.10                     | 0.65              |
| 1:A:314:ILE:HG23  | 4:D:58:TRP:CZ3     | 2.31                     | 0.65              |
| 2:B:17:GLY:O      | 2:B:20:ILE:HB      | 1.96                     | 0.65              |
| 3:C:128:GLY:HA2   | 11:C:1471:CLA:HBC2 | 1.78                     | 0.65              |
| 4:D:176:ALA:HA    | 4:D:179:PHE:CD2    | 2.32                     | 0.65              |
| 1:G:143:ILE:H     | 4:J:220:ASN:ND2    | 1.95                     | 0.65              |
| 2:H:109:LEU:O     | 2:H:112:CYS:HB2    | 1.97                     | 0.65              |
| 9:T:133:GLY:O     | 9:T:137:TYR:CB     | 2.42                     | 0.65              |
| 2:B:268:PHE:O     | 2:B:269:GLY:O      | 2.15                     | 0.65              |
| 4:D:236:ASN:C     | 4:D:238:THR:H      | 2.05                     | 0.65              |
| 1:G:141:PRO:O     | 1:G:143:ILE:N      | 2.29                     | 0.65              |
| 3:I:367:GLU:O     | 3:I:368:PRO:C      | 2.39                     | 0.65              |
| 5:K:26:THR:O      | 5:K:29:ALA:HB3     | 1.97                     | 0.65              |
| 10:Y:71:UNK:O     | 10:Y:73:UNK:N      | 2.29                     | 0.65              |
| 10:Y:506:UNK:O    | 10:Y:507:UNK:C     | 2.44                     | 0.65              |
| 2:B:79:SER:O      | 2:B:80:ILE:HG13    | 1.97                     | 0.64              |
| 4:D:91:LEU:HA     | 11:D:1353:CLA:O1D  | 1.97                     | 0.64              |
| 1:G:58:VAL:N      | 1:G:67:VAL:O       | 2.29                     | 0.64              |
| 1:G:83:VAL:HG22   | 4:J:314:PHE:HE1    | 1.62                     | 0.64              |
| 1:G:159:LEU:O     | 1:G:163:ILE:HG13   | 1.96                     | 0.64              |
| 4:J:39:PRO:O      | 4:J:43:LEU:HB2     | 1.96                     | 0.64              |
| 1:A:160:ILE:HD12  | 3:C:431:PHE:HE1    | 1.62                     | 0.64              |
| 1:A:258:LEU:HG    | 4:D:128:ARG:HH22   | 1.62                     | 0.64              |
| 11:A:1344:CLA:CED | 4:D:175:VAL:HG13   | 2.27                     | 0.64              |
| 3:C:235:GLY:O     | 3:C:238:ILE:HB     | 1.97                     | 0.64              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 3:C:304:PRO:O    | 3:C:305:THR:HG23   | 1.97                     | 0.64              |
| 4:D:274:VAL:CB   | 4:D:275:PRO:HD3    | 2.26                     | 0.64              |
| 1:G:166:GLY:O    | 1:G:167:SER:HB2    | 1.97                     | 0.64              |
| 2:H:452:THR:O    | 2:H:452:THR:HG22   | 1.96                     | 0.64              |
| 3:I:298:PRO:O    | 3:I:299:SER:CB     | 2.44                     | 0.64              |
| 4:J:161:PRO:HB3  | 4:J:167:TRP:HA     | 1.79                     | 0.64              |
| 6:L:16:PHE:HZ    | 10:Y:557:UNK:HA    | 1.63                     | 0.64              |
| 4:D:193:LEU:O    | 4:D:195:PRO:HD3    | 1.97                     | 0.64              |
| 1:G:289:GLY:O    | 1:G:292:THR:HB     | 1.97                     | 0.64              |
| 3:I:78:GLU:OE2   | 3:I:104:GLU:HA     | 1.98                     | 0.64              |
| 4:J:193:LEU:O    | 4:J:195:PRO:HD3    | 1.96                     | 0.64              |
| 5:K:62:SER:O     | 5:K:64:PRO:N       | 2.30                     | 0.64              |
| 9:T:55:ARG:HH21  | 9:T:128:ASP:HA     | 1.61                     | 0.64              |
| 1:A:60:ILE:HD12  | 1:A:83:VAL:CG1     | 2.27                     | 0.64              |
| 2:B:158:LEU:HB3  | 2:B:199:VAL:HG22   | 1.80                     | 0.64              |
| 2:B:235:GLU:OE1  | 2:B:472:ARG:HD3    | 1.97                     | 0.64              |
| 1:G:217:SER:HG   | 4:J:142:ASN:HA     | 1.63                     | 0.64              |
| 3:I:43:ILE:HG22  | 11:I:1467:CLA:HMC3 | 1.79                     | 0.64              |
| 3:I:162:GLY:HA2  | 3:I:248:GLY:HA2    | 1.78                     | 0.64              |
| 10:X:507:UNK:O   | 10:X:509:UNK:N     | 2.31                     | 0.64              |
| 1:A:161:TYR:HB3  | 1:A:162:PRO:HD3    | 1.77                     | 0.64              |
| 2:B:362:PHE:CE2  | 4:D:184:PHE:HZ     | 2.15                     | 0.64              |
| 4:D:347:PRO:O    | 4:D:348:ARG:CB     | 2.46                     | 0.64              |
| 1:G:36:ILE:O     | 1:G:39:PRO:HD2     | 1.96                     | 0.64              |
| 2:H:223:GLN:O    | 2:H:227:LYS:N      | 2.31                     | 0.64              |
| 2:H:236:THR:HB   | 2:H:473:THR:HG21   | 1.79                     | 0.64              |
| 4:J:7:ARG:O      | 4:J:8:ALA:O        | 2.14                     | 0.64              |
| 1:A:309:ALA:O    | 9:V:2:GLU:HB3      | 1.95                     | 0.64              |
| 2:B:135:LEU:O    | 2:B:138:MET:N      | 2.31                     | 0.64              |
| 1:G:137:LEU:CD1  | 1:G:139:MET:HE1    | 2.25                     | 0.64              |
| 1:G:180:PHE:CE2  | 4:J:192:THR:HB     | 2.32                     | 0.64              |
| 10:X:331:UNK:O   | 10:X:334:UNK:N     | 2.31                     | 0.64              |
| 1:A:269:ARG:NE   | 4:D:222:LEU:HD13   | 2.12                     | 0.64              |
| 3:C:49:LEU:O     | 3:C:50:LEU:C       | 2.40                     | 0.64              |
| 4:D:152:VAL:HG21 | 4:D:279:LEU:HD13   | 1.80                     | 0.64              |
| 4:D:235:PHE:O    | 4:D:235:PHE:CD1    | 2.50                     | 0.64              |
| 6:F:29:PRO:O     | 6:F:32:PHE:HB3     | 1.97                     | 0.64              |
| 3:I:122:SER:O    | 3:I:125:LEU:N      | 2.31                     | 0.64              |
| 3:C:40:ALA:O     | 3:C:43:ILE:HG23    | 1.96                     | 0.64              |
| 5:E:58:GLN:HE22  | 9:V:4:THR:HG23     | 1.63                     | 0.64              |
| 1:G:309:ALA:O    | 9:T:2:GLU:CA       | 2.46                     | 0.64              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:H:354:LEU:CD1   | 2:H:378:LYS:CB     | 2.75                     | 0.64              |
| 11:H:1496:CLA:ND  | 11:H:1497:CLA:HBB2 | 2.13                     | 0.64              |
| 5:E:8:ARG:HB2     | 5:E:9:PRO:CD       | 2.28                     | 0.64              |
| 6:F:16:PHE:HZ     | 10:X:557:UNK:HA    | 1.62                     | 0.64              |
| 1:G:117:PHE:HZ    | 1:G:168:PHE:CZ     | 2.16                     | 0.64              |
| 1:G:326:LEU:O     | 1:G:329:GLU:N      | 2.31                     | 0.64              |
| 3:I:35:TRP:C      | 3:I:37:ALA:H       | 2.04                     | 0.64              |
| 3:I:260:ALA:CB    | 11:I:1464:CLA:HAA2 | 2.28                     | 0.64              |
| 5:K:37:PHE:CE1    | 5:K:42:LEU:HB2     | 2.33                     | 0.64              |
| 6:L:29:PRO:O      | 6:L:32:PHE:HB3     | 1.97                     | 0.64              |
| 8:U:55:UNK:O      | 8:U:56:UNK:C       | 2.46                     | 0.64              |
| 3:C:164:HIS:HA    | 3:C:167:VAL:HG23   | 1.80                     | 0.64              |
| 4:D:7:ARG:O       | 4:D:8:ALA:O        | 2.16                     | 0.64              |
| 4:D:57:SER:O      | 4:D:59:TYR:N       | 2.31                     | 0.64              |
| 5:E:42:LEU:O      | 5:E:43:ALA:C       | 2.41                     | 0.64              |
| 1:G:78:ILE:HG23   | 1:G:176:ILE:HG21   | 1.79                     | 0.64              |
| 2:B:214:LEU:O     | 2:B:217:ILE:HG22   | 1.97                     | 0.63              |
| 3:C:54:VAL:O      | 3:C:57:ALA:HB3     | 1.99                     | 0.63              |
| 5:E:13:ILE:HG22   | 5:E:19:TYR:HD2     | 1.59                     | 0.63              |
| 4:J:184:PHE:HA    | 4:J:329:MET:HE1    | 1.80                     | 0.63              |
| 4:J:253:TRP:CB    | 4:J:260:ALA:HB2    | 2.27                     | 0.63              |
| 1:A:34:GLY:O      | 1:A:36:ILE:N       | 2.32                     | 0.63              |
| 3:C:176:VAL:HG13  | 3:C:177:ALA:N      | 2.13                     | 0.63              |
| 4:D:289:LEU:CD2   | 4:D:294:ARG:HB3    | 2.28                     | 0.63              |
| 1:G:269:ARG:NE    | 4:J:222:LEU:HD13   | 2.12                     | 0.63              |
| 3:I:189:TRP:CH2   | 3:I:363:GLY:HA2    | 2.32                     | 0.63              |
| 4:J:74:LEU:CD2    | 4:J:175:VAL:HG11   | 2.29                     | 0.63              |
| 1:A:161:TYR:CE2   | 1:A:186:PHE:HE1    | 2.16                     | 0.63              |
| 1:A:210:LEU:C     | 1:A:210:LEU:HD12   | 2.24                     | 0.63              |
| 3:C:287:THR:HG22  | 3:C:430:HIS:HB3    | 1.79                     | 0.63              |
| 1:G:85:SER:OG     | 1:G:113:GLN:HG3    | 1.99                     | 0.63              |
| 2:H:145:LEU:O     | 2:H:146:ALA:C      | 2.41                     | 0.63              |
| 4:J:145:ALA:HA    | 4:J:276:VAL:CG2    | 2.27                     | 0.63              |
| 11:B:1496:CLA:H13 | 11:B:1497:CLA:HMD1 | 1.80                     | 0.63              |
| 3:C:289:PHE:O     | 3:C:293:ASN:CB     | 2.47                     | 0.63              |
| 1:G:258:LEU:O     | 4:J:128:ARG:NH2    | 2.32                     | 0.63              |
| 1:G:331:MET:CE    | 4:J:346:LEU:O      | 2.46                     | 0.63              |
| 4:J:330:ALA:O     | 4:J:332:GLN:N      | 2.30                     | 0.63              |
| 1:A:104:GLU:HG2   | 1:A:108:ASN:ND2    | 2.14                     | 0.63              |
| 2:B:194:ASN:OD1   | 2:B:196:GLY:N      | 2.31                     | 0.63              |
| 3:C:362:ARG:HH11  | 3:C:362:ARG:HG3    | 1.64                     | 0.63              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 2:H:139:PHE:CG   | 2:H:139:PHE:O      | 2.51                     | 0.63              |
| 8:U:59:UNK:O     | 8:U:60:UNK:C       | 2.46                     | 0.63              |
| 10:X:71:UNK:O    | 10:X:73:UNK:N      | 2.32                     | 0.63              |
| 1:A:310:LYS:HA   | 9:V:2:GLU:CA       | 2.27                     | 0.63              |
| 4:D:45:LEU:HD22  | 4:D:49:LEU:HD11    | 1.81                     | 0.63              |
| 4:D:65:SER:HB2   | 4:D:77:ALA:O       | 1.98                     | 0.63              |
| 1:G:98:GLU:O     | 1:G:99:ALA:HB3     | 1.99                     | 0.63              |
| 1:G:104:GLU:OE2  | 7:P:36:UNK:CB      | 2.46                     | 0.63              |
| 2:H:197:GLY:O    | 2:H:198:VAL:C      | 2.42                     | 0.63              |
| 2:H:233:ASN:O    | 2:H:233:ASN:ND2    | 2.32                     | 0.63              |
| 3:I:50:LEU:O     | 3:I:54:VAL:HG23    | 1.99                     | 0.63              |
| 1:A:84:PRO:HA    | 1:A:112:TYR:CG     | 2.34                     | 0.63              |
| 4:D:16:ASP:O     | 4:D:17:ILE:C       | 2.41                     | 0.63              |
| 4:D:263:ASN:O    | 4:D:266:TRP:N      | 2.28                     | 0.63              |
| 1:A:297:LEU:HD22 | 3:C:428:THR:HG21   | 1.79                     | 0.63              |
| 2:B:217:ILE:O    | 2:B:217:ILE:HG12   | 1.97                     | 0.63              |
| 2:B:233:ASN:O    | 2:B:233:ASN:ND2    | 2.32                     | 0.63              |
| 2:B:391:SER:O    | 2:B:392:PHE:CB     | 2.46                     | 0.63              |
| 1:G:60:ILE:HB    | 1:G:83:VAL:CG1     | 2.28                     | 0.63              |
| 1:G:84:PRO:HG2   | 1:G:173:PRO:HD3    | 1.78                     | 0.63              |
| 1:G:85:SER:HA    | 1:G:109:GLY:O      | 1.97                     | 0.63              |
| 3:I:188:THR:HG21 | 3:I:298:PRO:HB3    | 1.81                     | 0.63              |
| 4:J:16:ASP:O     | 4:J:17:ILE:C       | 2.42                     | 0.63              |
| 1:A:117:PHE:HZ   | 1:A:168:PHE:CZ     | 2.17                     | 0.63              |
| 11:B:1496:CLA:ND | 11:B:1497:CLA:HBB2 | 2.13                     | 0.63              |
| 3:I:97:TRP:CZ3   | 3:I:178:LYS:NZ     | 2.66                     | 0.63              |
| 5:K:37:PHE:CD1   | 5:K:42:LEU:HB2     | 2.33                     | 0.63              |
| 8:S:55:UNK:O     | 8:S:56:UNK:C       | 2.47                     | 0.63              |
| 1:A:201:GLY:HA3  | 1:A:286:THR:OG1    | 1.98                     | 0.62              |
| 2:B:263:THR:O    | 2:B:263:THR:CG2    | 2.43                     | 0.62              |
| 3:I:186:TYR:HE2  | 3:I:188:THR:HG23   | 1.64                     | 0.62              |
| 4:J:62:GLY:HA3   | 5:K:63:ILE:CG2     | 2.29                     | 0.62              |
| 4:J:91:LEU:C     | 4:J:93:TRP:H       | 2.06                     | 0.62              |
| 4:J:171:PRO:CD   | 4:J:181:PHE:CZ     | 2.82                     | 0.62              |
| 3:C:264:PHE:HD1  | 3:C:274:TYR:HE1    | 1.48                     | 0.62              |
| 4:D:63:LEU:HD12  | 4:D:63:LEU:N       | 2.14                     | 0.62              |
| 4:D:253:TRP:CB   | 4:D:260:ALA:HB2    | 2.29                     | 0.62              |
| 3:I:95:LEU:HD23  | 3:I:97:TRP:CZ3     | 2.32                     | 0.62              |
| 3:I:202:PRO:CA   | 3:I:235:GLY:HA3    | 2.29                     | 0.62              |
| 7:O:51:UNK:O     | 7:O:82:UNK:HA      | 1.99                     | 0.62              |
| 9:T:129:LYS:CE   | 9:T:135:VAL:HG21   | 2.23                     | 0.62              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:A:137:LEU:HD12 | 1:A:139:MET:CE     | 2.29                     | 0.62              |
| 1:A:331:MET:HE2  | 4:D:346:LEU:O      | 1.98                     | 0.62              |
| 6:F:43:ILE:HG23  | 6:F:45:ARG:O       | 1.99                     | 0.62              |
| 1:G:201:GLY:HA3  | 1:G:286:THR:OG1    | 2.00                     | 0.62              |
| 3:I:91:HIS:HE1   | 11:I:1460:CLA:O1D  | 1.81                     | 0.62              |
| 7:P:99:UNK:O     | 7:P:102:UNK:N      | 2.31                     | 0.62              |
| 9:V:129:LYS:CE   | 9:V:135:VAL:HG21   | 2.26                     | 0.62              |
| 1:A:309:ALA:C    | 9:V:2:GLU:HG2      | 2.24                     | 0.62              |
| 2:B:452:THR:O    | 2:B:452:THR:HG22   | 1.98                     | 0.62              |
| 3:C:91:HIS:HE1   | 11:C:1460:CLA:O1D  | 1.81                     | 0.62              |
| 2:H:288:VAL:O    | 2:H:292:LEU:CB     | 2.48                     | 0.62              |
| 3:I:49:LEU:O     | 3:I:50:LEU:C       | 2.39                     | 0.62              |
| 3:I:69:LEU:CD1   | 3:I:115:GLY:HA3    | 2.30                     | 0.62              |
| 4:J:263:ASN:O    | 4:J:264:LYS:C      | 2.42                     | 0.62              |
| 10:X:225:UNK:C   | 10:X:227:UNK:N     | 2.62                     | 0.62              |
| 2:B:16:PRO:HG3   | 2:B:132:ALA:O      | 2.00                     | 0.62              |
| 2:B:338:GLN:O    | 2:B:339:ALA:O      | 2.17                     | 0.62              |
| 3:C:250:TRP:HA   | 3:C:253:LEU:HD12   | 1.80                     | 0.62              |
| 3:C:260:ALA:O    | 3:C:264:PHE:HD2    | 1.82                     | 0.62              |
| 4:D:126:MET:HE3  | 4:D:146:PHE:CD2    | 2.31                     | 0.62              |
| 4:D:235:PHE:CE1  | 4:D:237:PRO:HB3    | 2.33                     | 0.62              |
| 1:G:192:ILE:HG23 | 1:G:293:MET:HE1    | 1.81                     | 0.62              |
| 2:H:201:HIS:HD2  | 2:H:202:HIS:ND1    | 1.98                     | 0.62              |
| 3:I:424:SER:O    | 3:I:428:THR:OG1    | 2.15                     | 0.62              |
| 10:X:6:UNK:O     | 10:X:7:UNK:C       | 2.48                     | 0.62              |
| 1:G:112:TYR:CZ   | 1:G:116:ILE:HD11   | 2.34                     | 0.62              |
| 2:H:150:CYS:HB2  | 11:H:1484:CLA:HMC3 | 1.82                     | 0.62              |
| 3:I:312:ALA:O    | 3:I:316:THR:HG23   | 1.99                     | 0.62              |
| 5:K:8:ARG:HB2    | 5:K:9:PRO:CD       | 2.30                     | 0.62              |
| 10:Y:200:UNK:O   | 10:Y:204:UNK:N     | 2.32                     | 0.62              |
| 1:A:107:TYR:C    | 1:A:109:GLY:N      | 2.56                     | 0.62              |
| 3:C:250:TRP:CD1  | 3:C:250:TRP:C      | 2.77                     | 0.62              |
| 3:C:307:PRO:HA   | 3:C:358:PHE:CD1    | 2.34                     | 0.62              |
| 1:G:151:LEU:HG   | 1:G:155:PHE:CE2    | 2.35                     | 0.62              |
| 2:H:158:LEU:HB3  | 2:H:199:VAL:HG22   | 1.81                     | 0.62              |
| 3:I:189:TRP:HE1  | 3:I:295:THR:CG2    | 2.13                     | 0.62              |
| 4:J:167:TRP:O    | 4:J:168:PHE:HB2    | 1.98                     | 0.62              |
| 4:J:274:VAL:CB   | 4:J:275:PRO:HD3    | 2.30                     | 0.62              |
| 7:O:88:UNK:O     | 7:O:139:UNK:HA     | 2.00                     | 0.62              |
| 1:A:96:ILE:HG22  | 11:A:1346:CLA:OBD  | 1.99                     | 0.62              |
| 2:B:397:VAL:HA   | 2:B:417:VAL:CG2    | 2.29                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:C:161:LEU:O      | 3:C:164:HIS:HB2    | 1.99                     | 0.62              |
| 3:C:318:LEU:HD12   | 3:C:318:LEU:C      | 2.24                     | 0.62              |
| 3:I:269:GLU:O      | 3:I:272:LEU:HB3    | 1.99                     | 0.62              |
| 3:I:287:THR:HG22   | 3:I:430:HIS:HB3    | 1.79                     | 0.62              |
| 8:U:90:UNK:O       | 8:U:91:UNK:C       | 2.43                     | 0.62              |
| 3:C:287:THR:HG22   | 3:C:430:HIS:HB2    | 1.81                     | 0.62              |
| 4:D:15:PHE:O       | 4:D:16:ASP:C       | 2.43                     | 0.62              |
| 4:D:238:THR:O      | 4:D:239:GLN:CB     | 2.48                     | 0.62              |
| 1:G:131:TRP:CH2    | 11:I:1463:CLA:HAA2 | 2.35                     | 0.62              |
| 3:I:63:TRP:HE1     | 11:I:1462:CLA:C2C  | 2.12                     | 0.62              |
| 3:I:240:ILE:HD12   | 11:I:1465:CLA:H91  | 1.81                     | 0.62              |
| 3:I:279:LEU:O      | 3:I:280:SER:C      | 2.43                     | 0.62              |
| 4:J:110:LEU:O      | 4:J:114:ILE:HG13   | 1.99                     | 0.62              |
| 10:Y:6:UNK:O       | 10:Y:7:UNK:C       | 2.48                     | 0.62              |
| 2:B:354:LEU:CD1    | 2:B:378:LYS:CB     | 2.78                     | 0.62              |
| 3:I:58:GLY:HA2     | 3:I:125:LEU:HD12   | 1.82                     | 0.62              |
| 4:J:323:GLU:CG     | 4:J:326:ARG:HH21   | 2.10                     | 0.62              |
| 4:J:345:VAL:O      | 4:J:345:VAL:CG1    | 2.41                     | 0.62              |
| 3:C:276:LEU:CD1    | 11:C:1466:CLA:HBB1 | 2.29                     | 0.61              |
| 1:G:311:GLY:HA3    | 9:T:125:ILE:HG21   | 1.80                     | 0.61              |
| 2:H:403:GLY:H      | 2:H:407:ASN:HB2    | 1.65                     | 0.61              |
| 10:X:224:UNK:O     | 10:X:227:UNK:N     | 2.33                     | 0.61              |
| 1:A:276:ALA:HB2    | 4:D:215:GLY:C      | 2.26                     | 0.61              |
| 4:J:152:VAL:HG21   | 4:J:279:LEU:HD13   | 1.82                     | 0.61              |
| 4:D:46:GLY:HA2     | 4:D:49:LEU:HD12    | 1.82                     | 0.61              |
| 1:G:96:ILE:O       | 1:G:96:ILE:HG12    | 1.99                     | 0.61              |
| 3:I:188:THR:CG2    | 3:I:298:PRO:HB3    | 2.30                     | 0.61              |
| 4:J:104:TRP:CE2    | 4:J:109:GLY:HA3    | 2.35                     | 0.61              |
| 11:A:1342:CLA:H122 | 12:A:1345:PHO:H3A  | 1.82                     | 0.61              |
| 3:C:58:GLY:HA2     | 3:C:125:LEU:HD12   | 1.81                     | 0.61              |
| 4:D:91:LEU:C       | 4:D:93:TRP:H       | 2.08                     | 0.61              |
| 1:G:63:ILE:CG1     | 3:I:335:THR:HG23   | 2.30                     | 0.61              |
| 1:G:160:ILE:HD12   | 3:I:431:PHE:HE1    | 1.65                     | 0.61              |
| 2:H:270:PRO:C      | 2:H:271:THR:HG23   | 2.24                     | 0.61              |
| 3:I:176:VAL:HG13   | 3:I:177:ALA:N      | 2.15                     | 0.61              |
| 2:B:54:PRO:O       | 2:B:55:MET:C       | 2.42                     | 0.61              |
| 3:C:260:ALA:CB     | 11:C:1464:CLA:HAA2 | 2.30                     | 0.61              |
| 5:E:16:SER:O       | 5:E:17:VAL:HB      | 2.00                     | 0.61              |
| 1:G:63:ILE:CG1     | 3:I:335:THR:CG2    | 2.74                     | 0.61              |
| 1:G:133:LEU:HD12   | 4:J:256:ILE:HG13   | 1.83                     | 0.61              |
| 1:G:278:TRP:HB3    | 1:G:279:PRO:CD     | 2.24                     | 0.61              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:H:18:ARG:NH1    | 2:H:115:TRP:CZ2    | 2.69                     | 0.61              |
| 3:I:284:PHE:HE1   | 3:I:431:PHE:CD1    | 2.18                     | 0.61              |
| 3:I:390:ARG:CD    | 9:T:100:ILE:HD12   | 2.30                     | 0.61              |
| 4:J:126:MET:HE1   | 4:J:147:SER:CA     | 2.30                     | 0.61              |
| 1:A:102:LEU:HD11  | 1:A:105:TRP:CE3    | 2.35                     | 0.61              |
| 1:A:180:PHE:CE2   | 4:D:192:THR:HB     | 2.36                     | 0.61              |
| 2:B:316:GLY:HA2   | 2:B:443:PHE:HD1    | 1.62                     | 0.61              |
| 2:B:403:GLY:H     | 2:B:407:ASN:HB2    | 1.64                     | 0.61              |
| 3:C:102:GLY:H     | 3:C:193:GLY:CA     | 2.13                     | 0.61              |
| 4:D:104:TRP:CE2   | 4:D:109:GLY:HA3    | 2.35                     | 0.61              |
| 4:D:189:HIS:HA    | 4:D:294:ARG:HH11   | 1.65                     | 0.61              |
| 2:H:235:GLU:OE1   | 2:H:472:ARG:HD3    | 2.01                     | 0.61              |
| 2:H:263:THR:O     | 2:H:263:THR:CG2    | 2.47                     | 0.61              |
| 3:I:54:VAL:HB     | 3:I:129:GLY:HA2    | 1.81                     | 0.61              |
| 3:I:116:VAL:CG2   | 3:I:117:VAL:N      | 2.64                     | 0.61              |
| 3:C:315:MET:HG3   | 3:C:365:TRP:CZ3    | 2.36                     | 0.61              |
| 1:G:289:GLY:O     | 1:G:293:MET:HG3    | 2.00                     | 0.61              |
| 2:H:24:LEU:HB3    | 2:H:111:ALA:HB2    | 1.82                     | 0.61              |
| 9:T:87:GLU:CD     | 9:T:96:ARG:HH22    | 2.07                     | 0.61              |
| 1:A:58:VAL:N      | 1:A:67:VAL:O       | 2.33                     | 0.61              |
| 1:A:218:LEU:HD11  | 1:A:255:PHE:HD2    | 1.66                     | 0.61              |
| 1:A:295:PHE:O     | 3:C:291:TRP:CZ3    | 2.53                     | 0.61              |
| 11:A:1342:CLA:HBD | 11:A:1343:CLA:HAC2 | 1.83                     | 0.61              |
| 2:B:31:ALA:CB     | 11:B:1486:CLA:HBC3 | 2.30                     | 0.61              |
| 3:C:82:TYR:CD2    | 3:C:302:TYR:O      | 2.53                     | 0.61              |
| 1:G:267:ASN:O     | 1:G:268:SER:C      | 2.44                     | 0.61              |
| 2:H:54:PRO:O      | 2:H:55:MET:C       | 2.43                     | 0.61              |
| 2:H:135:LEU:O     | 2:H:138:MET:N      | 2.34                     | 0.61              |
| 3:I:176:VAL:HG22  | 3:I:180:MET:HE3    | 1.80                     | 0.61              |
| 4:J:89:LEU:O      | 4:J:90:LEU:C       | 2.44                     | 0.61              |
| 2:H:316:GLY:HA2   | 2:H:443:PHE:HD1    | 1.66                     | 0.61              |
| 3:I:259:TRP:HZ3   | 11:I:1464:CLA:H12  | 1.66                     | 0.61              |
| 7:P:51:UNK:O      | 7:P:82:UNK:HA      | 1.99                     | 0.61              |
| 9:T:48:THR:OG1    | 18:T:1138:HEC:HMD2 | 2.01                     | 0.61              |
| 4:D:111:TRP:O     | 4:D:114:ILE:N      | 2.34                     | 0.61              |
| 2:H:364:GLU:OE1   | 4:J:296:TYR:CD2    | 2.54                     | 0.61              |
| 3:I:230:LEU:O     | 3:I:234:VAL:HG23   | 2.01                     | 0.61              |
| 4:J:37:LEU:C      | 4:J:37:LEU:CD2     | 2.74                     | 0.61              |
| 4:J:126:MET:HE2   | 4:J:143:ALA:O      | 2.00                     | 0.61              |
| 4:J:171:PRO:HD2   | 4:J:181:PHE:CZ     | 2.36                     | 0.61              |
| 4:J:223:PHE:HE2   | 4:J:245:SER:HB3    | 1.63                     | 0.61              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 7:P:10:UNK:O     | 7:P:173:UNK:CB     | 2.49                     | 0.61              |
| 1:A:157:VAL:O    | 1:A:157:VAL:HG12   | 2.01                     | 0.60              |
| 1:A:306:VAL:HG23 | 1:A:308:ASP:H      | 1.65                     | 0.60              |
| 3:C:120:ILE:C    | 3:C:122:SER:N      | 2.57                     | 0.60              |
| 3:C:162:GLY:HA2  | 3:C:248:GLY:HA2    | 1.82                     | 0.60              |
| 1:G:266:ASN:O    | 1:G:267:ASN:C      | 2.44                     | 0.60              |
| 2:H:288:VAL:O    | 2:H:292:LEU:N      | 2.25                     | 0.60              |
| 3:I:51:GLY:O     | 3:I:52:ALA:C       | 2.44                     | 0.60              |
| 7:O:105:UNK:O    | 7:O:106:UNK:CB     | 2.49                     | 0.60              |
| 8:S:27:UNK:O     | 8:S:28:UNK:C       | 2.48                     | 0.60              |
| 10:Y:468:UNK:O   | 10:Y:469:UNK:C     | 2.49                     | 0.60              |
| 1:A:183:MET:HE1  | 11:A:1343:CLA:HHD  | 1.84                     | 0.60              |
| 2:B:68:ARG:HB3   | 2:B:267:LEU:HD13   | 1.83                     | 0.60              |
| 2:B:445:THR:OG1  | 2:B:446:SER:N      | 2.33                     | 0.60              |
| 3:C:376:ASP:C    | 3:C:378:ASN:N      | 2.58                     | 0.60              |
| 4:D:337:GLU:HG3  | 4:D:339:PHE:HE2    | 1.65                     | 0.60              |
| 5:E:41:GLY:O     | 5:E:44:TYR:HB2     | 2.01                     | 0.60              |
| 1:G:99:ALA:HB2   | 1:G:104:GLU:OE1    | 2.01                     | 0.60              |
| 1:G:297:LEU:HD22 | 3:I:428:THR:HG21   | 1.82                     | 0.60              |
| 2:H:268:PHE:HB2  | 2:H:448:ARG:HH11   | 1.66                     | 0.60              |
| 3:I:315:MET:HG3  | 3:I:365:TRP:CZ3    | 2.36                     | 0.60              |
| 1:A:151:LEU:HG   | 1:A:155:PHE:CE2    | 2.36                     | 0.60              |
| 2:B:285:ASN:O    | 2:B:289:GLN:HB2    | 2.01                     | 0.60              |
| 4:D:87:HIS:HE1   | 4:D:162:LEU:HA     | 1.64                     | 0.60              |
| 1:G:156:ALA:HA   | 1:G:160:ILE:HB     | 1.83                     | 0.60              |
| 8:S:1:UNK:O      | 8:S:3:UNK:N        | 2.32                     | 0.60              |
| 8:S:12:UNK:C     | 8:S:14:UNK:N       | 2.60                     | 0.60              |
| 2:B:318:ASN:C    | 2:B:318:ASN:OD1    | 2.44                     | 0.60              |
| 3:C:73:ALA:HB3   | 3:C:74:HIS:HD2     | 1.66                     | 0.60              |
| 1:G:121:LEU:HD23 | 1:G:121:LEU:O      | 2.01                     | 0.60              |
| 7:O:75:UNK:O     | 7:O:76:UNK:C       | 2.50                     | 0.60              |
| 2:B:92:SER:O     | 2:B:93:PHE:C       | 2.44                     | 0.60              |
| 2:B:149:LEU:HG   | 11:B:1484:CLA:CBC  | 2.28                     | 0.60              |
| 3:I:128:GLY:HA2  | 11:I:1471:CLA:HBC2 | 1.83                     | 0.60              |
| 10:Y:225:UNK:C   | 10:Y:227:UNK:N     | 2.62                     | 0.60              |
| 10:Y:560:UNK:O   | 10:Y:561:UNK:C     | 2.50                     | 0.60              |
| 1:A:143:ILE:N    | 4:D:220:ASN:HD21   | 1.99                     | 0.60              |
| 1:A:207:GLY:O    | 1:A:210:LEU:HB3    | 2.02                     | 0.60              |
| 2:B:223:GLN:O    | 2:B:227:LYS:N      | 2.34                     | 0.60              |
| 3:C:43:ILE:HG22  | 11:C:1467:CLA:CMC  | 2.31                     | 0.60              |
| 6:F:36:ALA:O     | 6:F:39:ALA:HB3     | 2.01                     | 0.60              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 2:H:352:GLU:O    | 2:H:354:LEU:N      | 2.35                     | 0.60              |
| 5:K:42:LEU:O     | 5:K:43:ALA:C       | 2.45                     | 0.60              |
| 2:B:33:TRP:HE1   | 11:B:1488:CLA:HBC2 | 1.65                     | 0.60              |
| 2:B:318:ASN:O    | 2:B:320:ALA:N      | 2.35                     | 0.60              |
| 2:B:346:PHE:O    | 2:B:354:LEU:HB3    | 2.02                     | 0.60              |
| 3:C:56:HIS:O     | 3:C:57:ALA:C       | 2.44                     | 0.60              |
| 4:D:253:TRP:O    | 4:D:256:ILE:N      | 2.29                     | 0.60              |
| 6:F:33:PHE:O     | 6:F:36:ALA:N       | 2.34                     | 0.60              |
| 3:I:225:VAL:HG22 | 3:I:289:PHE:HD1    | 1.67                     | 0.60              |
| 4:J:102:THR:O    | 4:J:105:CYS:HB2    | 2.02                     | 0.60              |
| 4:J:191:TRP:HZ3  | 4:J:194:ASN:ND2    | 1.98                     | 0.60              |
| 9:T:134:LYS:C    | 9:T:137:TYR:H      | 2.10                     | 0.60              |
| 1:A:166:GLY:O    | 1:A:167:SER:HB2    | 2.02                     | 0.60              |
| 3:C:226:SER:OG   | 3:C:227:VAL:N      | 2.34                     | 0.60              |
| 4:D:74:LEU:CD2   | 4:D:175:VAL:HG11   | 2.32                     | 0.60              |
| 4:D:263:ASN:O    | 4:D:264:LYS:C      | 2.45                     | 0.60              |
| 1:G:310:LYS:HD2  | 5:K:58:GLN:HG3     | 1.83                     | 0.60              |
| 1:G:331:MET:HE2  | 4:J:346:LEU:O      | 2.02                     | 0.60              |
| 3:I:264:PHE:HD1  | 3:I:274:TYR:HE1    | 1.50                     | 0.60              |
| 3:C:362:ARG:HG3  | 3:C:362:ARG:NH1    | 2.16                     | 0.60              |
| 4:D:102:THR:O    | 4:D:105:CYS:HB2    | 2.02                     | 0.60              |
| 1:G:314:ILE:HG23 | 4:J:58:TRP:HZ3     | 1.67                     | 0.60              |
| 4:J:126:MET:HE1  | 4:J:147:SER:HA     | 1.83                     | 0.60              |
| 5:K:8:ARG:HB2    | 5:K:9:PRO:HD2      | 1.84                     | 0.60              |
| 5:K:13:ILE:HA    | 5:K:16:SER:HB2     | 1.84                     | 0.60              |
| 8:U:30:UNK:O     | 8:U:31:UNK:C       | 2.49                     | 0.60              |
| 1:A:331:MET:O    | 1:A:332:HIS:C      | 2.45                     | 0.60              |
| 2:B:238:LEU:HD21 | 2:B:469:HIS:CD2    | 2.37                     | 0.60              |
| 3:C:319:ILE:HD11 | 3:C:384:ILE:HD11   | 1.83                     | 0.60              |
| 4:D:62:GLY:HA3   | 5:E:63:ILE:CG2     | 2.32                     | 0.60              |
| 4:D:152:VAL:HG13 | 11:D:1351:CLA:HED3 | 1.83                     | 0.60              |
| 1:G:127:MET:O    | 1:G:130:GLN:HB3    | 2.02                     | 0.60              |
| 1:G:244:GLU:OE2  | 1:G:246:TYR:CE1    | 2.55                     | 0.60              |
| 2:H:92:SER:O     | 2:H:93:PHE:C       | 2.45                     | 0.60              |
| 3:I:363:GLY:O    | 3:I:364:PRO:O      | 2.20                     | 0.60              |
| 4:J:331:PRO:HG2  | 4:J:339:PHE:CB     | 2.07                     | 0.60              |
| 1:A:217:SER:HG   | 4:D:142:ASN:HA     | 1.65                     | 0.59              |
| 4:D:223:PHE:HE2  | 4:D:245:SER:HB3    | 1.67                     | 0.59              |
| 5:E:58:GLN:CD    | 9:V:2:GLU:N        | 2.61                     | 0.59              |
| 1:G:211:PHE:CE2  | 1:G:274:PHE:HE2    | 2.19                     | 0.59              |
| 1:G:267:ASN:O    | 1:G:270:SER:N      | 2.34                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:H:24:LEU:HD23    | 2:H:110:ALA:C      | 2.26                     | 0.59              |
| 2:H:362:PHE:CE2    | 4:J:184:PHE:HZ     | 2.19                     | 0.59              |
| 4:J:61:HIS:CB      | 4:J:63:LEU:HD13    | 2.30                     | 0.59              |
| 6:L:33:PHE:O       | 6:L:35:GLY:N       | 2.34                     | 0.59              |
| 1:A:60:ILE:HD12    | 1:A:84:PRO:HD2     | 1.83                     | 0.59              |
| 1:A:180:PHE:CD2    | 4:D:192:THR:HB     | 2.37                     | 0.59              |
| 1:A:220:THR:C      | 1:A:222:SER:H      | 2.10                     | 0.59              |
| 4:D:37:LEU:C       | 4:D:37:LEU:CD2     | 2.75                     | 0.59              |
| 4:D:235:PHE:O      | 4:D:237:PRO:HD3    | 2.02                     | 0.59              |
| 1:G:62:GLY:O       | 1:G:63:ILE:HB      | 2.01                     | 0.59              |
| 2:H:135:LEU:HD12   | 2:H:232:GLY:HA2    | 1.83                     | 0.59              |
| 2:H:445:THR:OG1    | 2:H:446:SER:N      | 2.34                     | 0.59              |
| 3:I:287:THR:HG22   | 3:I:430:HIS:HB2    | 1.82                     | 0.59              |
| 4:J:62:GLY:C       | 4:J:63:LEU:HD12    | 2.27                     | 0.59              |
| 4:J:235:PHE:O      | 4:J:237:PRO:HD3    | 2.01                     | 0.59              |
| 1:A:104:GLU:OE2    | 7:O:36:UNK:CB      | 2.50                     | 0.59              |
| 2:B:25:MET:HE1     | 2:B:108:PHE:CD1    | 2.36                     | 0.59              |
| 3:C:284:PHE:O      | 3:C:285:ILE:C      | 2.45                     | 0.59              |
| 3:C:390:ARG:HD2    | 9:V:100:ILE:HD12   | 1.84                     | 0.59              |
| 1:G:143:ILE:HG13   | 4:J:220:ASN:ND2    | 2.08                     | 0.59              |
| 1:G:175:GLY:N      | 12:G:1345:PHO:H192 | 2.13                     | 0.59              |
| 1:G:220:THR:C      | 1:G:222:SER:H      | 2.10                     | 0.59              |
| 11:G:1344:CLA:HED3 | 4:J:175:VAL:HG13   | 1.82                     | 0.59              |
| 2:H:135:LEU:HD22   | 2:H:237:VAL:HG21   | 1.83                     | 0.59              |
| 2:H:272:ARG:HG2    | 2:H:273:TYR:CD2    | 2.36                     | 0.59              |
| 1:A:99:ALA:HB2     | 1:A:104:GLU:OE1    | 2.02                     | 0.59              |
| 2:B:172:TYR:HA     | 2:B:280:PHE:CE1    | 2.37                     | 0.59              |
| 3:C:54:VAL:HB      | 3:C:129:GLY:HA2    | 1.84                     | 0.59              |
| 2:H:113:TRP:HD1    | 11:H:1496:CLA:H191 | 1.67                     | 0.59              |
| 2:H:446:SER:HB2    | 2:H:447:PRO:HD2    | 1.85                     | 0.59              |
| 3:I:297:TYR:HD1    | 3:I:302:TYR:CZ     | 2.20                     | 0.59              |
| 4:J:46:GLY:O       | 4:J:47:GLY:C       | 2.45                     | 0.59              |
| 6:L:16:PHE:CZ      | 10:Y:557:UNK:HA    | 2.37                     | 0.59              |
| 10:X:200:UNK:O     | 10:X:204:UNK:N     | 2.35                     | 0.59              |
| 1:A:159:LEU:O      | 1:A:163:ILE:HG13   | 2.03                     | 0.59              |
| 1:A:311:GLY:HA3    | 9:V:125:ILE:HG21   | 1.83                     | 0.59              |
| 3:C:35:TRP:C       | 3:C:37:ALA:N       | 2.57                     | 0.59              |
| 3:C:63:TRP:HE1     | 11:C:1462:CLA:C2C  | 2.15                     | 0.59              |
| 2:H:347:ARG:HD2    | 2:H:398:THR:CB     | 2.32                     | 0.59              |
| 10:X:182:UNK:O     | 10:X:184:UNK:N     | 2.36                     | 0.59              |
| 10:Y:331:UNK:O     | 10:Y:334:UNK:N     | 2.35                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:192:ILE:O      | 1:A:195:HIS:N      | 2.35                     | 0.59              |
| 1:A:214:MET:HA     | 1:A:217:SER:HB3    | 1.85                     | 0.59              |
| 2:B:313:ASP:O      | 2:B:314:TYR:O      | 2.18                     | 0.59              |
| 2:B:347:ARG:HD2    | 2:B:398:THR:CB     | 2.33                     | 0.59              |
| 3:C:188:THR:HG21   | 3:C:298:PRO:HB3    | 1.84                     | 0.59              |
| 5:E:37:PHE:CE1     | 5:E:42:LEU:HB3     | 2.38                     | 0.59              |
| 1:G:104:GLU:HG2    | 1:G:108:ASN:ND2    | 2.18                     | 0.59              |
| 1:G:297:LEU:HD23   | 3:I:428:THR:HG21   | 1.84                     | 0.59              |
| 2:H:106:LEU:HD22   | 11:H:1496:CLA:H143 | 1.84                     | 0.59              |
| 11:H:1488:CLA:H171 | 4:J:281:MET:CE     | 2.30                     | 0.59              |
| 11:H:1496:CLA:H152 | 11:H:1497:CLA:HMD2 | 1.85                     | 0.59              |
| 4:J:87:HIS:HE1     | 4:J:161:PRO:O      | 1.85                     | 0.59              |
| 5:K:10:PHE:CD2     | 6:L:19:ARG:NH2     | 2.70                     | 0.59              |
| 7:O:82:UNK:O       | 7:O:90:UNK:CB      | 2.50                     | 0.59              |
| 10:Y:357:UNK:O     | 10:Y:361:UNK:N     | 2.36                     | 0.59              |
| 1:A:96:ILE:O       | 1:A:96:ILE:HG12    | 2.01                     | 0.59              |
| 2:B:236:THR:HB     | 2:B:473:THR:HG21   | 1.85                     | 0.59              |
| 2:B:270:PRO:C      | 2:B:271:THR:HG23   | 2.27                     | 0.59              |
| 2:B:415:PRO:O      | 2:B:419:SER:N      | 2.32                     | 0.59              |
| 3:C:248:GLY:O      | 3:C:252:ILE:HG13   | 2.03                     | 0.59              |
| 4:D:61:HIS:CB      | 4:D:63:LEU:HD13    | 2.32                     | 0.59              |
| 4:D:152:VAL:CG2    | 4:D:279:LEU:HB3    | 2.32                     | 0.59              |
| 5:E:74:GLN:O       | 5:E:77:GLU:N       | 2.36                     | 0.59              |
| 2:H:166:MET:HE1    | 2:H:198:VAL:HG11   | 1.85                     | 0.59              |
| 2:H:396:GLY:C      | 2:H:398:THR:N      | 2.60                     | 0.59              |
| 3:I:318:LEU:HD12   | 3:I:318:LEU:C      | 2.27                     | 0.59              |
| 7:O:123:UNK:O      | 7:O:124:UNK:C      | 2.50                     | 0.59              |
| 1:A:78:ILE:HG23    | 1:A:176:ILE:HG21   | 1.84                     | 0.59              |
| 1:A:83:VAL:HG22    | 4:D:314:PHE:HE1    | 1.66                     | 0.59              |
| 2:B:193:TYR:CE1    | 2:B:259:GLY:HA2    | 2.38                     | 0.59              |
| 2:B:220:ARG:HB3    | 2:B:221:PRO:HD2    | 1.83                     | 0.59              |
| 3:C:150:ASP:O      | 3:C:151:TRP:C      | 2.46                     | 0.59              |
| 3:C:433:LEU:O      | 3:C:434:ALA:C      | 2.44                     | 0.59              |
| 4:D:89:LEU:O       | 4:D:90:LEU:C       | 2.46                     | 0.59              |
| 6:F:16:PHE:CZ      | 10:X:557:UNK:HA    | 2.38                     | 0.59              |
| 11:G:1342:CLA:HBD  | 11:G:1343:CLA:HAC2 | 1.85                     | 0.59              |
| 3:I:116:VAL:O      | 3:I:117:VAL:C      | 2.46                     | 0.59              |
| 7:P:75:UNK:O       | 7:P:76:UNK:C       | 2.51                     | 0.59              |
| 8:S:30:UNK:O       | 8:S:31:UNK:C       | 2.51                     | 0.59              |
| 10:Y:357:UNK:O     | 10:Y:360:UNK:N     | 2.35                     | 0.59              |
| 1:A:267:ASN:O      | 1:A:268:SER:C      | 2.45                     | 0.59              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 3:C:126:GLY:O    | 3:C:130:VAL:HG23   | 2.03                     | 0.59              |
| 3:C:188:THR:CG2  | 3:C:298:PRO:HB3    | 2.32                     | 0.59              |
| 4:D:161:PRO:HB3  | 4:D:167:TRP:HA     | 1.85                     | 0.59              |
| 4:D:209:LEU:HD21 | 4:D:213:ILE:HD11   | 1.85                     | 0.59              |
| 1:G:49:VAL:O     | 1:G:53:ILE:HG13    | 2.03                     | 0.59              |
| 1:G:131:TRP:HB2  | 1:G:144:CYS:HB2    | 1.85                     | 0.59              |
| 1:G:134:SER:HA   | 1:G:139:MET:HB3    | 1.84                     | 0.59              |
| 2:H:275:TRP:CD1  | 2:H:318:ASN:HD22   | 2.20                     | 0.59              |
| 3:I:116:VAL:HG23 | 3:I:117:VAL:H      | 1.68                     | 0.59              |
| 3:I:266:TRP:N    | 3:I:266:TRP:CD1    | 2.71                     | 0.59              |
| 10:Y:118:UNK:O   | 10:Y:119:UNK:C     | 2.49                     | 0.59              |
| 1:A:90:GLY:O     | 1:A:167:SER:HA     | 2.02                     | 0.59              |
| 2:B:194:ASN:O    | 2:B:195:PRO:C      | 2.43                     | 0.59              |
| 2:B:353:GLU:O    | 2:B:354:LEU:O      | 2.21                     | 0.59              |
| 1:G:84:PRO:HA    | 1:G:112:TYR:CG     | 2.38                     | 0.59              |
| 4:J:347:PRO:O    | 4:J:348:ARG:CB     | 2.51                     | 0.59              |
| 6:L:18:VAL:O     | 6:L:21:VAL:N       | 2.36                     | 0.59              |
| 7:P:88:UNK:O     | 7:P:139:UNK:HA     | 2.02                     | 0.59              |
| 8:S:44:UNK:O     | 8:S:45:UNK:C       | 2.50                     | 0.59              |
| 1:A:60:ILE:HB    | 1:A:83:VAL:HG12    | 1.85                     | 0.58              |
| 1:A:63:ILE:CG1   | 1:A:64:ARG:N       | 2.64                     | 0.58              |
| 1:A:85:SER:HA    | 1:A:109:GLY:O      | 2.03                     | 0.58              |
| 2:B:229:LEU:C    | 2:B:231:MET:N      | 2.50                     | 0.58              |
| 2:B:470:GLY:O    | 2:B:473:THR:HB     | 2.03                     | 0.58              |
| 3:C:250:TRP:CD1  | 3:C:250:TRP:O      | 2.56                     | 0.58              |
| 2:H:398:THR:C    | 2:H:400:SER:N      | 2.57                     | 0.58              |
| 3:I:163:PHE:O    | 11:I:1470:CLA:HBB1 | 2.03                     | 0.58              |
| 4:J:171:PRO:HG3  | 4:J:181:PHE:CD1    | 2.38                     | 0.58              |
| 5:K:58:GLN:HE22  | 9:T:4:THR:CG2      | 2.15                     | 0.58              |
| 1:A:326:LEU:C    | 1:A:328:MET:H      | 2.09                     | 0.58              |
| 2:B:24:LEU:HD23  | 2:B:110:ALA:C      | 2.28                     | 0.58              |
| 2:B:31:ALA:N     | 11:B:1486:CLA:HBC3 | 2.18                     | 0.58              |
| 2:B:63:LEU:O     | 2:B:64:PRO:C       | 2.45                     | 0.58              |
| 2:B:167:TRP:CB   | 2:B:267:LEU:HD11   | 2.33                     | 0.58              |
| 3:C:116:VAL:O    | 3:C:117:VAL:C      | 2.46                     | 0.58              |
| 4:D:274:VAL:HB   | 4:D:275:PRO:CD     | 2.32                     | 0.58              |
| 4:D:313:THR:C    | 4:D:315:TYR:N      | 2.60                     | 0.58              |
| 5:E:58:GLN:HE22  | 9:V:4:THR:CG2      | 2.16                     | 0.58              |
| 1:G:114:LEU:HA   | 11:G:1346:CLA:CED  | 2.24                     | 0.58              |
| 2:H:351:GLY:O    | 2:H:353:GLU:N      | 2.36                     | 0.58              |
| 4:J:46:GLY:HA2   | 4:J:49:LEU:HD12    | 1.85                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:J:52:THR:CG2     | 4:J:67:TYR:HE1     | 2.01                     | 0.58              |
| 9:T:4:THR:HB       | 9:T:5:PRO:CD       | 2.33                     | 0.58              |
| 10:Y:224:UNK:O     | 10:Y:227:UNK:N     | 2.36                     | 0.58              |
| 1:A:131:TRP:O      | 1:A:134:SER:HB2    | 2.04                     | 0.58              |
| 1:A:134:SER:C      | 1:A:136:ARG:H      | 2.10                     | 0.58              |
| 2:B:109:LEU:O      | 2:B:112:CYS:HB2    | 2.03                     | 0.58              |
| 3:C:264:PHE:HD1    | 3:C:274:TYR:CE1    | 2.21                     | 0.58              |
| 4:D:183:LEU:O      | 4:D:184:PHE:C      | 2.46                     | 0.58              |
| 1:G:137:LEU:HB2    | 1:G:139:MET:CE     | 2.33                     | 0.58              |
| 2:H:172:TYR:O      | 2:H:174:LEU:HG     | 2.03                     | 0.58              |
| 2:H:353:GLU:O      | 2:H:354:LEU:O      | 2.21                     | 0.58              |
| 3:I:276:LEU:CD1    | 11:I:1466:CLA:HBB1 | 2.33                     | 0.58              |
| 2:B:76:SER:O       | 7:P:66:UNK:CA      | 2.52                     | 0.58              |
| 2:B:201:HIS:CD2    | 2:B:202:HIS:ND1    | 2.71                     | 0.58              |
| 3:C:228:ASN:OD1    | 3:C:229:ASN:N      | 2.36                     | 0.58              |
| 4:D:79:SER:HA      | 4:D:172:SER:HB3    | 1.85                     | 0.58              |
| 4:D:191:TRP:CZ2    | 4:D:286:VAL:HG22   | 2.39                     | 0.58              |
| 4:D:302:GLU:OE1    | 7:O:114:UNK:CB     | 2.52                     | 0.58              |
| 5:E:10:PHE:CD2     | 6:F:19:ARG:NH2     | 2.72                     | 0.58              |
| 1:G:90:GLY:O       | 1:G:167:SER:HA     | 2.03                     | 0.58              |
| 2:H:17:GLY:O       | 2:H:20:ILE:HB      | 2.03                     | 0.58              |
| 2:H:332:LYS:O      | 2:H:439:SER:CA     | 2.51                     | 0.58              |
| 3:I:82:TYR:HB3     | 3:I:302:TYR:C      | 2.28                     | 0.58              |
| 3:I:250:TRP:CD1    | 3:I:250:TRP:C      | 2.81                     | 0.58              |
| 4:J:126:MET:HE1    | 4:J:147:SER:N      | 2.19                     | 0.58              |
| 4:J:152:VAL:HG11   | 11:J:1351:CLA:HBA1 | 1.84                     | 0.58              |
| 7:P:105:UNK:O      | 7:P:106:UNK:CB     | 2.50                     | 0.58              |
| 10:X:578:UNK:C     | 10:X:580:UNK:N     | 2.64                     | 0.58              |
| 3:C:320:ARG:NH1    | 9:V:49:ASN:OD1     | 2.36                     | 0.58              |
| 4:D:36:LEU:HD23    | 11:D:1353:CLA:HBB2 | 1.84                     | 0.58              |
| 11:G:1342:CLA:H143 | 12:G:1345:PHO:H62  | 1.85                     | 0.58              |
| 2:H:318:ASN:C      | 2:H:318:ASN:OD1    | 2.47                     | 0.58              |
| 3:I:156:LYS:O      | 3:I:160:ILE:HG13   | 2.03                     | 0.58              |
| 4:J:40:CYS:O       | 4:J:41:ALA:C       | 2.46                     | 0.58              |
| 4:J:65:SER:HB2     | 4:J:77:ALA:O       | 2.02                     | 0.58              |
| 4:J:87:HIS:HE1     | 4:J:162:LEU:HA     | 1.66                     | 0.58              |
| 4:J:191:TRP:CZ2    | 4:J:286:VAL:HG22   | 2.39                     | 0.58              |
| 1:A:157:VAL:CG1    | 1:A:172:MET:HB3    | 2.34                     | 0.58              |
| 2:B:372:ASP:N      | 2:B:376:VAL:O      | 2.31                     | 0.58              |
| 2:B:435:GLU:O      | 2:B:436:THR:CB     | 2.48                     | 0.58              |
| 4:D:126:MET:HE2    | 4:D:143:ALA:O      | 2.03                     | 0.58              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 5:E:59:GLU:O     | 5:E:60:GLN:CB      | 2.49                     | 0.58              |
| 1:G:157:VAL:CG1  | 1:G:172:MET:HB3    | 2.34                     | 0.58              |
| 1:G:161:TYR:CE2  | 1:G:186:PHE:CE1    | 2.89                     | 0.58              |
| 1:G:161:TYR:HB3  | 1:G:162:PRO:HD3    | 1.86                     | 0.58              |
| 2:H:53:ASN:N     | 2:H:54:PRO:CD      | 2.62                     | 0.58              |
| 3:I:291:TRP:HD1  | 3:I:292:PHE:CD2    | 2.21                     | 0.58              |
| 3:I:362:ARG:HH11 | 3:I:362:ARG:HG3    | 1.69                     | 0.58              |
| 9:V:134:LYS:C    | 9:V:137:TYR:H      | 2.12                     | 0.58              |
| 1:A:244:GLU:OE2  | 1:A:246:TYR:CE1    | 2.57                     | 0.58              |
| 3:C:36:TRP:O     | 11:C:1466:CLA:H43  | 2.04                     | 0.58              |
| 3:C:82:TYR:HB3   | 3:C:302:TYR:C      | 2.29                     | 0.58              |
| 1:G:107:TYR:C    | 1:G:109:GLY:N      | 2.59                     | 0.58              |
| 1:A:85:SER:OG    | 1:A:113:GLN:HG3    | 2.04                     | 0.58              |
| 1:A:98:GLU:O     | 1:A:99:ALA:HB3     | 2.02                     | 0.58              |
| 3:C:283:GLY:O    | 3:C:286:ALA:HB3    | 2.02                     | 0.58              |
| 3:C:315:MET:O    | 3:C:319:ILE:CG1    | 2.52                     | 0.58              |
| 4:D:93:TRP:HH2   | 11:D:1353:CLA:HBA2 | 1.69                     | 0.58              |
| 1:G:137:LEU:HD12 | 1:G:139:MET:CE     | 2.29                     | 0.58              |
| 2:H:163:GLY:O    | 2:H:165:GLY:N      | 2.35                     | 0.58              |
| 5:K:15:THR:O     | 5:K:15:THR:HG22    | 2.02                     | 0.58              |
| 6:L:33:PHE:C     | 6:L:35:GLY:N       | 2.60                     | 0.58              |
| 10:Y:519:UNK:O   | 10:Y:522:UNK:N     | 2.36                     | 0.58              |
| 1:A:207:GLY:O    | 1:A:210:LEU:N      | 2.37                     | 0.58              |
| 2:B:425:ILE:O    | 2:B:426:PHE:HB3    | 2.03                     | 0.58              |
| 3:C:56:HIS:ND1   | 11:C:1467:CLA:HHB  | 2.18                     | 0.58              |
| 3:C:235:GLY:HA2  | 3:C:238:ILE:HD12   | 1.84                     | 0.58              |
| 3:C:363:GLY:O    | 3:C:364:PRO:O      | 2.21                     | 0.58              |
| 1:G:131:TRP:O    | 1:G:134:SER:HB2    | 2.03                     | 0.58              |
| 1:G:176:ILE:HG23 | 1:G:180:PHE:CE1    | 2.39                     | 0.58              |
| 1:G:328:MET:HE2  | 4:J:325:ILE:CD1    | 2.34                     | 0.58              |
| 2:H:30:VAL:HB    | 11:H:1486:CLA:HBC1 | 1.86                     | 0.58              |
| 2:H:31:ALA:HA    | 2:H:34:ALA:CB      | 2.29                     | 0.58              |
| 3:I:73:ALA:HB3   | 3:I:74:HIS:HD2     | 1.69                     | 0.58              |
| 3:I:109:PHE:HB3  | 3:I:110:PRO:HD3    | 1.85                     | 0.58              |
| 4:J:148:ALA:HB3  | 4:J:149:PRO:CD     | 2.30                     | 0.58              |
| 1:A:63:ILE:CG1   | 3:C:335:THR:CG2    | 2.75                     | 0.58              |
| 1:A:215:HIS:HB3  | 4:D:271:MET:HE1    | 1.85                     | 0.58              |
| 4:D:52:THR:CG2   | 4:D:67:TYR:HE1     | 2.00                     | 0.58              |
| 4:D:184:PHE:C    | 4:D:184:PHE:CD1    | 2.80                     | 0.58              |
| 4:D:209:LEU:C    | 4:D:209:LEU:CD2    | 2.77                     | 0.58              |
| 5:E:63:ILE:HG22  | 5:E:63:ILE:O       | 2.03                     | 0.58              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:H:243:ALA:O     | 2:H:246:PHE:HB3    | 2.04                     | 0.58              |
| 2:H:425:ILE:O     | 2:H:426:PHE:HB3    | 2.02                     | 0.58              |
| 3:I:248:GLY:O     | 3:I:252:ILE:HG13   | 2.03                     | 0.58              |
| 4:J:225:ASP:OD1   | 4:J:225:ASP:O      | 2.21                     | 0.58              |
| 7:O:64:UNK:HA     | 7:O:70:UNK:O       | 2.04                     | 0.58              |
| 9:V:4:THR:HB      | 9:V:5:PRO:CD       | 2.33                     | 0.58              |
| 2:B:53:ASN:N      | 2:B:54:PRO:CD      | 2.62                     | 0.57              |
| 2:B:394:GLN:O     | 2:B:395:GLN:CB     | 2.51                     | 0.57              |
| 1:G:310:LYS:HA    | 9:T:2:GLU:CA       | 2.27                     | 0.57              |
| 2:H:161:LEU:O     | 2:H:162:PHE:CB     | 2.52                     | 0.57              |
| 2:H:280:PHE:CZ    | 2:H:312:TYR:HD2    | 2.22                     | 0.57              |
| 8:U:1:UNK:O       | 8:U:3:UNK:N        | 2.36                     | 0.57              |
| 9:V:48:THR:OG1    | 18:V:1138:HEC:HMD3 | 2.04                     | 0.57              |
| 2:B:161:LEU:O     | 2:B:162:PHE:CB     | 2.51                     | 0.57              |
| 3:C:21:ILE:O      | 3:C:22:PHE:CB      | 2.53                     | 0.57              |
| 3:C:97:TRP:CZ3    | 3:C:178:LYS:NZ     | 2.72                     | 0.57              |
| 3:C:116:VAL:CG2   | 3:C:117:VAL:N      | 2.67                     | 0.57              |
| 4:D:160:TYR:HB3   | 4:D:161:PRO:CD     | 2.28                     | 0.57              |
| 1:G:288:LEU:HD13  | 3:I:432:VAL:HG22   | 1.86                     | 0.57              |
| 12:G:1345:PHO:CBB | 4:J:205:LEU:HD21   | 2.34                     | 0.57              |
| 2:H:94:GLU:CG     | 2:H:95:GLY:N       | 2.66                     | 0.57              |
| 2:H:265:ILE:HD12  | 2:H:270:PRO:HA     | 1.87                     | 0.57              |
| 2:H:313:ASP:O     | 2:H:314:TYR:O      | 2.21                     | 0.57              |
| 3:I:225:VAL:HG22  | 3:I:289:PHE:CD1    | 2.39                     | 0.57              |
| 3:I:252:ILE:O     | 3:I:253:LEU:C      | 2.46                     | 0.57              |
| 4:J:152:VAL:CG2   | 4:J:279:LEU:HB3    | 2.34                     | 0.57              |
| 1:A:126:TYR:O     | 1:A:130:GLN:HB2    | 2.05                     | 0.57              |
| 1:A:131:TRP:HB2   | 1:A:144:CYS:HB2    | 1.86                     | 0.57              |
| 1:A:142:TRP:CH2   | 1:A:273:PHE:CE1    | 2.92                     | 0.57              |
| 2:B:398:THR:C     | 2:B:400:SER:N      | 2.60                     | 0.57              |
| 4:D:46:GLY:O      | 4:D:47:GLY:C       | 2.46                     | 0.57              |
| 4:D:56:THR:N      | 5:E:49:THR:HG22    | 2.19                     | 0.57              |
| 4:D:148:ALA:HB3   | 4:D:149:PRO:CD     | 2.32                     | 0.57              |
| 4:D:235:PHE:HD2   | 4:D:243:THR:CG2    | 2.17                     | 0.57              |
| 4:D:330:ALA:O     | 4:D:332:GLN:N      | 2.37                     | 0.57              |
| 2:H:18:ARG:O      | 2:H:21:ALA:HB3     | 2.05                     | 0.57              |
| 2:H:68:ARG:HB3    | 2:H:267:LEU:HD13   | 1.85                     | 0.57              |
| 2:H:221:PRO:HB3   | 11:H:1490:CLA:HED3 | 1.85                     | 0.57              |
| 3:I:433:LEU:O     | 3:I:434:ALA:C      | 2.47                     | 0.57              |
| 4:J:302:GLU:OE1   | 7:P:114:UNK:CB     | 2.51                     | 0.57              |
| 9:T:100:ILE:C     | 9:T:102:PRO:HD3    | 2.29                     | 0.57              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 4:D:52:THR:O     | 4:D:66:SER:HA      | 2.04                     | 0.57              |
| 4:D:267:LEU:O    | 4:D:271:MET:HG3    | 2.04                     | 0.57              |
| 1:G:98:GLU:O     | 1:G:99:ALA:CB      | 2.52                     | 0.57              |
| 1:G:142:TRP:CH2  | 1:G:273:PHE:CE1    | 2.93                     | 0.57              |
| 2:H:27:THR:O     | 11:H:1486:CLA:HBC1 | 2.05                     | 0.57              |
| 4:J:179:PHE:HA   | 4:J:182:LEU:HD12   | 1.87                     | 0.57              |
| 7:O:10:UNK:O     | 7:O:173:UNK:CB     | 2.53                     | 0.57              |
| 8:S:59:UNK:C     | 8:S:61:UNK:N       | 2.67                     | 0.57              |
| 1:A:34:GLY:C     | 1:A:36:ILE:H       | 2.12                     | 0.57              |
| 1:A:35:VAL:O     | 1:A:35:VAL:HG12    | 2.04                     | 0.57              |
| 1:A:97:TRP:O     | 1:A:98:GLU:C       | 2.47                     | 0.57              |
| 1:A:114:LEU:HA   | 11:A:1346:CLA:CED  | 2.28                     | 0.57              |
| 1:A:183:MET:HE2  | 11:A:1343:CLA:HAC1 | 1.85                     | 0.57              |
| 2:B:24:LEU:HB3   | 2:B:111:ALA:HB2    | 1.87                     | 0.57              |
| 2:B:113:TRP:HD1  | 11:B:1496:CLA:H191 | 1.69                     | 0.57              |
| 3:C:163:PHE:O    | 11:C:1470:CLA:HBB1 | 2.05                     | 0.57              |
| 4:D:152:VAL:CG2  | 4:D:279:LEU:HD13   | 2.34                     | 0.57              |
| 1:G:290:ILE:C    | 1:G:292:THR:N      | 2.59                     | 0.57              |
| 2:H:424:ALA:O    | 2:H:426:PHE:N      | 2.37                     | 0.57              |
| 4:J:156:VAL:O    | 4:J:156:VAL:HG12   | 2.04                     | 0.57              |
| 7:P:24:UNK:O     | 7:P:25:UNK:O       | 2.23                     | 0.57              |
| 8:U:27:UNK:O     | 8:U:28:UNK:C       | 2.51                     | 0.57              |
| 2:B:293:ALA:O    | 2:B:295:GLY:N      | 2.37                     | 0.57              |
| 2:B:360:PRO:O    | 2:B:361:ALA:HB3    | 2.05                     | 0.57              |
| 1:G:246:TYR:O    | 1:G:247:ASN:CG     | 2.47                     | 0.57              |
| 2:H:24:LEU:HD23  | 2:H:111:ALA:CA     | 2.33                     | 0.57              |
| 3:I:235:GLY:O    | 3:I:238:ILE:HB     | 2.05                     | 0.57              |
| 4:J:296:TYR:HE1  | 4:J:322:ASN:HD22   | 1.51                     | 0.57              |
| 7:O:107:UNK:O    | 7:O:108:UNK:CB     | 2.52                     | 0.57              |
| 8:S:90:UNK:O     | 8:S:91:UNK:C       | 2.51                     | 0.57              |
| 10:X:468:UNK:O   | 10:X:469:UNK:C     | 2.52                     | 0.57              |
| 1:A:219:VAL:HG21 | 4:D:268:HIS:HD2    | 1.68                     | 0.57              |
| 2:B:272:ARG:HG2  | 2:B:273:TYR:CD2    | 2.39                     | 0.57              |
| 3:C:259:TRP:HZ3  | 11:C:1464:CLA:H12  | 1.69                     | 0.57              |
| 4:D:191:TRP:HZ3  | 4:D:194:ASN:ND2    | 2.03                     | 0.57              |
| 4:D:313:THR:C    | 4:D:315:TYR:H      | 2.12                     | 0.57              |
| 4:D:323:GLU:CG   | 4:D:326:ARG:HH21   | 2.13                     | 0.57              |
| 1:G:192:ILE:O    | 1:G:195:HIS:N      | 2.38                     | 0.57              |
| 1:G:298:ASN:OD1  | 1:G:298:ASN:N      | 2.38                     | 0.57              |
| 1:G:331:MET:O    | 1:G:332:HIS:O      | 2.21                     | 0.57              |
| 3:I:161:LEU:O    | 3:I:164:HIS:HB2    | 2.04                     | 0.57              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:J:63:LEU:HD12   | 4:J:63:LEU:N       | 2.19                     | 0.57              |
| 4:J:111:TRP:O     | 4:J:112:THR:C      | 2.47                     | 0.57              |
| 4:J:235:PHE:HD2   | 4:J:243:THR:CG2    | 2.16                     | 0.57              |
| 1:G:207:GLY:O     | 1:G:210:LEU:N      | 2.38                     | 0.57              |
| 12:G:1345:PHO:CAB | 4:J:205:LEU:HD21   | 2.34                     | 0.57              |
| 2:H:435:GLU:O     | 2:H:436:THR:CB     | 2.50                     | 0.57              |
| 3:I:21:ILE:O      | 3:I:22:PHE:CB      | 2.52                     | 0.57              |
| 3:I:228:ASN:OD1   | 3:I:229:ASN:N      | 2.38                     | 0.57              |
| 3:I:264:PHE:HD1   | 3:I:274:TYR:CE1    | 2.23                     | 0.57              |
| 4:J:57:SER:O      | 4:J:59:TYR:N       | 2.38                     | 0.57              |
| 8:S:64:UNK:O      | 8:S:65:UNK:C       | 2.52                     | 0.57              |
| 8:U:92:UNK:O      | 8:U:93:UNK:CB      | 2.52                     | 0.57              |
| 1:A:116:ILE:HG22  | 1:A:117:PHE:N      | 2.19                     | 0.57              |
| 3:C:276:LEU:HD12  | 3:C:276:LEU:O      | 2.05                     | 0.57              |
| 2:H:458:PHE:HB3   | 11:H:1485:CLA:HBC2 | 1.86                     | 0.57              |
| 3:I:377:LEU:O     | 3:I:381:LYS:HD3    | 2.05                     | 0.57              |
| 4:J:325:ILE:O     | 4:J:329:MET:HB3    | 2.05                     | 0.57              |
| 4:J:331:PRO:CG    | 4:J:339:PHE:HB2    | 2.24                     | 0.57              |
| 6:L:36:ALA:O      | 6:L:39:ALA:HB3     | 2.05                     | 0.57              |
| 1:A:137:LEU:CD1   | 1:A:139:MET:HE1    | 2.30                     | 0.57              |
| 2:B:275:TRP:CD1   | 2:B:318:ASN:HD22   | 2.22                     | 0.57              |
| 3:C:266:TRP:N     | 3:C:266:TRP:CD1    | 2.73                     | 0.57              |
| 4:D:191:TRP:CE3   | 4:D:191:TRP:HA     | 2.40                     | 0.57              |
| 6:F:33:PHE:O      | 6:F:35:GLY:N       | 2.37                     | 0.57              |
| 2:H:474:LEU:HG    | 11:H:1489:CLA:HED1 | 1.86                     | 0.57              |
| 3:I:116:VAL:CG2   | 3:I:117:VAL:H      | 2.18                     | 0.57              |
| 3:I:283:GLY:O     | 3:I:286:ALA:HB3    | 2.04                     | 0.57              |
| 4:J:152:VAL:CG2   | 4:J:279:LEU:HD13   | 2.34                     | 0.57              |
| 7:P:82:UNK:O      | 7:P:90:UNK:CB      | 2.53                     | 0.57              |
| 8:U:12:UNK:C      | 8:U:14:UNK:N       | 2.66                     | 0.57              |
| 9:V:133:GLY:O     | 9:V:137:TYR:CA     | 2.53                     | 0.57              |
| 1:A:156:ALA:HA    | 1:A:160:ILE:HB     | 1.87                     | 0.56              |
| 2:B:309:LEU:O     | 2:B:310:ALA:C      | 2.48                     | 0.56              |
| 1:G:151:LEU:HG    | 1:G:155:PHE:HE2    | 1.70                     | 0.56              |
| 1:G:248:ILE:CD1   | 4:J:235:PHE:CZ     | 2.88                     | 0.56              |
| 1:G:331:MET:O     | 1:G:332:HIS:C      | 2.46                     | 0.56              |
| 2:H:360:PRO:O     | 2:H:361:ALA:HB3    | 2.05                     | 0.56              |
| 5:K:59:GLU:O      | 5:K:60:GLN:CB      | 2.50                     | 0.56              |
| 8:S:57:UNK:C      | 8:S:59:UNK:N       | 2.62                     | 0.56              |
| 8:U:40:UNK:O      | 8:U:41:UNK:C       | 2.53                     | 0.56              |
| 8:U:71:UNK:O      | 8:U:74:UNK:N       | 2.38                     | 0.56              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:A:107:TYR:O    | 1:A:109:GLY:N      | 2.38                     | 0.56              |
| 2:B:27:THR:O     | 11:B:1486:CLA:HBC1 | 2.05                     | 0.56              |
| 2:B:474:LEU:HG   | 11:B:1489:CLA:HED1 | 1.86                     | 0.56              |
| 4:D:235:PHE:HE1  | 4:D:237:PRO:HB3    | 1.70                     | 0.56              |
| 1:G:207:GLY:O    | 1:G:210:LEU:HB3    | 2.05                     | 0.56              |
| 1:G:214:MET:O    | 1:G:217:SER:N      | 2.38                     | 0.56              |
| 2:H:330:MET:CE   | 2:H:446:SER:HB3    | 2.18                     | 0.56              |
| 2:H:397:VAL:O    | 2:H:411:PHE:O      | 2.23                     | 0.56              |
| 4:J:263:ASN:O    | 4:J:265:ARG:N      | 2.38                     | 0.56              |
| 6:L:37:ILE:HG12  | 6:L:40:MET:CE      | 2.35                     | 0.56              |
| 8:S:92:UNK:O     | 8:S:93:UNK:CB      | 2.51                     | 0.56              |
| 8:U:59:UNK:C     | 8:U:61:UNK:N       | 2.69                     | 0.56              |
| 10:X:357:UNK:O   | 10:X:361:UNK:N     | 2.38                     | 0.56              |
| 1:A:132:GLU:C    | 1:A:134:SER:H      | 2.13                     | 0.56              |
| 1:A:248:ILE:CD1  | 4:D:235:PHE:CZ     | 2.88                     | 0.56              |
| 2:B:144:PHE:HE1  | 2:B:210:ILE:HG23   | 1.69                     | 0.56              |
| 2:B:364:GLU:OE1  | 4:D:296:TYR:CD2    | 2.58                     | 0.56              |
| 2:B:450:TRP:NE1  | 11:B:1488:CLA:HBA1 | 2.19                     | 0.56              |
| 2:B:458:PHE:HB3  | 11:B:1485:CLA:HBC2 | 1.87                     | 0.56              |
| 2:B:473:THR:HG21 | 11:B:1489:CLA:HED3 | 1.86                     | 0.56              |
| 3:C:252:ILE:O    | 3:C:253:LEU:C      | 2.49                     | 0.56              |
| 3:C:284:PHE:HE1  | 3:C:431:PHE:CD1    | 2.24                     | 0.56              |
| 3:C:297:TYR:HD1  | 3:C:302:TYR:CZ     | 2.23                     | 0.56              |
| 4:D:57:SER:O     | 4:D:58:TRP:C       | 2.47                     | 0.56              |
| 5:E:62:SER:C     | 5:E:64:PRO:HD3     | 2.30                     | 0.56              |
| 1:G:116:ILE:CD1  | 1:G:158:PHE:HD1    | 2.18                     | 0.56              |
| 1:G:157:VAL:O    | 1:G:157:VAL:HG12   | 2.05                     | 0.56              |
| 1:G:258:LEU:HG   | 4:J:128:ARG:HH22   | 1.69                     | 0.56              |
| 2:H:172:TYR:HA   | 2:H:280:PHE:CE1    | 2.37                     | 0.56              |
| 2:H:174:LEU:HD11 | 2:H:309:LEU:HD21   | 1.87                     | 0.56              |
| 2:H:369:ILE:O    | 2:H:379:ALA:O      | 2.23                     | 0.56              |
| 2:H:394:GLN:O    | 2:H:395:GLN:CB     | 2.53                     | 0.56              |
| 3:I:297:TYR:HD1  | 3:I:302:TYR:CE2    | 2.23                     | 0.56              |
| 4:J:313:THR:C    | 4:J:315:TYR:N      | 2.61                     | 0.56              |
| 4:J:337:GLU:HG3  | 4:J:339:PHE:HE2    | 1.69                     | 0.56              |
| 8:S:69:UNK:O     | 8:S:70:UNK:C       | 2.53                     | 0.56              |
| 8:U:57:UNK:C     | 8:U:59:UNK:N       | 2.65                     | 0.56              |
| 10:Y:404:UNK:O   | 10:Y:408:UNK:CB    | 2.54                     | 0.56              |
| 1:A:34:GLY:C     | 1:A:36:ILE:N       | 2.62                     | 0.56              |
| 1:A:310:LYS:NZ   | 5:E:58:GLN:HG2     | 2.20                     | 0.56              |
| 2:B:150:CYS:HB2  | 11:B:1484:CLA:HMC3 | 1.88                     | 0.56              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:B:475:PHE:CE1   | 4:D:140:PRO:HG3    | 2.39                     | 0.56              |
| 11:B:1482:CLA:HBD | 11:B:1482:CLA:CGA  | 2.35                     | 0.56              |
| 3:C:258:GLY:O     | 3:C:262:ARG:NE     | 2.37                     | 0.56              |
| 2:H:144:PHE:HE1   | 2:H:210:ILE:HG23   | 1.69                     | 0.56              |
| 2:H:236:THR:CB    | 2:H:473:THR:HG21   | 2.35                     | 0.56              |
| 3:I:258:GLY:O     | 3:I:262:ARG:NE     | 2.39                     | 0.56              |
| 3:I:362:ARG:HG3   | 3:I:362:ARG:NH1    | 2.21                     | 0.56              |
| 4:J:96:GLU:OE1    | 4:J:96:GLU:HA      | 2.05                     | 0.56              |
| 4:J:236:ASN:C     | 4:J:238:THR:H      | 2.12                     | 0.56              |
| 4:J:289:LEU:HD22  | 4:J:294:ARG:HB3    | 1.87                     | 0.56              |
| 2:B:25:MET:HE1    | 2:B:108:PHE:CE1    | 2.41                     | 0.56              |
| 2:B:149:LEU:C     | 11:B:1484:CLA:HBC2 | 2.30                     | 0.56              |
| 4:D:164:GLN:NE2   | 4:D:189:HIS:HE1    | 1.95                     | 0.56              |
| 2:H:270:PRO:O     | 2:H:271:THR:CG2    | 2.53                     | 0.56              |
| 2:H:392:PHE:O     | 2:H:395:GLN:HA     | 2.05                     | 0.56              |
| 3:I:35:TRP:C      | 3:I:37:ALA:N       | 2.59                     | 0.56              |
| 10:Y:182:UNK:O    | 10:Y:184:UNK:N     | 2.39                     | 0.56              |
| 1:A:298:ASN:OD1   | 1:A:298:ASN:N      | 2.38                     | 0.56              |
| 2:B:332:LYS:O     | 2:B:439:SER:CA     | 2.54                     | 0.56              |
| 3:C:270:ALA:O     | 3:C:274:TYR:HD2    | 1.86                     | 0.56              |
| 3:C:355:THR:O     | 3:C:355:THR:HG22   | 2.04                     | 0.56              |
| 4:D:48:TRP:O      | 4:D:52:THR:OG1     | 2.20                     | 0.56              |
| 1:G:134:SER:C     | 1:G:136:ARG:H      | 2.12                     | 0.56              |
| 1:G:218:LEU:CD1   | 1:G:255:PHE:HD2    | 2.18                     | 0.56              |
| 2:H:285:ASN:O     | 2:H:289:GLN:HB2    | 2.06                     | 0.56              |
| 3:I:367:GLU:HB2   | 3:I:368:PRO:HD3    | 1.87                     | 0.56              |
| 7:P:107:UNK:O     | 7:P:108:UNK:CB     | 2.52                     | 0.56              |
| 1:A:133:LEU:HD12  | 4:D:256:ILE:HG13   | 1.87                     | 0.56              |
| 3:C:69:LEU:CD1    | 3:C:115:GLY:HA3    | 2.35                     | 0.56              |
| 1:G:93:PHE:CE1    | 1:G:95:PRO:CG      | 2.88                     | 0.56              |
| 2:H:134:ASP:O     | 2:H:136:PRO:CD     | 2.53                     | 0.56              |
| 6:L:37:ILE:HG22   | 6:L:41:GLN:HE21    | 1.69                     | 0.56              |
| 8:S:5:UNK:O       | 8:S:7:UNK:N        | 2.37                     | 0.56              |
| 8:U:90:UNK:C      | 8:U:91:UNK:O       | 2.52                     | 0.56              |
| 1:A:151:LEU:HG    | 1:A:155:PHE:HE2    | 1.71                     | 0.56              |
| 3:C:189:TRP:NE1   | 3:C:295:THR:HG22   | 2.18                     | 0.56              |
| 4:D:171:PRO:HG3   | 4:D:181:PHE:CG     | 2.40                     | 0.56              |
| 1:G:34:GLY:O      | 1:G:36:ILE:N       | 2.39                     | 0.56              |
| 1:G:69:GLY:C      | 1:G:75:ASN:OD1     | 2.49                     | 0.56              |
| 2:H:61:PHE:HZ     | 11:H:1488:CLA:HBB1 | 1.71                     | 0.56              |
| 3:I:39:ASN:ND2    | 11:I:1466:CLA:H11  | 2.20                     | 0.56              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 10:X:118:UNK:O   | 10:X:119:UNK:C     | 2.51                     | 0.56              |
| 1:A:93:PHE:C     | 1:A:95:PRO:HD3     | 2.31                     | 0.56              |
| 4:D:184:PHE:O    | 4:D:188:PHE:HB2    | 2.06                     | 0.56              |
| 1:G:315:ASN:HA   | 1:G:319:ASP:OD2    | 2.05                     | 0.56              |
| 4:J:16:ASP:O     | 4:J:19:ASP:N       | 2.39                     | 0.56              |
| 4:J:329:MET:O    | 4:J:330:ALA:C      | 2.47                     | 0.56              |
| 3:C:367:GLU:O    | 3:C:370:ARG:HB2    | 2.06                     | 0.56              |
| 4:D:45:LEU:CD2   | 4:D:49:LEU:HD11    | 2.37                     | 0.56              |
| 4:D:126:MET:HE1  | 4:D:147:SER:N      | 2.21                     | 0.56              |
| 4:D:263:ASN:O    | 4:D:265:ARG:N      | 2.39                     | 0.56              |
| 4:D:292:ASN:O    | 4:D:294:ARG:HG2    | 2.05                     | 0.56              |
| 1:G:210:LEU:C    | 1:G:210:LEU:HD12   | 2.31                     | 0.56              |
| 2:H:40:TYR:O     | 2:H:41:GLU:C       | 2.48                     | 0.56              |
| 2:H:293:ALA:O    | 2:H:295:GLY:N      | 2.39                     | 0.56              |
| 2:H:413:ASP:OD1  | 2:H:413:ASP:N      | 2.33                     | 0.56              |
| 8:S:40:UNK:O     | 8:S:41:UNK:C       | 2.54                     | 0.56              |
| 1:A:62:GLY:O     | 1:A:63:ILE:HB      | 2.04                     | 0.55              |
| 1:A:290:ILE:C    | 1:A:292:THR:N      | 2.62                     | 0.55              |
| 2:B:462:PHE:HA   | 11:B:1492:CLA:HMC2 | 1.86                     | 0.55              |
| 3:C:36:TRP:O     | 3:C:36:TRP:HE3     | 1.89                     | 0.55              |
| 3:C:72:LEU:O     | 3:C:75:PHE:N       | 2.38                     | 0.55              |
| 3:C:297:TYR:HD1  | 3:C:302:TYR:CE2    | 2.24                     | 0.55              |
| 4:D:62:GLY:C     | 4:D:63:LEU:HD12    | 2.31                     | 0.55              |
| 1:G:126:TYR:O    | 1:G:130:GLN:HB2    | 2.06                     | 0.55              |
| 1:G:132:GLU:C    | 1:G:134:SER:H      | 2.15                     | 0.55              |
| 2:H:278:SER:O    | 2:H:281:GLN:HG2    | 2.06                     | 0.55              |
| 2:H:338:GLN:O    | 2:H:339:ALA:O      | 2.23                     | 0.55              |
| 2:H:338:GLN:O    | 2:H:431:GLU:O      | 2.24                     | 0.55              |
| 4:J:160:TYR:HB3  | 4:J:161:PRO:CD     | 2.29                     | 0.55              |
| 4:J:171:PRO:HD2  | 4:J:181:PHE:CE2    | 2.36                     | 0.55              |
| 9:T:55:ARG:NH2   | 9:T:128:ASP:OD1    | 2.39                     | 0.55              |
| 10:X:404:UNK:O   | 10:X:408:UNK:CB    | 2.54                     | 0.55              |
| 3:C:424:SER:O    | 3:C:428:THR:OG1    | 2.23                     | 0.55              |
| 1:G:132:GLU:C    | 1:G:134:SER:N      | 2.63                     | 0.55              |
| 1:G:210:LEU:O    | 1:G:213:ALA:HB3    | 2.06                     | 0.55              |
| 2:H:238:LEU:HD21 | 2:H:469:HIS:CD2    | 2.41                     | 0.55              |
| 3:I:43:ILE:HG22  | 11:I:1467:CLA:CMC  | 2.35                     | 0.55              |
| 3:I:377:LEU:O    | 3:I:381:LYS:HB2    | 2.07                     | 0.55              |
| 4:J:209:LEU:C    | 4:J:209:LEU:CD2    | 2.80                     | 0.55              |
| 4:J:216:ALA:O    | 4:J:220:ASN:ND2    | 2.39                     | 0.55              |
| 8:U:5:UNK:O      | 8:U:7:UNK:N        | 2.38                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:174:LEU:HD22   | 12:A:1345:PHO:H151 | 1.88                     | 0.55              |
| 1:A:195:HIS:HE1    | 1:A:197:PHE:CD1    | 2.25                     | 0.55              |
| 2:B:138:MET:HA     | 2:B:141:ILE:HG22   | 1.89                     | 0.55              |
| 2:B:338:GLN:O      | 2:B:431:GLU:O      | 2.23                     | 0.55              |
| 3:C:227:VAL:HG11   | 3:C:233:VAL:HG23   | 1.88                     | 0.55              |
| 3:C:281:MET:O      | 3:C:282:MET:C      | 2.49                     | 0.55              |
| 5:E:74:GLN:O       | 5:E:75:GLN:C       | 2.47                     | 0.55              |
| 1:G:141:PRO:HG2    | 3:I:446:GLY:C      | 2.30                     | 0.55              |
| 1:G:207:GLY:O      | 1:G:208:GLY:C      | 2.49                     | 0.55              |
| 2:H:144:PHE:CE1    | 2:H:210:ILE:HG23   | 2.41                     | 0.55              |
| 3:I:93:ALA:O       | 3:I:94:THR:C       | 2.49                     | 0.55              |
| 3:I:186:TYR:HE2    | 3:I:188:THR:CG2    | 2.20                     | 0.55              |
| 3:I:307:PRO:HA     | 3:I:358:PHE:CD1    | 2.42                     | 0.55              |
| 2:B:61:PHE:O       | 2:B:62:VAL:C       | 2.48                     | 0.55              |
| 2:B:194:ASN:OD1    | 2:B:194:ASN:C      | 2.50                     | 0.55              |
| 11:B:1496:CLA:H152 | 11:B:1497:CLA:HMD2 | 1.88                     | 0.55              |
| 3:C:72:LEU:O       | 3:C:73:ALA:C       | 2.49                     | 0.55              |
| 3:C:284:PHE:HE1    | 3:C:431:PHE:CE1    | 2.25                     | 0.55              |
| 5:E:15:THR:HG22    | 5:E:15:THR:O       | 2.05                     | 0.55              |
| 1:G:93:PHE:C       | 1:G:95:PRO:HD3     | 2.32                     | 0.55              |
| 2:H:103:LEU:N      | 2:H:103:LEU:HD23   | 2.20                     | 0.55              |
| 2:H:424:ALA:C      | 2:H:426:PHE:H      | 2.13                     | 0.55              |
| 11:H:1488:CLA:C17  | 4:J:281:MET:HE1    | 2.31                     | 0.55              |
| 4:J:169:PHE:O      | 4:J:181:PHE:HE2    | 1.90                     | 0.55              |
| 4:J:189:HIS:HA     | 4:J:294:ARG:HH11   | 1.71                     | 0.55              |
| 4:J:213:ILE:O      | 4:J:214:HIS:C      | 2.49                     | 0.55              |
| 1:A:331:MET:HE3    | 4:D:346:LEU:O      | 2.06                     | 0.55              |
| 3:C:230:LEU:O      | 3:C:234:VAL:HG23   | 2.06                     | 0.55              |
| 3:I:67:MET:O       | 3:I:71:GLU:N       | 2.39                     | 0.55              |
| 3:I:156:LYS:O      | 3:I:157:MET:C      | 2.50                     | 0.55              |
| 9:V:87:GLU:CD      | 9:V:96:ARG:HH22    | 2.15                     | 0.55              |
| 2:B:426:PHE:O      | 2:B:426:PHE:HD1    | 1.90                     | 0.55              |
| 3:C:135:ARG:C      | 3:C:136:GLY:O      | 2.44                     | 0.55              |
| 4:D:345:VAL:O      | 4:D:346:LEU:CB     | 2.54                     | 0.55              |
| 1:G:157:VAL:HG13   | 1:G:172:MET:HB3    | 1.89                     | 0.55              |
| 1:G:195:HIS:HE1    | 1:G:197:PHE:CD1    | 2.24                     | 0.55              |
| 3:I:164:HIS:HA     | 3:I:167:VAL:HG23   | 1.87                     | 0.55              |
| 4:J:36:LEU:HD23    | 11:J:1353:CLA:HBB2 | 1.88                     | 0.55              |
| 4:J:313:THR:C      | 4:J:315:TYR:H      | 2.13                     | 0.55              |
| 5:K:37:PHE:CE1     | 5:K:42:LEU:CB      | 2.89                     | 0.55              |
| 5:K:74:GLN:O       | 5:K:75:GLN:C       | 2.49                     | 0.55              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 10:Y:568:UNK:O   | 10:Y:569:UNK:C     | 2.54                     | 0.55              |
| 1:A:176:ILE:HG23 | 1:A:180:PHE:CE1    | 2.41                     | 0.55              |
| 3:C:37:ALA:CA    | 11:C:1466:CLA:HBA2 | 2.30                     | 0.55              |
| 3:C:135:ARG:HG3  | 3:C:136:GLY:H      | 1.70                     | 0.55              |
| 3:C:202:PRO:CA   | 3:C:235:GLY:HA3    | 2.37                     | 0.55              |
| 6:F:18:VAL:O     | 6:F:21:VAL:N       | 2.39                     | 0.55              |
| 6:F:33:PHE:C     | 6:F:35:GLY:N       | 2.62                     | 0.55              |
| 1:G:116:ILE:HG12 | 1:G:158:PHE:HD1    | 1.72                     | 0.55              |
| 3:I:56:HIS:O     | 3:I:57:ALA:C       | 2.50                     | 0.55              |
| 3:I:276:LEU:O    | 3:I:276:LEU:HD12   | 2.06                     | 0.55              |
| 3:I:320:ARG:NH1  | 9:T:49:ASN:OD1     | 2.39                     | 0.55              |
| 4:J:238:THR:O    | 4:J:239:GLN:CB     | 2.54                     | 0.55              |
| 7:P:123:UNK:O    | 7:P:124:UNK:C      | 2.55                     | 0.55              |
| 9:V:136:TYR:O    | 9:V:137:TYR:CG     | 2.59                     | 0.55              |
| 2:B:172:TYR:O    | 2:B:174:LEU:HG     | 2.06                     | 0.55              |
| 2:B:193:TYR:OH   | 2:B:259:GLY:HA2    | 2.07                     | 0.55              |
| 3:C:77:PRO:C     | 3:C:79:LYS:N       | 2.64                     | 0.55              |
| 4:D:56:THR:CB    | 5:E:49:THR:HG22    | 2.37                     | 0.55              |
| 1:G:116:ILE:HG22 | 1:G:117:PHE:N      | 2.21                     | 0.55              |
| 1:G:288:LEU:O    | 1:G:289:GLY:C      | 2.48                     | 0.55              |
| 2:H:94:GLU:CG    | 2:H:95:GLY:H       | 2.20                     | 0.55              |
| 2:H:201:HIS:HB2  | 11:H:1483:CLA:C1B  | 2.37                     | 0.55              |
| 3:I:56:HIS:ND1   | 11:I:1467:CLA:HBB  | 2.22                     | 0.55              |
| 3:I:189:TRP:NE1  | 3:I:295:THR:HG22   | 2.22                     | 0.55              |
| 3:I:226:SER:OG   | 3:I:227:VAL:N      | 2.38                     | 0.55              |
| 3:I:281:MET:O    | 3:I:282:MET:C      | 2.50                     | 0.55              |
| 5:K:16:SER:O     | 5:K:17:VAL:HB      | 2.07                     | 0.55              |
| 5:K:35:TRP:CE3   | 6:L:39:ALA:HB2     | 2.42                     | 0.55              |
| 10:Y:214:UNK:O   | 10:Y:218:UNK:N     | 2.40                     | 0.55              |
| 2:B:330:MET:CE   | 2:B:446:SER:HB3    | 2.21                     | 0.55              |
| 2:B:397:VAL:C    | 2:B:399:VAL:H      | 2.15                     | 0.55              |
| 3:C:166:ILE:HD11 | 3:C:249:ILE:HD13   | 1.88                     | 0.55              |
| 4:D:58:TRP:HA    | 4:D:62:GLY:HA2     | 1.89                     | 0.55              |
| 4:D:159:ILE:O    | 4:D:160:TYR:C      | 2.50                     | 0.55              |
| 1:G:37:MET:O     | 1:G:38:ILE:C       | 2.49                     | 0.55              |
| 2:H:271:THR:HG22 | 2:H:448:ARG:HE     | 1.70                     | 0.55              |
| 3:I:36:TRP:O     | 3:I:36:TRP:HE3     | 1.89                     | 0.55              |
| 3:I:135:ARG:HG3  | 3:I:136:GLY:H      | 1.72                     | 0.55              |
| 4:J:183:LEU:O    | 4:J:184:PHE:C      | 2.49                     | 0.55              |
| 7:O:99:UNK:O     | 7:O:102:UNK:N      | 2.39                     | 0.55              |
| 8:U:44:UNK:O     | 8:U:45:UNK:C       | 2.54                     | 0.55              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:A:332:HIS:HD2  | 1:A:333:GLU:H      | 1.54                     | 0.55              |
| 2:B:94:GLU:CG    | 2:B:95:GLY:N       | 2.69                     | 0.55              |
| 2:B:193:TYR:CZ   | 2:B:259:GLY:HA2    | 2.42                     | 0.55              |
| 3:C:298:PRO:O    | 3:C:299:SER:HB3    | 2.06                     | 0.55              |
| 4:D:190:ASN:HB2  | 4:D:296:TYR:HD1    | 1.71                     | 0.55              |
| 1:G:89:ILE:HD11  | 1:G:108:ASN:HB3    | 1.89                     | 0.55              |
| 1:G:95:PRO:O     | 1:G:105:TRP:NE1    | 2.40                     | 0.55              |
| 2:H:30:VAL:HG12  | 11:H:1486:CLA:HHD  | 1.87                     | 0.55              |
| 2:H:37:MET:O     | 2:H:40:TYR:N       | 2.40                     | 0.55              |
| 2:H:397:VAL:C    | 2:H:399:VAL:H      | 2.15                     | 0.55              |
| 8:S:73:UNK:O     | 8:S:74:UNK:C       | 2.54                     | 0.55              |
| 10:X:13:UNK:O    | 10:X:14:UNK:C      | 2.54                     | 0.55              |
| 10:X:225:UNK:O   | 10:X:226:UNK:C     | 2.55                     | 0.55              |
| 1:A:331:MET:O    | 1:A:332:HIS:O      | 2.25                     | 0.54              |
| 2:B:246:PHE:CZ   | 2:B:463:PHE:HD1    | 2.24                     | 0.54              |
| 4:D:56:THR:HB    | 5:E:49:THR:HG22    | 1.90                     | 0.54              |
| 4:D:152:VAL:HG11 | 11:D:1351:CLA:HBA1 | 1.89                     | 0.54              |
| 1:G:198:HIS:O    | 1:G:201:GLY:N      | 2.37                     | 0.54              |
| 2:H:323:GLY:CA   | 4:J:293:LEU:HD22   | 2.38                     | 0.54              |
| 3:I:330:SER:HB3  | 7:P:56:UNK:O       | 2.07                     | 0.54              |
| 10:X:420:UNK:O   | 10:X:421:UNK:C     | 2.55                     | 0.54              |
| 1:A:118:HIS:O    | 1:A:119:PHE:C      | 2.47                     | 0.54              |
| 2:B:153:PHE:O    | 2:B:157:HIS:HB3    | 2.07                     | 0.54              |
| 3:C:33:PHE:O     | 3:C:34:ALA:HB3     | 2.07                     | 0.54              |
| 3:C:119:LEU:O    | 3:C:122:SER:OG     | 2.25                     | 0.54              |
| 3:C:240:ILE:HA   | 3:C:243:ILE:HB     | 1.89                     | 0.54              |
| 3:C:284:PHE:O    | 3:C:286:ALA:N      | 2.40                     | 0.54              |
| 4:D:72:ASN:O     | 4:D:72:ASN:OD1     | 2.24                     | 0.54              |
| 4:D:239:GLN:O    | 4:D:240:ALA:HB3    | 2.06                     | 0.54              |
| 1:G:13:LEU:O     | 1:G:17:PHE:N       | 2.39                     | 0.54              |
| 2:H:63:LEU:O     | 2:H:64:PRO:C       | 2.48                     | 0.54              |
| 2:H:346:PHE:O    | 2:H:354:LEU:HB3    | 2.07                     | 0.54              |
| 2:H:418:LYS:O    | 2:H:419:SER:C      | 2.48                     | 0.54              |
| 3:I:120:ILE:O    | 3:I:122:SER:N      | 2.40                     | 0.54              |
| 3:I:259:TRP:CZ3  | 11:I:1464:CLA:H12  | 2.42                     | 0.54              |
| 3:I:447:ARG:HH11 | 3:I:447:ARG:HG2    | 1.72                     | 0.54              |
| 9:V:133:GLY:O    | 9:V:137:TYR:N      | 2.40                     | 0.54              |
| 1:A:114:LEU:O    | 1:A:115:ILE:C      | 2.49                     | 0.54              |
| 1:A:132:GLU:C    | 1:A:134:SER:N      | 2.63                     | 0.54              |
| 4:D:272:LEU:HD23 | 4:D:272:LEU:O      | 2.06                     | 0.54              |
| 1:G:248:ILE:CD1  | 4:J:235:PHE:HZ     | 2.18                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:G:276:ALA:HB2    | 4:J:215:GLY:C      | 2.32                     | 0.54              |
| 11:G:1342:CLA:H122 | 12:G:1345:PHO:H3A  | 1.88                     | 0.54              |
| 4:J:56:THR:HB      | 5:K:49:THR:HG22    | 1.88                     | 0.54              |
| 5:K:10:PHE:HD2     | 6:L:19:ARG:NH2     | 2.06                     | 0.54              |
| 8:S:27:UNK:O       | 8:S:28:UNK:O       | 2.24                     | 0.54              |
| 1:A:65:GLU:CD      | 4:D:312:GLU:OE1    | 2.50                     | 0.54              |
| 1:A:310:LYS:HD2    | 5:E:58:GLN:HG3     | 1.89                     | 0.54              |
| 2:B:52:LEU:HD23    | 2:B:311:PHE:CD2    | 2.42                     | 0.54              |
| 2:B:107:LEU:HD23   | 11:B:1497:CLA:HBC1 | 1.88                     | 0.54              |
| 2:B:144:PHE:CE1    | 2:B:210:ILE:HG23   | 2.42                     | 0.54              |
| 2:B:359:MET:HB3    | 2:B:426:PHE:HB3    | 1.88                     | 0.54              |
| 3:C:74:HIS:H       | 3:C:74:HIS:CD2     | 2.26                     | 0.54              |
| 3:C:279:LEU:O      | 3:C:280:SER:C      | 2.50                     | 0.54              |
| 3:C:377:LEU:O      | 3:C:381:LYS:HB2    | 2.08                     | 0.54              |
| 4:D:126:MET:HE1    | 4:D:147:SER:CA     | 2.37                     | 0.54              |
| 1:G:278:TRP:CB     | 1:G:279:PRO:HD3    | 2.27                     | 0.54              |
| 2:H:193:TYR:CE1    | 2:H:259:GLY:HA2    | 2.42                     | 0.54              |
| 2:H:450:TRP:NE1    | 11:H:1488:CLA:HBA1 | 2.22                     | 0.54              |
| 3:I:137:PRO:O      | 3:I:138:GLU:HB2    | 2.08                     | 0.54              |
| 3:I:376:ASP:C      | 3:I:378:ASN:N      | 2.59                     | 0.54              |
| 8:U:64:UNK:O       | 8:U:65:UNK:C       | 2.55                     | 0.54              |
| 9:V:55:ARG:HG3     | 9:V:131:GLY:HA2    | 1.90                     | 0.54              |
| 1:A:122:GLY:C      | 1:A:124:SER:N      | 2.64                     | 0.54              |
| 2:B:68:ARG:NH1     | 2:B:262:THR:O      | 2.40                     | 0.54              |
| 3:C:75:PHE:CZ      | 3:C:77:PRO:HG3     | 2.42                     | 0.54              |
| 1:G:135:TYR:O      | 1:G:136:ARG:HG2    | 2.07                     | 0.54              |
| 1:G:311:GLY:HA3    | 9:T:125:ILE:CG2    | 2.38                     | 0.54              |
| 1:G:326:LEU:C      | 1:G:328:MET:N      | 2.64                     | 0.54              |
| 2:H:446:SER:HB2    | 2:H:447:PRO:CD     | 2.37                     | 0.54              |
| 2:H:475:PHE:CE1    | 4:J:140:PRO:HG3    | 2.42                     | 0.54              |
| 3:I:272:LEU:O      | 3:I:273:SER:C      | 2.49                     | 0.54              |
| 5:K:12:ASP:O       | 5:K:16:SER:N       | 2.40                     | 0.54              |
| 2:B:31:ALA:H       | 11:B:1486:CLA:CBC  | 2.19                     | 0.54              |
| 2:B:134:ASP:O      | 2:B:136:PRO:CD     | 2.55                     | 0.54              |
| 2:B:271:THR:HG22   | 2:B:448:ARG:HE     | 1.72                     | 0.54              |
| 2:B:446:SER:HB2    | 2:B:447:PRO:HD2    | 1.90                     | 0.54              |
| 3:C:440:GLY:O      | 3:C:441:HIS:C      | 2.50                     | 0.54              |
| 4:D:279:LEU:HD11   | 12:D:1352:PHO:HBC3 | 1.90                     | 0.54              |
| 1:G:34:GLY:C       | 1:G:36:ILE:H       | 2.15                     | 0.54              |
| 1:G:310:LYS:HZ1    | 5:K:58:GLN:HG2     | 1.71                     | 0.54              |
| 2:H:422:ARG:O      | 2:H:425:ILE:HG22   | 2.07                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:H:1482:CLA:CGA  | 11:H:1482:CLA:HBD  | 2.38                     | 0.54              |
| 3:I:77:PRO:C       | 3:I:79:LYS:N       | 2.66                     | 0.54              |
| 3:I:284:PHE:O      | 3:I:285:ILE:C      | 2.50                     | 0.54              |
| 4:J:45:LEU:HD22    | 4:J:49:LEU:HD11    | 1.88                     | 0.54              |
| 4:J:191:TRP:HA     | 4:J:191:TRP:CE3    | 2.42                     | 0.54              |
| 7:O:148:UNK:O      | 7:O:149:UNK:CB     | 2.53                     | 0.54              |
| 8:S:57:UNK:O       | 8:S:58:UNK:C       | 2.56                     | 0.54              |
| 8:U:67:UNK:O       | 8:U:68:UNK:C       | 2.55                     | 0.54              |
| 1:A:142:TRP:O      | 1:A:143:ILE:C      | 2.50                     | 0.54              |
| 1:A:210:LEU:O      | 1:A:213:ALA:HB3    | 2.08                     | 0.54              |
| 2:B:145:LEU:O      | 2:B:146:ALA:C      | 2.50                     | 0.54              |
| 2:B:205:ALA:O      | 2:B:209:GLY:N      | 2.41                     | 0.54              |
| 3:C:170:ILE:CG2    | 3:C:171:GLY:N      | 2.71                     | 0.54              |
| 3:C:186:TYR:HE2    | 3:C:188:THR:CG2    | 2.21                     | 0.54              |
| 3:C:270:ALA:C      | 3:C:274:TYR:HD2    | 2.16                     | 0.54              |
| 2:H:31:ALA:N       | 11:H:1486:CLA:CBC  | 2.66                     | 0.54              |
| 2:H:468:TRP:HD1    | 4:J:144:ILE:HD11   | 1.71                     | 0.54              |
| 2:H:470:GLY:O      | 2:H:473:THR:HB     | 2.07                     | 0.54              |
| 10:X:5:UNK:O       | 10:X:6:UNK:C       | 2.56                     | 0.54              |
| 10:X:17:UNK:O      | 10:X:18:UNK:C      | 2.55                     | 0.54              |
| 10:X:506:UNK:O     | 10:X:507:UNK:C     | 2.55                     | 0.54              |
| 11:A:1344:CLA:HED3 | 4:D:175:VAL:HG13   | 1.89                     | 0.54              |
| 2:B:211:ILE:O      | 2:B:214:LEU:HG     | 2.08                     | 0.54              |
| 2:B:280:PHE:CZ     | 2:B:312:TYR:HD2    | 2.26                     | 0.54              |
| 2:B:346:PHE:O      | 2:B:353:GLU:O      | 2.25                     | 0.54              |
| 2:B:424:ALA:C      | 2:B:426:PHE:H      | 2.16                     | 0.54              |
| 3:C:291:TRP:HD1    | 3:C:292:PHE:CD2    | 2.26                     | 0.54              |
| 3:C:318:LEU:CD1    | 3:C:328:VAL:HG21   | 2.38                     | 0.54              |
| 5:E:13:ILE:HA      | 5:E:16:SER:HB2     | 1.89                     | 0.54              |
| 1:G:34:GLY:C       | 1:G:36:ILE:N       | 2.65                     | 0.54              |
| 2:H:167:TRP:CB     | 2:H:267:LEU:HD11   | 2.38                     | 0.54              |
| 2:H:202:HIS:HE1    | 11:H:1484:CLA:NB   | 2.04                     | 0.54              |
| 11:H:1496:CLA:H13  | 11:H:1497:CLA:HMD1 | 1.89                     | 0.54              |
| 3:I:120:ILE:C      | 3:I:122:SER:N      | 2.66                     | 0.54              |
| 1:A:141:PRO:HG2    | 3:C:446:GLY:C      | 2.33                     | 0.54              |
| 1:A:184:ILE:O      | 1:A:185:VAL:C      | 2.51                     | 0.54              |
| 2:B:138:MET:C      | 2:B:140:GLY:N      | 2.65                     | 0.54              |
| 3:C:156:LYS:O      | 3:C:157:MET:C      | 2.51                     | 0.54              |
| 4:D:199:MET:O      | 4:D:200:GLY:C      | 2.51                     | 0.54              |
| 4:D:209:LEU:HD23   | 4:D:209:LEU:O      | 2.07                     | 0.54              |
| 6:F:40:MET:O       | 6:F:43:ILE:HG13    | 2.07                     | 0.54              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:H:149:LEU:C     | 11:H:1484:CLA:HBC2 | 2.32                     | 0.54              |
| 3:I:127:PHE:CE2   | 11:I:1471:CLA:HBC1 | 2.43                     | 0.54              |
| 3:I:449:ARG:NH1   | 11:I:1463:CLA:O1D  | 2.41                     | 0.54              |
| 4:J:139:ARG:HB3   | 4:J:141:TYR:HD1    | 1.73                     | 0.54              |
| 8:S:55:UNK:O      | 8:S:58:UNK:N       | 2.40                     | 0.54              |
| 8:S:67:UNK:O      | 8:S:68:UNK:C       | 2.56                     | 0.54              |
| 9:V:134:LYS:O     | 9:V:137:TYR:O      | 2.26                     | 0.54              |
| 1:A:69:GLY:C      | 1:A:75:ASN:OD1     | 2.51                     | 0.54              |
| 1:A:78:ILE:HD12   | 1:A:78:ILE:H       | 1.73                     | 0.54              |
| 1:A:98:GLU:O      | 1:A:99:ALA:CB      | 2.56                     | 0.54              |
| 1:A:258:LEU:CD1   | 4:D:128:ARG:NH2    | 2.71                     | 0.54              |
| 12:A:1345:PHO:CBB | 4:D:205:LEU:HD21   | 2.37                     | 0.54              |
| 2:B:24:LEU:HD23   | 2:B:111:ALA:CA     | 2.36                     | 0.54              |
| 4:D:253:TRP:O     | 4:D:254:SER:C      | 2.51                     | 0.54              |
| 2:H:269:GLY:H     | 2:H:448:ARG:HB2    | 1.73                     | 0.54              |
| 2:H:309:LEU:O     | 2:H:310:ALA:C      | 2.50                     | 0.54              |
| 4:J:253:TRP:O     | 4:J:254:SER:C      | 2.50                     | 0.54              |
| 5:K:16:SER:HB3    | 5:K:19:TYR:HB3     | 1.90                     | 0.54              |
| 2:B:33:TRP:NE1    | 11:B:1488:CLA:HBC2 | 2.22                     | 0.53              |
| 11:B:1494:CLA:OBD | 11:B:1495:CLA:HHC  | 2.08                     | 0.53              |
| 3:C:259:TRP:O     | 3:C:260:ALA:C      | 2.52                     | 0.53              |
| 1:G:210:LEU:HD13  | 12:J:1352:PHO:ND   | 2.24                     | 0.53              |
| 2:H:230:ARG:O     | 2:H:231:MET:C      | 2.51                     | 0.53              |
| 2:H:280:PHE:O     | 2:H:283:GLU:HB3    | 2.07                     | 0.53              |
| 3:I:37:ALA:CA     | 11:I:1466:CLA:HBA2 | 2.29                     | 0.53              |
| 3:I:126:GLY:O     | 3:I:130:VAL:HG23   | 2.08                     | 0.53              |
| 4:J:33:SER:OG     | 4:J:128:ARG:HA     | 2.08                     | 0.53              |
| 4:J:263:ASN:C     | 4:J:265:ARG:N      | 2.66                     | 0.53              |
| 9:V:13:ASN:HD21   | 9:V:17:LYS:CG      | 2.22                     | 0.53              |
| 10:X:59:UNK:O     | 10:X:61:UNK:N      | 2.41                     | 0.53              |
| 10:X:59:UNK:C     | 10:X:61:UNK:N      | 2.70                     | 0.53              |
| 10:X:270:UNK:O    | 10:X:271:UNK:C     | 2.57                     | 0.53              |
| 10:Y:425:UNK:O    | 10:Y:429:UNK:CB    | 2.56                     | 0.53              |
| 10:Y:578:UNK:C    | 10:Y:580:UNK:N     | 2.65                     | 0.53              |
| 1:A:288:LEU:O     | 1:A:290:ILE:N      | 2.41                     | 0.53              |
| 2:B:201:HIS:HB2   | 11:B:1483:CLA:C1B  | 2.38                     | 0.53              |
| 2:B:396:GLY:C     | 2:B:398:THR:N      | 2.60                     | 0.53              |
| 4:D:74:LEU:HA     | 4:D:175:VAL:HG11   | 1.90                     | 0.53              |
| 4:D:179:PHE:HA    | 4:D:182:LEU:HD12   | 1.89                     | 0.53              |
| 5:E:41:GLY:O      | 5:E:42:LEU:C       | 2.50                     | 0.53              |
| 5:E:56:TYR:O      | 5:E:57:ALA:CB      | 2.55                     | 0.53              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:G:84:PRO:O     | 1:G:85:SER:O       | 2.26                     | 0.53              |
| 1:G:219:VAL:HG11 | 4:J:268:HIS:CD2    | 2.44                     | 0.53              |
| 1:G:302:PHE:HE1  | 4:J:74:LEU:HD12    | 1.73                     | 0.53              |
| 2:H:27:THR:O     | 2:H:30:VAL:N       | 2.37                     | 0.53              |
| 2:H:462:PHE:CE1  | 11:H:1494:CLA:HMB2 | 2.43                     | 0.53              |
| 3:I:33:PHE:O     | 3:I:34:ALA:HB3     | 2.09                     | 0.53              |
| 4:J:57:SER:O     | 4:J:58:TRP:C       | 2.50                     | 0.53              |
| 4:J:199:MET:O    | 4:J:200:GLY:C      | 2.51                     | 0.53              |
| 7:P:64:UNK:HA    | 7:P:70:UNK:O       | 2.09                     | 0.53              |
| 9:V:4:THR:HB     | 9:V:5:PRO:HD2      | 1.89                     | 0.53              |
| 10:X:435:UNK:O   | 10:X:438:UNK:N     | 2.41                     | 0.53              |
| 2:B:323:GLY:CA   | 4:D:293:LEU:HD22   | 2.39                     | 0.53              |
| 2:B:475:PHE:CZ   | 4:D:134:ARG:HB2    | 2.43                     | 0.53              |
| 3:C:56:HIS:HE1   | 11:C:1467:CLA:HMA1 | 1.74                     | 0.53              |
| 3:C:179:ALA:O    | 3:C:184:GLY:HA2    | 2.09                     | 0.53              |
| 3:C:290:VAL:HA   | 3:C:297:TYR:CD2    | 2.43                     | 0.53              |
| 4:D:110:LEU:O    | 4:D:114:ILE:HG13   | 2.09                     | 0.53              |
| 1:G:26:ASN:CA    | 4:J:255:GLN:NE2    | 2.72                     | 0.53              |
| 1:G:174:LEU:HD22 | 12:G:1345:PHO:H151 | 1.89                     | 0.53              |
| 2:H:462:PHE:HA   | 11:H:1492:CLA:HMC2 | 1.91                     | 0.53              |
| 3:I:304:PRO:C    | 3:I:305:THR:CG2    | 2.81                     | 0.53              |
| 4:J:279:LEU:HD11 | 12:J:1352:PHO:HBC3 | 1.90                     | 0.53              |
| 8:S:31:UNK:O     | 8:S:32:UNK:C       | 2.57                     | 0.53              |
| 10:X:519:UNK:O   | 10:X:522:UNK:N     | 2.41                     | 0.53              |
| 10:Y:336:UNK:O   | 10:Y:337:UNK:CB    | 2.56                     | 0.53              |
| 1:A:201:GLY:HA2  | 1:A:282:GLY:O      | 2.07                     | 0.53              |
| 2:B:309:LEU:O    | 2:B:312:TYR:N      | 2.42                     | 0.53              |
| 2:B:314:TYR:OH   | 2:B:334:ASP:OD1    | 2.25                     | 0.53              |
| 5:E:16:SER:HB3   | 5:E:19:TYR:HB3     | 1.90                     | 0.53              |
| 1:G:132:GLU:O    | 1:G:134:SER:N      | 2.41                     | 0.53              |
| 1:G:133:LEU:HB2  | 4:J:252:PHE:CE2    | 2.43                     | 0.53              |
| 1:G:301:ASN:C    | 1:G:301:ASN:OD1    | 2.51                     | 0.53              |
| 2:H:139:PHE:HB2  | 11:H:1491:CLA:CHD  | 2.38                     | 0.53              |
| 3:I:173:LEU:O    | 3:I:176:VAL:CG1    | 2.51                     | 0.53              |
| 4:J:56:THR:N     | 5:K:49:THR:HG22    | 2.23                     | 0.53              |
| 4:J:184:PHE:C    | 4:J:184:PHE:CD1    | 2.86                     | 0.53              |
| 4:J:184:PHE:O    | 4:J:188:PHE:HB2    | 2.09                     | 0.53              |
| 5:K:17:VAL:O     | 5:K:21:VAL:HG23    | 2.08                     | 0.53              |
| 1:A:186:PHE:CD2  | 1:A:192:ILE:CD1    | 2.84                     | 0.53              |
| 1:A:218:LEU:CD1  | 1:A:255:PHE:HD2    | 2.20                     | 0.53              |
| 1:A:218:LEU:HA   | 1:A:221:SER:OG     | 2.09                     | 0.53              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:A:301:ASN:C    | 1:A:301:ASN:OD1    | 2.51                     | 0.53              |
| 3:C:72:LEU:O     | 3:C:75:PHE:HB3     | 2.08                     | 0.53              |
| 3:C:376:ASP:HB2  | 3:C:379:LYS:CG     | 2.34                     | 0.53              |
| 3:C:455:PHE:O    | 3:C:456:GLU:CG     | 2.56                     | 0.53              |
| 4:D:181:PHE:CZ   | 4:D:185:PHE:HE1    | 2.27                     | 0.53              |
| 4:D:191:TRP:HA   | 4:D:191:TRP:HE3    | 1.74                     | 0.53              |
| 4:D:263:ASN:C    | 4:D:265:ARG:N      | 2.65                     | 0.53              |
| 4:D:296:TYR:HE1  | 4:D:322:ASN:HD22   | 1.56                     | 0.53              |
| 1:G:118:HIS:O    | 1:G:119:PHE:C      | 2.49                     | 0.53              |
| 1:G:255:PHE:CZ   | 1:G:259:ILE:HD12   | 2.44                     | 0.53              |
| 2:H:33:TRP:HE1   | 11:H:1488:CLA:HBC2 | 1.73                     | 0.53              |
| 2:H:135:LEU:CD1  | 2:H:232:GLY:HA2    | 2.38                     | 0.53              |
| 2:H:220:ARG:HD2  | 2:H:221:PRO:HD2    | 1.90                     | 0.53              |
| 2:H:415:PRO:O    | 2:H:416:THR:C      | 2.49                     | 0.53              |
| 3:I:284:PHE:HE1  | 3:I:431:PHE:CE1    | 2.25                     | 0.53              |
| 3:I:355:THR:O    | 3:I:355:THR:HG22   | 2.07                     | 0.53              |
| 4:J:210:LEU:HD11 | 4:J:270:PHE:CD2    | 2.43                     | 0.53              |
| 9:V:55:ARG:NH2   | 9:V:128:ASP:OD1    | 2.41                     | 0.53              |
| 2:B:220:ARG:HD2  | 2:B:221:PRO:HD2    | 1.90                     | 0.53              |
| 2:B:446:SER:HB2  | 2:B:447:PRO:CD     | 2.39                     | 0.53              |
| 3:C:39:ASN:ND2   | 11:C:1466:CLA:H11  | 2.23                     | 0.53              |
| 3:C:288:CYS:O    | 3:C:289:PHE:C      | 2.50                     | 0.53              |
| 1:G:122:GLY:C    | 1:G:124:SER:N      | 2.64                     | 0.53              |
| 1:G:140:ARG:O    | 4:J:220:ASN:HB3    | 2.08                     | 0.53              |
| 1:G:142:TRP:O    | 1:G:143:ILE:C      | 2.52                     | 0.53              |
| 1:G:271:LEU:O    | 1:G:271:LEU:HG     | 2.09                     | 0.53              |
| 1:G:285:PHE:O    | 1:G:289:GLY:N      | 2.33                     | 0.53              |
| 2:H:98:LEU:O     | 2:H:101:ILE:N      | 2.41                     | 0.53              |
| 3:I:40:ALA:HA    | 3:I:43:ILE:HG23    | 1.91                     | 0.53              |
| 3:I:154:LYS:HZ3  | 3:I:261:ARG:HD3    | 1.74                     | 0.53              |
| 3:I:270:ALA:O    | 3:I:274:TYR:HD2    | 1.91                     | 0.53              |
| 6:L:37:ILE:CA    | 6:L:40:MET:HE2     | 2.31                     | 0.53              |
| 9:V:78:ASN:OD1   | 9:V:96:ARG:NH2     | 2.41                     | 0.53              |
| 1:A:36:ILE:O     | 1:A:39:PRO:HD2     | 2.09                     | 0.53              |
| 1:A:326:LEU:C    | 1:A:328:MET:N      | 2.66                     | 0.53              |
| 2:B:15:ASP:CA    | 2:B:16:PRO:CD      | 2.87                     | 0.53              |
| 2:B:106:LEU:HD22 | 11:B:1496:CLA:H143 | 1.89                     | 0.53              |
| 2:B:135:LEU:HD12 | 2:B:232:GLY:HA2    | 1.90                     | 0.53              |
| 3:C:358:PHE:C    | 3:C:360:ASP:H      | 2.17                     | 0.53              |
| 3:C:367:GLU:HB2  | 3:C:368:PRO:HD3    | 1.89                     | 0.53              |
| 4:D:289:LEU:HD22 | 4:D:294:ARG:HB3    | 1.90                     | 0.53              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 5:E:17:VAL:O     | 5:E:21:VAL:HG23    | 2.09                     | 0.53              |
| 1:G:168:PHE:O    | 1:G:170:ASP:O      | 2.26                     | 0.53              |
| 1:G:214:MET:HE1  | 12:J:1352:PHO:CED  | 2.38                     | 0.53              |
| 2:H:107:LEU:HD23 | 11:H:1497:CLA:HBC1 | 1.90                     | 0.53              |
| 2:H:393:GLU:C    | 2:H:395:GLN:N      | 2.64                     | 0.53              |
| 3:I:122:SER:O    | 3:I:123:ALA:C      | 2.52                     | 0.53              |
| 3:I:287:THR:OG1  | 3:I:288:CYS:N      | 2.41                     | 0.53              |
| 3:I:318:LEU:CD1  | 3:I:328:VAL:HG21   | 2.38                     | 0.53              |
| 3:I:320:ARG:HD2  | 9:T:49:ASN:ND2     | 2.24                     | 0.53              |
| 3:I:440:GLY:O    | 3:I:441:HIS:C      | 2.51                     | 0.53              |
| 10:Y:262:UNK:O   | 10:Y:263:UNK:C     | 2.57                     | 0.53              |
| 1:A:132:GLU:O    | 1:A:134:SER:N      | 2.42                     | 0.53              |
| 1:A:211:PHE:CE2  | 1:A:274:PHE:HE2    | 2.26                     | 0.53              |
| 1:A:288:LEU:O    | 1:A:291:SER:N      | 2.42                     | 0.53              |
| 2:B:236:THR:CB   | 2:B:473:THR:HG21   | 2.39                     | 0.53              |
| 3:C:240:ILE:HD12 | 11:C:1465:CLA:C9   | 2.39                     | 0.53              |
| 4:D:71:CYS:CB    | 4:D:76:VAL:HG22    | 2.38                     | 0.53              |
| 4:D:148:ALA:HA   | 4:D:280:TRP:HE1    | 1.73                     | 0.53              |
| 4:D:272:LEU:CD2  | 4:D:276:VAL:HG21   | 2.39                     | 0.53              |
| 4:D:283:ALA:O    | 4:D:287:VAL:HG23   | 2.09                     | 0.53              |
| 2:H:52:LEU:HD23  | 2:H:311:PHE:CD2    | 2.44                     | 0.53              |
| 2:H:65:PHE:O     | 2:H:66:MET:C       | 2.50                     | 0.53              |
| 2:H:220:ARG:HB3  | 2:H:221:PRO:HD2    | 1.90                     | 0.53              |
| 3:I:79:LYS:HE2   | 3:I:83:GLU:HG2     | 1.90                     | 0.53              |
| 3:I:290:VAL:HA   | 3:I:297:TYR:CD2    | 2.43                     | 0.53              |
| 4:J:339:PHE:HD1  | 4:J:341:PHE:CE1    | 2.27                     | 0.53              |
| 8:S:71:UNK:O     | 8:S:74:UNK:N       | 2.41                     | 0.53              |
| 1:A:271:LEU:HG   | 1:A:271:LEU:O      | 2.08                     | 0.53              |
| 3:C:156:LYS:O    | 3:C:160:ILE:HG13   | 2.09                     | 0.53              |
| 4:D:216:ALA:O    | 4:D:220:ASN:ND2    | 2.42                     | 0.53              |
| 1:G:255:PHE:CE1  | 1:G:259:ILE:HD12   | 2.44                     | 0.53              |
| 3:I:171:GLY:O    | 3:I:172:ALA:C      | 2.50                     | 0.53              |
| 9:T:13:ASN:HD21  | 9:T:17:LYS:CG      | 2.22                     | 0.53              |
| 10:X:357:UNK:O   | 10:X:360:UNK:N     | 2.41                     | 0.53              |
| 10:Y:5:UNK:O     | 10:Y:6:UNK:C       | 2.56                     | 0.53              |
| 10:Y:13:UNK:O    | 10:Y:14:UNK:C      | 2.57                     | 0.53              |
| 10:Y:184:UNK:O   | 10:Y:185:UNK:C     | 2.57                     | 0.53              |
| 1:A:302:PHE:HE1  | 4:D:74:LEU:HD12    | 1.73                     | 0.53              |
| 1:A:314:ILE:HG23 | 4:D:58:TRP:HZ3     | 1.74                     | 0.53              |
| 2:B:49:ASP:OD2   | 2:B:52:LEU:N       | 2.41                     | 0.53              |
| 2:B:135:LEU:HD22 | 2:B:237:VAL:HG21   | 1.91                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:362:PHE:HE2    | 4:D:184:PHE:HZ     | 1.57                     | 0.53              |
| 2:B:471:ALA:O      | 2:B:472:ARG:C      | 2.51                     | 0.53              |
| 4:D:139:ARG:HB3    | 4:D:141:TYR:HD1    | 1.74                     | 0.53              |
| 5:E:16:SER:O       | 5:E:17:VAL:CB      | 2.57                     | 0.53              |
| 1:G:142:TRP:O      | 1:G:145:VAL:N      | 2.41                     | 0.53              |
| 2:H:76:SER:O       | 7:O:66:UNK:CA      | 2.57                     | 0.53              |
| 11:H:1496:CLA:H171 | 11:H:1497:CLA:CMD  | 2.37                     | 0.53              |
| 4:J:283:ALA:O      | 4:J:287:VAL:HG23   | 2.08                     | 0.53              |
| 1:A:289:GLY:O      | 1:A:292:THR:HB     | 2.09                     | 0.52              |
| 3:C:81:MET:HE3     | 3:C:301:PHE:HA     | 1.91                     | 0.52              |
| 1:G:76:ASN:C       | 1:G:76:ASN:OD1     | 2.51                     | 0.52              |
| 2:H:246:PHE:CZ     | 2:H:463:PHE:HD1    | 2.27                     | 0.52              |
| 2:H:473:THR:HG21   | 11:H:1489:CLA:HED3 | 1.92                     | 0.52              |
| 3:I:318:LEU:HD11   | 3:I:328:VAL:HG21   | 1.90                     | 0.52              |
| 4:J:52:THR:O       | 4:J:67:TYR:HD1     | 1.92                     | 0.52              |
| 4:J:58:TRP:HA      | 4:J:62:GLY:HA2     | 1.90                     | 0.52              |
| 4:J:76:VAL:HG12    | 4:J:77:ALA:N       | 2.23                     | 0.52              |
| 4:J:159:ILE:O      | 4:J:160:TYR:C      | 2.51                     | 0.52              |
| 8:S:99:UNK:O       | 8:S:100:UNK:C      | 2.58                     | 0.52              |
| 8:U:14:UNK:C       | 8:U:16:UNK:N       | 2.70                     | 0.52              |
| 10:X:200:UNK:O     | 10:X:201:UNK:C     | 2.57                     | 0.52              |
| 10:Y:420:UNK:O     | 10:Y:421:UNK:C     | 2.56                     | 0.52              |
| 1:A:93:PHE:CE1     | 1:A:95:PRO:CG      | 2.92                     | 0.52              |
| 1:A:142:TRP:O      | 1:A:145:VAL:N      | 2.42                     | 0.52              |
| 3:C:67:MET:O       | 3:C:71:GLU:N       | 2.42                     | 0.52              |
| 3:C:259:TRP:CZ3    | 11:C:1464:CLA:H12  | 2.44                     | 0.52              |
| 2:H:247:PHE:HB2    | 11:H:1489:CLA:HBC1 | 1.91                     | 0.52              |
| 4:J:32:TRP:O       | 4:J:35:ILE:N       | 2.43                     | 0.52              |
| 4:J:56:THR:CB      | 5:K:49:THR:HG22    | 2.39                     | 0.52              |
| 9:T:4:THR:HB       | 9:T:5:PRO:HD2      | 1.90                     | 0.52              |
| 10:X:356:UNK:O     | 10:X:357:UNK:C     | 2.57                     | 0.52              |
| 3:C:376:ASP:C      | 3:C:378:ASN:H      | 2.17                     | 0.52              |
| 4:D:16:ASP:O       | 4:D:19:ASP:N       | 2.42                     | 0.52              |
| 4:D:103:ARG:O      | 4:D:104:TRP:C      | 2.50                     | 0.52              |
| 4:D:111:TRP:O      | 4:D:112:THR:C      | 2.52                     | 0.52              |
| 4:D:213:ILE:O      | 4:D:214:HIS:C      | 2.52                     | 0.52              |
| 4:D:340:VAL:O      | 4:D:342:PRO:HD3    | 2.07                     | 0.52              |
| 6:F:19:ARG:O       | 6:F:23:VAL:CG2     | 2.54                     | 0.52              |
| 1:G:330:VAL:HG12   | 4:J:347:PRO:CA     | 2.35                     | 0.52              |
| 3:I:74:HIS:CD2     | 3:I:74:HIS:N       | 2.77                     | 0.52              |
| 4:J:239:GLN:O      | 4:J:240:ALA:HB3    | 2.09                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:P:148:UNK:O     | 7:P:149:UNK:CB     | 2.57                     | 0.52              |
| 1:A:288:LEU:O     | 1:A:289:GLY:C      | 2.52                     | 0.52              |
| 2:B:40:TYR:O      | 2:B:41:GLU:C       | 2.50                     | 0.52              |
| 2:B:61:PHE:HZ     | 11:B:1488:CLA:HBB1 | 1.73                     | 0.52              |
| 2:B:62:VAL:HG13   | 11:B:1486:CLA:O2D  | 2.10                     | 0.52              |
| 3:C:137:PRO:O     | 3:C:138:GLU:HB2    | 2.08                     | 0.52              |
| 6:F:15:ILE:O      | 6:F:15:ILE:HG22    | 2.09                     | 0.52              |
| 2:H:194:ASN:O     | 2:H:195:PRO:C      | 2.51                     | 0.52              |
| 2:H:263:THR:CG2   | 2:H:448:ARG:CZ     | 2.87                     | 0.52              |
| 6:L:18:VAL:O      | 6:L:19:ARG:C       | 2.51                     | 0.52              |
| 10:Y:272:UNK:O    | 10:Y:273:UNK:C     | 2.57                     | 0.52              |
| 1:A:294:ALA:O     | 1:A:296:ASN:N      | 2.43                     | 0.52              |
| 4:D:32:TRP:O      | 4:D:35:ILE:N       | 2.42                     | 0.52              |
| 4:D:80:THR:HB     | 4:D:168:PHE:HA     | 1.91                     | 0.52              |
| 1:G:193:LEU:HD13  | 4:J:179:PHE:HB3    | 1.92                     | 0.52              |
| 12:G:1345:PHO:HAB | 4:J:205:LEU:HD21   | 1.90                     | 0.52              |
| 3:I:183:GLY:O     | 3:I:184:GLY:O      | 2.28                     | 0.52              |
| 4:J:127:LEU:C     | 4:J:129:GLN:H      | 2.18                     | 0.52              |
| 5:K:55:TYR:O      | 5:K:56:TYR:HB2     | 2.07                     | 0.52              |
| 9:V:100:ILE:C     | 9:V:102:PRO:HD3    | 2.34                     | 0.52              |
| 10:Y:459:UNK:O    | 10:Y:460:UNK:C     | 2.56                     | 0.52              |
| 1:A:49:VAL:O      | 1:A:53:ILE:HG13    | 2.10                     | 0.52              |
| 1:A:122:GLY:O     | 1:A:125:CYS:N      | 2.42                     | 0.52              |
| 3:C:35:TRP:O      | 3:C:37:ALA:N       | 2.43                     | 0.52              |
| 3:C:116:VAL:HG23  | 3:C:117:VAL:H      | 1.73                     | 0.52              |
| 2:H:372:ASP:C     | 2:H:374:ASN:H      | 2.18                     | 0.52              |
| 2:H:415:PRO:O     | 2:H:418:LYS:N      | 2.43                     | 0.52              |
| 3:I:376:ASP:HB3   | 3:I:379:LYS:H      | 1.75                     | 0.52              |
| 4:J:72:ASN:O      | 4:J:72:ASN:OD1     | 2.27                     | 0.52              |
| 4:J:80:THR:HB     | 4:J:168:PHE:HA     | 1.92                     | 0.52              |
| 4:J:174:GLY:O     | 4:J:178:ILE:HG13   | 2.10                     | 0.52              |
| 7:P:37:UNK:O      | 7:P:38:UNK:CB      | 2.58                     | 0.52              |
| 8:U:31:UNK:O      | 8:U:32:UNK:C       | 2.55                     | 0.52              |
| 8:U:46:UNK:O      | 8:U:47:UNK:C       | 2.55                     | 0.52              |
| 4:D:88:SER:O      | 4:D:167:TRP:HZ3    | 1.92                     | 0.52              |
| 4:D:126:MET:HE1   | 4:D:147:SER:HA     | 1.92                     | 0.52              |
| 1:G:183:MET:HE1   | 11:G:1343:CLA:CMD  | 2.39                     | 0.52              |
| 1:G:309:ALA:HB2   | 5:K:52:PRO:O       | 2.10                     | 0.52              |
| 2:H:66:MET:O      | 2:H:71:VAL:HB      | 2.10                     | 0.52              |
| 3:I:39:ASN:HB2    | 11:I:1466:CLA:HAA2 | 1.90                     | 0.52              |
| 3:I:282:MET:HE1   | 11:I:1465:CLA:C4   | 2.40                     | 0.52              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 4:J:45:LEU:CD2   | 4:J:49:LEU:HD11    | 2.40                     | 0.52              |
| 4:J:88:SER:O     | 4:J:90:LEU:N       | 2.43                     | 0.52              |
| 4:J:167:TRP:O    | 4:J:168:PHE:CB     | 2.58                     | 0.52              |
| 9:V:2:GLU:O      | 9:V:4:THR:N        | 2.41                     | 0.52              |
| 10:X:158:UNK:O   | 10:X:162:UNK:N     | 2.42                     | 0.52              |
| 10:Y:3:UNK:O     | 10:Y:6:UNK:N       | 2.43                     | 0.52              |
| 2:B:18:ARG:NH1   | 2:B:115:TRP:CZ2    | 2.78                     | 0.52              |
| 2:B:37:MET:O     | 2:B:40:TYR:N       | 2.43                     | 0.52              |
| 6:F:28:VAL:HB    | 6:F:29:PRO:CD      | 2.37                     | 0.52              |
| 1:G:102:LEU:HD11 | 1:G:105:TRP:CE3    | 2.45                     | 0.52              |
| 2:H:314:TYR:H    | 2:H:427:GLY:HA3    | 1.75                     | 0.52              |
| 3:I:69:LEU:HD13  | 3:I:115:GLY:HA3    | 1.91                     | 0.52              |
| 4:J:91:LEU:O     | 4:J:93:TRP:N       | 2.42                     | 0.52              |
| 4:J:235:PHE:CD1  | 4:J:235:PHE:C      | 2.87                     | 0.52              |
| 10:Y:59:UNK:O    | 10:Y:61:UNK:N      | 2.43                     | 0.52              |
| 10:Y:219:UNK:O   | 10:Y:220:UNK:C     | 2.58                     | 0.52              |
| 1:A:142:TRP:CH2  | 1:A:273:PHE:HE1    | 2.28                     | 0.52              |
| 2:B:94:GLU:CG    | 2:B:95:GLY:H       | 2.23                     | 0.52              |
| 3:C:25:ASN:O     | 3:C:26:ARG:CB      | 2.58                     | 0.52              |
| 3:C:127:PHE:C    | 3:C:129:GLY:H      | 2.17                     | 0.52              |
| 4:D:54:PHE:HB3   | 5:E:47:PHE:CG      | 2.44                     | 0.52              |
| 5:E:51:ARG:O     | 5:E:53:ASP:N       | 2.43                     | 0.52              |
| 1:G:129:ARG:HH22 | 4:J:256:ILE:CA     | 2.22                     | 0.52              |
| 1:G:310:LYS:HZ2  | 5:K:58:GLN:HG2     | 1.75                     | 0.52              |
| 2:H:64:PRO:HG3   | 2:H:267:LEU:O      | 2.09                     | 0.52              |
| 2:H:79:SER:O     | 2:H:80:ILE:HG13    | 2.09                     | 0.52              |
| 2:H:279:TYR:O    | 2:H:281:GLN:N      | 2.43                     | 0.52              |
| 2:H:425:ILE:HG23 | 2:H:426:PHE:HD2    | 1.75                     | 0.52              |
| 3:I:364:PRO:O    | 3:I:365:TRP:C      | 2.51                     | 0.52              |
| 3:I:429:SER:O    | 3:I:432:VAL:HB     | 2.10                     | 0.52              |
| 4:J:72:ASN:C     | 4:J:76:VAL:HG23    | 2.35                     | 0.52              |
| 6:L:15:ILE:HG22  | 6:L:15:ILE:O       | 2.09                     | 0.52              |
| 1:A:151:LEU:CG   | 1:A:155:PHE:HE2    | 2.23                     | 0.52              |
| 1:A:183:MET:HA   | 11:A:1342:CLA:HMD2 | 1.92                     | 0.52              |
| 2:B:103:LEU:HD23 | 2:B:103:LEU:N      | 2.24                     | 0.52              |
| 2:B:247:PHE:HB2  | 11:B:1489:CLA:HBC1 | 1.92                     | 0.52              |
| 2:B:362:PHE:HE2  | 4:D:184:PHE:CZ     | 2.27                     | 0.52              |
| 3:C:304:PRO:C    | 3:C:305:THR:CG2    | 2.83                     | 0.52              |
| 3:C:450:ALA:O    | 3:C:455:PHE:N      | 2.41                     | 0.52              |
| 4:D:279:LEU:CD1  | 12:D:1352:PHO:HBC3 | 2.40                     | 0.52              |
| 1:G:184:ILE:HA   | 11:G:1342:CLA:HBC1 | 1.92                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:H:33:TRP:O     | 2:H:36:SER:HB3    | 2.10                     | 0.52              |
| 2:H:243:ALA:C    | 2:H:246:PHE:HB3   | 2.34                     | 0.52              |
| 3:I:227:VAL:HG11 | 3:I:233:VAL:HG23  | 1.92                     | 0.52              |
| 10:X:268:UNK:O   | 10:X:269:UNK:C    | 2.58                     | 0.52              |
| 10:Y:200:UNK:O   | 10:Y:201:UNK:C    | 2.58                     | 0.52              |
| 1:A:246:TYR:O    | 1:A:247:ASN:CG    | 2.52                     | 0.51              |
| 1:A:323:ARG:HG3  | 4:D:329:MET:HA    | 1.91                     | 0.51              |
| 2:B:415:PRO:O    | 2:B:416:THR:C     | 2.54                     | 0.51              |
| 3:C:314:ALA:O    | 3:C:315:MET:C     | 2.53                     | 0.51              |
| 3:C:376:ASP:HB3  | 3:C:379:LYS:H     | 1.76                     | 0.51              |
| 6:F:37:ILE:HG22  | 6:F:41:GLN:HE21   | 1.75                     | 0.51              |
| 2:H:201:HIS:CD2  | 2:H:202:HIS:ND1   | 2.76                     | 0.51              |
| 2:H:314:TYR:HA   | 2:H:427:GLY:HA3   | 1.92                     | 0.51              |
| 2:H:426:PHE:HD1  | 2:H:426:PHE:O     | 1.93                     | 0.51              |
| 3:I:450:ALA:O    | 3:I:455:PHE:N     | 2.43                     | 0.51              |
| 10:Y:158:UNK:O   | 10:Y:162:UNK:N    | 2.43                     | 0.51              |
| 1:A:60:ILE:HG23  | 1:A:61:ASP:N      | 2.25                     | 0.51              |
| 1:A:129:ARG:HH22 | 4:D:256:ILE:CA    | 2.24                     | 0.51              |
| 1:A:248:ILE:O    | 1:A:251:ALA:N     | 2.38                     | 0.51              |
| 2:B:49:ASP:OD2   | 2:B:52:LEU:HB2    | 2.10                     | 0.51              |
| 2:B:138:MET:O    | 2:B:140:GLY:N     | 2.44                     | 0.51              |
| 2:B:164:PRO:CB   | 11:B:1487:CLA:O1D | 2.58                     | 0.51              |
| 3:C:176:VAL:HG23 | 3:C:234:VAL:HG12  | 1.92                     | 0.51              |
| 4:D:16:ASP:O     | 4:D:18:LEU:N      | 2.44                     | 0.51              |
| 5:E:37:PHE:CD1   | 5:E:42:LEU:HB2    | 2.46                     | 0.51              |
| 1:G:151:LEU:CG   | 1:G:155:PHE:HE2   | 2.23                     | 0.51              |
| 1:G:162:PRO:HB3  | 1:G:168:PHE:HA    | 1.93                     | 0.51              |
| 2:H:138:MET:C    | 2:H:140:GLY:N     | 2.63                     | 0.51              |
| 2:H:147:GLY:O    | 2:H:148:LEU:C     | 2.53                     | 0.51              |
| 3:I:162:GLY:CA   | 3:I:248:GLY:HA2   | 2.40                     | 0.51              |
| 5:K:63:ILE:N     | 5:K:64:PRO:CD     | 2.73                     | 0.51              |
| 9:V:28:GLU:HA    | 9:V:28:GLU:OE1    | 2.10                     | 0.51              |
| 1:A:84:PRO:HG2   | 1:A:173:PRO:HG3   | 1.92                     | 0.51              |
| 3:C:35:TRP:CE3   | 3:C:36:TRP:HB3    | 2.45                     | 0.51              |
| 3:C:176:VAL:CG1  | 3:C:177:ALA:N     | 2.73                     | 0.51              |
| 3:C:227:VAL:O    | 3:C:227:VAL:HG12  | 2.09                     | 0.51              |
| 3:C:282:MET:O    | 3:C:285:ILE:HB    | 2.10                     | 0.51              |
| 4:D:35:ILE:CG2   | 4:D:35:ILE:O      | 2.57                     | 0.51              |
| 4:D:100:ASP:CB   | 4:D:103:ARG:HB2   | 2.40                     | 0.51              |
| 1:G:60:ILE:HB    | 1:G:83:VAL:HG12   | 1.91                     | 0.51              |
| 1:G:277:ALA:O    | 1:G:278:TRP:C     | 2.50                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:G:320:ILE:O     | 1:G:321:ILE:C      | 2.53                     | 0.51              |
| 2:H:138:MET:HA    | 2:H:141:ILE:HG22   | 1.92                     | 0.51              |
| 3:I:80:PRO:HB2    | 3:I:83:GLU:HB3     | 1.92                     | 0.51              |
| 3:I:280:SER:O     | 3:I:434:ALA:HB1    | 2.10                     | 0.51              |
| 5:K:78:THR:O      | 5:K:79:PHE:C       | 2.53                     | 0.51              |
| 8:U:43:UNK:O      | 8:U:47:UNK:N       | 2.42                     | 0.51              |
| 8:U:55:UNK:O      | 8:U:58:UNK:N       | 2.43                     | 0.51              |
| 10:X:563:UNK:O    | 10:X:566:UNK:N     | 2.43                     | 0.51              |
| 2:B:164:PRO:HB2   | 11:B:1487:CLA:O1D  | 2.10                     | 0.51              |
| 2:B:263:THR:CG2   | 2:B:448:ARG:CZ     | 2.88                     | 0.51              |
| 3:C:57:ALA:O      | 3:C:58:GLY:C       | 2.52                     | 0.51              |
| 11:C:1466:CLA:HBD | 11:C:1466:CLA:HBA1 | 1.93                     | 0.51              |
| 4:D:190:ASN:CG    | 4:D:322:ASN:HD21   | 2.18                     | 0.51              |
| 5:E:37:PHE:CE1    | 5:E:42:LEU:CB      | 2.93                     | 0.51              |
| 2:H:110:ALA:HA    | 11:H:1496:CLA:C20  | 2.40                     | 0.51              |
| 2:H:220:ARG:CD    | 2:H:221:PRO:HD2    | 2.41                     | 0.51              |
| 3:I:418:ASN:CA    | 3:I:419:PHE:N      | 2.74                     | 0.51              |
| 4:J:291:LEU:N     | 4:J:291:LEU:CD1    | 2.73                     | 0.51              |
| 5:K:51:ARG:O      | 5:K:53:ASP:N       | 2.43                     | 0.51              |
| 9:V:30:LYS:HG2    | 9:V:118:HIS:CE1    | 2.45                     | 0.51              |
| 10:X:177:UNK:O    | 10:X:180:UNK:N     | 2.43                     | 0.51              |
| 10:X:516:UNK:O    | 10:X:518:UNK:N     | 2.44                     | 0.51              |
| 1:A:183:MET:HE2   | 11:A:1343:CLA:HHD  | 1.93                     | 0.51              |
| 2:B:37:MET:HG2    | 2:B:62:VAL:HG21    | 1.92                     | 0.51              |
| 3:C:109:PHE:O     | 3:C:113:VAL:HG23   | 2.11                     | 0.51              |
| 4:D:152:VAL:HG23  | 4:D:279:LEU:HB3    | 1.91                     | 0.51              |
| 1:G:60:ILE:HG23   | 1:G:61:ASP:N       | 2.25                     | 0.51              |
| 2:H:138:MET:O     | 2:H:140:GLY:N      | 2.44                     | 0.51              |
| 2:H:150:CYS:HB2   | 11:H:1484:CLA:CMC  | 2.40                     | 0.51              |
| 3:I:280:SER:HA    | 3:I:434:ALA:HA     | 1.92                     | 0.51              |
| 4:J:87:HIS:C      | 4:J:167:TRP:CZ3    | 2.88                     | 0.51              |
| 4:J:111:TRP:C     | 4:J:113:PHE:N      | 2.66                     | 0.51              |
| 4:J:274:VAL:HB    | 4:J:275:PRO:CD     | 2.37                     | 0.51              |
| 5:K:8:ARG:CB      | 5:K:9:PRO:CD       | 2.88                     | 0.51              |
| 6:L:29:PRO:O      | 6:L:33:PHE:HD1     | 1.92                     | 0.51              |
| 7:P:160:UNK:O     | 7:P:161:UNK:C      | 2.59                     | 0.51              |
| 1:A:54:ALA:CB     | 1:A:72:LEU:HD12    | 2.40                     | 0.51              |
| 1:A:122:GLY:C     | 1:A:124:SER:H      | 2.19                     | 0.51              |
| 1:A:159:LEU:HD11  | 1:A:163:ILE:HD11   | 1.91                     | 0.51              |
| 1:A:326:LEU:O     | 1:A:329:GLU:N      | 2.43                     | 0.51              |
| 2:B:288:VAL:HG23  | 2:B:289:GLN:H      | 1.75                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:C:74:HIS:CD2   | 3:C:74:HIS:N      | 2.78                     | 0.51              |
| 3:C:116:VAL:CG2  | 3:C:117:VAL:H     | 2.23                     | 0.51              |
| 4:D:152:VAL:HG12 | 11:D:1351:CLA:H43 | 1.92                     | 0.51              |
| 4:D:181:PHE:CZ   | 4:D:185:PHE:CE1   | 2.98                     | 0.51              |
| 1:G:32:TRP:O     | 1:G:35:VAL:N      | 2.42                     | 0.51              |
| 1:G:193:LEU:HB3  | 4:J:179:PHE:CE1   | 2.45                     | 0.51              |
| 4:J:9:PRO:O      | 4:J:10:ALA:CB     | 2.58                     | 0.51              |
| 4:J:136:VAL:O    | 4:J:136:VAL:HG12  | 2.09                     | 0.51              |
| 5:K:31:PHE:CE1   | 6:L:35:GLY:HA2    | 2.46                     | 0.51              |
| 5:K:35:TRP:CD2   | 6:L:39:ALA:HB2    | 2.45                     | 0.51              |
| 9:T:30:LYS:O     | 9:T:34:GLN:HG3    | 2.10                     | 0.51              |
| 10:X:422:UNK:O   | 10:X:423:UNK:C    | 2.58                     | 0.51              |
| 1:A:83:VAL:HG22  | 4:D:314:PHE:CE1   | 2.45                     | 0.51              |
| 1:A:93:PHE:O     | 1:A:95:PRO:HD3    | 2.11                     | 0.51              |
| 2:B:450:TRP:O    | 2:B:451:PHE:C     | 2.51                     | 0.51              |
| 3:C:430:HIS:NE2  | 11:C:1460:CLA:ND  | 2.59                     | 0.51              |
| 4:D:330:ALA:O    | 4:D:333:ASP:N     | 2.37                     | 0.51              |
| 1:G:65:GLU:CD    | 4:J:312:GLU:OE1   | 2.54                     | 0.51              |
| 1:G:120:LEU:O    | 1:G:124:SER:N     | 2.44                     | 0.51              |
| 1:G:143:ILE:N    | 4:J:220:ASN:HD21  | 2.08                     | 0.51              |
| 2:H:68:ARG:CG    | 2:H:69:LEU:N      | 2.74                     | 0.51              |
| 2:H:471:ALA:O    | 2:H:472:ARG:C     | 2.54                     | 0.51              |
| 3:I:72:LEU:O     | 3:I:73:ALA:C      | 2.54                     | 0.51              |
| 3:I:367:GLU:O    | 3:I:370:ARG:HB2   | 2.11                     | 0.51              |
| 4:J:296:TYR:CD2  | 4:J:296:TYR:O     | 2.63                     | 0.51              |
| 4:J:296:TYR:CE1  | 4:J:319:LEU:HD23  | 2.46                     | 0.51              |
| 7:O:160:UNK:O    | 7:O:161:UNK:C     | 2.59                     | 0.51              |
| 10:X:184:UNK:O   | 10:X:185:UNK:C    | 2.59                     | 0.51              |
| 10:Y:59:UNK:C    | 10:Y:61:UNK:N     | 2.72                     | 0.51              |
| 10:Y:422:UNK:O   | 10:Y:423:UNK:C    | 2.59                     | 0.51              |
| 1:A:59:ASP:O     | 1:A:60:ILE:C      | 2.52                     | 0.51              |
| 1:A:192:ILE:HG23 | 1:A:293:MET:HE1   | 1.93                     | 0.51              |
| 2:B:246:PHE:CE1  | 2:B:463:PHE:HB2   | 2.40                     | 0.51              |
| 3:C:80:PRO:HB2   | 3:C:83:GLU:CB     | 2.41                     | 0.51              |
| 3:C:225:VAL:HG22 | 3:C:289:PHE:HD1   | 1.76                     | 0.51              |
| 3:C:330:SER:HB3  | 7:O:56:UNK:O      | 2.10                     | 0.51              |
| 3:I:235:GLY:HA2  | 3:I:238:ILE:HD12  | 1.93                     | 0.51              |
| 3:I:270:ALA:C    | 3:I:274:TYR:HD2   | 2.19                     | 0.51              |
| 10:X:568:UNK:O   | 10:X:569:UNK:C    | 2.58                     | 0.51              |
| 10:Y:264:UNK:O   | 10:Y:265:UNK:C    | 2.57                     | 0.51              |
| 1:A:54:ALA:HB2   | 1:A:72:LEU:HD12   | 1.93                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:112:TYR:CE1    | 1:A:116:ILE:CD1    | 2.93                     | 0.51              |
| 1:A:140:ARG:O      | 4:D:220:ASN:HB3    | 2.10                     | 0.51              |
| 2:B:463:PHE:C      | 2:B:465:GLY:N      | 2.66                     | 0.51              |
| 3:C:93:ALA:O       | 3:C:94:THR:C       | 2.52                     | 0.51              |
| 3:C:322:GLN:HE22   | 3:C:381:LYS:HA     | 1.76                     | 0.51              |
| 3:C:385:GLN:HB3    | 3:C:386:PRO:HD2    | 1.93                     | 0.51              |
| 4:D:210:LEU:HD11   | 4:D:270:PHE:CD2    | 2.46                     | 0.51              |
| 2:H:61:PHE:CZ      | 11:H:1488:CLA:HBB1 | 2.45                     | 0.51              |
| 2:H:280:PHE:CE2    | 2:H:312:TYR:HB3    | 2.46                     | 0.51              |
| 2:H:475:PHE:CZ     | 4:J:134:ARG:HB2    | 2.46                     | 0.51              |
| 3:I:35:TRP:O       | 3:I:37:ALA:N       | 2.43                     | 0.51              |
| 3:I:52:ALA:HA      | 11:I:1469:CLA:CMB  | 2.41                     | 0.51              |
| 3:I:449:ARG:CG     | 3:I:449:ARG:NH1    | 2.53                     | 0.51              |
| 5:K:19:TYR:CD1     | 5:K:19:TYR:C       | 2.88                     | 0.51              |
| 8:U:63:UNK:O       | 8:U:64:UNK:CB      | 2.58                     | 0.51              |
| 10:X:203:UNK:O     | 10:X:204:UNK:C     | 2.58                     | 0.51              |
| 10:X:459:UNK:O     | 10:X:460:UNK:C     | 2.56                     | 0.51              |
| 1:A:220:THR:O      | 4:D:139:ARG:HD2    | 2.11                     | 0.51              |
| 2:B:67:ALA:HA      | 2:B:71:VAL:O       | 2.11                     | 0.51              |
| 2:B:220:ARG:CB     | 2:B:221:PRO:HD2    | 2.41                     | 0.51              |
| 2:B:314:TYR:HA     | 2:B:427:GLY:HA3    | 1.92                     | 0.51              |
| 3:C:127:PHE:CE2    | 11:C:1471:CLA:HBC1 | 2.45                     | 0.51              |
| 4:D:83:ASN:CG      | 4:D:336:HIS:CD2    | 2.81                     | 0.51              |
| 4:D:172:SER:O      | 4:D:173:PHE:HB2    | 2.11                     | 0.51              |
| 1:G:317:TRP:CG     | 4:J:177:ALA:HB2    | 2.46                     | 0.51              |
| 3:I:36:TRP:O       | 11:I:1466:CLA:H43  | 2.10                     | 0.51              |
| 3:I:455:PHE:O      | 3:I:456:GLU:CG     | 2.59                     | 0.51              |
| 10:X:64:UNK:O      | 10:X:65:UNK:C      | 2.57                     | 0.51              |
| 10:X:264:UNK:O     | 10:X:265:UNK:C     | 2.59                     | 0.51              |
| 1:A:315:ASN:HA     | 1:A:319:ASP:OD2    | 2.11                     | 0.50              |
| 2:B:202:HIS:HE1    | 11:B:1484:CLA:NB   | 2.09                     | 0.50              |
| 11:C:1463:CLA:HAC1 | 11:C:1463:CLA:H92  | 1.92                     | 0.50              |
| 4:D:39:PRO:O       | 4:D:43:LEU:CB      | 2.59                     | 0.50              |
| 6:F:27:ALA:O       | 6:F:28:VAL:C       | 2.54                     | 0.50              |
| 1:G:32:TRP:O       | 1:G:33:PHE:C       | 2.54                     | 0.50              |
| 1:G:97:TRP:O       | 1:G:98:GLU:C       | 2.53                     | 0.50              |
| 1:G:114:LEU:O      | 1:G:115:ILE:C      | 2.54                     | 0.50              |
| 2:H:24:LEU:HB3     | 2:H:111:ALA:CB     | 2.41                     | 0.50              |
| 2:H:135:LEU:O      | 2:H:136:PRO:C      | 2.54                     | 0.50              |
| 2:H:194:ASN:OD1    | 2:H:194:ASN:C      | 2.54                     | 0.50              |
| 3:I:24:THR:O       | 3:I:25:ASN:CB      | 2.58                     | 0.50              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 4:J:52:THR:O     | 4:J:66:SER:HA      | 2.10                     | 0.50              |
| 5:K:38:VAL:HG11  | 6:L:40:MET:HG2     | 1.91                     | 0.50              |
| 5:K:41:GLY:O     | 5:K:42:LEU:C       | 2.54                     | 0.50              |
| 7:O:127:UNK:O    | 7:O:129:UNK:N      | 2.44                     | 0.50              |
| 10:X:262:UNK:O   | 10:X:263:UNK:C     | 2.58                     | 0.50              |
| 10:Y:201:UNK:O   | 10:Y:202:UNK:C     | 2.59                     | 0.50              |
| 10:Y:412:UNK:C   | 10:Y:414:UNK:N     | 2.72                     | 0.50              |
| 1:A:76:ASN:C     | 1:A:76:ASN:OD1     | 2.54                     | 0.50              |
| 1:A:116:ILE:CD1  | 1:A:158:PHE:HD1    | 2.24                     | 0.50              |
| 1:A:145:VAL:HA   | 1:A:148:SER:HB3    | 1.93                     | 0.50              |
| 1:A:193:LEU:HD13 | 4:D:179:PHE:HB3    | 1.91                     | 0.50              |
| 1:A:248:ILE:CD1  | 4:D:235:PHE:HZ     | 2.17                     | 0.50              |
| 3:C:39:ASN:HB2   | 11:C:1466:CLA:HAA2 | 1.92                     | 0.50              |
| 3:C:171:GLY:O    | 3:C:172:ALA:C      | 2.55                     | 0.50              |
| 3:C:270:ALA:O    | 3:C:271:TYR:C      | 2.53                     | 0.50              |
| 3:C:455:PHE:O    | 3:C:456:GLU:CB     | 2.59                     | 0.50              |
| 4:D:126:MET:CE   | 4:D:146:PHE:HB3    | 2.42                     | 0.50              |
| 1:G:176:ILE:HG23 | 1:G:180:PHE:HE1    | 1.76                     | 0.50              |
| 1:G:211:PHE:CE2  | 1:G:274:PHE:CE2    | 2.99                     | 0.50              |
| 3:I:370:ARG:HA   | 3:I:375:LEU:H      | 1.76                     | 0.50              |
| 3:I:376:ASP:HB2  | 3:I:379:LYS:CG     | 2.35                     | 0.50              |
| 4:J:16:ASP:O     | 4:J:18:LEU:N       | 2.45                     | 0.50              |
| 9:V:64:PRO:HD2   | 9:V:66:ARG:NH2     | 2.26                     | 0.50              |
| 2:B:27:THR:CG2   | 2:B:107:LEU:HD13   | 2.37                     | 0.50              |
| 2:B:37:MET:HG2   | 2:B:62:VAL:CG2     | 2.42                     | 0.50              |
| 2:B:293:ALA:O    | 2:B:294:SER:C      | 2.54                     | 0.50              |
| 3:C:150:ASP:CB   | 3:C:271:TYR:HE2    | 2.25                     | 0.50              |
| 3:C:308:GLU:O    | 3:C:311:GLN:HB2    | 2.12                     | 0.50              |
| 5:E:18:ARG:O     | 5:E:21:VAL:HB      | 2.11                     | 0.50              |
| 1:G:172:MET:HE1  | 11:G:1343:CLA:CHC  | 2.42                     | 0.50              |
| 2:H:193:TYR:CZ   | 2:H:259:GLY:HA2    | 2.46                     | 0.50              |
| 3:I:180:MET:HG3  | 3:I:181:PHE:N      | 2.27                     | 0.50              |
| 3:I:288:CYS:O    | 3:I:289:PHE:C      | 2.55                     | 0.50              |
| 4:J:93:TRP:HH2   | 11:J:1353:CLA:HBA2 | 1.76                     | 0.50              |
| 4:J:222:LEU:HA   | 4:J:244:TYR:HA     | 1.93                     | 0.50              |
| 7:P:163:UNK:O    | 7:P:164:UNK:O      | 2.29                     | 0.50              |
| 9:T:134:LYS:O    | 9:T:137:TYR:N      | 2.43                     | 0.50              |
| 10:Y:270:UNK:O   | 10:Y:271:UNK:C     | 2.60                     | 0.50              |
| 1:A:60:ILE:HB    | 1:A:83:VAL:HG11    | 1.91                     | 0.50              |
| 2:B:197:GLY:O    | 2:B:199:VAL:N      | 2.43                     | 0.50              |
| 2:B:270:PRO:O    | 2:B:271:THR:CG2    | 2.59                     | 0.50              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 2:B:397:VAL:O    | 2:B:399:VAL:N      | 2.44                     | 0.50              |
| 4:D:32:TRP:O     | 4:D:33:SER:C       | 2.54                     | 0.50              |
| 1:G:177:SER:O    | 1:G:180:PHE:N      | 2.44                     | 0.50              |
| 3:I:56:HIS:HE1   | 11:I:1467:CLA:HMA1 | 1.76                     | 0.50              |
| 3:I:431:PHE:O    | 3:I:432:VAL:C      | 2.54                     | 0.50              |
| 5:K:10:PHE:HE2   | 6:L:19:ARG:CZ      | 2.24                     | 0.50              |
| 8:U:66:UNK:O     | 8:U:70:UNK:N       | 2.45                     | 0.50              |
| 10:Y:356:UNK:O   | 10:Y:357:UNK:C     | 2.59                     | 0.50              |
| 10:Y:573:UNK:O   | 10:Y:574:UNK:C     | 2.60                     | 0.50              |
| 1:A:305:SER:O    | 1:A:313:VAL:HG13   | 2.11                     | 0.50              |
| 2:B:62:VAL:HG12  | 2:B:66:MET:HE2     | 1.93                     | 0.50              |
| 2:B:278:SER:C    | 2:B:279:TYR:O      | 2.50                     | 0.50              |
| 2:H:68:ARG:HH22  | 11:H:1485:CLA:HED3 | 1.76                     | 0.50              |
| 2:H:463:PHE:C    | 2:H:465:GLY:N      | 2.68                     | 0.50              |
| 3:I:53:HIS:NE2   | 11:I:1467:CLA:NB   | 2.60                     | 0.50              |
| 3:I:188:THR:HG21 | 3:I:298:PRO:CB     | 2.41                     | 0.50              |
| 3:I:298:PRO:O    | 3:I:299:SER:HB3    | 2.10                     | 0.50              |
| 4:J:330:ALA:O    | 4:J:333:ASP:N      | 2.37                     | 0.50              |
| 6:L:21:VAL:O     | 6:L:25:THR:HG23    | 2.12                     | 0.50              |
| 8:S:14:UNK:C     | 8:S:16:UNK:N       | 2.72                     | 0.50              |
| 10:X:68:UNK:C    | 10:X:70:UNK:N      | 2.74                     | 0.50              |
| 1:A:255:PHE:CZ   | 1:A:259:ILE:HD12   | 2.46                     | 0.50              |
| 1:A:311:GLY:HA3  | 9:V:125:ILE:CG2    | 2.41                     | 0.50              |
| 3:C:52:ALA:HA    | 11:C:1469:CLA:CMB  | 2.41                     | 0.50              |
| 3:C:188:THR:CG2  | 3:C:300:GLU:OE1    | 2.60                     | 0.50              |
| 3:C:230:LEU:O    | 3:C:230:LEU:HD12   | 2.12                     | 0.50              |
| 3:C:242:LEU:O    | 3:C:243:ILE:C      | 2.55                     | 0.50              |
| 4:D:88:SER:O     | 4:D:167:TRP:CZ3    | 2.65                     | 0.50              |
| 4:D:272:LEU:HD21 | 4:D:276:VAL:HG21   | 1.93                     | 0.50              |
| 5:E:8:ARG:CB     | 5:E:9:PRO:CD       | 2.87                     | 0.50              |
| 5:E:37:PHE:CE2   | 5:E:43:ALA:HA      | 2.47                     | 0.50              |
| 1:G:142:TRP:CH2  | 1:G:273:PHE:HE1    | 2.30                     | 0.50              |
| 1:G:258:LEU:CD1  | 4:J:128:ARG:NH2    | 2.75                     | 0.50              |
| 1:G:323:ARG:HG3  | 4:J:329:MET:HA     | 1.94                     | 0.50              |
| 2:H:15:ASP:CA    | 2:H:16:PRO:CD      | 2.88                     | 0.50              |
| 2:H:68:ARG:HG3   | 2:H:69:LEU:N       | 2.27                     | 0.50              |
| 2:H:290:ALA:O    | 2:H:294:SER:HB3    | 2.12                     | 0.50              |
| 3:I:80:PRO:HB2   | 3:I:83:GLU:CB      | 2.40                     | 0.50              |
| 3:I:358:PHE:C    | 3:I:360:ASP:H      | 2.18                     | 0.50              |
| 7:P:127:UNK:O    | 7:P:129:UNK:N      | 2.45                     | 0.50              |
| 10:X:168:UNK:O   | 10:X:169:UNK:C     | 2.59                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:X:412:UNK:C     | 10:X:414:UNK:N     | 2.73                     | 0.50              |
| 1:A:84:PRO:HG3     | 1:A:112:TYR:CE2    | 2.47                     | 0.50              |
| 1:A:288:LEU:HD13   | 3:C:432:VAL:HG22   | 1.92                     | 0.50              |
| 2:B:366:PHE:HD2    | 2:B:425:ILE:HD11   | 1.75                     | 0.50              |
| 5:E:82:GLN:O       | 5:E:84:LYS:N       | 2.43                     | 0.50              |
| 5:E:82:GLN:O       | 5:E:83:LEU:C       | 2.54                     | 0.50              |
| 1:G:60:ILE:HB      | 1:G:83:VAL:HG11    | 1.93                     | 0.50              |
| 3:I:178:LYS:CA     | 3:I:182:PHE:HB2    | 2.40                     | 0.50              |
| 3:I:366:LEU:O      | 3:I:366:LEU:HD12   | 2.12                     | 0.50              |
| 4:J:190:ASN:HB2    | 4:J:296:TYR:HD1    | 1.76                     | 0.50              |
| 4:J:209:LEU:HD21   | 4:J:213:ILE:HD11   | 1.92                     | 0.50              |
| 6:L:33:PHE:HA      | 6:L:36:ALA:HB3     | 1.94                     | 0.50              |
| 7:O:123:UNK:O      | 7:O:126:UNK:N      | 2.45                     | 0.50              |
| 8:S:29:UNK:O       | 8:S:30:UNK:C       | 2.59                     | 0.50              |
| 10:Y:168:UNK:O     | 10:Y:169:UNK:C     | 2.60                     | 0.50              |
| 11:A:1342:CLA:H143 | 12:A:1345:PHO:H62  | 1.93                     | 0.50              |
| 2:B:135:LEU:O      | 2:B:137:LYS:N      | 2.45                     | 0.50              |
| 2:B:204:ALA:O      | 2:B:205:ALA:C      | 2.55                     | 0.50              |
| 2:B:351:GLY:O      | 2:B:353:GLU:N      | 2.45                     | 0.50              |
| 3:C:55:ALA:O       | 3:C:56:HIS:C       | 2.55                     | 0.50              |
| 1:G:266:ASN:O      | 1:G:267:ASN:O      | 2.30                     | 0.50              |
| 2:H:346:PHE:O      | 2:H:353:GLU:O      | 2.29                     | 0.50              |
| 4:J:103:ARG:O      | 4:J:104:TRP:C      | 2.55                     | 0.50              |
| 4:J:264:LYS:C      | 4:J:266:TRP:H      | 2.20                     | 0.50              |
| 10:Y:17:UNK:O      | 10:Y:18:UNK:C      | 2.59                     | 0.50              |
| 10:Y:203:UNK:O     | 10:Y:204:UNK:C     | 2.59                     | 0.50              |
| 10:Y:526:UNK:O     | 10:Y:529:UNK:N     | 2.45                     | 0.50              |
| 1:A:32:TRP:O       | 1:A:33:PHE:C       | 2.55                     | 0.50              |
| 1:A:184:ILE:HA     | 11:A:1342:CLA:HBC1 | 1.94                     | 0.50              |
| 1:A:290:ILE:CD1    | 11:A:1342:CLA:OBD  | 2.58                     | 0.50              |
| 12:A:1345:PHO:CAB  | 4:D:205:LEU:HD21   | 2.41                     | 0.50              |
| 2:B:152:GLY:O      | 2:B:153:PHE:C      | 2.53                     | 0.50              |
| 2:B:220:ARG:CD     | 2:B:221:PRO:HD2    | 2.41                     | 0.50              |
| 2:B:400:SER:HB3    | 2:B:410:THR:CB     | 2.27                     | 0.50              |
| 3:C:84:GLN:O       | 3:C:85:GLY:C       | 2.55                     | 0.50              |
| 3:C:159:THR:HA     | 3:C:252:ILE:HA     | 1.94                     | 0.50              |
| 3:C:318:LEU:HD11   | 3:C:328:VAL:HG21   | 1.93                     | 0.50              |
| 4:D:53:THR:HG21    | 6:F:37:ILE:HD11    | 1.93                     | 0.50              |
| 4:D:273:PHE:O      | 4:D:277:THR:OG1    | 2.24                     | 0.50              |
| 5:E:10:PHE:HE2     | 6:F:19:ARG:HE      | 1.60                     | 0.50              |
| 5:E:10:PHE:HD2     | 6:F:19:ARG:NH2     | 2.09                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:E:18:ARG:NH1     | 10:X:564:UNK:CB    | 2.75                     | 0.50              |
| 1:G:107:TYR:O      | 1:G:109:GLY:N      | 2.44                     | 0.50              |
| 2:H:178:VAL:O      | 2:H:179:GLN:HG3    | 2.11                     | 0.50              |
| 3:I:120:ILE:C      | 3:I:122:SER:H      | 2.18                     | 0.50              |
| 3:I:322:GLN:HE22   | 3:I:381:LYS:HA     | 1.77                     | 0.50              |
| 4:J:209:LEU:HD23   | 4:J:209:LEU:O      | 2.12                     | 0.50              |
| 5:K:41:GLY:O       | 5:K:44:TYR:HB2     | 2.11                     | 0.50              |
| 6:L:14:PRO:O       | 6:L:15:ILE:HB      | 2.12                     | 0.50              |
| 10:X:423:UNK:O     | 10:X:424:UNK:C     | 2.60                     | 0.50              |
| 10:Y:225:UNK:O     | 10:Y:226:UNK:C     | 2.59                     | 0.50              |
| 1:A:210:LEU:HD12   | 1:A:210:LEU:O      | 2.12                     | 0.49              |
| 2:B:236:THR:HG23   | 2:B:237:VAL:N      | 2.27                     | 0.49              |
| 2:B:408:GLY:O      | 2:B:409:GLN:HB2    | 2.12                     | 0.49              |
| 3:C:37:ALA:C       | 3:C:39:ASN:H       | 2.19                     | 0.49              |
| 3:C:449:ARG:NH1    | 11:C:1463:CLA:O1D  | 2.45                     | 0.49              |
| 4:D:40:CYS:O       | 4:D:41:ALA:C       | 2.54                     | 0.49              |
| 2:H:211:ILE:O      | 2:H:214:LEU:HG     | 2.10                     | 0.49              |
| 2:H:415:PRO:O      | 2:H:419:SER:N      | 2.37                     | 0.49              |
| 2:H:437:LEU:O      | 2:H:439:SER:N      | 2.43                     | 0.49              |
| 3:I:74:HIS:CD2     | 3:I:74:HIS:H       | 2.28                     | 0.49              |
| 3:I:169:GLY:CA     | 3:I:244:CYS:SG     | 3.00                     | 0.49              |
| 3:I:170:ILE:CG2    | 3:I:171:GLY:N      | 2.75                     | 0.49              |
| 3:I:270:ALA:O      | 3:I:271:TYR:C      | 2.54                     | 0.49              |
| 4:J:276:VAL:O      | 4:J:280:TRP:HD1    | 1.95                     | 0.49              |
| 5:K:27:ILE:O       | 5:K:28:PRO:C       | 2.54                     | 0.49              |
| 5:K:37:PHE:CE2     | 5:K:43:ALA:HA      | 2.47                     | 0.49              |
| 8:S:72:UNK:O       | 8:S:73:UNK:C       | 2.57                     | 0.49              |
| 10:X:263:UNK:O     | 10:X:264:UNK:C     | 2.60                     | 0.49              |
| 10:X:526:UNK:C     | 10:X:528:UNK:N     | 2.73                     | 0.49              |
| 10:Y:405:UNK:O     | 10:Y:409:UNK:N     | 2.44                     | 0.49              |
| 1:A:133:LEU:HB2    | 4:D:252:PHE:CE2    | 2.47                     | 0.49              |
| 1:A:279:PRO:HB2    | 12:A:1345:PHO:HBC1 | 1.94                     | 0.49              |
| 2:B:139:PHE:HB2    | 11:B:1491:CLA:CHD  | 2.42                     | 0.49              |
| 2:B:372:ASP:C      | 2:B:374:ASN:H      | 2.19                     | 0.49              |
| 2:B:468:TRP:HD1    | 4:D:144:ILE:HD11   | 1.73                     | 0.49              |
| 2:B:478:VAL:O      | 2:B:481:GLY:N      | 2.45                     | 0.49              |
| 11:B:1485:CLA:HMC2 | 11:B:1492:CLA:H191 | 1.94                     | 0.49              |
| 3:C:40:ALA:HA      | 3:C:43:ILE:HG23    | 1.94                     | 0.49              |
| 4:D:87:HIS:C       | 4:D:167:TRP:CZ3    | 2.90                     | 0.49              |
| 6:F:29:PRO:O       | 6:F:33:PHE:HD1     | 1.95                     | 0.49              |
| 1:G:60:ILE:HD12    | 1:G:84:PRO:HD2     | 1.94                     | 0.49              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 12:G:1345:PHO:HBB2 | 4:J:205:LEU:HD21  | 1.93                     | 0.49              |
| 3:I:127:PHE:C      | 3:I:129:GLY:H     | 2.20                     | 0.49              |
| 3:I:166:ILE:HD11   | 3:I:249:ILE:HD13  | 1.95                     | 0.49              |
| 4:J:191:TRP:HA     | 4:J:191:TRP:HE3   | 1.76                     | 0.49              |
| 4:J:235:PHE:CD2    | 4:J:243:THR:HG21  | 2.47                     | 0.49              |
| 5:K:51:ARG:O       | 5:K:52:PRO:C      | 2.56                     | 0.49              |
| 10:X:24:UNK:O      | 10:X:25:UNK:C     | 2.61                     | 0.49              |
| 10:X:214:UNK:O     | 10:X:218:UNK:N    | 2.44                     | 0.49              |
| 10:Y:221:UNK:O     | 10:Y:222:UNK:C    | 2.60                     | 0.49              |
| 10:Y:225:UNK:O     | 10:Y:227:UNK:N    | 2.46                     | 0.49              |
| 10:Y:255:UNK:O     | 10:Y:256:UNK:C    | 2.61                     | 0.49              |
| 10:Y:418:UNK:O     | 10:Y:419:UNK:C    | 2.59                     | 0.49              |
| 1:A:110:GLY:O      | 1:A:111:PRO:C     | 2.53                     | 0.49              |
| 1:A:172:MET:SD     | 1:A:179:THR:HG23  | 2.53                     | 0.49              |
| 1:A:183:MET:HE1    | 11:A:1343:CLA:CMD | 2.41                     | 0.49              |
| 1:A:285:PHE:O      | 1:A:289:GLY:N     | 2.35                     | 0.49              |
| 3:C:242:LEU:HD12   | 3:C:245:ILE:HD11  | 1.95                     | 0.49              |
| 3:C:364:PRO:O      | 3:C:365:TRP:C     | 2.55                     | 0.49              |
| 4:D:276:VAL:O      | 4:D:280:TRP:HD1   | 1.95                     | 0.49              |
| 4:D:296:TYR:O      | 4:D:297:ASP:HB3   | 2.12                     | 0.49              |
| 6:F:35:GLY:O       | 6:F:36:ALA:C      | 2.52                     | 0.49              |
| 1:G:35:VAL:O       | 1:G:35:VAL:HG12   | 2.11                     | 0.49              |
| 1:G:331:MET:HE3    | 4:J:346:LEU:O     | 2.11                     | 0.49              |
| 2:H:69:LEU:HB3     | 11:H:1487:CLA:CMA | 2.42                     | 0.49              |
| 2:H:264:PRO:HB2    | 2:H:267:LEU:HD12  | 1.94                     | 0.49              |
| 8:S:91:UNK:O       | 8:S:92:UNK:CB     | 2.59                     | 0.49              |
| 9:V:122:GLU:N      | 9:V:123:PRO:HD2   | 2.27                     | 0.49              |
| 10:X:426:UNK:O     | 10:X:427:UNK:C    | 2.60                     | 0.49              |
| 10:Y:526:UNK:C     | 10:Y:528:UNK:N    | 2.72                     | 0.49              |
| 1:A:330:VAL:HG12   | 4:D:347:PRO:CA    | 2.36                     | 0.49              |
| 2:B:45:PHE:C       | 2:B:47:PRO:HD2    | 2.37                     | 0.49              |
| 2:B:397:VAL:O      | 2:B:411:PHE:O     | 2.30                     | 0.49              |
| 3:C:370:ARG:HE     | 3:C:371:GLY:N     | 2.06                     | 0.49              |
| 4:D:96:GLU:OE1     | 4:D:96:GLU:HA     | 2.12                     | 0.49              |
| 1:G:48:PHE:C       | 1:G:48:PHE:CD2    | 2.90                     | 0.49              |
| 1:G:145:VAL:HA     | 1:G:148:SER:HB3   | 1.93                     | 0.49              |
| 2:H:94:GLU:HG3     | 2:H:95:GLY:H      | 1.76                     | 0.49              |
| 9:T:136:TYR:O      | 9:T:137:TYR:CG    | 2.65                     | 0.49              |
| 1:A:207:GLY:O      | 1:A:208:GLY:C     | 2.54                     | 0.49              |
| 2:B:136:PRO:HG2    | 2:B:221:PRO:HG3   | 1.94                     | 0.49              |
| 2:B:243:ALA:O      | 2:B:246:PHE:HB3   | 2.13                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:280:PHE:O      | 2:B:283:GLU:HB3    | 2.13                     | 0.49              |
| 3:C:109:PHE:HD2    | 3:C:110:PRO:HD3    | 1.77                     | 0.49              |
| 3:C:235:GLY:HA2    | 3:C:238:ILE:CD1    | 2.43                     | 0.49              |
| 3:C:287:THR:OG1    | 3:C:288:CYS:N      | 2.46                     | 0.49              |
| 3:C:299:SER:HB2    | 3:C:303:GLY:O      | 2.11                     | 0.49              |
| 3:C:387:TRP:O      | 3:C:390:ARG:HG2    | 2.11                     | 0.49              |
| 4:D:296:TYR:CD2    | 4:D:296:TYR:O      | 2.65                     | 0.49              |
| 17:F:1046:BCR:H331 | 17:F:1046:BCR:H343 | 1.94                     | 0.49              |
| 1:G:309:ALA:O      | 9:T:2:GLU:CB       | 2.60                     | 0.49              |
| 2:H:49:ASP:CG      | 2:H:49:ASP:O       | 2.55                     | 0.49              |
| 3:I:240:ILE:HA     | 3:I:243:ILE:HB     | 1.93                     | 0.49              |
| 3:I:299:SER:HB2    | 3:I:303:GLY:O      | 2.13                     | 0.49              |
| 3:I:305:THR:O      | 3:I:306:GLY:C      | 2.55                     | 0.49              |
| 4:J:181:PHE:CZ     | 4:J:185:PHE:HE1    | 2.31                     | 0.49              |
| 4:J:186:GLN:HB2    | 11:J:1351:CLA:HBC1 | 1.93                     | 0.49              |
| 1:A:58:VAL:HB      | 1:A:83:VAL:HB      | 1.94                     | 0.49              |
| 1:A:219:VAL:HG11   | 4:D:268:HIS:CD2    | 2.47                     | 0.49              |
| 1:A:278:TRP:CB     | 1:A:279:PRO:HD3    | 2.36                     | 0.49              |
| 2:B:263:THR:O      | 2:B:448:ARG:NH1    | 2.45                     | 0.49              |
| 2:B:278:SER:O      | 2:B:281:GLN:HG2    | 2.13                     | 0.49              |
| 3:C:109:PHE:CD2    | 3:C:110:PRO:HD3    | 2.47                     | 0.49              |
| 3:C:431:PHE:O      | 3:C:432:VAL:C      | 2.53                     | 0.49              |
| 4:D:191:TRP:CE3    | 4:D:289:LEU:HD11   | 2.48                     | 0.49              |
| 4:D:235:PHE:CD1    | 4:D:235:PHE:C      | 2.90                     | 0.49              |
| 4:D:313:THR:OG1    | 4:D:315:TYR:HB3    | 2.13                     | 0.49              |
| 1:G:93:PHE:CE1     | 1:G:95:PRO:HG2     | 2.48                     | 0.49              |
| 1:G:122:GLY:C      | 1:G:124:SER:H      | 2.20                     | 0.49              |
| 2:H:160:GLY:HA2    | 2:H:163:GLY:HA2    | 1.94                     | 0.49              |
| 2:H:272:ARG:NH1    | 4:J:164:GLN:HA     | 2.27                     | 0.49              |
| 3:I:88:LEU:O       | 3:I:89:ILE:C       | 2.56                     | 0.49              |
| 6:L:17:THR:O       | 6:L:20:TRP:HB3     | 2.13                     | 0.49              |
| 10:X:418:UNK:O     | 10:X:419:UNK:C     | 2.61                     | 0.49              |
| 1:A:26:ASN:CA      | 4:D:255:GLN:NE2    | 2.76                     | 0.49              |
| 1:A:320:ILE:O      | 1:A:321:ILE:C      | 2.56                     | 0.49              |
| 2:B:18:ARG:O       | 2:B:21:ALA:HB3     | 2.13                     | 0.49              |
| 2:B:24:LEU:HD12    | 11:B:1496:CLA:HED2 | 1.94                     | 0.49              |
| 2:B:418:LYS:O      | 2:B:419:SER:C      | 2.53                     | 0.49              |
| 2:B:466:HIS:O      | 2:B:468:TRP:N      | 2.45                     | 0.49              |
| 11:C:1471:CLA:HBC3 | 11:C:1471:CLA:HHD  | 1.95                     | 0.49              |
| 4:D:291:LEU:N      | 4:D:291:LEU:CD1    | 2.76                     | 0.49              |
| 1:G:330:VAL:HG11   | 4:J:328:TRP:HZ2    | 1.78                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:I:430:HIS:NE2    | 11:I:1460:CLA:ND   | 2.61                     | 0.49              |
| 4:J:126:MET:CE     | 4:J:146:PHE:HB3    | 2.43                     | 0.49              |
| 7:O:163:UNK:O      | 7:O:164:UNK:O      | 2.31                     | 0.49              |
| 10:X:170:UNK:O     | 10:X:171:UNK:C     | 2.61                     | 0.49              |
| 1:A:47:CYS:HG      | 1:A:114:LEU:HD23   | 1.75                     | 0.49              |
| 1:A:89:ILE:HD11    | 1:A:108:ASN:HB3    | 1.95                     | 0.49              |
| 1:A:330:VAL:HG11   | 4:D:328:TRP:HZ2    | 1.76                     | 0.49              |
| 1:A:330:VAL:HG21   | 4:D:328:TRP:CZ2    | 2.48                     | 0.49              |
| 3:C:250:TRP:O      | 3:C:250:TRP:HD1    | 1.94                     | 0.49              |
| 1:G:83:VAL:HG13    | 4:J:314:PHE:CZ     | 2.47                     | 0.49              |
| 2:H:205:ALA:O      | 2:H:209:GLY:N      | 2.45                     | 0.49              |
| 3:I:176:VAL:HG23   | 3:I:234:VAL:HG12   | 1.94                     | 0.49              |
| 3:I:319:ILE:HD11   | 3:I:384:ILE:HD11   | 1.95                     | 0.49              |
| 4:J:186:GLN:CB     | 11:J:1351:CLA:HBC1 | 2.43                     | 0.49              |
| 4:J:188:PHE:CE1    | 4:J:326:ARG:HG2    | 2.48                     | 0.49              |
| 9:T:55:ARG:HG3     | 9:T:131:GLY:HA2    | 1.95                     | 0.49              |
| 8:U:20:UNK:C       | 8:U:22:UNK:H       | 2.26                     | 0.49              |
| 10:Y:357:UNK:O     | 10:Y:358:UNK:C     | 2.60                     | 0.49              |
| 1:A:137:LEU:HB2    | 1:A:139:MET:CE     | 2.42                     | 0.49              |
| 1:A:330:VAL:CG1    | 4:D:347:PRO:CA     | 2.89                     | 0.49              |
| 2:B:61:PHE:CZ      | 11:B:1488:CLA:HBB1 | 2.48                     | 0.49              |
| 2:B:347:ARG:HB3    | 2:B:351:GLY:CA     | 2.28                     | 0.49              |
| 11:B:1496:CLA:H171 | 11:B:1497:CLA:CMD  | 2.39                     | 0.49              |
| 3:C:129:GLY:C      | 3:C:131:TYR:N      | 2.70                     | 0.49              |
| 3:C:177:ALA:O      | 3:C:178:LYS:C      | 2.56                     | 0.49              |
| 3:C:429:SER:O      | 3:C:432:VAL:HB     | 2.12                     | 0.49              |
| 4:D:91:LEU:C       | 4:D:93:TRP:N       | 2.71                     | 0.49              |
| 4:D:174:GLY:O      | 4:D:178:ILE:HG13   | 2.12                     | 0.49              |
| 4:D:236:ASN:C      | 4:D:238:THR:N      | 2.71                     | 0.49              |
| 5:E:63:ILE:N       | 5:E:64:PRO:HD3     | 2.28                     | 0.49              |
| 6:F:33:PHE:C       | 6:F:35:GLY:H       | 2.21                     | 0.49              |
| 1:G:58:VAL:HB      | 1:G:83:VAL:HB      | 1.95                     | 0.49              |
| 1:G:186:PHE:CD2    | 1:G:192:ILE:CD1    | 2.86                     | 0.49              |
| 2:H:196:GLY:O      | 2:H:197:GLY:C      | 2.54                     | 0.49              |
| 3:I:27:ASP:O       | 3:I:31:SER:HB2     | 2.12                     | 0.49              |
| 4:J:53:THR:HG21    | 6:L:37:ILE:HD11    | 1.95                     | 0.49              |
| 4:J:122:LEU:CD2    | 11:J:1351:CLA:H92  | 2.28                     | 0.49              |
| 4:J:166:SER:O      | 4:J:167:TRP:C      | 2.50                     | 0.49              |
| 4:J:181:PHE:CZ     | 4:J:185:PHE:CE1    | 3.01                     | 0.49              |
| 9:T:128:ASP:HB3    | 9:T:134:LYS:HG3    | 1.95                     | 0.49              |
| 10:X:168:UNK:O     | 10:X:170:UNK:N     | 2.46                     | 0.49              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 10:Y:64:UNK:O    | 10:Y:65:UNK:C      | 2.60                     | 0.49              |
| 1:A:13:LEU:O     | 1:A:14:TRP:C       | 2.55                     | 0.49              |
| 1:A:134:SER:C    | 1:A:136:ARG:N      | 2.71                     | 0.49              |
| 2:B:69:LEU:HB3   | 11:B:1487:CLA:CMA  | 2.43                     | 0.49              |
| 3:C:51:GLY:O     | 3:C:52:ALA:C       | 2.56                     | 0.49              |
| 3:C:91:HIS:O     | 3:C:92:ILE:C       | 2.56                     | 0.49              |
| 3:C:172:ALA:O    | 3:C:173:LEU:C      | 2.56                     | 0.49              |
| 4:D:116:LEU:O    | 4:D:119:ALA:HB3    | 2.12                     | 0.49              |
| 1:G:290:ILE:O    | 1:G:292:THR:N      | 2.45                     | 0.49              |
| 2:H:24:LEU:HD23  | 2:H:111:ALA:HA     | 1.94                     | 0.49              |
| 2:H:52:LEU:HD23  | 2:H:311:PHE:CE2    | 2.48                     | 0.49              |
| 2:H:397:VAL:O    | 2:H:399:VAL:N      | 2.43                     | 0.49              |
| 3:I:35:TRP:CE3   | 3:I:36:TRP:HB3     | 2.47                     | 0.49              |
| 3:I:159:THR:HA   | 3:I:252:ILE:HA     | 1.94                     | 0.49              |
| 3:I:442:LEU:HD21 | 11:I:1463:CLA:C1B  | 2.43                     | 0.49              |
| 4:J:54:PHE:HB3   | 5:K:47:PHE:CG      | 2.48                     | 0.49              |
| 6:L:11:VAL:CG1   | 6:L:12:SER:N       | 2.76                     | 0.49              |
| 7:O:141:UNK:O    | 7:O:149:UNK:CB     | 2.61                     | 0.49              |
| 8:S:43:UNK:O     | 8:S:47:UNK:N       | 2.46                     | 0.49              |
| 8:U:4:UNK:O      | 8:U:7:UNK:CB       | 2.61                     | 0.49              |
| 8:U:99:UNK:O     | 8:U:100:UNK:C      | 2.59                     | 0.49              |
| 10:X:219:UNK:O   | 10:X:220:UNK:C     | 2.60                     | 0.49              |
| 10:X:405:UNK:O   | 10:X:409:UNK:N     | 2.46                     | 0.49              |
| 10:X:573:UNK:O   | 10:X:574:UNK:C     | 2.61                     | 0.49              |
| 1:A:278:TRP:HB3  | 1:A:279:PRO:CD     | 2.34                     | 0.48              |
| 2:B:65:PHE:O     | 2:B:66:MET:C       | 2.56                     | 0.48              |
| 2:B:263:THR:O    | 2:B:448:ARG:NH2    | 2.46                     | 0.48              |
| 2:B:415:PRO:O    | 2:B:418:LYS:N      | 2.46                     | 0.48              |
| 2:B:462:PHE:HA   | 11:B:1492:CLA:CMC  | 2.43                     | 0.48              |
| 3:C:28:GLN:O     | 3:C:30:SER:N       | 2.46                     | 0.48              |
| 3:C:178:LYS:CA   | 3:C:182:PHE:HB2    | 2.42                     | 0.48              |
| 3:C:271:TYR:O    | 3:C:272:LEU:C      | 2.54                     | 0.48              |
| 3:C:445:ALA:CB   | 11:C:1463:CLA:HED1 | 2.36                     | 0.48              |
| 4:D:51:GLY:O     | 4:D:52:THR:C       | 2.56                     | 0.48              |
| 4:D:235:PHE:CD2  | 4:D:243:THR:HG21   | 2.47                     | 0.48              |
| 1:G:122:GLY:O    | 1:G:125:CYS:N      | 2.45                     | 0.48              |
| 1:G:248:ILE:O    | 1:G:249:VAL:C      | 2.55                     | 0.48              |
| 2:H:113:TRP:CD1  | 11:H:1496:CLA:H191 | 2.48                     | 0.48              |
| 3:I:46:SER:O     | 3:I:47:GLY:C       | 2.56                     | 0.48              |
| 3:I:82:TYR:HD2   | 3:I:302:TYR:O      | 1.96                     | 0.48              |
| 4:J:279:LEU:CD1  | 12:J:1352:PHO:HBC3 | 2.42                     | 0.48              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 5:K:63:ILE:O     | 5:K:63:ILE:HG22    | 2.12                     | 0.48              |
| 8:S:63:UNK:O     | 8:S:64:UNK:CB      | 2.60                     | 0.48              |
| 10:Y:59:UNK:O    | 10:Y:62:UNK:N      | 2.46                     | 0.48              |
| 1:A:142:TRP:CZ2  | 1:A:273:PHE:CE1    | 3.01                     | 0.48              |
| 1:A:161:TYR:HA   | 1:A:294:ALA:HB1    | 1.95                     | 0.48              |
| 1:A:273:PHE:C    | 1:A:273:PHE:CD2    | 2.92                     | 0.48              |
| 1:A:311:GLY:O    | 1:A:312:ASN:C      | 2.56                     | 0.48              |
| 2:B:24:LEU:HB3   | 2:B:111:ALA:CB     | 2.43                     | 0.48              |
| 2:B:393:GLU:C    | 2:B:395:GLN:N      | 2.69                     | 0.48              |
| 3:C:449:ARG:HH12 | 11:C:1463:CLA:HAA1 | 1.78                     | 0.48              |
| 4:D:335:PRO:O    | 4:D:336:HIS:C      | 2.56                     | 0.48              |
| 1:G:214:MET:CE   | 12:J:1352:PHO:CED  | 2.91                     | 0.48              |
| 2:H:263:THR:O    | 2:H:448:ARG:NH2    | 2.45                     | 0.48              |
| 3:I:242:LEU:O    | 3:I:243:ILE:C      | 2.56                     | 0.48              |
| 6:L:40:MET:O     | 6:L:43:ILE:HG13    | 2.13                     | 0.48              |
| 9:T:69:ILE:O     | 9:T:70:GLU:C       | 2.56                     | 0.48              |
| 10:X:64:UNK:C    | 10:X:66:UNK:N      | 2.74                     | 0.48              |
| 10:X:425:UNK:O   | 10:X:429:UNK:CB    | 2.61                     | 0.48              |
| 10:Y:410:UNK:O   | 10:Y:411:UNK:C     | 2.60                     | 0.48              |
| 2:B:135:LEU:O    | 2:B:136:PRO:C      | 2.53                     | 0.48              |
| 2:B:178:VAL:O    | 2:B:179:GLN:HG3    | 2.12                     | 0.48              |
| 2:B:314:TYR:H    | 2:B:427:GLY:HA3    | 1.79                     | 0.48              |
| 4:D:57:SER:HB2   | 4:D:63:LEU:O       | 2.13                     | 0.48              |
| 4:D:72:ASN:C     | 4:D:76:VAL:HG23    | 2.38                     | 0.48              |
| 4:D:171:PRO:HG3  | 4:D:181:PHE:CD1    | 2.48                     | 0.48              |
| 4:D:225:ASP:OD1  | 4:D:225:ASP:O      | 2.32                     | 0.48              |
| 5:E:10:PHE:HE2   | 6:F:19:ARG:CZ      | 2.25                     | 0.48              |
| 5:E:19:TYR:C     | 5:E:19:TYR:CD1     | 2.90                     | 0.48              |
| 5:E:51:ARG:O     | 5:E:52:PRO:C       | 2.54                     | 0.48              |
| 1:G:21:VAL:O     | 1:G:22:THR:C       | 2.56                     | 0.48              |
| 1:G:83:VAL:HG22  | 4:J:314:PHE:CE1    | 2.44                     | 0.48              |
| 1:G:201:GLY:HA2  | 1:G:282:GLY:O      | 2.13                     | 0.48              |
| 2:H:97:ALA:O     | 2:H:98:LEU:C       | 2.52                     | 0.48              |
| 2:H:135:LEU:CB   | 2:H:136:PRO:CD     | 2.86                     | 0.48              |
| 2:H:149:LEU:HG   | 11:H:1484:CLA:CBC  | 2.34                     | 0.48              |
| 2:H:360:PRO:HB2  | 2:H:363:PHE:CD2    | 2.44                     | 0.48              |
| 2:H:396:GLY:O    | 2:H:397:VAL:C      | 2.56                     | 0.48              |
| 3:I:43:ILE:HG22  | 11:I:1467:CLA:HBC2 | 1.96                     | 0.48              |
| 3:I:75:PHE:CZ    | 3:I:77:PRO:HG3     | 2.48                     | 0.48              |
| 3:I:97:TRP:O     | 3:I:98:GLY:C       | 2.56                     | 0.48              |
| 3:I:150:ASP:CB   | 3:I:271:TYR:HE2    | 2.25                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 11:I:1466:CLA:HBD | 11:I:1466:CLA:HBA1 | 1.94                     | 0.48              |
| 4:J:9:PRO:O       | 4:J:10:ALA:HB2     | 2.12                     | 0.48              |
| 5:K:74:GLN:O      | 5:K:77:GLU:N       | 2.45                     | 0.48              |
| 8:S:39:UNK:O      | 8:S:40:UNK:O       | 2.31                     | 0.48              |
| 8:S:69:UNK:C      | 8:S:71:UNK:N       | 2.77                     | 0.48              |
| 10:Y:268:UNK:O    | 10:Y:269:UNK:C     | 2.61                     | 0.48              |
| 10:Y:426:UNK:O    | 10:Y:427:UNK:C     | 2.60                     | 0.48              |
| 2:B:213:GLY:O     | 2:B:214:LEU:C      | 2.57                     | 0.48              |
| 3:C:225:VAL:HG22  | 3:C:289:PHE:CD1    | 2.48                     | 0.48              |
| 3:C:382:ASN:O     | 3:C:383:ASP:HB2    | 2.13                     | 0.48              |
| 3:C:442:LEU:HD21  | 11:C:1463:CLA:C1B  | 2.43                     | 0.48              |
| 4:D:192:THR:OG1   | 4:D:193:LEU:N      | 2.46                     | 0.48              |
| 4:D:222:LEU:HA    | 4:D:244:TYR:HA     | 1.94                     | 0.48              |
| 1:G:142:TRP:CG    | 4:J:220:ASN:OD1    | 2.67                     | 0.48              |
| 1:G:307:ILE:O     | 1:G:308:ASP:C      | 2.53                     | 0.48              |
| 1:G:332:HIS:HD2   | 1:G:333:GLU:H      | 1.60                     | 0.48              |
| 2:H:236:THR:CB    | 2:H:473:THR:CG2    | 2.88                     | 0.48              |
| 3:I:28:GLN:O      | 3:I:30:SER:N       | 2.46                     | 0.48              |
| 7:P:42:UNK:CB     | 7:P:52:UNK:O       | 2.61                     | 0.48              |
| 8:S:71:UNK:O      | 8:S:72:UNK:C       | 2.58                     | 0.48              |
| 8:U:73:UNK:O      | 8:U:74:UNK:C       | 2.59                     | 0.48              |
| 8:U:74:UNK:O      | 8:U:75:UNK:C       | 2.61                     | 0.48              |
| 1:A:255:PHE:CE1   | 1:A:259:ILE:HD12   | 2.47                     | 0.48              |
| 1:A:258:LEU:HD12  | 4:D:128:ARG:NH2    | 2.28                     | 0.48              |
| 2:B:114:HIS:NE2   | 11:B:1497:CLA:NB   | 2.62                     | 0.48              |
| 3:C:81:MET:O      | 3:C:84:GLN:N       | 2.37                     | 0.48              |
| 4:D:48:TRP:HB2    | 4:D:114:ILE:HD13   | 1.95                     | 0.48              |
| 4:D:218:VAL:O     | 4:D:219:GLU:C      | 2.55                     | 0.48              |
| 2:H:222:PRO:O     | 2:H:223:GLN:C      | 2.56                     | 0.48              |
| 2:H:263:THR:H     | 2:H:264:PRO:HD3    | 1.72                     | 0.48              |
| 2:H:362:PHE:HE2   | 4:J:184:PHE:CZ     | 2.32                     | 0.48              |
| 4:J:81:PRO:O      | 4:J:168:PHE:HD1    | 1.97                     | 0.48              |
| 4:J:95:PRO:O      | 4:J:96:GLU:O       | 2.31                     | 0.48              |
| 5:K:16:SER:O      | 5:K:17:VAL:CB      | 2.61                     | 0.48              |
| 10:X:567:UNK:O    | 10:X:571:UNK:N     | 2.47                     | 0.48              |
| 10:Y:435:UNK:O    | 10:Y:438:UNK:N     | 2.46                     | 0.48              |
| 2:B:309:LEU:C     | 2:B:311:PHE:N      | 2.68                     | 0.48              |
| 3:C:46:SER:O      | 3:C:47:GLY:C       | 2.56                     | 0.48              |
| 3:C:170:ILE:O     | 3:C:171:GLY:C      | 2.56                     | 0.48              |
| 3:C:274:TYR:CD1   | 11:C:1463:CLA:HMD1 | 2.47                     | 0.48              |
| 4:D:46:GLY:O      | 4:D:49:LEU:N       | 2.47                     | 0.48              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 4:D:53:THR:HG22  | 4:D:67:TYR:CE1     | 2.48                     | 0.48              |
| 4:D:76:VAL:HG12  | 4:D:77:ALA:N       | 2.28                     | 0.48              |
| 4:D:200:GLY:O    | 4:D:201:VAL:C      | 2.56                     | 0.48              |
| 6:F:33:PHE:HA    | 6:F:36:ALA:HB3     | 1.96                     | 0.48              |
| 1:G:221:SER:HB2  | 4:J:139:ARG:O      | 2.14                     | 0.48              |
| 3:I:49:LEU:O     | 3:I:52:ALA:N       | 2.47                     | 0.48              |
| 3:I:382:ASN:O    | 3:I:383:ASP:HB2    | 2.12                     | 0.48              |
| 4:J:46:GLY:O     | 4:J:49:LEU:N       | 2.45                     | 0.48              |
| 4:J:88:SER:O     | 4:J:167:TRP:HZ3    | 1.96                     | 0.48              |
| 4:J:218:VAL:O    | 4:J:219:GLU:C      | 2.56                     | 0.48              |
| 7:P:127:UNK:O    | 7:P:128:UNK:C      | 2.61                     | 0.48              |
| 8:S:46:UNK:O     | 8:S:47:UNK:C       | 2.61                     | 0.48              |
| 10:X:272:UNK:O   | 10:X:273:UNK:C     | 2.61                     | 0.48              |
| 10:Y:263:UNK:O   | 10:Y:264:UNK:C     | 2.61                     | 0.48              |
| 1:A:127:MET:HB2  | 1:A:147:TYR:HD1    | 1.77                     | 0.48              |
| 2:B:30:VAL:HG12  | 11:B:1486:CLA:HHD  | 1.96                     | 0.48              |
| 4:D:87:HIS:HE1   | 4:D:161:PRO:O      | 1.96                     | 0.48              |
| 4:D:159:ILE:O    | 4:D:162:LEU:N      | 2.46                     | 0.48              |
| 6:F:22:ALA:O     | 6:F:24:HIS:N       | 2.47                     | 0.48              |
| 1:G:121:LEU:HD23 | 1:G:121:LEU:C      | 2.39                     | 0.48              |
| 1:G:330:VAL:CG1  | 4:J:347:PRO:CA     | 2.90                     | 0.48              |
| 2:H:372:ASP:O    | 2:H:374:ASN:N      | 2.43                     | 0.48              |
| 3:I:92:ILE:O     | 3:I:93:ALA:C       | 2.55                     | 0.48              |
| 3:I:161:LEU:HD21 | 11:I:1464:CLA:HBB1 | 1.95                     | 0.48              |
| 3:I:178:LYS:HD3  | 3:I:178:LYS:O      | 2.14                     | 0.48              |
| 3:I:385:GLN:HB3  | 3:I:386:PRO:HD2    | 1.96                     | 0.48              |
| 4:J:54:PHE:HE1   | 6:L:33:PHE:CE2     | 2.32                     | 0.48              |
| 4:J:91:LEU:C     | 4:J:93:TRP:N       | 2.69                     | 0.48              |
| 4:J:298:PHE:O    | 10:Y:129:UNK:O     | 2.31                     | 0.48              |
| 4:J:340:VAL:O    | 4:J:340:VAL:HG12   | 2.14                     | 0.48              |
| 8:U:71:UNK:C     | 8:U:73:UNK:N       | 2.76                     | 0.48              |
| 10:Y:218:UNK:O   | 10:Y:219:UNK:C     | 2.62                     | 0.48              |
| 1:A:35:VAL:O     | 1:A:35:VAL:CG1     | 2.62                     | 0.48              |
| 1:A:214:MET:O    | 1:A:217:SER:N      | 2.47                     | 0.48              |
| 2:B:24:LEU:HD23  | 2:B:111:ALA:HA     | 1.95                     | 0.48              |
| 2:B:98:LEU:O     | 2:B:101:ILE:N      | 2.46                     | 0.48              |
| 2:B:426:PHE:O    | 2:B:426:PHE:CD1    | 2.67                     | 0.48              |
| 3:C:227:VAL:CG1  | 3:C:233:VAL:HG23   | 2.44                     | 0.48              |
| 4:D:298:PHE:O    | 4:D:299:ILE:HB     | 2.14                     | 0.48              |
| 1:G:32:TRP:O     | 1:G:35:VAL:HB      | 2.14                     | 0.48              |
| 1:G:137:LEU:HB2  | 1:G:139:MET:HE3    | 1.96                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:G:159:LEU:HD11   | 1:G:163:ILE:HD11   | 1.95                     | 0.48              |
| 1:G:222:SER:O      | 1:G:246:TYR:CB     | 2.62                     | 0.48              |
| 2:H:52:LEU:O       | 2:H:337:ALA:HB3    | 2.13                     | 0.48              |
| 2:H:258:TYR:O      | 2:H:259:GLY:O      | 2.32                     | 0.48              |
| 2:H:263:THR:O      | 2:H:448:ARG:NH1    | 2.46                     | 0.48              |
| 3:I:32:GLY:O       | 3:I:34:ALA:N       | 2.43                     | 0.48              |
| 3:I:115:GLY:O      | 3:I:116:VAL:C      | 2.56                     | 0.48              |
| 4:J:224:GLN:HE21   | 4:J:227:GLU:CB     | 2.27                     | 0.48              |
| 8:S:57:UNK:O       | 8:S:59:UNK:N       | 2.47                     | 0.48              |
| 1:A:198:HIS:O      | 1:A:201:GLY:N      | 2.47                     | 0.48              |
| 1:A:258:LEU:O      | 4:D:128:ARG:NH2    | 2.46                     | 0.48              |
| 2:B:230:ARG:O      | 2:B:231:MET:C      | 2.57                     | 0.48              |
| 2:B:396:GLY:O      | 2:B:397:VAL:C      | 2.56                     | 0.48              |
| 3:C:69:LEU:HD13    | 3:C:115:GLY:HA3    | 1.94                     | 0.48              |
| 3:C:75:PHE:CE2     | 3:C:77:PRO:HG3     | 2.49                     | 0.48              |
| 4:D:129:GLN:OE1    | 4:D:143:ALA:HA     | 2.14                     | 0.48              |
| 5:E:27:ILE:O       | 5:E:28:PRO:C       | 2.56                     | 0.48              |
| 1:G:59:ASP:O       | 1:G:60:ILE:C       | 2.57                     | 0.48              |
| 1:G:110:GLY:O      | 1:G:111:PRO:C      | 2.53                     | 0.48              |
| 11:H:1494:CLA:OBD  | 11:H:1495:CLA:HHC  | 2.13                     | 0.48              |
| 3:I:176:VAL:CG1    | 3:I:177:ALA:N      | 2.77                     | 0.48              |
| 4:J:116:LEU:O      | 4:J:119:ALA:HB3    | 2.14                     | 0.48              |
| 4:J:152:VAL:HG23   | 4:J:279:LEU:HB3    | 1.95                     | 0.48              |
| 5:K:18:ARG:O       | 5:K:21:VAL:HB      | 2.14                     | 0.48              |
| 7:P:141:UNK:O      | 7:P:149:UNK:CB     | 2.62                     | 0.48              |
| 8:U:71:UNK:O       | 8:U:72:UNK:C       | 2.61                     | 0.48              |
| 10:X:331:UNK:O     | 10:X:332:UNK:C     | 2.61                     | 0.48              |
| 10:Y:168:UNK:O     | 10:Y:170:UNK:N     | 2.47                     | 0.48              |
| 10:Y:578:UNK:O     | 10:Y:579:UNK:C     | 2.62                     | 0.48              |
| 2:B:52:LEU:O       | 2:B:337:ALA:HB3    | 2.13                     | 0.48              |
| 3:C:53:HIS:NE2     | 11:C:1467:CLA:NB   | 2.62                     | 0.48              |
| 3:C:115:GLY:O      | 3:C:116:VAL:C      | 2.56                     | 0.48              |
| 3:C:170:ILE:HG23   | 3:C:171:GLY:H      | 1.78                     | 0.48              |
| 4:D:113:PHE:CZ     | 17:F:1046:BCR:HC41 | 2.49                     | 0.48              |
| 4:D:185:PHE:O      | 4:D:186:GLN:C      | 2.56                     | 0.48              |
| 1:G:133:LEU:HB2    | 4:J:252:PHE:HE2    | 1.79                     | 0.48              |
| 1:G:330:VAL:HG21   | 4:J:328:TRP:CZ2    | 2.49                     | 0.48              |
| 2:H:152:GLY:O      | 2:H:153:PHE:C      | 2.55                     | 0.48              |
| 2:H:204:ALA:O      | 2:H:205:ALA:C      | 2.56                     | 0.48              |
| 2:H:234:ILE:O      | 2:H:237:VAL:N      | 2.46                     | 0.48              |
| 11:H:1485:CLA:HMC2 | 11:H:1492:CLA:H191 | 1.96                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:I:109:PHE:O      | 3:I:113:VAL:HG23   | 2.14                     | 0.48              |
| 3:I:150:ASP:O      | 3:I:151:TRP:C      | 2.56                     | 0.48              |
| 3:I:188:THR:HG21   | 3:I:298:PRO:CA     | 2.44                     | 0.48              |
| 4:J:313:THR:OG1    | 4:J:315:TYR:HB3    | 2.12                     | 0.48              |
| 5:K:18:ARG:NH1     | 10:Y:564:UNK:CB    | 2.77                     | 0.48              |
| 8:U:90:UNK:O       | 8:U:91:UNK:O       | 2.32                     | 0.48              |
| 10:X:159:UNK:O     | 10:X:160:UNK:C     | 2.61                     | 0.48              |
| 1:A:134:SER:O      | 1:A:136:ARG:N      | 2.42                     | 0.47              |
| 2:B:195:PRO:O      | 2:B:197:GLY:N      | 2.46                     | 0.47              |
| 3:C:185:LEU:O      | 3:C:186:TYR:O      | 2.31                     | 0.47              |
| 4:D:272:LEU:C      | 4:D:272:LEU:CD2    | 2.87                     | 0.47              |
| 4:D:342:PRO:O      | 4:D:345:VAL:CG2    | 2.62                     | 0.47              |
| 1:G:58:VAL:CG1     | 1:G:109:GLY:HA3    | 2.44                     | 0.47              |
| 1:G:192:ILE:C      | 1:G:194:MET:N      | 2.69                     | 0.47              |
| 1:G:258:LEU:HD12   | 4:J:128:ARG:NH2    | 2.29                     | 0.47              |
| 1:G:279:PRO:HB2    | 12:G:1345:PHO:HBC1 | 1.96                     | 0.47              |
| 11:G:1344:CLA:HBB2 | 12:J:1352:PHO:H91  | 1.96                     | 0.47              |
| 3:I:51:GLY:HA2     | 3:I:54:VAL:HB      | 1.96                     | 0.47              |
| 3:I:72:LEU:O       | 3:I:75:PHE:HB3     | 2.14                     | 0.47              |
| 3:I:188:THR:CG2    | 3:I:300:GLU:OE1    | 2.61                     | 0.47              |
| 4:J:101:PHE:O      | 4:J:104:TRP:HB3    | 2.13                     | 0.47              |
| 7:P:26:UNK:O       | 7:P:27:UNK:C       | 2.62                     | 0.47              |
| 10:X:405:UNK:O     | 10:X:406:UNK:C     | 2.61                     | 0.47              |
| 10:Y:404:UNK:O     | 10:Y:405:UNK:CB    | 2.62                     | 0.47              |
| 1:A:121:LEU:HD23   | 1:A:121:LEU:C      | 2.38                     | 0.47              |
| 2:B:33:TRP:O       | 2:B:36:SER:HB3     | 2.14                     | 0.47              |
| 3:C:118:HIS:HA     | 3:C:121:SER:HB3    | 1.95                     | 0.47              |
| 3:C:276:LEU:HD11   | 11:C:1466:CLA:HBB1 | 1.94                     | 0.47              |
| 4:D:73:PHE:CE2     | 4:D:175:VAL:HG21   | 2.48                     | 0.47              |
| 4:D:88:SER:O       | 4:D:90:LEU:N       | 2.48                     | 0.47              |
| 4:D:122:LEU:CD2    | 11:D:1351:CLA:H92  | 2.28                     | 0.47              |
| 4:D:189:HIS:ND1    | 4:D:294:ARG:NH1    | 2.62                     | 0.47              |
| 1:G:84:PRO:CG      | 1:G:173:PRO:HD3    | 2.43                     | 0.47              |
| 2:H:309:LEU:C      | 2:H:311:PHE:N      | 2.69                     | 0.47              |
| 2:H:345:VAL:HG23   | 2:H:345:VAL:O      | 2.13                     | 0.47              |
| 2:H:408:GLY:O      | 2:H:409:GLN:HB2    | 2.13                     | 0.47              |
| 3:I:284:PHE:O      | 3:I:286:ALA:N      | 2.48                     | 0.47              |
| 4:J:111:TRP:O      | 4:J:113:PHE:N      | 2.47                     | 0.47              |
| 4:J:279:LEU:O      | 4:J:283:ALA:HB2    | 2.14                     | 0.47              |
| 4:J:296:TYR:O      | 4:J:297:ASP:HB3    | 2.15                     | 0.47              |
| 6:L:24:HIS:HA      | 6:L:27:ALA:HB3     | 1.95                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:S:9:UNK:O        | 8:S:11:UNK:N       | 2.47                     | 0.47              |
| 9:T:41:HIS:HA      | 9:T:45:ILE:O       | 2.15                     | 0.47              |
| 8:U:27:UNK:O       | 8:U:28:UNK:O       | 2.32                     | 0.47              |
| 10:Y:8:UNK:O       | 10:Y:9:UNK:C       | 2.62                     | 0.47              |
| 1:A:112:TYR:OH     | 1:A:116:ILE:HD11   | 2.14                     | 0.47              |
| 1:A:127:MET:HB2    | 1:A:147:TYR:CD1    | 2.49                     | 0.47              |
| 1:A:142:TRP:C      | 1:A:144:CYS:N      | 2.70                     | 0.47              |
| 1:A:244:GLU:HG3    | 1:A:245:THR:N      | 2.30                     | 0.47              |
| 1:A:277:ALA:O      | 1:A:278:TRP:C      | 2.56                     | 0.47              |
| 3:C:390:ARG:CD     | 9:V:100:ILE:HD12   | 2.43                     | 0.47              |
| 5:E:31:PHE:CE1     | 6:F:35:GLY:HA2     | 2.49                     | 0.47              |
| 1:G:143:ILE:CG1    | 4:J:220:ASN:HD22   | 2.12                     | 0.47              |
| 1:G:328:MET:HE2    | 4:J:325:ILE:HD11   | 1.95                     | 0.47              |
| 2:H:76:SER:HA      | 7:O:69:UNK:CB      | 2.44                     | 0.47              |
| 3:I:243:ILE:HG22   | 3:I:244:CYS:N      | 2.30                     | 0.47              |
| 3:I:455:PHE:O      | 3:I:456:GLU:CB     | 2.61                     | 0.47              |
| 4:J:72:ASN:H       | 4:J:75:THR:HG1     | 1.60                     | 0.47              |
| 4:J:336:HIS:ND1    | 4:J:336:HIS:C      | 2.73                     | 0.47              |
| 5:K:41:GLY:O       | 5:K:44:TYR:N       | 2.47                     | 0.47              |
| 5:K:82:GLN:O       | 5:K:84:LYS:N       | 2.47                     | 0.47              |
| 6:L:33:PHE:C       | 6:L:35:GLY:H       | 2.22                     | 0.47              |
| 7:P:142:UNK:CA     | 7:P:149:UNK:CB     | 2.91                     | 0.47              |
| 10:Y:428:UNK:C     | 10:Y:430:UNK:N     | 2.77                     | 0.47              |
| 10:Y:526:UNK:O     | 10:Y:527:UNK:C     | 2.61                     | 0.47              |
| 10:Y:563:UNK:O     | 10:Y:566:UNK:N     | 2.47                     | 0.47              |
| 1:A:84:PRO:O       | 1:A:85:SER:O       | 2.31                     | 0.47              |
| 2:B:263:THR:N      | 2:B:264:PRO:CD     | 2.76                     | 0.47              |
| 2:B:424:ALA:O      | 2:B:426:PHE:N      | 2.44                     | 0.47              |
| 3:C:264:PHE:N      | 3:C:264:PHE:CD2    | 2.82                     | 0.47              |
| 4:D:52:THR:O       | 4:D:67:TYR:HD1     | 1.98                     | 0.47              |
| 4:D:111:TRP:C      | 4:D:113:PHE:N      | 2.68                     | 0.47              |
| 1:G:63:ILE:CG1     | 1:G:64:ARG:N       | 2.65                     | 0.47              |
| 1:G:84:PRO:HG3     | 1:G:112:TYR:CE2    | 2.49                     | 0.47              |
| 1:G:190:HIS:ND1    | 1:G:298:ASN:ND2    | 2.61                     | 0.47              |
| 2:H:33:TRP:NE1     | 11:H:1488:CLA:HBC2 | 2.28                     | 0.47              |
| 3:I:40:ALA:O       | 3:I:43:ILE:HG23    | 2.14                     | 0.47              |
| 3:I:119:LEU:O      | 3:I:122:SER:OG     | 2.30                     | 0.47              |
| 11:I:1464:CLA:HBA2 | 11:I:1464:CLA:H3A  | 1.49                     | 0.47              |
| 4:J:54:PHE:HE1     | 6:L:33:PHE:CD2     | 2.31                     | 0.47              |
| 4:J:126:MET:C      | 4:J:129:GLN:HG2    | 2.35                     | 0.47              |
| 4:J:149:PRO:O      | 4:J:150:ILE:C      | 2.57                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:X:115:UNK:O     | 10:X:119:UNK:N     | 2.47                     | 0.47              |
| 10:X:225:UNK:O     | 10:X:227:UNK:N     | 2.47                     | 0.47              |
| 10:X:526:UNK:O     | 10:X:527:UNK:C     | 2.63                     | 0.47              |
| 10:Y:24:UNK:O      | 10:Y:25:UNK:C      | 2.62                     | 0.47              |
| 12:A:1345:PHO:HBB2 | 4:D:205:LEU:HD21   | 1.95                     | 0.47              |
| 2:B:172:TYR:HB3    | 2:B:309:LEU:CD2    | 2.44                     | 0.47              |
| 3:C:167:VAL:HG13   | 11:C:1470:CLA:HMB1 | 1.97                     | 0.47              |
| 3:C:187:ASP:HB3    | 3:C:230:LEU:CD2    | 2.27                     | 0.47              |
| 5:E:35:TRP:CE3     | 6:F:39:ALA:HB2     | 2.49                     | 0.47              |
| 1:G:129:ARG:NH2    | 4:J:256:ILE:CA     | 2.74                     | 0.47              |
| 3:I:81:MET:SD      | 3:I:90:PRO:HG3     | 2.54                     | 0.47              |
| 4:J:191:TRP:CZ2    | 4:J:286:VAL:CG2    | 2.97                     | 0.47              |
| 7:P:79:UNK:O       | 7:P:80:UNK:C       | 2.62                     | 0.47              |
| 10:X:357:UNK:O     | 10:X:358:UNK:C     | 2.63                     | 0.47              |
| 10:Y:170:UNK:O     | 10:Y:171:UNK:C     | 2.60                     | 0.47              |
| 10:Y:334:UNK:O     | 10:Y:335:UNK:O     | 2.31                     | 0.47              |
| 1:A:290:ILE:HD11   | 11:A:1342:CLA:CAD  | 2.44                     | 0.47              |
| 1:A:292:THR:HG23   | 3:C:428:THR:CG2    | 2.44                     | 0.47              |
| 1:A:322:ASN:O      | 1:A:323:ARG:C      | 2.56                     | 0.47              |
| 2:B:425:ILE:HG23   | 2:B:426:PHE:HD2    | 1.79                     | 0.47              |
| 3:C:32:GLY:O       | 3:C:34:ALA:N       | 2.46                     | 0.47              |
| 3:C:376:ASP:OD2    | 3:C:379:LYS:HE3    | 2.14                     | 0.47              |
| 4:D:224:GLN:HE21   | 4:D:227:GLU:CB     | 2.27                     | 0.47              |
| 1:G:104:GLU:HG2    | 1:G:108:ASN:HD21   | 1.79                     | 0.47              |
| 1:G:248:ILE:O      | 1:G:250:ALA:N      | 2.47                     | 0.47              |
| 1:G:294:ALA:O      | 1:G:296:ASN:N      | 2.48                     | 0.47              |
| 2:H:137:LYS:O      | 2:H:141:ILE:HG22   | 2.14                     | 0.47              |
| 2:H:213:GLY:O      | 2:H:214:LEU:C      | 2.57                     | 0.47              |
| 3:I:226:SER:O      | 3:I:227:VAL:C      | 2.57                     | 0.47              |
| 3:I:244:CYS:HA     | 11:I:1464:CLA:CMC  | 2.45                     | 0.47              |
| 3:I:311:GLN:HA     | 3:I:355:THR:HG21   | 1.95                     | 0.47              |
| 3:I:398:HIS:O      | 3:I:399:ALA:CA     | 2.63                     | 0.47              |
| 5:K:15:THR:O       | 5:K:15:THR:CG2     | 2.63                     | 0.47              |
| 10:X:470:UNK:O     | 10:X:471:UNK:C     | 2.62                     | 0.47              |
| 1:A:53:ILE:O       | 1:A:71:LEU:HB2     | 2.14                     | 0.47              |
| 1:A:104:GLU:HG2    | 1:A:108:ASN:HD21   | 1.80                     | 0.47              |
| 1:A:127:MET:O      | 1:A:130:GLN:HB3    | 2.14                     | 0.47              |
| 1:A:153:SER:HB3    | 11:A:1342:CLA:H43  | 1.96                     | 0.47              |
| 2:B:68:ARG:CG      | 2:B:69:LEU:N       | 2.76                     | 0.47              |
| 2:B:207:ILE:CG1    | 2:B:208:VAL:N      | 2.78                     | 0.47              |
| 2:B:243:ALA:C      | 2:B:246:PHE:HB3    | 2.39                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:288:VAL:CG2    | 2:B:289:GLN:N      | 2.78                     | 0.47              |
| 2:B:392:PHE:O      | 2:B:395:GLN:HA     | 2.14                     | 0.47              |
| 3:C:88:LEU:O       | 3:C:89:ILE:C       | 2.57                     | 0.47              |
| 3:C:272:LEU:O      | 3:C:273:SER:C      | 2.55                     | 0.47              |
| 3:C:370:ARG:HA     | 3:C:375:LEU:H      | 1.79                     | 0.47              |
| 4:D:55:VAL:O       | 4:D:66:SER:HB3     | 2.15                     | 0.47              |
| 4:D:156:VAL:O      | 4:D:156:VAL:HG12   | 2.14                     | 0.47              |
| 4:D:188:PHE:CE1    | 4:D:326:ARG:HG2    | 2.48                     | 0.47              |
| 4:D:337:GLU:HG3    | 4:D:339:PHE:CE2    | 2.49                     | 0.47              |
| 1:G:54:ALA:HB2     | 1:G:72:LEU:HD12    | 1.97                     | 0.47              |
| 1:G:259:ILE:O      | 1:G:260:PHE:CB     | 2.62                     | 0.47              |
| 1:G:290:ILE:C      | 1:G:292:THR:H      | 2.23                     | 0.47              |
| 2:H:192:PRO:HG3    | 11:H:1483:CLA:HBA2 | 1.95                     | 0.47              |
| 2:H:310:ALA:O      | 2:H:428:GLU:HB2    | 2.15                     | 0.47              |
| 11:H:1488:CLA:H162 | 4:J:281:MET:HE1    | 1.97                     | 0.47              |
| 3:I:50:LEU:O       | 3:I:54:VAL:N       | 2.46                     | 0.47              |
| 3:I:55:ALA:O       | 3:I:56:HIS:C       | 2.57                     | 0.47              |
| 3:I:188:THR:HG21   | 3:I:298:PRO:HA     | 1.96                     | 0.47              |
| 3:I:274:TYR:CD1    | 11:I:1463:CLA:HMD2 | 2.50                     | 0.47              |
| 3:I:299:SER:C      | 3:I:301:PHE:N      | 2.70                     | 0.47              |
| 3:I:305:THR:C      | 3:I:307:PRO:HD2    | 2.40                     | 0.47              |
| 3:I:387:TRP:O      | 3:I:390:ARG:HG2    | 2.15                     | 0.47              |
| 3:I:425:TRP:CZ2    | 11:I:1462:CLA:O1A  | 2.68                     | 0.47              |
| 4:J:39:PRO:O       | 4:J:43:LEU:CB      | 2.62                     | 0.47              |
| 4:J:339:PHE:CD1    | 4:J:341:PHE:CE1    | 3.03                     | 0.47              |
| 6:L:28:VAL:HB      | 6:L:29:PRO:CD      | 2.39                     | 0.47              |
| 7:O:42:UNK:CB      | 7:O:52:UNK:O       | 2.63                     | 0.47              |
| 7:O:79:UNK:O       | 7:O:80:UNK:C       | 2.62                     | 0.47              |
| 8:U:69:UNK:O       | 8:U:70:UNK:C       | 2.63                     | 0.47              |
| 10:X:560:UNK:O     | 10:X:561:UNK:C     | 2.62                     | 0.47              |
| 10:X:578:UNK:O     | 10:X:579:UNK:C     | 2.63                     | 0.47              |
| 10:Y:115:UNK:O     | 10:Y:119:UNK:N     | 2.47                     | 0.47              |
| 1:A:58:VAL:CG1     | 1:A:109:GLY:HA3    | 2.45                     | 0.47              |
| 1:A:64:ARG:C       | 1:A:66:PRO:HD3     | 2.38                     | 0.47              |
| 3:C:160:ILE:O      | 3:C:161:LEU:C      | 2.58                     | 0.47              |
| 3:C:162:GLY:CA     | 3:C:248:GLY:HA2    | 2.43                     | 0.47              |
| 3:C:286:ALA:O      | 3:C:287:THR:C      | 2.58                     | 0.47              |
| 4:D:43:LEU:HG      | 4:D:113:PHE:CZ     | 2.50                     | 0.47              |
| 4:D:56:THR:OG1     | 4:D:57:SER:N       | 2.48                     | 0.47              |
| 1:G:79:THR:O       | 1:G:80:GLY:O       | 2.32                     | 0.47              |
| 2:H:63:LEU:HA      | 2:H:66:MET:HE3     | 1.97                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:H:132:ALA:O      | 2:H:133:LEU:CB     | 2.62                     | 0.47              |
| 2:H:203:ILE:O      | 2:H:207:ILE:HG23   | 2.14                     | 0.47              |
| 3:I:245:ILE:O      | 3:I:249:ILE:HG12   | 2.15                     | 0.47              |
| 4:J:92:LEU:C       | 4:J:93:TRP:CD1     | 2.93                     | 0.47              |
| 4:J:127:LEU:C      | 4:J:129:GLN:N      | 2.72                     | 0.47              |
| 5:K:30:LEU:HD13    | 6:L:28:VAL:HG13    | 1.97                     | 0.47              |
| 1:A:129:ARG:NH2    | 4:D:256:ILE:CA     | 2.75                     | 0.47              |
| 1:A:196:PRO:O      | 1:A:199:GLN:HB2    | 2.14                     | 0.47              |
| 1:A:221:SER:HB2    | 4:D:139:ARG:O      | 2.15                     | 0.47              |
| 11:A:1342:CLA:HBB1 | 11:D:1351:CLA:NC   | 2.30                     | 0.47              |
| 2:B:179:GLN:HB3    | 2:B:180:PRO:HD2    | 1.96                     | 0.47              |
| 2:B:372:ASP:O      | 2:B:374:ASN:N      | 2.46                     | 0.47              |
| 3:C:172:ALA:O      | 3:C:175:LEU:N      | 2.47                     | 0.47              |
| 1:G:218:LEU:HD11   | 1:G:255:PHE:CD2    | 2.45                     | 0.47              |
| 2:H:24:LEU:HD12    | 11:H:1496:CLA:HED2 | 1.97                     | 0.47              |
| 2:H:155:ALA:O      | 2:H:159:THR:CB     | 2.63                     | 0.47              |
| 3:I:52:ALA:O       | 11:I:1469:CLA:HMB2 | 2.15                     | 0.47              |
| 3:I:82:TYR:HB3     | 3:I:302:TYR:O      | 2.14                     | 0.47              |
| 3:I:265:ILE:C      | 3:I:266:TRP:CD1    | 2.93                     | 0.47              |
| 4:J:57:SER:HB2     | 4:J:63:LEU:O       | 2.15                     | 0.47              |
| 4:J:74:LEU:HA      | 4:J:175:VAL:HG11   | 1.97                     | 0.47              |
| 4:J:159:ILE:O      | 4:J:162:LEU:N      | 2.45                     | 0.47              |
| 4:J:190:ASN:CG     | 4:J:322:ASN:HD21   | 2.23                     | 0.47              |
| 9:T:122:GLU:N      | 9:T:123:PRO:HD2    | 2.29                     | 0.47              |
| 10:Y:177:UNK:O     | 10:Y:180:UNK:N     | 2.47                     | 0.47              |
| 4:D:264:LYS:C      | 4:D:266:TRP:H      | 2.23                     | 0.47              |
| 1:G:62:GLY:CA      | 1:G:87:ASN:CB      | 2.90                     | 0.47              |
| 1:G:93:PHE:O       | 1:G:95:PRO:HD3     | 2.14                     | 0.47              |
| 1:G:181:ASN:O      | 1:G:183:MET:N      | 2.48                     | 0.47              |
| 2:H:98:LEU:O       | 2:H:99:ALA:C       | 2.58                     | 0.47              |
| 2:H:136:PRO:HG2    | 2:H:221:PRO:HG3    | 1.97                     | 0.47              |
| 2:H:309:LEU:O      | 2:H:312:TYR:N      | 2.48                     | 0.47              |
| 2:H:330:MET:O      | 2:H:331:ASN:CB     | 2.63                     | 0.47              |
| 3:I:436:PHE:O      | 3:I:439:VAL:HB     | 2.15                     | 0.47              |
| 4:J:189:HIS:ND1    | 4:J:294:ARG:NH1    | 2.63                     | 0.47              |
| 6:L:27:ALA:O       | 6:L:28:VAL:C       | 2.58                     | 0.47              |
| 8:S:90:UNK:C       | 8:S:91:UNK:O       | 2.62                     | 0.47              |
| 9:T:133:GLY:O      | 9:T:137:TYR:CA     | 2.62                     | 0.47              |
| 8:U:7:UNK:O        | 8:U:9:UNK:N        | 2.48                     | 0.47              |
| 2:B:174:LEU:O      | 2:B:175:THR:O      | 2.32                     | 0.46              |
| 2:B:214:LEU:O      | 2:B:217:ILE:CG2    | 2.63                     | 0.46              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 2:B:222:PRO:O    | 2:B:223:GLN:C      | 2.57                     | 0.46              |
| 6:F:17:THR:O     | 6:F:20:TRP:HB3     | 2.15                     | 0.46              |
| 1:G:45:THR:HA    | 12:G:1345:PHO:H93  | 1.97                     | 0.46              |
| 1:G:57:PRO:HA    | 1:G:67:VAL:O       | 2.14                     | 0.46              |
| 3:I:178:LYS:C    | 3:I:178:LYS:CD     | 2.85                     | 0.46              |
| 3:I:229:ASN:CB   | 3:I:232:ASP:OD1    | 2.64                     | 0.46              |
| 3:I:314:ALA:O    | 3:I:315:MET:C      | 2.58                     | 0.46              |
| 4:J:48:TRP:HB2   | 4:J:114:ILE:HD13   | 1.97                     | 0.46              |
| 4:J:113:PHE:CZ   | 17:L:1047:BCR:HC41 | 2.50                     | 0.46              |
| 4:J:192:THR:OG1  | 4:J:193:LEU:N      | 2.48                     | 0.46              |
| 4:J:342:PRO:O    | 4:J:345:VAL:CG2    | 2.63                     | 0.46              |
| 5:K:10:PHE:CE2   | 6:L:19:ARG:CZ      | 2.98                     | 0.46              |
| 8:U:39:UNK:O     | 8:U:40:UNK:O       | 2.33                     | 0.46              |
| 10:X:221:UNK:O   | 10:X:222:UNK:C     | 2.63                     | 0.46              |
| 1:A:13:LEU:O     | 1:A:17:PHE:N       | 2.40                     | 0.46              |
| 1:A:79:THR:O     | 1:A:80:GLY:O       | 2.33                     | 0.46              |
| 1:A:206:PHE:HE1  | 11:A:1342:CLA:HMB3 | 1.79                     | 0.46              |
| 2:B:113:TRP:CD1  | 11:B:1496:CLA:H191 | 2.49                     | 0.46              |
| 3:C:122:SER:O    | 3:C:125:LEU:N      | 2.48                     | 0.46              |
| 3:C:188:THR:HG21 | 3:C:298:PRO:CB     | 2.45                     | 0.46              |
| 4:D:127:LEU:C    | 4:D:129:GLN:H      | 2.22                     | 0.46              |
| 4:D:274:VAL:CB   | 4:D:275:PRO:CD     | 2.91                     | 0.46              |
| 4:D:335:PRO:O    | 4:D:337:GLU:N      | 2.48                     | 0.46              |
| 2:H:193:TYR:CE1  | 2:H:260:SER:N      | 2.84                     | 0.46              |
| 2:H:462:PHE:HA   | 11:H:1492:CLA:CMC  | 2.45                     | 0.46              |
| 3:I:135:ARG:O    | 3:I:136:GLY:O      | 2.34                     | 0.46              |
| 3:I:179:ALA:O    | 3:I:184:GLY:HA2    | 2.14                     | 0.46              |
| 3:I:225:VAL:O    | 3:I:225:VAL:CG1    | 2.62                     | 0.46              |
| 3:I:242:LEU:HD12 | 3:I:245:ILE:HD11   | 1.97                     | 0.46              |
| 3:I:273:SER:CB   | 3:I:445:ALA:HB2    | 2.37                     | 0.46              |
| 4:J:191:TRP:HZ2  | 4:J:286:VAL:CG2    | 2.29                     | 0.46              |
| 7:O:99:UNK:O     | 7:O:100:UNK:C      | 2.62                     | 0.46              |
| 9:T:2:GLU:O      | 9:T:4:THR:N        | 2.45                     | 0.46              |
| 2:B:61:PHE:O     | 2:B:63:LEU:N       | 2.48                     | 0.46              |
| 2:B:193:TYR:CE1  | 2:B:260:SER:N      | 2.83                     | 0.46              |
| 3:C:245:ILE:O    | 3:C:249:ILE:HG12   | 2.15                     | 0.46              |
| 5:E:12:ASP:O     | 5:E:16:SER:N       | 2.48                     | 0.46              |
| 5:E:35:TRP:CD2   | 6:F:39:ALA:HB2     | 2.50                     | 0.46              |
| 5:E:37:PHE:HE1   | 5:E:42:LEU:HB3     | 1.79                     | 0.46              |
| 5:E:82:GLN:C     | 5:E:84:LYS:N       | 2.72                     | 0.46              |
| 1:G:166:GLY:O    | 1:G:167:SER:CB     | 2.59                     | 0.46              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:G:327:GLY:O    | 4:J:324:GLY:HA3    | 2.16                     | 0.46              |
| 2:H:45:PHE:C     | 2:H:47:PRO:HD2     | 2.40                     | 0.46              |
| 2:H:293:ALA:O    | 2:H:294:SER:C      | 2.56                     | 0.46              |
| 3:I:37:ALA:C     | 3:I:39:ASN:H       | 2.22                     | 0.46              |
| 3:I:160:ILE:O    | 3:I:161:LEU:C      | 2.57                     | 0.46              |
| 3:I:207:ARG:HA   | 3:I:210:PHE:CB     | 2.45                     | 0.46              |
| 3:I:267:SER:O    | 3:I:271:TYR:N      | 2.40                     | 0.46              |
| 3:I:370:ARG:HE   | 3:I:371:GLY:N      | 2.09                     | 0.46              |
| 4:J:148:ALA:HB2  | 4:J:276:VAL:HG13   | 1.97                     | 0.46              |
| 10:X:336:UNK:O   | 10:X:337:UNK:CB    | 2.64                     | 0.46              |
| 10:X:410:UNK:O   | 10:X:411:UNK:C     | 2.64                     | 0.46              |
| 10:X:580:UNK:C   | 10:X:582:UNK:N     | 2.77                     | 0.46              |
| 1:A:87:ASN:O     | 1:A:87:ASN:ND2     | 2.48                     | 0.46              |
| 1:A:127:MET:HE1  | 1:A:151:LEU:CD2    | 2.45                     | 0.46              |
| 1:A:166:GLY:O    | 1:A:167:SER:CB     | 2.63                     | 0.46              |
| 1:A:167:SER:OG   | 1:A:169:SER:HB2    | 2.15                     | 0.46              |
| 1:A:181:ASN:O    | 1:A:183:MET:N      | 2.48                     | 0.46              |
| 1:A:248:ILE:O    | 1:A:250:ALA:N      | 2.48                     | 0.46              |
| 2:B:50:PRO:O     | 2:B:54:PRO:HG3     | 2.15                     | 0.46              |
| 3:C:61:VAL:HG21  | 3:C:125:LEU:HD12   | 1.97                     | 0.46              |
| 3:C:95:LEU:HD23  | 3:C:97:TRP:CZ3     | 2.42                     | 0.46              |
| 3:C:276:LEU:CD2  | 11:C:1466:CLA:HBB1 | 2.46                     | 0.46              |
| 3:C:418:ASN:CA   | 3:C:419:PHE:N      | 2.78                     | 0.46              |
| 4:D:298:PHE:O    | 10:X:129:UNK:O     | 2.33                     | 0.46              |
| 1:G:292:THR:HG23 | 3:I:428:THR:CG2    | 2.44                     | 0.46              |
| 2:H:397:VAL:C    | 2:H:399:VAL:N      | 2.73                     | 0.46              |
| 2:H:463:PHE:C    | 2:H:465:GLY:H      | 2.23                     | 0.46              |
| 3:I:52:ALA:HA    | 11:I:1469:CLA:HMB1 | 1.97                     | 0.46              |
| 3:I:170:ILE:HG23 | 3:I:171:GLY:H      | 1.78                     | 0.46              |
| 3:I:259:TRP:O    | 3:I:260:ALA:C      | 2.58                     | 0.46              |
| 3:I:318:LEU:HD21 | 3:I:380:ILE:HG21   | 1.97                     | 0.46              |
| 8:S:66:UNK:O     | 8:S:70:UNK:N       | 2.48                     | 0.46              |
| 9:V:53:ASP:C     | 9:V:53:ASP:OD1     | 2.58                     | 0.46              |
| 10:X:182:UNK:O   | 10:X:183:UNK:C     | 2.62                     | 0.46              |
| 10:Y:158:UNK:O   | 10:Y:159:UNK:C     | 2.62                     | 0.46              |
| 1:A:32:TRP:O     | 1:A:35:VAL:HB      | 2.15                     | 0.46              |
| 1:A:142:TRP:CZ2  | 1:A:273:PHE:CD1    | 3.04                     | 0.46              |
| 2:B:31:ALA:HA    | 2:B:34:ALA:CB      | 2.41                     | 0.46              |
| 2:B:68:ARG:HG3   | 2:B:69:LEU:N       | 2.30                     | 0.46              |
| 2:B:419:SER:HA   | 2:B:422:ARG:HE     | 1.80                     | 0.46              |
| 3:C:52:ALA:HA    | 11:C:1469:CLA:HMB1 | 1.96                     | 0.46              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 4:D:9:PRO:O      | 4:D:10:ALA:CB      | 2.64                     | 0.46              |
| 4:D:149:PRO:O    | 4:D:150:ILE:C      | 2.57                     | 0.46              |
| 4:D:279:LEU:O    | 4:D:283:ALA:HB2    | 2.15                     | 0.46              |
| 1:G:142:TRP:CZ2  | 1:G:273:PHE:CE1    | 3.04                     | 0.46              |
| 1:G:220:THR:O    | 4:J:139:ARG:HD2    | 2.15                     | 0.46              |
| 3:I:257:PHE:HB3  | 3:I:258:GLY:H      | 1.58                     | 0.46              |
| 4:J:57:SER:O     | 4:J:60:THR:HG22    | 2.16                     | 0.46              |
| 4:J:88:SER:O     | 4:J:167:TRP:CZ3    | 2.68                     | 0.46              |
| 4:J:154:VAL:O    | 4:J:159:ILE:HG13   | 2.15                     | 0.46              |
| 4:J:180:ARG:CD   | 4:J:180:ARG:C      | 2.88                     | 0.46              |
| 4:J:286:VAL:O    | 4:J:287:VAL:C      | 2.55                     | 0.46              |
| 4:J:335:PRO:O    | 4:J:336:HIS:C      | 2.58                     | 0.46              |
| 5:K:27:ILE:HB    | 5:K:28:PRO:CD      | 2.40                     | 0.46              |
| 5:K:38:VAL:CG1   | 6:L:40:MET:HG2     | 2.46                     | 0.46              |
| 1:A:160:ILE:HD12 | 3:C:431:PHE:CE1    | 2.47                     | 0.46              |
| 2:B:219:VAL:O    | 2:B:219:VAL:HG12   | 2.16                     | 0.46              |
| 3:C:280:SER:HA   | 3:C:434:ALA:HA     | 1.96                     | 0.46              |
| 3:C:370:ARG:O    | 3:C:375:LEU:N      | 2.49                     | 0.46              |
| 4:D:83:ASN:O     | 4:D:84:SER:C       | 2.59                     | 0.46              |
| 1:G:116:ILE:CG1  | 1:G:158:PHE:HD1    | 2.29                     | 0.46              |
| 3:I:150:ASP:CB   | 3:I:271:TYR:CE2    | 2.99                     | 0.46              |
| 5:K:37:PHE:CZ    | 5:K:43:ALA:HA      | 2.50                     | 0.46              |
| 8:S:71:UNK:C     | 8:S:73:UNK:N       | 2.74                     | 0.46              |
| 10:Y:412:UNK:O   | 10:Y:414:UNK:N     | 2.49                     | 0.46              |
| 1:A:157:VAL:O    | 1:A:157:VAL:CG1    | 2.64                     | 0.46              |
| 2:B:462:PHE:CE1  | 11:B:1494:CLA:HMB2 | 2.50                     | 0.46              |
| 3:C:41:ARG:HB2   | 11:C:1469:CLA:O1D  | 2.16                     | 0.46              |
| 4:D:92:LEU:HA    | 4:D:104:TRP:CD1    | 2.51                     | 0.46              |
| 4:D:180:ARG:C    | 4:D:180:ARG:CD     | 2.89                     | 0.46              |
| 1:G:142:TRP:CZ2  | 1:G:273:PHE:CD1    | 3.04                     | 0.46              |
| 1:G:153:SER:HB3  | 11:G:1342:CLA:H43  | 1.98                     | 0.46              |
| 1:G:255:PHE:O    | 1:G:256:GLY:C      | 2.58                     | 0.46              |
| 2:H:174:LEU:O    | 2:H:175:THR:O      | 2.34                     | 0.46              |
| 3:I:282:MET:O    | 3:I:285:ILE:HB     | 2.16                     | 0.46              |
| 3:I:376:ASP:C    | 3:I:378:ASN:H      | 2.22                     | 0.46              |
| 8:S:74:UNK:O     | 8:S:75:UNK:C       | 2.61                     | 0.46              |
| 9:T:134:LYS:O    | 9:T:137:TYR:O      | 2.34                     | 0.46              |
| 9:V:62:ALA:HB2   | 9:V:82:TYR:CE1     | 2.50                     | 0.46              |
| 10:Y:160:UNK:O   | 10:Y:164:UNK:CB    | 2.64                     | 0.46              |
| 10:Y:534:UNK:O   | 10:Y:535:UNK:C     | 2.64                     | 0.46              |
| 1:A:248:ILE:O    | 1:A:249:VAL:C      | 2.59                     | 0.46              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 2:B:422:ARG:O    | 2:B:425:ILE:HG22   | 2.16                     | 0.46              |
| 3:C:265:ILE:C    | 3:C:266:TRP:CD1    | 2.94                     | 0.46              |
| 1:G:273:PHE:C    | 1:G:273:PHE:CD2    | 2.93                     | 0.46              |
| 2:H:69:LEU:HD23  | 11:H:1487:CLA:CMA  | 2.46                     | 0.46              |
| 2:H:218:LEU:HD12 | 2:H:218:LEU:O      | 2.16                     | 0.46              |
| 2:H:246:PHE:CE1  | 2:H:463:PHE:HB2    | 2.40                     | 0.46              |
| 2:H:278:SER:C    | 2:H:279:TYR:O      | 2.56                     | 0.46              |
| 3:I:47:GLY:O     | 3:I:48:LYS:C       | 2.56                     | 0.46              |
| 3:I:91:HIS:CE1   | 11:I:1460:CLA:O1D  | 2.66                     | 0.46              |
| 3:I:273:SER:OG   | 3:I:274:TYR:N      | 2.49                     | 0.46              |
| 4:J:73:PHE:CE2   | 4:J:175:VAL:HG21   | 2.51                     | 0.46              |
| 4:J:93:TRP:N     | 4:J:93:TRP:CD1     | 2.83                     | 0.46              |
| 4:J:132:ILE:O    | 4:J:133:ALA:C      | 2.58                     | 0.46              |
| 4:J:164:GLN:NE2  | 4:J:189:HIS:HE1    | 2.01                     | 0.46              |
| 4:J:272:LEU:CD2  | 4:J:276:VAL:HG21   | 2.44                     | 0.46              |
| 6:L:33:PHE:O     | 6:L:34:LEU:C       | 2.57                     | 0.46              |
| 9:V:83:ASP:OD1   | 9:V:85:GLU:HB2     | 2.16                     | 0.46              |
| 10:X:428:UNK:C   | 10:X:430:UNK:N     | 2.77                     | 0.46              |
| 1:A:176:ILE:HG23 | 1:A:180:PHE:HE1    | 1.79                     | 0.46              |
| 1:A:187:GLN:NE2  | 1:A:325:ASN:OD1    | 2.49                     | 0.46              |
| 1:A:193:LEU:HB3  | 4:D:179:PHE:CE1    | 2.50                     | 0.46              |
| 1:A:210:LEU:HD13 | 12:D:1352:PHO:ND   | 2.31                     | 0.46              |
| 3:C:164:HIS:O    | 3:C:167:VAL:N      | 2.49                     | 0.46              |
| 4:D:71:CYS:HB2   | 4:D:76:VAL:HG22    | 1.98                     | 0.46              |
| 4:D:71:CYS:HB3   | 4:D:76:VAL:HG22    | 1.98                     | 0.46              |
| 4:D:286:VAL:C    | 4:D:288:GLY:N      | 2.69                     | 0.46              |
| 1:G:54:ALA:CB    | 1:G:72:LEU:HD12    | 2.46                     | 0.46              |
| 1:G:206:PHE:CD1  | 11:G:1342:CLA:HMB1 | 2.51                     | 0.46              |
| 1:G:244:GLU:HG3  | 1:G:245:THR:N      | 2.31                     | 0.46              |
| 1:G:320:ILE:C    | 1:G:322:ASN:N      | 2.73                     | 0.46              |
| 2:H:197:GLY:O    | 2:H:199:VAL:N      | 2.49                     | 0.46              |
| 3:I:95:LEU:C     | 3:I:185:LEU:HA     | 2.39                     | 0.46              |
| 3:I:240:ILE:HD12 | 11:I:1465:CLA:C9   | 2.46                     | 0.46              |
| 4:J:139:ARG:HH11 | 4:J:141:TYR:HE1    | 1.64                     | 0.46              |
| 4:J:224:GLN:O    | 4:J:225:ASP:C      | 2.58                     | 0.46              |
| 6:L:19:ARG:O     | 6:L:23:VAL:CG2     | 2.59                     | 0.46              |
| 8:S:27:UNK:C     | 8:S:28:UNK:O       | 2.64                     | 0.46              |
| 9:V:77:LYS:HG2   | 9:V:95:LEU:HD22    | 1.97                     | 0.46              |
| 10:X:218:UNK:O   | 10:X:219:UNK:C     | 2.64                     | 0.46              |
| 10:X:469:UNK:O   | 10:X:470:UNK:C     | 2.63                     | 0.46              |
| 10:X:580:UNK:O   | 10:X:581:UNK:C     | 2.64                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 10:Y:365:UNK:O    | 10:Y:366:UNK:C     | 2.64                     | 0.46              |
| 10:Y:516:UNK:O    | 10:Y:518:UNK:N     | 2.49                     | 0.46              |
| 1:A:32:TRP:O      | 1:A:35:VAL:N       | 2.49                     | 0.46              |
| 1:A:48:PHE:C      | 1:A:48:PHE:CD2     | 2.94                     | 0.46              |
| 1:A:134:SER:CA    | 1:A:139:MET:HB3    | 2.44                     | 0.46              |
| 1:A:191:ASN:O     | 1:A:192:ILE:C      | 2.59                     | 0.46              |
| 1:A:244:GLU:HG3   | 1:A:245:THR:H      | 1.81                     | 0.46              |
| 2:B:52:LEU:HD23   | 2:B:311:PHE:CE2    | 2.51                     | 0.46              |
| 2:B:466:HIS:C     | 2:B:468:TRP:N      | 2.73                     | 0.46              |
| 3:C:92:ILE:O      | 3:C:93:ALA:C       | 2.59                     | 0.46              |
| 3:C:305:THR:C     | 3:C:307:PRO:HD2    | 2.41                     | 0.46              |
| 3:C:381:LYS:O     | 3:C:382:ASN:HB3    | 2.15                     | 0.46              |
| 4:D:9:PRO:O       | 4:D:10:ALA:HB2     | 2.16                     | 0.46              |
| 4:D:52:THR:CG2    | 4:D:76:VAL:HG11    | 2.46                     | 0.46              |
| 4:D:91:LEU:O      | 4:D:93:TRP:N       | 2.49                     | 0.46              |
| 4:D:139:ARG:HH11  | 4:D:141:TYR:HE1    | 1.64                     | 0.46              |
| 2:H:49:ASP:OD2    | 2:H:52:LEU:HB2     | 2.16                     | 0.46              |
| 2:H:207:ILE:CG1   | 2:H:208:VAL:N      | 2.78                     | 0.46              |
| 2:H:386:ALA:O     | 2:H:387:GLU:C      | 2.58                     | 0.46              |
| 11:H:1488:CLA:C16 | 4:J:281:MET:HE1    | 2.45                     | 0.46              |
| 3:I:449:ARG:HH12  | 11:I:1463:CLA:HAA1 | 1.81                     | 0.46              |
| 4:J:10:ALA:O      | 4:J:11:GLU:CB      | 2.64                     | 0.46              |
| 4:J:55:VAL:O      | 4:J:66:SER:HB3     | 2.16                     | 0.46              |
| 4:J:156:VAL:O     | 4:J:156:VAL:CG1    | 2.64                     | 0.46              |
| 6:L:35:GLY:O      | 6:L:36:ALA:C       | 2.58                     | 0.46              |
| 8:U:72:UNK:O      | 8:U:73:UNK:C       | 2.62                     | 0.46              |
| 10:X:3:UNK:O      | 10:X:6:UNK:N       | 2.49                     | 0.46              |
| 10:Y:3:UNK:C      | 10:Y:5:UNK:N       | 2.77                     | 0.46              |
| 1:A:141:PRO:CG    | 3:C:446:GLY:O      | 2.58                     | 0.45              |
| 2:B:69:LEU:HD23   | 11:B:1487:CLA:CMA  | 2.46                     | 0.45              |
| 2:B:70:GLY:HA2    | 2:B:178:VAL:HG11   | 1.97                     | 0.45              |
| 2:B:272:ARG:NH1   | 4:D:164:GLN:HA     | 2.31                     | 0.45              |
| 3:C:164:HIS:O     | 3:C:167:VAL:HG23   | 2.15                     | 0.45              |
| 4:D:57:SER:O      | 4:D:60:THR:HG22    | 2.16                     | 0.45              |
| 4:D:203:GLY:O     | 4:D:207:GLY:N      | 2.46                     | 0.45              |
| 1:G:65:GLU:O      | 1:G:65:GLU:HG2     | 2.15                     | 0.45              |
| 1:G:202:VAL:O     | 1:G:203:ALA:C      | 2.59                     | 0.45              |
| 2:H:27:THR:CG2    | 2:H:107:LEU:HD13   | 2.43                     | 0.45              |
| 2:H:95:GLY:O      | 2:H:96:VAL:C       | 2.58                     | 0.45              |
| 3:I:57:ALA:O      | 3:I:58:GLY:C       | 2.58                     | 0.45              |
| 3:I:84:GLN:O      | 3:I:85:GLY:C       | 2.58                     | 0.45              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 3:I:118:HIS:HA   | 3:I:121:SER:HB3    | 1.98                     | 0.45              |
| 4:J:139:ARG:NH1  | 4:J:141:TYR:HE1    | 2.13                     | 0.45              |
| 8:S:9:UNK:O      | 8:S:10:UNK:C       | 2.55                     | 0.45              |
| 10:X:266:UNK:O   | 10:X:267:UNK:C     | 2.63                     | 0.45              |
| 1:A:184:ILE:HD11 | 4:D:186:GLN:CD     | 2.42                     | 0.45              |
| 1:A:192:ILE:C    | 1:A:194:MET:N      | 2.71                     | 0.45              |
| 2:B:132:ALA:O    | 2:B:133:LEU:CB     | 2.64                     | 0.45              |
| 2:B:450:TRP:O    | 2:B:453:PHE:N      | 2.29                     | 0.45              |
| 3:C:39:ASN:O     | 3:C:40:ALA:C       | 2.59                     | 0.45              |
| 3:C:66:ALA:HB1   | 10:X:517:UNK:HA    | 1.97                     | 0.45              |
| 3:C:245:ILE:HD12 | 3:C:245:ILE:C      | 2.41                     | 0.45              |
| 3:C:398:HIS:O    | 3:C:399:ALA:CA     | 2.62                     | 0.45              |
| 4:D:64:ALA:HB1   | 4:D:69:GLU:HB3     | 1.98                     | 0.45              |
| 4:D:186:GLN:CB   | 11:D:1351:CLA:HBC1 | 2.47                     | 0.45              |
| 1:G:131:TRP:O    | 1:G:134:SER:CB     | 2.64                     | 0.45              |
| 1:G:171:GLY:HA2  | 1:G:182:PHE:CE1    | 2.51                     | 0.45              |
| 1:G:176:ILE:CG2  | 1:G:180:PHE:HE1    | 2.29                     | 0.45              |
| 1:G:215:HIS:O    | 1:G:219:VAL:HG23   | 2.16                     | 0.45              |
| 1:G:288:LEU:O    | 1:G:290:ILE:N      | 2.50                     | 0.45              |
| 3:I:376:ASP:OD2  | 3:I:379:LYS:HE3    | 2.16                     | 0.45              |
| 4:J:87:HIS:CE1   | 4:J:161:PRO:O      | 2.69                     | 0.45              |
| 5:K:61:ARG:O     | 5:K:62:SER:HB2     | 2.15                     | 0.45              |
| 8:U:86:UNK:O     | 8:U:87:UNK:C       | 2.65                     | 0.45              |
| 10:Y:331:UNK:O   | 10:Y:334:UNK:CB    | 2.64                     | 0.45              |
| 10:Y:419:UNK:O   | 10:Y:423:UNK:N     | 2.49                     | 0.45              |
| 10:Y:567:UNK:O   | 10:Y:571:UNK:N     | 2.48                     | 0.45              |
| 1:A:172:MET:HE1  | 11:A:1343:CLA:CHC  | 2.46                     | 0.45              |
| 1:A:172:MET:HA   | 1:A:173:PRO:HD3    | 1.44                     | 0.45              |
| 1:A:190:HIS:ND1  | 1:A:298:ASN:ND2    | 2.63                     | 0.45              |
| 1:A:290:ILE:O    | 1:A:292:THR:N      | 2.50                     | 0.45              |
| 2:B:110:ALA:HA   | 11:B:1496:CLA:C20  | 2.45                     | 0.45              |
| 2:B:196:GLY:O    | 2:B:197:GLY:C      | 2.59                     | 0.45              |
| 2:B:395:GLN:CB   | 2:B:397:VAL:CB     | 2.95                     | 0.45              |
| 2:B:450:TRP:CE2  | 11:B:1488:CLA:HBA1 | 2.51                     | 0.45              |
| 3:C:24:THR:O     | 3:C:25:ASN:CB      | 2.64                     | 0.45              |
| 4:D:33:SER:OG    | 4:D:128:ARG:HA     | 2.16                     | 0.45              |
| 4:D:286:VAL:O    | 4:D:287:VAL:C      | 2.58                     | 0.45              |
| 6:F:9:GLU:N      | 6:F:10:PRO:CD      | 2.79                     | 0.45              |
| 1:G:206:PHE:CZ   | 11:J:1351:CLA:HAA1 | 2.51                     | 0.45              |
| 2:H:214:LEU:HD12 | 2:H:215:PHE:N      | 2.31                     | 0.45              |
| 3:I:250:TRP:CD1  | 3:I:250:TRP:O      | 2.69                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:I:304:PRO:O      | 3:I:305:THR:CG2    | 2.63                     | 0.45              |
| 3:I:354:GLU:C      | 3:I:356:MET:N      | 2.70                     | 0.45              |
| 4:J:42:TYR:O       | 4:J:43:LEU:C       | 2.60                     | 0.45              |
| 5:K:82:GLN:O       | 5:K:83:LEU:C       | 2.58                     | 0.45              |
| 9:T:64:PRO:HD2     | 9:T:66:ARG:NH2     | 2.30                     | 0.45              |
| 10:X:202:UNK:O     | 10:X:203:UNK:C     | 2.64                     | 0.45              |
| 10:Y:531:UNK:O     | 10:Y:532:UNK:C     | 2.62                     | 0.45              |
| 1:A:290:ILE:C      | 1:A:292:THR:H      | 2.25                     | 0.45              |
| 2:B:37:MET:O       | 2:B:38:ALA:C       | 2.59                     | 0.45              |
| 2:B:309:LEU:O      | 2:B:311:PHE:N      | 2.50                     | 0.45              |
| 3:C:133:ALA:C      | 3:C:134:ILE:HG13   | 2.40                     | 0.45              |
| 3:C:238:ILE:O      | 3:C:239:TRP:C      | 2.58                     | 0.45              |
| 4:D:81:PRO:O       | 4:D:168:PHE:HD1    | 1.99                     | 0.45              |
| 4:D:83:ASN:OD1     | 4:D:336:HIS:HD2    | 1.98                     | 0.45              |
| 4:D:199:MET:O      | 4:D:202:ALA:N      | 2.50                     | 0.45              |
| 5:E:37:PHE:CZ      | 5:E:43:ALA:HA      | 2.52                     | 0.45              |
| 1:G:131:TRP:CD2    | 1:G:131:TRP:C      | 2.91                     | 0.45              |
| 1:G:222:SER:O      | 1:G:246:TYR:O      | 2.34                     | 0.45              |
| 1:G:324:ALA:HB2    | 4:J:329:MET:HE3    | 1.98                     | 0.45              |
| 2:H:193:TYR:OH     | 2:H:259:GLY:HA2    | 2.15                     | 0.45              |
| 2:H:396:GLY:O      | 2:H:398:THR:N      | 2.50                     | 0.45              |
| 11:H:1488:CLA:H203 | 4:J:281:MET:SD     | 2.57                     | 0.45              |
| 3:I:25:ASN:O       | 3:I:26:ARG:CB      | 2.64                     | 0.45              |
| 4:J:72:ASN:O       | 4:J:73:PHE:C       | 2.60                     | 0.45              |
| 4:J:191:TRP:O      | 4:J:194:ASN:N      | 2.38                     | 0.45              |
| 1:A:44:ALA:O       | 1:A:45:THR:C       | 2.58                     | 0.45              |
| 1:A:171:GLY:HA2    | 1:A:182:PHE:CE1    | 2.51                     | 0.45              |
| 1:A:176:ILE:CG2    | 1:A:180:PHE:HE1    | 2.29                     | 0.45              |
| 3:C:161:LEU:HD21   | 11:C:1464:CLA:HBB1 | 1.98                     | 0.45              |
| 3:C:366:LEU:HD12   | 3:C:366:LEU:O      | 2.17                     | 0.45              |
| 4:D:56:THR:HG22    | 5:E:49:THR:HG22    | 1.99                     | 0.45              |
| 4:D:186:GLN:HB2    | 11:D:1351:CLA:HBC1 | 1.99                     | 0.45              |
| 4:D:335:PRO:C      | 4:D:337:GLU:N      | 2.74                     | 0.45              |
| 1:G:180:PHE:CZ     | 4:J:192:THR:HB     | 2.51                     | 0.45              |
| 2:H:193:TYR:HD1    | 2:H:260:SER:CB     | 2.29                     | 0.45              |
| 3:I:228:ASN:HA     | 3:I:295:THR:CG2    | 2.25                     | 0.45              |
| 3:I:267:SER:H      | 3:I:270:ALA:HB3    | 1.82                     | 0.45              |
| 4:J:129:GLN:OE1    | 4:J:143:ALA:HA     | 2.16                     | 0.45              |
| 7:O:127:UNK:O      | 7:O:128:UNK:C      | 2.64                     | 0.45              |
| 7:O:154:UNK:HA     | 7:O:170:UNK:HA     | 1.98                     | 0.45              |
| 10:Y:64:UNK:C      | 10:Y:66:UNK:N      | 2.75                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:Y:202:UNK:O     | 10:Y:203:UNK:C     | 2.64                     | 0.45              |
| 10:Y:503:UNK:O     | 10:Y:504:UNK:C     | 2.65                     | 0.45              |
| 1:A:62:GLY:CA      | 1:A:87:ASN:CB      | 2.92                     | 0.45              |
| 1:A:104:GLU:HG2    | 1:A:104:GLU:O      | 2.17                     | 0.45              |
| 2:B:75:TRP:C       | 2:B:77:GLY:H       | 2.11                     | 0.45              |
| 2:B:192:PRO:HG3    | 11:B:1483:CLA:HBA2 | 1.98                     | 0.45              |
| 2:B:234:ILE:O      | 2:B:237:VAL:N      | 2.49                     | 0.45              |
| 2:B:280:PHE:CE2    | 2:B:312:TYR:HB3    | 2.52                     | 0.45              |
| 3:C:82:TYR:CA      | 3:C:422:PRO:HG2    | 2.38                     | 0.45              |
| 3:C:164:HIS:C      | 3:C:166:ILE:N      | 2.74                     | 0.45              |
| 3:C:273:SER:CB     | 3:C:445:ALA:HB2    | 2.42                     | 0.45              |
| 4:D:35:ILE:O       | 4:D:35:ILE:HG22    | 2.15                     | 0.45              |
| 1:G:141:PRO:CG     | 3:I:446:GLY:O      | 2.60                     | 0.45              |
| 2:H:64:PRO:CB      | 2:H:268:PHE:CZ     | 2.99                     | 0.45              |
| 2:H:114:HIS:NE2    | 11:H:1497:CLA:NB   | 2.65                     | 0.45              |
| 2:H:267:LEU:H      | 2:H:267:LEU:HG     | 1.57                     | 0.45              |
| 2:H:464:PHE:CE1    | 4:J:144:ILE:HG23   | 2.51                     | 0.45              |
| 3:I:56:HIS:O       | 3:I:59:LEU:HB3     | 2.16                     | 0.45              |
| 3:I:227:VAL:CG1    | 3:I:233:VAL:HG23   | 2.47                     | 0.45              |
| 4:J:53:THR:HG22    | 4:J:67:TYR:CE1     | 2.52                     | 0.45              |
| 4:J:83:ASN:CG      | 4:J:336:HIS:CD2    | 2.83                     | 0.45              |
| 4:J:315:TYR:CE1    | 4:J:319:LEU:HD12   | 2.52                     | 0.45              |
| 17:L:1047:BCR:H331 | 17:L:1047:BCR:H343 | 1.98                     | 0.45              |
| 7:O:63:UNK:O       | 7:O:72:UNK:N       | 2.49                     | 0.45              |
| 9:T:30:LYS:HG2     | 9:T:118:HIS:CE1    | 2.51                     | 0.45              |
| 9:T:53:ASP:C       | 9:T:53:ASP:OD1     | 2.59                     | 0.45              |
| 9:T:93:PRO:HG3     | 9:T:101:PHE:CD1    | 2.52                     | 0.45              |
| 10:X:213:UNK:O     | 10:X:214:UNK:C     | 2.65                     | 0.45              |
| 1:A:119:PHE:O      | 1:A:120:LEU:C      | 2.57                     | 0.45              |
| 1:A:157:VAL:HG13   | 1:A:172:MET:HB3    | 1.99                     | 0.45              |
| 1:A:215:HIS:HB3    | 4:D:271:MET:CE     | 2.46                     | 0.45              |
| 1:A:317:TRP:CG     | 4:D:177:ALA:HB2    | 2.51                     | 0.45              |
| 2:B:386:ALA:O      | 2:B:387:GLU:C      | 2.60                     | 0.45              |
| 3:C:109:PHE:HB3    | 3:C:110:PRO:CD     | 2.47                     | 0.45              |
| 3:C:244:CYS:HA     | 11:C:1464:CLA:CMC  | 2.47                     | 0.45              |
| 3:C:402:GLY:CA     | 3:C:420:VAL:HG13   | 2.47                     | 0.45              |
| 4:D:139:ARG:NH1    | 4:D:141:TYR:HE1    | 2.14                     | 0.45              |
| 4:D:148:ALA:CB     | 4:D:276:VAL:HA     | 2.46                     | 0.45              |
| 4:D:171:PRO:HG3    | 4:D:181:PHE:CD2    | 2.52                     | 0.45              |
| 1:G:290:ILE:HD11   | 11:G:1342:CLA:CAD  | 2.46                     | 0.45              |
| 1:G:320:ILE:O      | 1:G:322:ASN:N      | 2.50                     | 0.45              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 2:H:18:ARG:O     | 2:H:21:ALA:N       | 2.48                     | 0.45              |
| 2:H:67:ALA:HA    | 2:H:71:VAL:O       | 2.17                     | 0.45              |
| 2:H:68:ARG:NH1   | 2:H:262:THR:O      | 2.49                     | 0.45              |
| 2:H:150:CYS:N    | 11:H:1484:CLA:HBC2 | 2.32                     | 0.45              |
| 2:H:215:PHE:CD2  | 2:H:216:HIS:N      | 2.84                     | 0.45              |
| 2:H:220:ARG:CB   | 2:H:221:PRO:HD2    | 2.47                     | 0.45              |
| 2:H:407:ASN:O    | 2:H:408:GLY:C      | 2.60                     | 0.45              |
| 3:I:170:ILE:O    | 3:I:171:GLY:C      | 2.59                     | 0.45              |
| 3:I:227:VAL:O    | 3:I:227:VAL:HG12   | 2.13                     | 0.45              |
| 3:I:376:ASP:O    | 3:I:377:LEU:C      | 2.60                     | 0.45              |
| 4:J:48:TRP:O     | 4:J:52:THR:OG1     | 2.23                     | 0.45              |
| 4:J:185:PHE:O    | 4:J:186:GLN:C      | 2.59                     | 0.45              |
| 7:O:24:UNK:O     | 7:O:25:UNK:O       | 2.34                     | 0.45              |
| 7:O:142:UNK:CA   | 7:O:149:UNK:CB     | 2.93                     | 0.45              |
| 8:S:4:UNK:O      | 8:S:7:UNK:CB       | 2.65                     | 0.45              |
| 8:U:69:UNK:C     | 8:U:71:UNK:N       | 2.80                     | 0.45              |
| 10:X:200:UNK:O   | 10:X:203:UNK:N     | 2.50                     | 0.45              |
| 10:X:269:UNK:O   | 10:X:270:UNK:C     | 2.63                     | 0.45              |
| 10:X:470:UNK:C   | 10:X:472:UNK:N     | 2.78                     | 0.45              |
| 10:Y:519:UNK:C   | 10:Y:521:UNK:N     | 2.80                     | 0.45              |
| 1:A:283:VAL:O    | 1:A:284:TRP:C      | 2.60                     | 0.45              |
| 2:B:97:ALA:O     | 2:B:98:LEU:C       | 2.59                     | 0.45              |
| 2:B:150:CYS:HB2  | 11:B:1484:CLA:CMC  | 2.46                     | 0.45              |
| 2:B:310:ALA:O    | 2:B:428:GLU:HB2    | 2.17                     | 0.45              |
| 2:B:357:ARG:NH1  | 4:D:338:ASN:O      | 2.50                     | 0.45              |
| 3:C:80:PRO:HB2   | 3:C:83:GLU:HB2     | 1.99                     | 0.45              |
| 3:C:169:GLY:CA   | 3:C:244:CYS:SG     | 3.03                     | 0.45              |
| 4:D:54:PHE:HE1   | 6:F:33:PHE:CD2     | 2.34                     | 0.45              |
| 6:F:10:PRO:CB    | 6:F:19:ARG:HH11    | 2.20                     | 0.45              |
| 6:F:33:PHE:CE1   | 17:F:1046:BCR:H14C | 2.52                     | 0.45              |
| 2:H:451:PHE:C    | 2:H:451:PHE:CD2    | 2.94                     | 0.45              |
| 3:I:230:LEU:O    | 3:I:230:LEU:HD12   | 2.16                     | 0.45              |
| 4:J:83:ASN:OD1   | 4:J:83:ASN:O       | 2.34                     | 0.45              |
| 4:J:287:VAL:O    | 4:J:290:ALA:HB3    | 2.16                     | 0.45              |
| 8:U:57:UNK:O     | 8:U:58:UNK:C       | 2.63                     | 0.45              |
| 1:A:119:PHE:CD2  | 12:A:1345:PHO:H111 | 2.52                     | 0.45              |
| 2:B:345:VAL:HG23 | 2:B:345:VAL:O      | 2.17                     | 0.45              |
| 2:B:360:PRO:HB2  | 2:B:363:PHE:CD2    | 2.43                     | 0.45              |
| 2:B:396:GLY:O    | 2:B:398:THR:N      | 2.50                     | 0.45              |
| 3:C:62:PHE:O     | 3:C:63:TRP:C       | 2.59                     | 0.45              |
| 3:C:67:MET:O     | 3:C:68:THR:C       | 2.59                     | 0.45              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 3:C:125:LEU:O    | 3:C:126:GLY:C      | 2.59                     | 0.45              |
| 4:D:127:LEU:C    | 4:D:129:GLN:N      | 2.75                     | 0.45              |
| 4:D:315:TYR:CE1  | 4:D:319:LEU:HD12   | 2.51                     | 0.45              |
| 1:G:135:TYR:C    | 1:G:136:ARG:HG2    | 2.42                     | 0.45              |
| 1:G:180:PHE:CG   | 4:J:192:THR:HB     | 2.52                     | 0.45              |
| 2:H:31:ALA:CB    | 11:H:1486:CLA:HBC3 | 2.46                     | 0.45              |
| 2:H:238:LEU:CD2  | 2:H:469:HIS:CG     | 3.00                     | 0.45              |
| 2:H:426:PHE:O    | 2:H:426:PHE:CD1    | 2.70                     | 0.45              |
| 3:I:56:HIS:O     | 3:I:59:LEU:CB      | 2.65                     | 0.45              |
| 3:I:138:GLU:C    | 3:I:139:THR:CA     | 2.90                     | 0.45              |
| 3:I:238:ILE:O    | 3:I:239:TRP:C      | 2.59                     | 0.45              |
| 9:V:41:HIS:O     | 9:V:42:VAL:C       | 2.59                     | 0.45              |
| 10:X:201:UNK:O   | 10:X:202:UNK:C     | 2.63                     | 0.45              |
| 1:A:215:HIS:CD2  | 4:D:271:MET:HE1    | 2.52                     | 0.45              |
| 1:A:278:TRP:C    | 1:A:278:TRP:CD1    | 2.95                     | 0.45              |
| 5:E:18:ARG:NE    | 5:E:22:ILE:HD11    | 2.32                     | 0.45              |
| 2:H:16:PRO:O     | 2:H:17:GLY:C       | 2.58                     | 0.45              |
| 3:I:81:MET:HB3   | 3:I:301:PHE:O      | 2.17                     | 0.45              |
| 3:I:82:TYR:CA    | 3:I:422:PRO:HG2    | 2.39                     | 0.45              |
| 4:J:43:LEU:HG    | 4:J:113:PHE:CZ     | 2.52                     | 0.45              |
| 5:K:18:ARG:NE    | 5:K:22:ILE:HD11    | 2.32                     | 0.45              |
| 5:K:35:TRP:O     | 5:K:35:TRP:CD1     | 2.70                     | 0.45              |
| 6:L:14:PRO:O     | 6:L:15:ILE:CB      | 2.65                     | 0.45              |
| 7:P:142:UNK:C    | 7:P:149:UNK:CB     | 2.95                     | 0.45              |
| 10:Y:507:UNK:O   | 10:Y:508:UNK:C     | 2.64                     | 0.45              |
| 1:A:120:LEU:O    | 1:A:124:SER:N      | 2.49                     | 0.44              |
| 2:B:133:LEU:O    | 2:B:134:ASP:CB     | 2.65                     | 0.44              |
| 2:B:348:ASN:C    | 2:B:350:GLU:N      | 2.73                     | 0.44              |
| 2:B:358:ARG:O    | 2:B:360:PRO:HD3    | 2.17                     | 0.44              |
| 2:B:425:ILE:O    | 2:B:426:PHE:CB     | 2.65                     | 0.44              |
| 3:C:138:GLU:C    | 3:C:139:THR:CA     | 2.91                     | 0.44              |
| 4:D:74:LEU:HA    | 4:D:175:VAL:CG1    | 2.46                     | 0.44              |
| 4:D:191:TRP:O    | 4:D:192:THR:C      | 2.61                     | 0.44              |
| 4:D:294:ARG:HB2  | 4:D:295:SER:H      | 1.56                     | 0.44              |
| 5:E:49:THR:HA    | 5:E:50:PRO:HD3     | 1.79                     | 0.44              |
| 1:G:93:PHE:CZ    | 1:G:95:PRO:HG3     | 2.51                     | 0.44              |
| 1:G:157:VAL:C    | 1:G:158:PHE:CD2    | 2.95                     | 0.44              |
| 1:G:258:LEU:O    | 4:J:128:ARG:CZ     | 2.65                     | 0.44              |
| 2:H:174:LEU:HD23 | 2:H:308:LYS:HB3    | 1.98                     | 0.44              |
| 3:I:370:ARG:O    | 3:I:375:LEU:N      | 2.49                     | 0.44              |
| 3:I:447:ARG:HG2  | 3:I:447:ARG:NH1    | 2.32                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:J:32:TRP:O      | 4:J:35:ILE:HB      | 2.18                     | 0.44              |
| 10:Y:224:UNK:O    | 10:Y:225:UNK:C     | 2.64                     | 0.44              |
| 1:A:162:PRO:HB3   | 1:A:168:PHE:HA     | 2.00                     | 0.44              |
| 2:B:222:PRO:O     | 2:B:226:TYR:N      | 2.42                     | 0.44              |
| 2:B:421:ALA:O     | 2:B:422:ARG:C      | 2.60                     | 0.44              |
| 2:B:451:PHE:C     | 2:B:451:PHE:CD2    | 2.95                     | 0.44              |
| 3:C:35:TRP:CZ3    | 3:C:36:TRP:HB3     | 2.52                     | 0.44              |
| 3:C:150:ASP:CB    | 3:C:271:TYR:CE2    | 3.00                     | 0.44              |
| 3:C:164:HIS:HA    | 3:C:167:VAL:CG2    | 2.47                     | 0.44              |
| 3:C:311:GLN:HA    | 3:C:355:THR:HG21   | 1.99                     | 0.44              |
| 5:E:78:THR:O      | 5:E:79:PHE:C       | 2.57                     | 0.44              |
| 1:G:308:ASP:O     | 1:G:309:ALA:C      | 2.61                     | 0.44              |
| 2:H:280:PHE:O     | 2:H:283:GLU:N      | 2.50                     | 0.44              |
| 2:H:286:ARG:HG3   | 2:H:287:ARG:N      | 2.31                     | 0.44              |
| 3:I:188:THR:HG21  | 3:I:300:GLU:OE1    | 2.17                     | 0.44              |
| 3:I:229:ASN:HB2   | 3:I:232:ASP:OD1    | 2.18                     | 0.44              |
| 11:I:1471:CLA:HHD | 11:I:1471:CLA:HBC3 | 1.99                     | 0.44              |
| 4:J:96:GLU:OE1    | 4:J:96:GLU:CA      | 2.66                     | 0.44              |
| 4:J:288:GLY:C     | 4:J:290:ALA:H      | 2.24                     | 0.44              |
| 4:J:288:GLY:C     | 4:J:290:ALA:N      | 2.72                     | 0.44              |
| 4:J:302:GLU:HB3   | 7:P:114:UNK:CB     | 2.47                     | 0.44              |
| 5:K:10:PHE:HE2    | 6:L:19:ARG:HE      | 1.62                     | 0.44              |
| 7:P:11:UNK:CA     | 7:P:173:UNK:CB     | 2.90                     | 0.44              |
| 8:S:77:UNK:C      | 8:S:79:UNK:N       | 2.79                     | 0.44              |
| 10:Y:200:UNK:O    | 10:Y:203:UNK:N     | 2.51                     | 0.44              |
| 1:A:78:ILE:HB     | 4:D:298:PHE:HZ     | 1.81                     | 0.44              |
| 1:A:105:TRP:CZ3   | 1:A:111:PRO:HG3    | 2.53                     | 0.44              |
| 1:A:131:TRP:O     | 1:A:134:SER:CB     | 2.65                     | 0.44              |
| 1:A:179:THR:HG22  | 1:A:183:MET:HE3    | 1.99                     | 0.44              |
| 1:A:206:PHE:CZ    | 11:D:1351:CLA:HAA1 | 2.52                     | 0.44              |
| 2:B:139:PHE:O     | 2:B:139:PHE:CD1    | 2.70                     | 0.44              |
| 1:G:112:TYR:CE1   | 1:G:116:ILE:CD1    | 3.00                     | 0.44              |
| 1:G:176:ILE:CG1   | 11:G:1343:CLA:HED3 | 2.41                     | 0.44              |
| 1:G:279:PRO:CB    | 12:G:1345:PHO:HBC1 | 2.48                     | 0.44              |
| 1:G:288:LEU:O     | 1:G:291:SER:N      | 2.50                     | 0.44              |
| 2:H:425:ILE:O     | 2:H:426:PHE:CB     | 2.64                     | 0.44              |
| 3:I:237:HIS:O     | 3:I:238:ILE:C      | 2.59                     | 0.44              |
| 3:I:394:GLU:O     | 3:I:395:TYR:C      | 2.59                     | 0.44              |
| 4:J:203:GLY:O     | 4:J:207:GLY:N      | 2.48                     | 0.44              |
| 4:J:210:LEU:HD11  | 4:J:270:PHE:HD2    | 1.81                     | 0.44              |
| 4:J:272:LEU:HD23  | 4:J:272:LEU:O      | 2.17                     | 0.44              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 10:X:9:UNK:O     | 10:X:10:UNK:C      | 2.62                     | 0.44              |
| 10:X:223:UNK:O   | 10:X:224:UNK:C     | 2.65                     | 0.44              |
| 1:A:55:ALA:HA    | 1:A:56:PRO:HD3     | 1.75                     | 0.44              |
| 1:A:57:PRO:CG    | 1:A:68:SER:HB3     | 2.36                     | 0.44              |
| 2:B:172:TYR:HB3  | 2:B:309:LEU:HD21   | 1.98                     | 0.44              |
| 2:B:463:PHE:C    | 2:B:465:GLY:H      | 2.24                     | 0.44              |
| 3:C:49:LEU:O     | 3:C:52:ALA:N       | 2.51                     | 0.44              |
| 3:C:109:PHE:HB3  | 3:C:110:PRO:HD2    | 1.98                     | 0.44              |
| 3:C:243:ILE:HG22 | 3:C:244:CYS:N      | 2.32                     | 0.44              |
| 4:D:235:PHE:CD2  | 4:D:243:THR:CG2    | 2.99                     | 0.44              |
| 5:E:10:PHE:CE2   | 6:F:19:ARG:CZ      | 3.01                     | 0.44              |
| 2:H:106:LEU:O    | 2:H:107:LEU:C      | 2.60                     | 0.44              |
| 2:H:265:ILE:HD13 | 2:H:265:ILE:HA     | 1.77                     | 0.44              |
| 3:I:229:ASN:HD22 | 3:I:232:ASP:CG     | 2.25                     | 0.44              |
| 3:I:274:TYR:HD1  | 11:I:1463:CLA:HMD2 | 1.81                     | 0.44              |
| 7:O:142:UNK:C    | 7:O:149:UNK:CB     | 2.96                     | 0.44              |
| 1:A:167:SER:C    | 1:A:169:SER:N      | 2.73                     | 0.44              |
| 2:B:397:VAL:C    | 2:B:399:VAL:N      | 2.73                     | 0.44              |
| 3:C:354:GLU:C    | 3:C:356:MET:N      | 2.63                     | 0.44              |
| 4:D:224:GLN:O    | 4:D:225:ASP:C      | 2.59                     | 0.44              |
| 4:D:337:GLU:CG   | 4:D:339:PHE:HE2    | 2.28                     | 0.44              |
| 4:D:339:PHE:HD1  | 4:D:341:PHE:CE1    | 2.35                     | 0.44              |
| 5:E:23:HIS:HD2   | 16:E:1085:HEM:NB   | 2.14                     | 0.44              |
| 1:G:218:LEU:HA   | 1:G:221:SER:OG     | 2.17                     | 0.44              |
| 2:H:270:PRO:O    | 2:H:271:THR:CB     | 2.65                     | 0.44              |
| 4:J:52:THR:CG2   | 4:J:76:VAL:HG11    | 2.47                     | 0.44              |
| 4:J:82:ALA:H     | 4:J:85:MET:HE3     | 1.81                     | 0.44              |
| 10:X:158:UNK:O   | 10:X:159:UNK:C     | 2.63                     | 0.44              |
| 10:X:331:UNK:O   | 10:X:334:UNK:CB    | 2.65                     | 0.44              |
| 1:A:131:TRP:CD2  | 1:A:131:TRP:C      | 2.91                     | 0.44              |
| 2:B:272:ARG:CG   | 2:B:273:TYR:N      | 2.80                     | 0.44              |
| 3:C:38:GLY:HA3   | 11:C:1469:CLA:C2D  | 2.47                     | 0.44              |
| 3:C:188:THR:HG21 | 3:C:300:GLU:OE1    | 2.18                     | 0.44              |
| 3:C:269:GLU:N    | 11:C:1467:CLA:HBC1 | 2.32                     | 0.44              |
| 3:C:430:HIS:O    | 3:C:434:ALA:N      | 2.46                     | 0.44              |
| 4:D:180:ARG:C    | 4:D:180:ARG:HD3    | 2.43                     | 0.44              |
| 6:F:18:VAL:O     | 6:F:21:VAL:HB      | 2.17                     | 0.44              |
| 1:G:183:MET:HE1  | 11:G:1343:CLA:HMD1 | 1.98                     | 0.44              |
| 1:G:322:ASN:O    | 1:G:323:ARG:C      | 2.61                     | 0.44              |
| 2:H:31:ALA:HB2   | 11:H:1486:CLA:HBC3 | 1.99                     | 0.44              |
| 2:H:35:GLY:O     | 2:H:38:ALA:HB3     | 2.18                     | 0.44              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 2:H:172:TYR:CE1  | 2:H:279:TYR:CZ     | 3.05                     | 0.44              |
| 2:H:445:THR:HG23 | 2:H:450:TRP:NE1    | 2.33                     | 0.44              |
| 3:I:225:VAL:HA   | 3:I:289:PHE:CE1    | 2.52                     | 0.44              |
| 3:I:276:LEU:HD13 | 11:I:1466:CLA:HBB1 | 1.99                     | 0.44              |
| 4:J:93:TRP:HA    | 4:J:97:ALA:HB2     | 2.00                     | 0.44              |
| 9:T:28:GLU:OE1   | 9:T:28:GLU:HA      | 2.18                     | 0.44              |
| 9:T:77:LYS:HG2   | 9:T:95:LEU:HD22    | 1.99                     | 0.44              |
| 9:V:40:CYS:SG    | 9:V:47:LYS:HB2     | 2.58                     | 0.44              |
| 10:X:255:UNK:O   | 10:X:256:UNK:C     | 2.65                     | 0.44              |
| 10:Y:68:UNK:C    | 10:Y:70:UNK:N      | 2.74                     | 0.44              |
| 1:A:83:VAL:HG13  | 4:D:314:PHE:CZ     | 2.53                     | 0.44              |
| 1:A:222:SER:O    | 1:A:246:TYR:CB     | 2.65                     | 0.44              |
| 1:A:259:ILE:O    | 1:A:260:PHE:CB     | 2.65                     | 0.44              |
| 2:B:238:LEU:CD2  | 2:B:469:HIS:CG     | 3.01                     | 0.44              |
| 2:B:280:PHE:O    | 2:B:283:GLU:N      | 2.50                     | 0.44              |
| 2:B:445:THR:HG23 | 2:B:450:TRP:NE1    | 2.33                     | 0.44              |
| 2:B:468:TRP:O    | 2:B:471:ALA:CB     | 2.64                     | 0.44              |
| 3:C:56:HIS:O     | 3:C:59:LEU:HB3     | 2.18                     | 0.44              |
| 3:C:91:HIS:CE1   | 11:C:1460:CLA:O1D  | 2.67                     | 0.44              |
| 3:C:185:LEU:O    | 3:C:186:TYR:C      | 2.61                     | 0.44              |
| 3:C:189:TRP:C    | 3:C:190:ALA:O      | 2.60                     | 0.44              |
| 4:D:67:TYR:HB2   | 6:F:40:MET:HE1     | 2.00                     | 0.44              |
| 4:D:111:TRP:HB3  | 4:D:112:THR:H      | 1.67                     | 0.44              |
| 4:D:148:ALA:HB2  | 4:D:276:VAL:HA     | 2.00                     | 0.44              |
| 4:D:191:TRP:CZ2  | 4:D:286:VAL:CG2    | 3.01                     | 0.44              |
| 4:D:331:PRO:CG   | 4:D:339:PHE:CG     | 2.93                     | 0.44              |
| 1:G:258:LEU:HG   | 4:J:128:ARG:NH2    | 2.33                     | 0.44              |
| 2:H:309:LEU:O    | 2:H:311:PHE:N      | 2.50                     | 0.44              |
| 3:I:43:ILE:HG13  | 3:I:44:ASN:N       | 2.32                     | 0.44              |
| 3:I:320:ARG:HD2  | 9:T:49:ASN:CG      | 2.42                     | 0.44              |
| 4:J:56:THR:OG1   | 4:J:57:SER:N       | 2.50                     | 0.44              |
| 4:J:330:ALA:HB3  | 4:J:331:PRO:CD     | 2.00                     | 0.44              |
| 1:A:112:TYR:CE1  | 1:A:116:ILE:HD12   | 2.53                     | 0.44              |
| 1:A:112:TYR:CE1  | 1:A:116:ILE:HD11   | 2.53                     | 0.44              |
| 3:C:320:ARG:HH11 | 9:V:49:ASN:CG      | 2.26                     | 0.44              |
| 4:D:69:GLU:HG2   | 5:E:55:TYR:HH      | 1.82                     | 0.44              |
| 4:D:122:LEU:HD23 | 4:D:122:LEU:HA     | 1.80                     | 0.44              |
| 4:D:296:TYR:CE1  | 4:D:319:LEU:HD23   | 2.53                     | 0.44              |
| 1:G:47:CYS:SG    | 1:G:114:LEU:CD2    | 2.89                     | 0.44              |
| 1:G:52:PHE:C     | 1:G:52:PHE:CD2     | 2.96                     | 0.44              |
| 1:G:167:SER:OG   | 1:G:169:SER:HB2    | 2.18                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:H:45:PHE:CE2    | 2:H:47:PRO:CD      | 2.82                     | 0.44              |
| 2:H:195:PRO:O     | 2:H:198:VAL:N      | 2.50                     | 0.44              |
| 2:H:398:THR:O     | 2:H:400:SER:N      | 2.50                     | 0.44              |
| 2:H:425:ILE:CG2   | 2:H:426:PHE:CD2    | 3.01                     | 0.44              |
| 2:H:468:TRP:O     | 2:H:471:ALA:CB     | 2.64                     | 0.44              |
| 3:I:189:TRP:C     | 3:I:190:ALA:O      | 2.58                     | 0.44              |
| 7:P:154:UNK:HA    | 7:P:170:UNK:HA     | 2.00                     | 0.44              |
| 10:X:168:UNK:C    | 10:X:170:UNK:N     | 2.81                     | 0.44              |
| 10:X:463:UNK:O    | 10:X:464:UNK:C     | 2.66                     | 0.44              |
| 10:Y:159:UNK:O    | 10:Y:160:UNK:C     | 2.63                     | 0.44              |
| 1:A:57:PRO:HA     | 1:A:67:VAL:O       | 2.18                     | 0.44              |
| 1:A:258:LEU:HG    | 4:D:128:ARG:NH2    | 2.31                     | 0.44              |
| 2:B:149:LEU:O     | 2:B:150:CYS:C      | 2.61                     | 0.44              |
| 4:D:261:PHE:CD1   | 4:D:266:TRP:HD1    | 2.36                     | 0.44              |
| 4:D:342:PRO:O     | 4:D:345:VAL:HG23   | 2.17                     | 0.44              |
| 1:G:34:GLY:O      | 1:G:38:ILE:N       | 2.51                     | 0.44              |
| 1:G:157:VAL:CG1   | 1:G:157:VAL:O      | 2.65                     | 0.44              |
| 1:G:211:PHE:CD2   | 1:G:274:PHE:HE2    | 2.36                     | 0.44              |
| 1:G:258:LEU:O     | 4:J:128:ARG:NH1    | 2.51                     | 0.44              |
| 1:G:258:LEU:C     | 4:J:128:ARG:HH22   | 2.26                     | 0.44              |
| 1:G:320:ILE:HD11  | 4:J:63:LEU:HD21    | 1.98                     | 0.44              |
| 2:H:62:VAL:O      | 2:H:63:LEU:C       | 2.61                     | 0.44              |
| 3:I:420:VAL:HG12  | 3:I:421:SER:N      | 2.33                     | 0.44              |
| 4:J:160:TYR:CZ    | 4:J:164:GLN:OE1    | 2.70                     | 0.44              |
| 18:V:1138:HEC:HHA | 18:V:1138:HEC:HAD2 | 1.61                     | 0.44              |
| 1:A:12:ASN:C      | 1:A:14:TRP:N       | 2.75                     | 0.43              |
| 1:A:21:VAL:O      | 1:A:22:THR:C       | 2.61                     | 0.43              |
| 1:A:78:ILE:HD12   | 10:X:125:UNK:CB    | 2.48                     | 0.43              |
| 1:A:91:LEU:HD12   | 1:A:91:LEU:HA      | 1.88                     | 0.43              |
| 1:A:176:ILE:CG2   | 1:A:180:PHE:CE1    | 3.01                     | 0.43              |
| 1:A:290:ILE:O     | 1:A:291:SER:C      | 2.61                     | 0.43              |
| 2:B:176:GLY:O     | 2:B:177:SER:HB3    | 2.18                     | 0.43              |
| 2:B:425:ILE:CG2   | 2:B:426:PHE:CD2    | 3.00                     | 0.43              |
| 3:C:170:ILE:CG2   | 3:C:171:GLY:H      | 2.29                     | 0.43              |
| 3:C:189:TRP:HH2   | 3:C:363:GLY:HA2    | 1.80                     | 0.43              |
| 3:C:341:LEU:CD2   | 3:C:375:LEU:HD13   | 2.48                     | 0.43              |
| 3:C:395:TYR:O     | 3:C:398:HIS:N      | 2.37                     | 0.43              |
| 3:C:438:LEU:O     | 3:C:439:VAL:C      | 2.61                     | 0.43              |
| 12:G:1345:PHO:HAB | 4:J:205:LEU:CD2    | 2.47                     | 0.43              |
| 2:H:466:HIS:C     | 2:H:468:TRP:N      | 2.75                     | 0.43              |
| 3:I:267:SER:O     | 3:I:268:GLY:C      | 2.59                     | 0.43              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 3:I:318:LEU:HA   | 3:I:340:TYR:CD1    | 2.53                     | 0.43              |
| 4:J:61:HIS:CE1   | 4:J:80:THR:OG1     | 2.71                     | 0.43              |
| 4:J:148:ALA:HA   | 4:J:280:TRP:HE1    | 1.80                     | 0.43              |
| 4:J:320:LEU:HD23 | 4:J:320:LEU:HA     | 1.73                     | 0.43              |
| 8:S:20:UNK:C     | 8:S:22:UNK:H       | 2.29                     | 0.43              |
| 9:T:62:ALA:HB2   | 9:T:82:TYR:CE1     | 2.53                     | 0.43              |
| 10:Y:423:UNK:O   | 10:Y:424:UNK:C     | 2.65                     | 0.43              |
| 1:A:142:TRP:CG   | 4:D:220:ASN:OD1    | 2.71                     | 0.43              |
| 1:A:168:PHE:O    | 1:A:169:SER:C      | 2.60                     | 0.43              |
| 1:A:177:SER:O    | 1:A:180:PHE:N      | 2.51                     | 0.43              |
| 2:B:18:ARG:O     | 2:B:21:ALA:N       | 2.51                     | 0.43              |
| 2:B:19:LEU:O     | 2:B:22:ALA:HB3     | 2.18                     | 0.43              |
| 2:B:29:LEU:HD12  | 11:B:1495:CLA:HBB2 | 2.00                     | 0.43              |
| 2:B:98:LEU:O     | 2:B:99:ALA:C       | 2.61                     | 0.43              |
| 2:B:435:GLU:C    | 2:B:437:LEU:H      | 2.26                     | 0.43              |
| 3:C:127:PHE:C    | 3:C:129:GLY:N      | 2.76                     | 0.43              |
| 4:D:127:LEU:O    | 4:D:130:PHE:N      | 2.51                     | 0.43              |
| 4:D:148:ALA:HB2  | 4:D:276:VAL:HG13   | 1.98                     | 0.43              |
| 1:G:77:ILE:H     | 1:G:77:ILE:HG13    | 1.64                     | 0.43              |
| 2:H:153:PHE:O    | 2:H:157:HIS:HB3    | 2.19                     | 0.43              |
| 2:H:316:GLY:HA2  | 2:H:443:PHE:CE1    | 2.51                     | 0.43              |
| 2:H:450:TRP:CE2  | 11:H:1488:CLA:HBA1 | 2.54                     | 0.43              |
| 3:I:430:HIS:O    | 3:I:431:PHE:C      | 2.60                     | 0.43              |
| 4:J:236:ASN:C    | 4:J:238:THR:N      | 2.75                     | 0.43              |
| 4:J:335:PRO:C    | 4:J:337:GLU:N      | 2.77                     | 0.43              |
| 7:O:37:UNK:O     | 7:O:38:UNK:CB      | 2.66                     | 0.43              |
| 2:B:24:LEU:HD21  | 2:B:110:ALA:HB1    | 2.01                     | 0.43              |
| 2:B:218:LEU:HD12 | 2:B:218:LEU:O      | 2.18                     | 0.43              |
| 3:C:361:PHE:CD1  | 3:C:361:PHE:C      | 2.92                     | 0.43              |
| 1:G:47:CYS:HG    | 1:G:114:LEU:HD23   | 1.77                     | 0.43              |
| 1:G:116:ILE:HG12 | 1:G:158:PHE:CD1    | 2.51                     | 0.43              |
| 1:G:202:VAL:O    | 1:G:206:PHE:N      | 2.47                     | 0.43              |
| 2:H:62:VAL:HG13  | 11:H:1486:CLA:O2D  | 2.18                     | 0.43              |
| 2:H:400:SER:HB3  | 2:H:410:THR:CB     | 2.28                     | 0.43              |
| 4:J:103:ARG:HA   | 4:J:106:GLN:HG3    | 2.01                     | 0.43              |
| 9:V:134:LYS:O    | 9:V:137:TYR:N      | 2.50                     | 0.43              |
| 10:X:56:UNK:O    | 10:X:59:UNK:N      | 2.50                     | 0.43              |
| 10:Y:200:UNK:O   | 10:Y:203:UNK:CB    | 2.66                     | 0.43              |
| 10:Y:265:UNK:O   | 10:Y:266:UNK:C     | 2.66                     | 0.43              |
| 1:A:37:MET:O     | 1:A:38:ILE:C       | 2.60                     | 0.43              |
| 2:B:29:LEU:HA    | 2:B:29:LEU:HD23    | 1.70                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:135:LEU:CD1    | 2:B:232:GLY:HA2    | 2.48                     | 0.43              |
| 2:B:277:SER:C      | 2:B:279:TYR:N      | 2.76                     | 0.43              |
| 2:B:464:PHE:CE1    | 4:D:144:ILE:HG23   | 2.53                     | 0.43              |
| 3:C:61:VAL:HG21    | 3:C:125:LEU:CD1    | 2.48                     | 0.43              |
| 3:C:188:THR:HG21   | 3:C:298:PRO:CA     | 2.48                     | 0.43              |
| 3:C:319:ILE:CD1    | 3:C:384:ILE:HD11   | 2.47                     | 0.43              |
| 4:D:117:HIS:NE2    | 11:D:1353:CLA:NA   | 2.66                     | 0.43              |
| 4:D:252:PHE:O      | 4:D:256:ILE:HG13   | 2.17                     | 0.43              |
| 1:G:172:MET:N      | 1:G:182:PHE:CD1    | 2.75                     | 0.43              |
| 1:G:300:PHE:CE2    | 11:I:1462:CLA:H93  | 2.54                     | 0.43              |
| 2:H:18:ARG:NH2     | 2:H:118:TRP:CE3    | 2.87                     | 0.43              |
| 2:H:68:ARG:NH2     | 11:H:1485:CLA:CED  | 2.82                     | 0.43              |
| 2:H:162:PHE:HB3    | 11:H:1487:CLA:HHD  | 2.00                     | 0.43              |
| 3:I:165:LEU:O      | 3:I:169:GLY:N      | 2.50                     | 0.43              |
| 3:I:282:MET:SD     | 11:I:1465:CLA:H42  | 2.57                     | 0.43              |
| 3:I:445:ALA:CB     | 11:I:1463:CLA:HED1 | 2.45                     | 0.43              |
| 4:J:59:TYR:N       | 4:J:59:TYR:CD1     | 2.87                     | 0.43              |
| 6:L:34:LEU:HD12    | 6:L:34:LEU:HA      | 1.84                     | 0.43              |
| 9:T:41:HIS:O       | 9:T:42:VAL:C       | 2.60                     | 0.43              |
| 10:X:59:UNK:O      | 10:X:62:UNK:N      | 2.50                     | 0.43              |
| 10:X:470:UNK:O     | 10:X:472:UNK:N     | 2.51                     | 0.43              |
| 1:A:38:ILE:CB      | 1:A:39:PRO:HD3     | 2.46                     | 0.43              |
| 1:A:116:ILE:HG12   | 1:A:158:PHE:HD1    | 1.82                     | 0.43              |
| 1:A:218:LEU:HD11   | 1:A:255:PHE:CD2    | 2.50                     | 0.43              |
| 1:A:320:ILE:HD11   | 4:D:63:LEU:HD21    | 2.01                     | 0.43              |
| 11:A:1344:CLA:HBB2 | 12:D:1352:PHO:H91  | 2.00                     | 0.43              |
| 2:B:16:PRO:O       | 2:B:17:GLY:C       | 2.58                     | 0.43              |
| 2:B:63:LEU:CB      | 2:B:64:PRO:CD      | 2.97                     | 0.43              |
| 2:B:68:ARG:HH22    | 11:B:1485:CLA:HED3 | 1.84                     | 0.43              |
| 2:B:92:SER:O       | 2:B:95:GLY:N       | 2.50                     | 0.43              |
| 2:B:214:LEU:C      | 2:B:217:ILE:HG22   | 2.43                     | 0.43              |
| 3:C:32:GLY:O       | 3:C:33:PHE:HB2     | 2.17                     | 0.43              |
| 3:C:271:TYR:O      | 3:C:274:TYR:HB2    | 2.19                     | 0.43              |
| 3:C:272:LEU:O      | 3:C:276:LEU:N      | 2.51                     | 0.43              |
| 5:E:35:TRP:O       | 5:E:35:TRP:CD1     | 2.72                     | 0.43              |
| 1:G:12:ASN:C       | 1:G:14:TRP:N       | 2.75                     | 0.43              |
| 1:G:84:PRO:HD3     | 1:G:173:PRO:HB3    | 2.00                     | 0.43              |
| 1:G:210:LEU:HD12   | 1:G:210:LEU:O      | 2.19                     | 0.43              |
| 2:H:18:ARG:NH2     | 2:H:118:TRP:CZ3    | 2.86                     | 0.43              |
| 2:H:63:LEU:CB      | 2:H:64:PRO:CD      | 2.96                     | 0.43              |
| 3:I:241:GLY:O      | 3:I:245:ILE:HG23   | 2.18                     | 0.43              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 3:I:271:TYR:O    | 3:I:272:LEU:C      | 2.60                     | 0.43              |
| 4:J:334:GLN:C    | 4:J:336:HIS:H      | 2.27                     | 0.43              |
| 5:K:34:GLY:O     | 5:K:38:VAL:HG23    | 2.19                     | 0.43              |
| 10:X:160:UNK:O   | 10:X:164:UNK:CB    | 2.66                     | 0.43              |
| 2:B:288:VAL:O    | 2:B:289:GLN:C      | 2.59                     | 0.43              |
| 2:B:458:PHE:HB3  | 11:B:1485:CLA:HMC1 | 2.00                     | 0.43              |
| 3:C:47:GLY:HA3   | 3:C:138:GLU:C      | 2.44                     | 0.43              |
| 3:C:47:GLY:O     | 3:C:48:LYS:C       | 2.61                     | 0.43              |
| 3:C:225:VAL:HA   | 3:C:289:PHE:CE1    | 2.54                     | 0.43              |
| 3:C:240:ILE:CD1  | 11:C:1465:CLA:H91  | 2.48                     | 0.43              |
| 3:C:286:ALA:HB2  | 11:C:1460:CLA:CMD  | 2.49                     | 0.43              |
| 3:C:318:LEU:HA   | 3:C:340:TYR:CD1    | 2.54                     | 0.43              |
| 3:C:376:ASP:O    | 3:C:377:LEU:C      | 2.60                     | 0.43              |
| 3:C:376:ASP:O    | 3:C:378:ASN:N      | 2.51                     | 0.43              |
| 4:D:91:LEU:HD13  | 4:D:93:TRP:CZ3     | 2.52                     | 0.43              |
| 4:D:336:HIS:C    | 4:D:336:HIS:ND1    | 2.76                     | 0.43              |
| 5:E:13:ILE:CG2   | 5:E:19:TYR:HD2     | 2.29                     | 0.43              |
| 6:F:37:ILE:C     | 6:F:39:ALA:N       | 2.75                     | 0.43              |
| 1:G:142:TRP:C    | 1:G:144:CYS:N      | 2.74                     | 0.43              |
| 1:G:160:ILE:HD12 | 3:I:431:PHE:CE1    | 2.49                     | 0.43              |
| 1:G:161:TYR:HA   | 1:G:294:ALA:HB1    | 2.00                     | 0.43              |
| 1:G:191:ASN:O    | 1:G:192:ILE:C      | 2.61                     | 0.43              |
| 1:G:311:GLY:O    | 1:G:312:ASN:C      | 2.62                     | 0.43              |
| 2:H:242:ILE:HD11 | 11:H:1492:CLA:HBB1 | 2.00                     | 0.43              |
| 3:I:90:PRO:O     | 3:I:93:ALA:HB3     | 2.19                     | 0.43              |
| 3:I:118:HIS:O    | 3:I:122:SER:OG     | 2.37                     | 0.43              |
| 3:I:177:ALA:O    | 3:I:178:LYS:C      | 2.60                     | 0.43              |
| 3:I:290:VAL:HA   | 3:I:297:TYR:CE2    | 2.54                     | 0.43              |
| 3:I:320:ARG:HH11 | 9:T:49:ASN:CG      | 2.26                     | 0.43              |
| 4:J:249:ALA:O    | 4:J:252:PHE:HB3    | 2.17                     | 0.43              |
| 4:J:286:VAL:C    | 4:J:288:GLY:N      | 2.68                     | 0.43              |
| 4:J:298:PHE:O    | 4:J:299:ILE:HB     | 2.19                     | 0.43              |
| 7:O:11:UNK:CA    | 7:O:173:UNK:CB     | 2.93                     | 0.43              |
| 2:B:332:LYS:O    | 2:B:440:ASP:N      | 2.52                     | 0.43              |
| 2:B:446:SER:O    | 2:B:447:PRO:C      | 2.59                     | 0.43              |
| 3:C:82:TYR:HB3   | 3:C:302:TYR:O      | 2.18                     | 0.43              |
| 3:C:421:SER:HA   | 3:C:422:PRO:HD3    | 1.81                     | 0.43              |
| 4:D:56:THR:H     | 5:E:49:THR:HG22    | 1.82                     | 0.43              |
| 4:D:154:VAL:O    | 4:D:159:ILE:HG13   | 2.18                     | 0.43              |
| 5:E:10:PHE:CE2   | 6:F:19:ARG:NH2     | 2.87                     | 0.43              |
| 6:F:24:HIS:HA    | 6:F:27:ALA:HB3     | 1.99                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:G:105:TRP:CZ3    | 1:G:111:PRO:HG3    | 2.54                     | 0.43              |
| 1:G:222:SER:O      | 1:G:246:TYR:HB2    | 2.19                     | 0.43              |
| 2:H:424:ALA:C      | 2:H:426:PHE:N      | 2.77                     | 0.43              |
| 2:H:450:TRP:O      | 2:H:451:PHE:C      | 2.62                     | 0.43              |
| 3:I:38:GLY:HA3     | 11:I:1469:CLA:C2D  | 2.49                     | 0.43              |
| 3:I:85:GLY:N       | 3:I:419:PHE:CE2    | 2.87                     | 0.43              |
| 3:I:264:PHE:N      | 3:I:264:PHE:CD2    | 2.87                     | 0.43              |
| 4:J:127:LEU:O      | 4:J:130:PHE:N      | 2.51                     | 0.43              |
| 4:J:190:ASN:ND2    | 4:J:193:LEU:HD12   | 2.34                     | 0.43              |
| 6:L:33:PHE:HB2     | 17:L:1047:BCR:H363 | 2.00                     | 0.43              |
| 8:U:57:UNK:O       | 8:U:59:UNK:N       | 2.52                     | 0.43              |
| 10:Y:580:UNK:O     | 10:Y:581:UNK:C     | 2.66                     | 0.43              |
| 1:A:183:MET:HE2    | 11:A:1343:CLA:CAC  | 2.48                     | 0.43              |
| 1:A:214:MET:O      | 1:A:217:SER:HB3    | 2.19                     | 0.43              |
| 1:A:272:HIS:HD2    | 4:D:218:VAL:HG21   | 1.73                     | 0.43              |
| 2:B:279:TYR:O      | 2:B:281:GLN:N      | 2.51                     | 0.43              |
| 2:B:419:SER:OG     | 2:B:420:TYR:N      | 2.51                     | 0.43              |
| 3:C:27:ASP:O       | 3:C:31:SER:HB2     | 2.19                     | 0.43              |
| 4:D:279:LEU:HD22   | 11:D:1351:CLA:HBA2 | 2.01                     | 0.43              |
| 5:E:15:THR:O       | 5:E:15:THR:CG2     | 2.66                     | 0.43              |
| 6:F:14:PRO:O       | 6:F:15:ILE:HB      | 2.18                     | 0.43              |
| 1:G:44:ALA:O       | 1:G:45:THR:C       | 2.61                     | 0.43              |
| 1:G:119:PHE:CD2    | 12:G:1345:PHO:H111 | 2.54                     | 0.43              |
| 2:H:64:PRO:HB3     | 2:H:268:PHE:CZ     | 2.53                     | 0.43              |
| 3:I:187:ASP:OD1    | 3:I:187:ASP:C      | 2.62                     | 0.43              |
| 4:J:46:GLY:O       | 4:J:48:TRP:N       | 2.52                     | 0.43              |
| 4:J:51:GLY:O       | 4:J:52:THR:C       | 2.60                     | 0.43              |
| 6:L:11:VAL:HG12    | 6:L:12:SER:N       | 2.34                     | 0.43              |
| 8:U:77:UNK:C       | 8:U:79:UNK:N       | 2.80                     | 0.43              |
| 1:A:8:ARG:N        | 1:A:11:ALA:CB      | 2.80                     | 0.43              |
| 2:B:71:VAL:CG1     | 2:B:93:PHE:H       | 2.32                     | 0.43              |
| 2:B:94:GLU:O       | 2:B:97:ALA:HB3     | 2.19                     | 0.43              |
| 3:C:63:TRP:O       | 3:C:64:ALA:C       | 2.61                     | 0.43              |
| 3:C:188:THR:HG21   | 3:C:298:PRO:HA     | 2.00                     | 0.43              |
| 3:C:282:MET:HE1    | 11:C:1465:CLA:C4   | 2.48                     | 0.43              |
| 3:C:309:ALA:C      | 3:C:311:GLN:N      | 2.75                     | 0.43              |
| 3:C:425:TRP:CZ2    | 11:C:1462:CLA:O1A  | 2.72                     | 0.43              |
| 4:D:228:GLY:O      | 4:D:229:ALA:HB3    | 2.19                     | 0.43              |
| 1:G:75:ASN:HD22    | 1:G:75:ASN:HA      | 1.59                     | 0.43              |
| 1:G:131:TRP:CE3    | 1:G:132:GLU:N      | 2.86                     | 0.43              |
| 11:G:1342:CLA:HBB1 | 11:J:1351:CLA:NC   | 2.33                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:H:70:GLY:HA2     | 2:H:178:VAL:HG11   | 2.00                     | 0.43              |
| 3:I:75:PHE:CE1     | 3:I:76:ILE:O       | 2.72                     | 0.43              |
| 3:I:265:ILE:N      | 3:I:274:TYR:OH     | 2.47                     | 0.43              |
| 4:J:246:MET:O      | 4:J:249:ALA:HB3    | 2.19                     | 0.43              |
| 4:J:272:LEU:HD21   | 4:J:276:VAL:HG21   | 2.00                     | 0.43              |
| 18:T:1138:HEC:HAD2 | 18:T:1138:HEC:HHA  | 1.60                     | 0.43              |
| 1:A:180:PHE:CZ     | 4:D:192:THR:HB     | 2.54                     | 0.43              |
| 2:B:21:ALA:O       | 2:B:22:ALA:C       | 2.62                     | 0.43              |
| 3:C:237:HIS:O      | 3:C:238:ILE:C      | 2.62                     | 0.43              |
| 4:D:111:TRP:O      | 4:D:113:PHE:N      | 2.52                     | 0.43              |
| 4:D:190:ASN:HD22   | 4:D:193:LEU:HD12   | 1.84                     | 0.43              |
| 4:D:213:ILE:O      | 4:D:216:ALA:N      | 2.52                     | 0.43              |
| 1:G:84:PRO:C       | 1:G:85:SER:O       | 2.62                     | 0.43              |
| 1:G:187:GLN:CB     | 11:G:1342:CLA:HAC2 | 2.43                     | 0.43              |
| 2:H:96:VAL:O       | 2:H:99:ALA:HB3     | 2.19                     | 0.43              |
| 4:J:160:TYR:CB     | 4:J:161:PRO:HD3    | 2.34                     | 0.43              |
| 8:U:51:UNK:O       | 8:U:52:UNK:O       | 2.37                     | 0.43              |
| 9:V:13:ASN:HB2     | 9:V:15:GLU:OE1     | 2.19                     | 0.43              |
| 10:X:116:UNK:O     | 10:X:117:UNK:C     | 2.67                     | 0.43              |
| 1:A:211:PHE:CE2    | 1:A:274:PHE:CE2    | 3.06                     | 0.42              |
| 2:B:158:LEU:CB     | 2:B:199:VAL:HG22   | 2.48                     | 0.42              |
| 2:B:348:ASN:C      | 2:B:350:GLU:H      | 2.27                     | 0.42              |
| 3:C:35:TRP:CE2     | 3:C:36:TRP:CD1     | 2.96                     | 0.42              |
| 3:C:178:LYS:C      | 3:C:178:LYS:CD     | 2.88                     | 0.42              |
| 3:C:280:SER:O      | 3:C:434:ALA:HB1    | 2.19                     | 0.42              |
| 3:C:374:GLY:O      | 3:C:375:LEU:HB2    | 2.19                     | 0.42              |
| 6:F:33:PHE:HB2     | 17:F:1046:BCR:H363 | 2.00                     | 0.42              |
| 1:G:184:ILE:O      | 1:G:185:VAL:C      | 2.61                     | 0.42              |
| 1:G:210:LEU:HD13   | 12:J:1352:PHO:C1D  | 2.48                     | 0.42              |
| 2:H:36:SER:O       | 2:H:37:MET:C       | 2.61                     | 0.42              |
| 2:H:139:PHE:O      | 2:H:139:PHE:CD1    | 2.71                     | 0.42              |
| 2:H:347:ARG:O      | 2:H:396:GLY:HA2    | 2.19                     | 0.42              |
| 2:H:407:ASN:O      | 2:H:408:GLY:O      | 2.37                     | 0.42              |
| 2:H:466:HIS:O      | 2:H:468:TRP:N      | 2.52                     | 0.42              |
| 3:I:170:ILE:CG2    | 3:I:171:GLY:H      | 2.33                     | 0.42              |
| 9:T:133:GLY:O      | 9:T:137:TYR:N      | 2.51                     | 0.42              |
| 10:X:516:UNK:O     | 10:X:517:UNK:C     | 2.67                     | 0.42              |
| 1:A:93:PHE:CE1     | 1:A:95:PRO:HG2     | 2.54                     | 0.42              |
| 1:A:95:PRO:O       | 1:A:105:TRP:NE1    | 2.52                     | 0.42              |
| 1:A:151:LEU:O      | 1:A:152:ALA:C      | 2.61                     | 0.42              |
| 1:A:323:ARG:O      | 1:A:326:LEU:HB2    | 2.19                     | 0.42              |

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| Atom-1          | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|--------------------|--------------------------|-------------------|
| 3:C:269:GLU:OE1 | 3:C:447:ARG:HD3    | 2.19                     | 0.42              |
| 3:C:284:PHE:C   | 3:C:286:ALA:N      | 2.76                     | 0.42              |
| 3:C:322:GLN:NE2 | 3:C:381:LYS:HA     | 2.34                     | 0.42              |
| 4:D:16:ASP:C    | 4:D:18:LEU:N       | 2.77                     | 0.42              |
| 4:D:93:TRP:HA   | 4:D:97:ALA:HB2     | 2.00                     | 0.42              |
| 4:D:98:GLN:O    | 4:D:99:GLY:C       | 2.63                     | 0.42              |
| 5:E:23:HIS:C    | 5:E:25:ILE:N       | 2.74                     | 0.42              |
| 1:G:192:ILE:O   | 1:G:194:MET:N      | 2.52                     | 0.42              |
| 1:G:290:ILE:O   | 1:G:291:SER:C      | 2.60                     | 0.42              |
| 2:H:25:MET:HE1  | 2:H:108:PHE:CE1    | 2.54                     | 0.42              |
| 2:H:395:GLN:CB  | 2:H:397:VAL:CB     | 2.97                     | 0.42              |
| 2:H:412:THR:O   | 2:H:413:ASP:C      | 2.62                     | 0.42              |
| 2:H:458:PHE:HB3 | 11:H:1485:CLA:HMC1 | 2.00                     | 0.42              |
| 3:I:32:GLY:C    | 3:I:34:ALA:H       | 2.26                     | 0.42              |
| 3:I:85:GLY:N    | 3:I:419:PHE:HE2    | 2.18                     | 0.42              |
| 3:I:89:ILE:HB   | 3:I:90:PRO:CD      | 2.42                     | 0.42              |
| 3:I:172:ALA:O   | 3:I:173:LEU:C      | 2.62                     | 0.42              |
| 3:I:428:THR:H   | 3:I:428:THR:HG1    | 1.55                     | 0.42              |
| 4:J:272:LEU:C   | 4:J:272:LEU:CD2    | 2.90                     | 0.42              |
| 4:J:296:TYR:CZ  | 4:J:319:LEU:CD2    | 3.02                     | 0.42              |
| 7:P:86:UNK:O    | 7:P:87:UNK:CB      | 2.67                     | 0.42              |
| 9:V:41:HIS:HA   | 9:V:45:ILE:O       | 2.18                     | 0.42              |
| 10:X:412:UNK:O  | 10:X:414:UNK:N     | 2.52                     | 0.42              |
| 10:Y:266:UNK:O  | 10:Y:267:UNK:C     | 2.67                     | 0.42              |
| 1:A:95:PRO:HB3  | 11:A:1346:CLA:OBD  | 2.19                     | 0.42              |
| 1:A:204:GLY:HA3 | 1:A:282:GLY:HA3    | 2.00                     | 0.42              |
| 1:A:222:SER:O   | 1:A:246:TYR:O      | 2.37                     | 0.42              |
| 3:C:56:HIS:O    | 3:C:59:LEU:CB      | 2.67                     | 0.42              |
| 3:C:80:PRO:HB2  | 3:C:83:GLU:HB3     | 2.00                     | 0.42              |
| 3:C:178:LYS:O   | 3:C:182:PHE:HB2    | 2.19                     | 0.42              |
| 4:D:59:TYR:N    | 4:D:59:TYR:CD1     | 2.85                     | 0.42              |
| 4:D:161:PRO:HG2 | 4:D:170:ALA:HB2    | 2.02                     | 0.42              |
| 4:D:217:THR:O   | 4:D:218:VAL:C      | 2.62                     | 0.42              |
| 1:G:244:GLU:OE2 | 4:J:264:LYS:NZ     | 2.52                     | 0.42              |
| 2:H:275:TRP:HZ2 | 2:H:359:MET:O      | 2.03                     | 0.42              |
| 2:H:277:SER:C   | 2:H:279:TYR:N      | 2.76                     | 0.42              |
| 2:H:314:TYR:N   | 2:H:427:GLY:HA3    | 2.35                     | 0.42              |
| 2:H:332:LYS:O   | 2:H:440:ASP:N      | 2.52                     | 0.42              |
| 2:H:357:ARG:NH1 | 4:J:338:ASN:O      | 2.52                     | 0.42              |
| 3:I:272:LEU:O   | 3:I:276:LEU:N      | 2.52                     | 0.42              |
| 5:K:23:HIS:C    | 5:K:25:ILE:N       | 2.75                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:P:63:UNK:O      | 7:P:72:UNK:N       | 2.53                     | 0.42              |
| 10:X:531:UNK:O    | 10:X:532:UNK:C     | 2.66                     | 0.42              |
| 10:Y:52:UNK:O     | 10:Y:53:UNK:C      | 2.66                     | 0.42              |
| 10:Y:507:UNK:C    | 10:Y:509:UNK:N     | 2.80                     | 0.42              |
| 1:A:220:THR:C     | 1:A:222:SER:N      | 2.76                     | 0.42              |
| 1:A:258:LEU:CD1   | 4:D:128:ARG:CZ     | 2.95                     | 0.42              |
| 2:B:242:ILE:HD11  | 11:B:1492:CLA:HBB1 | 2.00                     | 0.42              |
| 2:B:425:ILE:HG23  | 2:B:426:PHE:CD2    | 2.54                     | 0.42              |
| 3:C:33:PHE:CZ     | 3:C:40:ALA:HB1     | 2.54                     | 0.42              |
| 3:C:186:TYR:CE2   | 3:C:188:THR:HG23   | 2.49                     | 0.42              |
| 3:C:226:SER:O     | 3:C:227:VAL:C      | 2.62                     | 0.42              |
| 3:C:420:VAL:HG12  | 3:C:421:SER:N      | 2.35                     | 0.42              |
| 4:D:43:LEU:O      | 4:D:113:PHE:HE1    | 2.03                     | 0.42              |
| 5:E:30:LEU:HD13   | 6:F:28:VAL:HG13    | 2.01                     | 0.42              |
| 5:E:58:GLN:NE2    | 9:V:4:THR:OG1      | 2.53                     | 0.42              |
| 6:F:23:VAL:O      | 6:F:23:VAL:HG12    | 2.19                     | 0.42              |
| 1:G:41:LEU:HD13   | 12:G:1345:PHO:C2   | 2.50                     | 0.42              |
| 2:H:195:PRO:O     | 2:H:197:GLY:N      | 2.52                     | 0.42              |
| 2:H:214:LEU:HG    | 2:H:215:PHE:H      | 1.85                     | 0.42              |
| 3:I:88:LEU:C      | 3:I:90:PRO:HD2     | 2.45                     | 0.42              |
| 3:I:264:PHE:CE2   | 11:I:1464:CLA:HBA1 | 2.53                     | 0.42              |
| 4:J:200:GLY:HA3   | 4:J:282:SER:HB3    | 2.02                     | 0.42              |
| 10:X:215:UNK:O    | 10:X:219:UNK:N     | 2.52                     | 0.42              |
| 10:Y:563:UNK:O    | 10:Y:564:UNK:C     | 2.68                     | 0.42              |
| 12:A:1345:PHO:HAB | 4:D:205:LEU:HD21   | 2.01                     | 0.42              |
| 2:B:214:LEU:HD12  | 2:B:215:PHE:N      | 2.34                     | 0.42              |
| 3:C:129:GLY:C     | 3:C:131:TYR:H      | 2.26                     | 0.42              |
| 3:C:163:PHE:CE2   | 3:C:252:ILE:HD13   | 2.53                     | 0.42              |
| 3:C:269:GLU:OE2   | 3:C:447:ARG:NH1    | 2.52                     | 0.42              |
| 3:C:445:ALA:HB1   | 11:C:1463:CLA:CED  | 2.41                     | 0.42              |
| 2:H:65:PHE:C      | 2:H:67:ALA:N       | 2.75                     | 0.42              |
| 2:H:135:LEU:O     | 2:H:137:LYS:N      | 2.52                     | 0.42              |
| 2:H:452:THR:O     | 2:H:452:THR:CG2    | 2.65                     | 0.42              |
| 3:I:113:VAL:O     | 3:I:116:VAL:HG22   | 2.19                     | 0.42              |
| 3:I:125:LEU:O     | 3:I:126:GLY:C      | 2.62                     | 0.42              |
| 3:I:185:LEU:O     | 3:I:186:TYR:C      | 2.62                     | 0.42              |
| 3:I:309:ALA:C     | 3:I:311:GLN:N      | 2.75                     | 0.42              |
| 4:J:98:GLN:O      | 4:J:99:GLY:C       | 2.61                     | 0.42              |
| 4:J:223:PHE:HD2   | 4:J:243:THR:O      | 2.03                     | 0.42              |
| 4:J:244:TYR:HB2   | 4:J:245:SER:H      | 1.66                     | 0.42              |
| 5:K:82:GLN:C      | 5:K:84:LYS:N       | 2.77                     | 0.42              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 6:L:9:GLU:N      | 6:L:10:PRO:HD2     | 2.34                     | 0.42              |
| 9:V:30:LYS:O     | 9:V:34:GLN:HG3     | 2.20                     | 0.42              |
| 9:V:40:CYS:SG    | 9:V:40:CYS:O       | 2.77                     | 0.42              |
| 1:A:102:LEU:O    | 1:A:105:TRP:HB3    | 2.20                     | 0.42              |
| 1:A:327:GLY:O    | 4:D:324:GLY:HA3    | 2.19                     | 0.42              |
| 2:B:248:ALA:O    | 2:B:251:VAL:CG2    | 2.63                     | 0.42              |
| 2:B:412:THR:O    | 2:B:413:ASP:C      | 2.62                     | 0.42              |
| 2:B:464:PHE:HD2  | 11:B:1492:CLA:HAC2 | 1.84                     | 0.42              |
| 2:B:468:TRP:CD1  | 4:D:144:ILE:CD1    | 2.99                     | 0.42              |
| 3:C:97:TRP:O     | 3:C:98:GLY:C       | 2.62                     | 0.42              |
| 3:C:187:ASP:C    | 3:C:189:TRP:H      | 2.28                     | 0.42              |
| 4:D:93:TRP:N     | 4:D:93:TRP:CD1     | 2.86                     | 0.42              |
| 4:D:193:LEU:HD11 | 4:D:315:TYR:HE2    | 1.83                     | 0.42              |
| 4:D:223:PHE:HB3  | 4:D:225:ASP:OD1    | 2.20                     | 0.42              |
| 6:F:18:VAL:O     | 6:F:19:ARG:C       | 2.61                     | 0.42              |
| 1:G:13:LEU:O     | 1:G:14:TRP:C       | 2.62                     | 0.42              |
| 1:G:167:SER:C    | 1:G:169:SER:N      | 2.76                     | 0.42              |
| 1:G:283:VAL:O    | 1:G:284:TRP:C      | 2.62                     | 0.42              |
| 2:H:47:PRO:O     | 2:H:48:SER:C       | 2.62                     | 0.42              |
| 2:H:176:GLY:O    | 2:H:177:SER:HB3    | 2.19                     | 0.42              |
| 2:H:263:THR:HG22 | 2:H:448:ARG:NH2    | 2.34                     | 0.42              |
| 2:H:425:ILE:HG23 | 2:H:426:PHE:CD2    | 2.52                     | 0.42              |
| 4:J:32:TRP:O     | 4:J:33:SER:C       | 2.61                     | 0.42              |
| 4:J:64:ALA:HB1   | 4:J:69:GLU:HB3     | 2.00                     | 0.42              |
| 4:J:191:TRP:CZ3  | 4:J:194:ASN:ND2    | 2.85                     | 0.42              |
| 7:P:123:UNK:O    | 7:P:126:UNK:N      | 2.53                     | 0.42              |
| 10:X:365:UNK:O   | 10:X:366:UNK:C     | 2.63                     | 0.42              |
| 1:A:120:LEU:C    | 1:A:122:GLY:N      | 2.77                     | 0.42              |
| 1:A:134:SER:HA   | 1:A:139:MET:CB     | 2.47                     | 0.42              |
| 2:B:151:PHE:O    | 2:B:152:GLY:C      | 2.62                     | 0.42              |
| 2:B:330:MET:O    | 2:B:331:ASN:CB     | 2.68                     | 0.42              |
| 3:C:43:ILE:HA    | 11:C:1467:CLA:HMC3 | 2.02                     | 0.42              |
| 3:C:51:GLY:HA2   | 3:C:54:VAL:CG2     | 2.50                     | 0.42              |
| 4:D:194:ASN:HA   | 4:D:195:PRO:HD3    | 1.84                     | 0.42              |
| 1:G:116:ILE:HD13 | 1:G:158:PHE:HB3    | 2.01                     | 0.42              |
| 1:G:134:SER:C    | 1:G:136:ARG:N      | 2.74                     | 0.42              |
| 1:G:176:ILE:CG2  | 1:G:180:PHE:CE1    | 3.02                     | 0.42              |
| 1:G:195:HIS:CE1  | 1:G:197:PHE:CD1    | 3.06                     | 0.42              |
| 2:H:69:LEU:HD23  | 11:H:1487:CLA:HMA2 | 2.01                     | 0.42              |
| 2:H:236:THR:N    | 2:H:473:THR:OG1    | 2.52                     | 0.42              |
| 3:I:450:ALA:HB1  | 3:I:455:PHE:HB2    | 2.02                     | 0.42              |

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| Atom-1          | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|--------------------|--------------------------|-------------------|
| 4:J:235:PHE:CZ  | 4:J:237:PRO:HA     | 2.55                     | 0.42              |
| 5:K:13:ILE:CG2  | 5:K:19:TYR:HD2     | 2.28                     | 0.42              |
| 8:U:31:UNK:O    | 8:U:33:UNK:N       | 2.53                     | 0.42              |
| 10:X:71:UNK:O   | 10:X:72:UNK:C      | 2.67                     | 0.42              |
| 10:X:507:UNK:C  | 10:X:509:UNK:N     | 2.83                     | 0.42              |
| 1:A:143:ILE:CA  | 4:D:220:ASN:ND2    | 2.83                     | 0.42              |
| 1:A:310:LYS:HZ1 | 5:E:58:GLN:HG2     | 1.84                     | 0.42              |
| 2:B:69:LEU:HD23 | 11:B:1487:CLA:HMA2 | 2.02                     | 0.42              |
| 2:B:362:PHE:CE2 | 4:D:184:PHE:CZ     | 3.00                     | 0.42              |
| 2:B:401:PHE:CD1 | 2:B:401:PHE:N      | 2.87                     | 0.42              |
| 2:B:464:PHE:HE1 | 4:D:144:ILE:HG23   | 1.85                     | 0.42              |
| 3:C:50:LEU:O    | 3:C:54:VAL:N       | 2.50                     | 0.42              |
| 3:C:50:LEU:C    | 3:C:54:VAL:HG23    | 2.45                     | 0.42              |
| 3:C:165:LEU:O   | 3:C:169:GLY:N      | 2.51                     | 0.42              |
| 3:C:172:ALA:N   | 11:C:1459:CLA:CAC  | 2.83                     | 0.42              |
| 3:C:187:ASP:CB  | 3:C:230:LEU:CD2    | 2.94                     | 0.42              |
| 3:C:225:VAL:O   | 3:C:225:VAL:CG1    | 2.64                     | 0.42              |
| 4:D:288:GLY:C   | 4:D:290:ALA:H      | 2.26                     | 0.42              |
| 5:E:27:ILE:HB   | 5:E:28:PRO:CD      | 2.45                     | 0.42              |
| 1:G:187:GLN:NE2 | 1:G:325:ASN:OD1    | 2.53                     | 0.42              |
| 3:I:107:ASP:O   | 3:I:110:PRO:CD     | 2.52                     | 0.42              |
| 4:J:148:ALA:CB  | 4:J:276:VAL:HA     | 2.50                     | 0.42              |
| 5:K:10:PHE:CE2  | 6:L:19:ARG:NH2     | 2.88                     | 0.42              |
| 5:K:58:GLN:NE2  | 9:T:2:GLU:O        | 2.53                     | 0.42              |
| 7:O:75:UNK:O    | 7:O:77:UNK:N       | 2.53                     | 0.42              |
| 10:X:266:UNK:O  | 10:X:268:UNK:N     | 2.53                     | 0.42              |
| 10:Y:16:UNK:O   | 10:Y:17:UNK:C      | 2.64                     | 0.42              |
| 10:Y:213:UNK:O  | 10:Y:214:UNK:C     | 2.67                     | 0.42              |
| 1:A:81:ALA:CB   | 1:A:174:LEU:O      | 2.56                     | 0.42              |
| 1:A:133:LEU:HB2 | 4:D:252:PHE:HE2    | 1.85                     | 0.42              |
| 2:B:30:VAL:HB   | 11:B:1486:CLA:HAC1 | 2.02                     | 0.42              |
| 2:B:167:TRP:HA  | 2:B:177:SER:O      | 2.19                     | 0.42              |
| 2:B:369:ILE:O   | 2:B:379:ALA:O      | 2.38                     | 0.42              |
| 3:C:41:ARG:NH1  | 11:C:1469:CLA:OBD  | 2.50                     | 0.42              |
| 3:C:95:LEU:HD12 | 3:C:95:LEU:HA      | 1.89                     | 0.42              |
| 3:C:367:GLU:HB2 | 3:C:368:PRO:CD     | 2.50                     | 0.42              |
| 4:D:92:LEU:C    | 4:D:93:TRP:CD1     | 2.98                     | 0.42              |
| 4:D:193:LEU:HB3 | 4:D:295:SER:HB3    | 2.02                     | 0.42              |
| 4:D:200:GLY:O   | 4:D:203:GLY:N      | 2.52                     | 0.42              |
| 1:G:83:VAL:HA   | 1:G:84:PRO:HD3     | 1.87                     | 0.42              |
| 1:G:244:GLU:HG3 | 1:G:245:THR:H      | 1.85                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:G:323:ARG:O      | 1:G:326:LEU:HB2   | 2.20                     | 0.42              |
| 2:H:167:TRP:CH2    | 2:H:177:SER:HA    | 2.55                     | 0.42              |
| 3:I:239:TRP:O      | 3:I:243:ILE:N     | 2.37                     | 0.42              |
| 3:I:305:THR:O      | 3:I:307:PRO:N     | 2.53                     | 0.42              |
| 3:I:315:MET:O      | 3:I:319:ILE:CB    | 2.68                     | 0.42              |
| 4:J:128:ARG:O      | 4:J:128:ARG:HG2   | 2.18                     | 0.42              |
| 4:J:213:ILE:O      | 4:J:216:ALA:N     | 2.53                     | 0.42              |
| 7:P:75:UNK:O       | 7:P:77:UNK:N      | 2.53                     | 0.42              |
| 9:T:106:ASN:N      | 9:T:106:ASN:HD22  | 2.18                     | 0.42              |
| 10:Y:9:UNK:O       | 10:Y:10:UNK:C     | 2.67                     | 0.42              |
| 10:Y:253:UNK:C     | 10:Y:255:UNK:N    | 2.82                     | 0.42              |
| 10:Y:405:UNK:O     | 10:Y:408:UNK:N    | 2.53                     | 0.42              |
| 10:Y:463:UNK:O     | 10:Y:464:UNK:C    | 2.68                     | 0.42              |
| 1:A:167:SER:OG     | 1:A:169:SER:CB    | 2.68                     | 0.42              |
| 1:A:330:VAL:HG21   | 4:D:328:TRP:CH2   | 2.55                     | 0.42              |
| 11:A:1344:CLA:HBC3 | 4:D:178:ILE:HG23  | 2.02                     | 0.42              |
| 2:B:18:ARG:NH2     | 2:B:115:TRP:O     | 2.52                     | 0.42              |
| 2:B:35:GLY:O       | 2:B:38:ALA:HB3    | 2.20                     | 0.42              |
| 2:B:240:SER:HB3    | 11:B:1491:CLA:C4B | 2.50                     | 0.42              |
| 2:B:466:HIS:O      | 2:B:467:ILE:C     | 2.63                     | 0.42              |
| 3:C:73:ALA:HB3     | 3:C:74:HIS:CD2    | 2.50                     | 0.42              |
| 4:D:63:LEU:CD1     | 4:D:63:LEU:N      | 2.80                     | 0.42              |
| 4:D:161:PRO:CG     | 4:D:170:ALA:HB2   | 2.50                     | 0.42              |
| 4:D:288:GLY:C      | 4:D:290:ALA:N     | 2.73                     | 0.42              |
| 1:G:150:PRO:HB3    | 11:G:1342:CLA:H62 | 2.01                     | 0.42              |
| 2:H:37:MET:HG2     | 2:H:62:VAL:HG21   | 2.01                     | 0.42              |
| 2:H:164:PRO:CB     | 11:H:1487:CLA:O1D | 2.68                     | 0.42              |
| 3:I:75:PHE:CE2     | 3:I:77:PRO:HG3    | 2.55                     | 0.42              |
| 3:I:373:ASN:OD1    | 3:I:373:ASN:N     | 2.53                     | 0.42              |
| 4:J:100:ASP:CB     | 4:J:103:ARG:H     | 2.33                     | 0.42              |
| 4:J:190:ASN:HD22   | 4:J:193:LEU:HD12  | 1.83                     | 0.42              |
| 5:K:19:TYR:HE2     | 16:L:1046:HEM:C2A | 2.38                     | 0.42              |
| 8:U:9:UNK:O        | 8:U:10:UNK:C      | 2.62                     | 0.42              |
| 10:X:224:UNK:O     | 10:X:225:UNK:C    | 2.68                     | 0.42              |
| 10:X:272:UNK:C     | 10:X:274:UNK:N    | 2.82                     | 0.42              |
| 10:Y:182:UNK:O     | 10:Y:183:UNK:C    | 2.67                     | 0.42              |
| 1:A:65:GLU:O       | 1:A:65:GLU:HG2    | 2.19                     | 0.41              |
| 3:C:299:SER:C      | 3:C:301:PHE:N     | 2.71                     | 0.41              |
| 4:D:54:PHE:HE1     | 6:F:33:PHE:CE2    | 2.38                     | 0.41              |
| 6:F:18:VAL:HA      | 6:F:21:VAL:HG23   | 2.02                     | 0.41              |
| 1:G:193:LEU:HD22   | 4:J:179:PHE:CD1   | 2.55                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:G:256:GLY:HA2   | 1:G:260:PHE:O      | 2.20                     | 0.41              |
| 2:H:174:LEU:C     | 2:H:175:THR:O      | 2.63                     | 0.41              |
| 11:H:1492:CLA:CMA | 11:H:1493:CLA:HBC2 | 2.49                     | 0.41              |
| 11:I:1463:CLA:CMD | 11:I:1465:CLA:HAB  | 2.50                     | 0.41              |
| 4:J:337:GLU:HG3   | 4:J:339:PHE:CE2    | 2.53                     | 0.41              |
| 5:K:19:TYR:HD1    | 5:K:20:TRP:N       | 2.18                     | 0.41              |
| 9:T:63:THR:O      | 9:T:84:GLY:HA3     | 2.20                     | 0.41              |
| 10:X:204:UNK:O    | 10:X:205:UNK:C     | 2.68                     | 0.41              |
| 1:A:21:VAL:O      | 1:A:24:THR:CB      | 2.68                     | 0.41              |
| 1:A:93:PHE:CZ     | 1:A:95:PRO:HG3     | 2.55                     | 0.41              |
| 2:B:468:TRP:HD1   | 4:D:144:ILE:CD1    | 2.34                     | 0.41              |
| 3:C:51:GLY:HA2    | 3:C:54:VAL:HB      | 2.01                     | 0.41              |
| 3:C:188:THR:HG22  | 3:C:300:GLU:CD     | 2.45                     | 0.41              |
| 4:D:20:ASP:O      | 4:D:21:TRP:C       | 2.63                     | 0.41              |
| 4:D:191:TRP:HZ2   | 4:D:286:VAL:CG2    | 2.32                     | 0.41              |
| 4:D:197:HIS:O     | 4:D:198:MET:C      | 2.63                     | 0.41              |
| 4:D:320:LEU:HA    | 4:D:320:LEU:HD23   | 1.78                     | 0.41              |
| 1:G:84:PRO:HD3    | 1:G:173:PRO:CB     | 2.50                     | 0.41              |
| 1:G:110:GLY:N     | 1:G:111:PRO:CD     | 2.82                     | 0.41              |
| 1:G:152:ALA:O     | 1:G:155:PHE:N      | 2.53                     | 0.41              |
| 1:G:290:ILE:CD1   | 11:G:1342:CLA:OBD  | 2.63                     | 0.41              |
| 1:G:323:ARG:HA    | 1:G:326:LEU:HD12   | 2.01                     | 0.41              |
| 2:H:62:VAL:CG1    | 2:H:66:MET:HE2     | 2.44                     | 0.41              |
| 2:H:201:HIS:CD2   | 2:H:201:HIS:C      | 2.96                     | 0.41              |
| 2:H:316:GLY:CA    | 2:H:443:PHE:CE1    | 3.04                     | 0.41              |
| 2:H:414:PRO:HB2   | 2:H:415:PRO:CD     | 2.41                     | 0.41              |
| 3:I:122:SER:O     | 3:I:126:GLY:N      | 2.48                     | 0.41              |
| 3:I:129:GLY:C     | 3:I:131:TYR:N      | 2.74                     | 0.41              |
| 4:J:100:ASP:CB    | 4:J:103:ARG:HB2    | 2.50                     | 0.41              |
| 4:J:191:TRP:CE3   | 4:J:289:LEU:HD11   | 2.55                     | 0.41              |
| 4:J:199:MET:O     | 4:J:202:ALA:N      | 2.53                     | 0.41              |
| 4:J:235:PHE:HD2   | 4:J:243:THR:HG21   | 1.83                     | 0.41              |
| 6:L:36:ALA:O      | 6:L:40:MET:HG3     | 2.21                     | 0.41              |
| 8:S:69:UNK:O      | 8:S:71:UNK:N       | 2.53                     | 0.41              |
| 10:X:578:UNK:O    | 10:X:580:UNK:N     | 2.54                     | 0.41              |
| 10:Y:470:UNK:O    | 10:Y:471:UNK:C     | 2.68                     | 0.41              |
| 1:A:192:ILE:O     | 1:A:194:MET:N      | 2.53                     | 0.41              |
| 2:B:18:ARG:O      | 2:B:19:LEU:C       | 2.59                     | 0.41              |
| 2:B:94:GLU:HG3    | 2:B:95:GLY:H       | 1.79                     | 0.41              |
| 3:C:244:CYS:HA    | 11:C:1464:CLA:HMC1 | 2.02                     | 0.41              |
| 3:C:267:SER:O     | 3:C:268:GLY:C      | 2.62                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:C:394:GLU:O      | 3:C:395:TYR:C      | 2.63                     | 0.41              |
| 4:D:10:ALA:O       | 4:D:11:GLU:CB      | 2.67                     | 0.41              |
| 1:G:102:LEU:O      | 1:G:105:TRP:HB3    | 2.20                     | 0.41              |
| 1:G:151:LEU:O      | 1:G:152:ALA:C      | 2.61                     | 0.41              |
| 1:G:157:VAL:HG21   | 11:G:1343:CLA:CMC  | 2.49                     | 0.41              |
| 2:H:21:ALA:O       | 2:H:22:ALA:C       | 2.64                     | 0.41              |
| 2:H:236:THR:HG23   | 2:H:237:VAL:N      | 2.34                     | 0.41              |
| 2:H:366:PHE:HD2    | 2:H:425:ILE:HD11   | 1.86                     | 0.41              |
| 3:I:276:LEU:HD13   | 3:I:276:LEU:HA     | 1.86                     | 0.41              |
| 11:I:1465:CLA:HBA1 | 11:I:1465:CLA:H3A  | 1.83                     | 0.41              |
| 4:J:16:ASP:C       | 4:J:18:LEU:N       | 2.78                     | 0.41              |
| 4:J:50:THR:O       | 4:J:54:PHE:N       | 2.45                     | 0.41              |
| 4:J:112:THR:O      | 4:J:113:PHE:C      | 2.63                     | 0.41              |
| 4:J:180:ARG:C      | 4:J:180:ARG:HD3    | 2.46                     | 0.41              |
| 4:J:337:GLU:CG     | 4:J:339:PHE:HE2    | 2.31                     | 0.41              |
| 6:L:37:ILE:C       | 6:L:39:ALA:N       | 2.78                     | 0.41              |
| 10:Y:331:UNK:O     | 10:Y:332:UNK:C     | 2.66                     | 0.41              |
| 1:A:157:VAL:HG21   | 11:A:1343:CLA:CMC  | 2.50                     | 0.41              |
| 2:B:162:PHE:HB3    | 11:B:1487:CLA:HHD  | 2.02                     | 0.41              |
| 2:B:201:HIS:HA     | 11:B:1483:CLA:C4B  | 2.49                     | 0.41              |
| 2:B:421:ALA:O      | 2:B:424:ALA:N      | 2.53                     | 0.41              |
| 3:C:105:VAL:O      | 3:C:107:ASP:N      | 2.54                     | 0.41              |
| 3:C:358:PHE:C      | 3:C:360:ASP:N      | 2.79                     | 0.41              |
| 3:C:382:ASN:N      | 3:C:382:ASN:OD1    | 2.52                     | 0.41              |
| 3:C:450:ALA:HB1    | 3:C:455:PHE:HB2    | 2.01                     | 0.41              |
| 4:D:42:TYR:O       | 4:D:43:LEU:C       | 2.63                     | 0.41              |
| 4:D:55:VAL:CG1     | 4:D:56:THR:N       | 2.82                     | 0.41              |
| 4:D:253:TRP:HE1    | 15:D:1354:PL9:C1   | 2.32                     | 0.41              |
| 4:D:262:SER:O      | 4:D:263:ASN:HB2    | 2.20                     | 0.41              |
| 1:G:267:ASN:O      | 1:G:271:LEU:N      | 2.38                     | 0.41              |
| 2:H:405:GLU:O      | 2:H:406:LEU:HB2    | 2.20                     | 0.41              |
| 3:I:91:HIS:O       | 3:I:92:ILE:C       | 2.64                     | 0.41              |
| 3:I:97:TRP:CE3     | 3:I:178:LYS:NZ     | 2.88                     | 0.41              |
| 3:I:156:LYS:HD2    | 3:I:156:LYS:HA     | 1.89                     | 0.41              |
| 3:I:251:HIS:O      | 3:I:252:ILE:C      | 2.62                     | 0.41              |
| 3:I:275:SER:HB2    | 11:I:1465:CLA:HAA1 | 2.03                     | 0.41              |
| 4:J:179:PHE:O      | 4:J:182:LEU:HB2    | 2.20                     | 0.41              |
| 4:J:264:LYS:C      | 4:J:266:TRP:N      | 2.78                     | 0.41              |
| 8:U:5:UNK:O        | 8:U:8:UNK:N        | 2.54                     | 0.41              |
| 10:Y:56:UNK:O      | 10:Y:59:UNK:N      | 2.54                     | 0.41              |
| 10:Y:116:UNK:O     | 10:Y:117:UNK:C     | 2.68                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:58:VAL:HG13    | 1:A:109:GLY:HA3    | 2.02                     | 0.41              |
| 1:A:300:PHE:CE2    | 11:C:1462:CLA:H93  | 2.56                     | 0.41              |
| 2:B:195:PRO:O      | 2:B:198:VAL:N      | 2.53                     | 0.41              |
| 3:C:56:HIS:O       | 3:C:57:ALA:O       | 2.39                     | 0.41              |
| 3:C:61:VAL:O       | 3:C:62:PHE:C       | 2.63                     | 0.41              |
| 3:C:153:ASP:OD1    | 3:C:155:ASN:N      | 2.51                     | 0.41              |
| 3:C:173:LEU:O      | 3:C:174:LEU:C      | 2.61                     | 0.41              |
| 4:D:126:MET:HE2    | 4:D:146:PHE:HB3    | 2.01                     | 0.41              |
| 5:E:58:GLN:OE1     | 9:V:2:GLU:HB2      | 2.19                     | 0.41              |
| 1:G:69:GLY:HA2     | 1:G:75:ASN:OD1     | 2.21                     | 0.41              |
| 1:G:84:PRO:CG      | 1:G:173:PRO:CD     | 2.88                     | 0.41              |
| 1:G:120:LEU:C      | 1:G:122:GLY:N      | 2.77                     | 0.41              |
| 2:H:59:GLY:CA      | 11:H:1488:CLA:CED  | 2.88                     | 0.41              |
| 2:H:251:VAL:O      | 2:H:252:VAL:C      | 2.62                     | 0.41              |
| 2:H:419:SER:OG     | 2:H:420:TYR:N      | 2.53                     | 0.41              |
| 11:H:1483:CLA:H143 | 11:H:1483:CLA:H111 | 1.94                     | 0.41              |
| 3:I:75:PHE:CD1     | 3:I:75:PHE:C       | 2.96                     | 0.41              |
| 3:I:119:LEU:C      | 3:I:122:SER:OG     | 2.64                     | 0.41              |
| 3:I:298:PRO:O      | 3:I:299:SER:OG     | 2.34                     | 0.41              |
| 3:I:395:TYR:O      | 3:I:398:HIS:N      | 2.37                     | 0.41              |
| 3:I:438:LEU:O      | 3:I:439:VAL:C      | 2.64                     | 0.41              |
| 4:J:152:VAL:CG1    | 11:J:1351:CLA:HBA1 | 2.51                     | 0.41              |
| 4:J:228:GLY:O      | 4:J:229:ALA:HB3    | 2.20                     | 0.41              |
| 7:P:99:UNK:O       | 7:P:100:UNK:C      | 2.68                     | 0.41              |
| 9:T:87:GLU:CD      | 9:T:96:ARG:NH2     | 2.77                     | 0.41              |
| 10:X:3:UNK:C       | 10:X:5:UNK:N       | 2.78                     | 0.41              |
| 1:A:23:SER:O       | 1:A:24:THR:C       | 2.63                     | 0.41              |
| 1:A:135:TYR:O      | 1:A:136:ARG:HG2    | 2.20                     | 0.41              |
| 1:A:168:PHE:O      | 1:A:170:ASP:O      | 2.38                     | 0.41              |
| 1:A:206:PHE:CE1    | 11:A:1342:CLA:HMB3 | 2.56                     | 0.41              |
| 11:A:1342:CLA:H201 | 12:A:1345:PHO:H43  | 2.03                     | 0.41              |
| 2:B:110:ALA:C      | 2:B:112:CYS:N      | 2.75                     | 0.41              |
| 2:B:471:ALA:O      | 2:B:473:THR:N      | 2.53                     | 0.41              |
| 11:B:1496:CLA:H13  | 11:B:1497:CLA:CMD  | 2.50                     | 0.41              |
| 3:C:188:THR:HG22   | 3:C:300:GLU:OE1    | 2.19                     | 0.41              |
| 4:D:166:SER:O      | 4:D:167:TRP:C      | 2.62                     | 0.41              |
| 4:D:186:GLN:C      | 4:D:186:GLN:CD     | 2.88                     | 0.41              |
| 4:D:194:ASN:OD1    | 4:D:196:PHE:HB2    | 2.20                     | 0.41              |
| 1:G:45:THR:CA      | 12:G:1345:PHO:H93  | 2.50                     | 0.41              |
| 2:H:21:ALA:CB      | 2:H:115:TRP:HD1    | 2.34                     | 0.41              |
| 2:H:24:LEU:HD21    | 2:H:110:ALA:HB1    | 2.01                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:H:71:VAL:CG1     | 2:H:93:PHE:H       | 2.34                     | 0.41              |
| 2:H:110:ALA:C      | 2:H:112:CYS:N      | 2.76                     | 0.41              |
| 2:H:464:PHE:HD2    | 11:H:1492:CLA:HAC2 | 1.86                     | 0.41              |
| 3:I:35:TRP:CZ3     | 3:I:36:TRP:HB3     | 2.56                     | 0.41              |
| 3:I:43:ILE:HA      | 11:I:1467:CLA:HMC3 | 2.03                     | 0.41              |
| 3:I:305:THR:C      | 3:I:307:PRO:CD     | 2.94                     | 0.41              |
| 3:I:395:TYR:O      | 3:I:396:MET:C      | 2.62                     | 0.41              |
| 7:O:118:UNK:O      | 7:O:119:UNK:C      | 2.68                     | 0.41              |
| 8:S:12:UNK:O       | 8:S:14:UNK:N       | 2.53                     | 0.41              |
| 9:T:128:ASP:HB3    | 9:T:134:LYS:CG     | 2.50                     | 0.41              |
| 8:U:29:UNK:O       | 8:U:30:UNK:C       | 2.67                     | 0.41              |
| 10:X:16:UNK:O      | 10:X:17:UNK:C      | 2.68                     | 0.41              |
| 10:X:256:UNK:O     | 10:X:257:UNK:C     | 2.69                     | 0.41              |
| 10:Y:71:UNK:O      | 10:Y:72:UNK:C      | 2.68                     | 0.41              |
| 1:A:255:PHE:O      | 1:A:256:GLY:C      | 2.63                     | 0.41              |
| 2:B:75:TRP:O       | 2:B:76:SER:CB      | 2.68                     | 0.41              |
| 2:B:157:HIS:CE1    | 2:B:164:PRO:O      | 2.73                     | 0.41              |
| 2:B:236:THR:CB     | 2:B:473:THR:CG2    | 2.89                     | 0.41              |
| 2:B:263:THR:HG22   | 2:B:448:ARG:NH2    | 2.36                     | 0.41              |
| 3:C:305:THR:O      | 3:C:306:GLY:C      | 2.63                     | 0.41              |
| 11:C:1464:CLA:HBA2 | 11:C:1464:CLA:H3A  | 1.46                     | 0.41              |
| 4:D:200:GLY:HA3    | 4:D:282:SER:HB3    | 2.03                     | 0.41              |
| 6:F:11:VAL:CG1     | 6:F:12:SER:N       | 2.83                     | 0.41              |
| 1:G:48:PHE:HA      | 1:G:115:ILE:HD11   | 2.02                     | 0.41              |
| 1:G:184:ILE:HD11   | 4:J:186:GLN:CD     | 2.46                     | 0.41              |
| 1:G:272:HIS:HD2    | 4:J:218:VAL:HG21   | 1.74                     | 0.41              |
| 2:H:224:ARG:O      | 2:H:228:ALA:HB2    | 2.19                     | 0.41              |
| 2:H:237:VAL:HG22   | 11:H:1491:CLA:C3C  | 2.50                     | 0.41              |
| 3:I:67:MET:O       | 3:I:68:THR:C       | 2.63                     | 0.41              |
| 3:I:308:GLU:O      | 3:I:311:GLN:HB2    | 2.21                     | 0.41              |
| 4:J:122:LEU:HA     | 4:J:122:LEU:HD23   | 1.76                     | 0.41              |
| 4:J:126:MET:HG2    | 4:J:130:PHE:HE1    | 1.85                     | 0.41              |
| 4:J:191:TRP:O      | 4:J:192:THR:C      | 2.63                     | 0.41              |
| 4:J:262:SER:O      | 4:J:263:ASN:HB2    | 2.21                     | 0.41              |
| 4:J:298:PHE:O      | 10:Y:129:UNK:CB    | 2.69                     | 0.41              |
| 7:P:88:UNK:CB      | 7:P:140:UNK:O      | 2.69                     | 0.41              |
| 8:S:7:UNK:O        | 8:S:9:UNK:N        | 2.53                     | 0.41              |
| 10:Y:215:UNK:O     | 10:Y:219:UNK:N     | 2.54                     | 0.41              |
| 1:A:45:THR:HA      | 12:A:1345:PHO:H93  | 2.02                     | 0.41              |
| 1:A:69:GLY:HA2     | 1:A:75:ASN:OD1     | 2.20                     | 0.41              |
| 1:A:84:PRO:CD      | 1:A:173:PRO:HB3    | 2.46                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:64:PRO:HG3     | 2:B:267:LEU:O      | 2.21                     | 0.41              |
| 3:C:187:ASP:OD1    | 3:C:187:ASP:C      | 2.64                     | 0.41              |
| 3:C:250:TRP:C      | 3:C:250:TRP:HD1    | 2.23                     | 0.41              |
| 3:C:251:HIS:O      | 3:C:252:ILE:C      | 2.64                     | 0.41              |
| 3:C:257:PHE:HB3    | 3:C:258:GLY:H      | 1.59                     | 0.41              |
| 4:D:101:PHE:O      | 4:D:104:TRP:HB3    | 2.20                     | 0.41              |
| 1:G:167:SER:OG     | 1:G:169:SER:CB     | 2.69                     | 0.41              |
| 2:H:37:MET:HG2     | 2:H:62:VAL:CG2     | 2.51                     | 0.41              |
| 2:H:64:PRO:HB2     | 2:H:268:PHE:CZ     | 2.55                     | 0.41              |
| 2:H:193:TYR:O      | 2:H:195:PRO:HD3    | 2.20                     | 0.41              |
| 2:H:349:LYS:HG3    | 2:H:394:GLN:O      | 2.21                     | 0.41              |
| 3:I:35:TRP:O       | 3:I:36:TRP:CG      | 2.74                     | 0.41              |
| 3:I:245:ILE:HD12   | 3:I:245:ILE:C      | 2.46                     | 0.41              |
| 3:I:272:LEU:HD21   | 11:I:1466:CLA:C1B  | 2.51                     | 0.41              |
| 4:J:308:ASP:C      | 4:J:310:GLU:N      | 2.79                     | 0.41              |
| 10:Y:223:UNK:O     | 10:Y:224:UNK:C     | 2.68                     | 0.41              |
| 1:A:142:TRP:HH2    | 1:A:273:PHE:CE1    | 2.38                     | 0.41              |
| 1:A:150:PRO:HB3    | 11:A:1342:CLA:H62  | 2.02                     | 0.41              |
| 1:A:176:ILE:HG23   | 11:A:1343:CLA:HED1 | 2.03                     | 0.41              |
| 2:B:18:ARG:NH2     | 2:B:118:TRP:CE3    | 2.89                     | 0.41              |
| 2:B:18:ARG:NH2     | 2:B:118:TRP:CZ3    | 2.89                     | 0.41              |
| 2:B:21:ALA:CB      | 2:B:115:TRP:HD1    | 2.34                     | 0.41              |
| 2:B:30:VAL:CG1     | 11:B:1486:CLA:HAC1 | 2.51                     | 0.41              |
| 2:B:31:ALA:HB3     | 2:B:104:SER:HB2    | 2.02                     | 0.41              |
| 2:B:63:LEU:HA      | 2:B:66:MET:CE      | 2.51                     | 0.41              |
| 2:B:106:LEU:O      | 2:B:107:LEU:C      | 2.64                     | 0.41              |
| 2:B:141:ILE:O      | 2:B:144:PHE:HB3    | 2.21                     | 0.41              |
| 2:B:214:LEU:HA     | 2:B:217:ILE:HG22   | 2.02                     | 0.41              |
| 2:B:220:ARG:CB     | 2:B:221:PRO:CD     | 2.99                     | 0.41              |
| 2:B:224:ARG:O      | 2:B:228:ALA:HB2    | 2.21                     | 0.41              |
| 2:B:263:THR:O      | 2:B:448:ARG:CZ     | 2.69                     | 0.41              |
| 2:B:268:PHE:O      | 2:B:269:GLY:C      | 2.64                     | 0.41              |
| 2:B:372:ASP:C      | 2:B:374:ASN:N      | 2.79                     | 0.41              |
| 3:C:122:SER:O      | 3:C:126:GLY:N      | 2.48                     | 0.41              |
| 3:C:183:GLY:O      | 3:C:184:GLY:O      | 2.38                     | 0.41              |
| 3:C:436:PHE:O      | 3:C:439:VAL:HB     | 2.21                     | 0.41              |
| 11:C:1465:CLA:HBA1 | 11:C:1465:CLA:H3A  | 1.80                     | 0.41              |
| 4:D:50:THR:O       | 4:D:54:PHE:HB2     | 2.21                     | 0.41              |
| 4:D:72:ASN:O       | 4:D:73:PHE:C       | 2.63                     | 0.41              |
| 4:D:100:ASP:CB     | 4:D:103:ARG:H      | 2.34                     | 0.41              |
| 4:D:190:ASN:ND2    | 4:D:193:LEU:HD12   | 2.36                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:D:298:PHE:O     | 10:X:129:UNK:CB    | 2.68                     | 0.41              |
| 1:G:60:ILE:HD12   | 1:G:83:VAL:HG12    | 1.99                     | 0.41              |
| 1:G:139:MET:HE3   | 1:G:139:MET:HB2    | 1.46                     | 0.41              |
| 1:G:214:MET:O     | 1:G:217:SER:HB3    | 2.20                     | 0.41              |
| 2:H:31:ALA:HB3    | 2:H:104:SER:HB2    | 2.03                     | 0.41              |
| 2:H:69:LEU:HA     | 2:H:69:LEU:HD12    | 1.84                     | 0.41              |
| 2:H:133:LEU:O     | 2:H:134:ASP:CB     | 2.68                     | 0.41              |
| 2:H:217:ILE:O     | 2:H:217:ILE:CG1    | 2.66                     | 0.41              |
| 2:H:238:LEU:HD23  | 2:H:469:HIS:CG     | 2.56                     | 0.41              |
| 2:H:263:THR:O     | 2:H:448:ARG:CZ     | 2.69                     | 0.41              |
| 2:H:358:ARG:O     | 2:H:360:PRO:HD3    | 2.21                     | 0.41              |
| 2:H:359:MET:HB3   | 2:H:426:PHE:HB3    | 2.02                     | 0.41              |
| 2:H:372:ASP:C     | 2:H:374:ASN:N      | 2.79                     | 0.41              |
| 2:H:421:ALA:O     | 2:H:422:ARG:C      | 2.62                     | 0.41              |
| 3:I:63:TRP:NE1    | 11:I:1462:CLA:C2C  | 2.83                     | 0.41              |
| 3:I:102:GLY:O     | 3:I:103:GLY:O      | 2.38                     | 0.41              |
| 3:I:186:TYR:C     | 3:I:186:TYR:CD2    | 2.98                     | 0.41              |
| 3:I:187:ASP:C     | 3:I:189:TRP:H      | 2.29                     | 0.41              |
| 3:I:322:GLN:NE2   | 3:I:381:LYS:HA     | 2.36                     | 0.41              |
| 3:I:394:GLU:OE2   | 3:I:398:HIS:CD2    | 2.74                     | 0.41              |
| 3:I:439:VAL:O     | 3:I:440:GLY:C      | 2.64                     | 0.41              |
| 11:I:1463:CLA:H93 | 11:I:1464:CLA:H51  | 2.02                     | 0.41              |
| 4:J:76:VAL:O      | 4:J:77:ALA:HB2     | 2.20                     | 0.41              |
| 4:J:83:ASN:O      | 4:J:84:SER:C       | 2.63                     | 0.41              |
| 4:J:144:ILE:O     | 4:J:145:ALA:C      | 2.62                     | 0.41              |
| 4:J:161:PRO:HG2   | 4:J:170:ALA:HB2    | 2.03                     | 0.41              |
| 4:J:188:PHE:CE2   | 4:J:326:ARG:HG2    | 2.56                     | 0.41              |
| 4:J:253:TRP:HE1   | 15:J:1354:PL9:C1   | 2.33                     | 0.41              |
| 4:J:313:THR:O     | 4:J:315:TYR:N      | 2.54                     | 0.41              |
| 10:X:258:UNK:O    | 10:X:259:UNK:C     | 2.68                     | 0.41              |
| 10:X:268:UNK:O    | 10:X:271:UNK:N     | 2.54                     | 0.41              |
| 10:X:519:UNK:C    | 10:X:521:UNK:N     | 2.82                     | 0.41              |
| 10:X:563:UNK:O    | 10:X:564:UNK:C     | 2.68                     | 0.41              |
| 10:Y:406:UNK:O    | 10:Y:407:UNK:C     | 2.68                     | 0.41              |
| 10:Y:532:UNK:C    | 10:Y:534:UNK:N     | 2.83                     | 0.41              |
| 10:Y:580:UNK:C    | 10:Y:582:UNK:N     | 2.79                     | 0.41              |
| 1:A:127:MET:HE1   | 1:A:151:LEU:HD23   | 2.03                     | 0.41              |
| 1:A:296:ASN:ND2   | 1:A:298:ASN:OD1    | 2.54                     | 0.41              |
| 2:B:147:GLY:O     | 2:B:148:LEU:C      | 2.64                     | 0.41              |
| 2:B:215:PHE:CZ    | 11:B:1490:CLA:CMD  | 3.04                     | 0.41              |
| 2:B:215:PHE:CZ    | 11:B:1490:CLA:HMD3 | 2.55                     | 0.41              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 2:B:238:LEU:HD23 | 2:B:469:HIS:CG     | 2.56                     | 0.41              |
| 2:B:347:ARG:H    | 2:B:398:THR:CB     | 2.34                     | 0.41              |
| 2:B:407:ASN:O    | 2:B:408:GLY:C      | 2.62                     | 0.41              |
| 3:C:36:TRP:O     | 3:C:36:TRP:CE3     | 2.73                     | 0.41              |
| 3:C:60:ILE:O     | 3:C:61:VAL:C       | 2.64                     | 0.41              |
| 3:C:164:HIS:C    | 3:C:166:ILE:H      | 2.29                     | 0.41              |
| 4:D:281:MET:C    | 4:D:283:ALA:N      | 2.78                     | 0.41              |
| 4:D:321:LEU:O    | 4:D:324:GLY:N      | 2.54                     | 0.41              |
| 6:F:33:PHE:O     | 6:F:34:LEU:C       | 2.64                     | 0.41              |
| 1:G:104:GLU:HG2  | 1:G:104:GLU:O      | 2.20                     | 0.41              |
| 1:G:120:LEU:O    | 1:G:121:LEU:C      | 2.62                     | 0.41              |
| 1:G:134:SER:HA   | 1:G:139:MET:CB     | 2.51                     | 0.41              |
| 1:G:151:LEU:CD2  | 1:G:155:PHE:HE2    | 2.33                     | 0.41              |
| 1:G:176:ILE:HG22 | 1:G:177:SER:N      | 2.36                     | 0.41              |
| 2:H:25:MET:HE1   | 2:H:108:PHE:HE1    | 1.86                     | 0.41              |
| 2:H:92:SER:O     | 2:H:95:GLY:N       | 2.54                     | 0.41              |
| 2:H:207:ILE:O    | 2:H:208:VAL:C      | 2.63                     | 0.41              |
| 2:H:222:PRO:O    | 2:H:226:TYR:N      | 2.45                     | 0.41              |
| 2:H:469:HIS:O    | 2:H:470:GLY:C      | 2.63                     | 0.41              |
| 3:I:161:LEU:O    | 3:I:164:HIS:N      | 2.46                     | 0.41              |
| 3:I:167:VAL:HG13 | 11:I:1470:CLA:HMB1 | 2.02                     | 0.41              |
| 4:J:294:ARG:HB2  | 4:J:295:SER:H      | 1.51                     | 0.41              |
| 4:J:307:GLU:C    | 4:J:309:PRO:HD3    | 2.42                     | 0.41              |
| 8:U:47:UNK:O     | 8:U:48:UNK:C       | 2.69                     | 0.41              |
| 2:B:174:LEU:C    | 2:B:175:THR:O      | 2.64                     | 0.40              |
| 3:C:241:GLY:O    | 3:C:245:ILE:HG23   | 2.21                     | 0.40              |
| 3:C:250:TRP:HA   | 3:C:253:LEU:CD1    | 2.50                     | 0.40              |
| 4:D:32:TRP:O     | 4:D:35:ILE:HB      | 2.21                     | 0.40              |
| 4:D:62:GLY:HA3   | 5:E:63:ILE:HG23    | 2.03                     | 0.40              |
| 1:G:248:ILE:O    | 1:G:251:ALA:N      | 2.48                     | 0.40              |
| 1:G:256:GLY:O    | 1:G:260:PHE:O      | 2.38                     | 0.40              |
| 1:G:307:ILE:O    | 1:G:310:LYS:N      | 2.40                     | 0.40              |
| 3:I:33:PHE:CZ    | 3:I:40:ALA:HB1     | 2.56                     | 0.40              |
| 3:I:73:ALA:HB3   | 3:I:74:HIS:CD2     | 2.52                     | 0.40              |
| 3:I:298:PRO:HB3  | 3:I:300:GLU:OE1    | 2.22                     | 0.40              |
| 3:I:365:TRP:CG   | 3:I:366:LEU:N      | 2.90                     | 0.40              |
| 3:I:382:ASN:N    | 3:I:382:ASN:OD1    | 2.53                     | 0.40              |
| 5:K:37:PHE:CE1   | 5:K:42:LEU:HB3     | 2.56                     | 0.40              |
| 5:K:51:ARG:C     | 5:K:53:ASP:N       | 2.78                     | 0.40              |
| 8:S:86:UNK:O     | 8:S:87:UNK:C       | 2.68                     | 0.40              |
| 10:X:162:UNK:O   | 10:X:163:UNK:C     | 2.65                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:X:519:UNK:O     | 10:X:520:UNK:C     | 2.69                     | 0.40              |
| 10:Y:268:UNK:O     | 10:Y:271:UNK:N     | 2.53                     | 0.40              |
| 1:A:67:VAL:HG21    | 4:D:317:LYS:NZ     | 2.35                     | 0.40              |
| 1:A:133:LEU:HD12   | 4:D:256:ILE:HG12   | 1.99                     | 0.40              |
| 1:A:137:LEU:HB2    | 1:A:139:MET:HE3    | 2.03                     | 0.40              |
| 2:B:150:CYS:N      | 11:B:1484:CLA:HBC2 | 2.36                     | 0.40              |
| 2:B:290:ALA:O      | 2:B:294:SER:HB3    | 2.21                     | 0.40              |
| 3:C:81:MET:HE3     | 3:C:81:MET:HB2     | 1.89                     | 0.40              |
| 3:C:439:VAL:O      | 3:C:440:GLY:C      | 2.62                     | 0.40              |
| 11:C:1462:CLA:HMB1 | 11:C:1462:CLA:CBB  | 2.51                     | 0.40              |
| 4:D:56:THR:CG2     | 5:E:49:THR:HG22    | 2.51                     | 0.40              |
| 4:D:281:MET:HA     | 4:D:281:MET:HE3    | 2.03                     | 0.40              |
| 1:G:142:TRP:HH2    | 1:G:273:PHE:CE1    | 2.38                     | 0.40              |
| 2:H:18:ARG:HH21    | 2:H:118:TRP:HE3    | 1.69                     | 0.40              |
| 2:H:193:TYR:CD1    | 2:H:260:SER:CB     | 3.03                     | 0.40              |
| 2:H:347:ARG:CB     | 2:H:398:THR:CB     | 2.95                     | 0.40              |
| 2:H:393:GLU:O      | 2:H:394:GLN:C      | 2.64                     | 0.40              |
| 2:H:416:THR:O      | 2:H:420:TYR:HB2    | 2.21                     | 0.40              |
| 3:I:185:LEU:O      | 3:I:186:TYR:O      | 2.38                     | 0.40              |
| 3:I:282:MET:HE1    | 11:I:1465:CLA:H43  | 2.02                     | 0.40              |
| 4:J:56:THR:H       | 5:K:49:THR:HG22    | 1.86                     | 0.40              |
| 4:J:186:GLN:C      | 4:J:186:GLN:CD     | 2.89                     | 0.40              |
| 7:O:88:UNK:CB      | 7:O:140:UNK:O      | 2.69                     | 0.40              |
| 7:P:159:UNK:C      | 7:P:161:UNK:N      | 2.81                     | 0.40              |
| 1:A:110:GLY:N      | 1:A:111:PRO:CD     | 2.85                     | 0.40              |
| 1:A:115:ILE:O      | 1:A:116:ILE:C      | 2.63                     | 0.40              |
| 2:B:346:PHE:O      | 2:B:354:LEU:CB     | 2.68                     | 0.40              |
| 11:B:1483:CLA:H62  | 11:B:1483:CLA:H41  | 1.92                     | 0.40              |
| 3:C:297:TYR:CD1    | 3:C:302:TYR:CZ     | 3.05                     | 0.40              |
| 1:G:87:ASN:ND2     | 1:G:87:ASN:O       | 2.55                     | 0.40              |
| 11:G:1344:CLA:HED1 | 4:J:179:PHE:CZ     | 2.56                     | 0.40              |
| 2:H:190:PHE:O      | 2:H:191:ASN:C      | 2.64                     | 0.40              |
| 2:H:468:TRP:CD1    | 4:J:144:ILE:CD1    | 3.02                     | 0.40              |
| 3:I:275:SER:HA     | 3:I:278:ALA:HB2    | 2.03                     | 0.40              |
| 4:J:91:LEU:HD13    | 4:J:93:TRP:CZ3     | 2.56                     | 0.40              |
| 5:K:39:SER:O       | 5:K:40:THR:C       | 2.63                     | 0.40              |
| 10:Y:168:UNK:C     | 10:Y:170:UNK:N     | 2.82                     | 0.40              |
| 1:A:192:ILE:O      | 1:A:193:LEU:C      | 2.64                     | 0.40              |
| 1:A:254:TYR:CE2    | 4:D:133:ALA:HB2    | 2.56                     | 0.40              |
| 1:A:316:THR:O      | 1:A:318:ALA:N      | 2.55                     | 0.40              |
| 2:B:156:PHE:CB     | 11:B:1487:CLA:HAC1 | 2.51                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:237:VAL:HG22   | 11:B:1491:CLA:C3C  | 2.50                     | 0.40              |
| 3:C:52:ALA:O       | 11:C:1469:CLA:HMB2 | 2.22                     | 0.40              |
| 1:G:112:TYR:OH     | 1:G:116:ILE:HD11   | 2.20                     | 0.40              |
| 1:G:180:PHE:CD2    | 4:J:192:THR:CG2    | 3.04                     | 0.40              |
| 1:G:326:LEU:O      | 1:G:328:MET:N      | 2.53                     | 0.40              |
| 2:H:99:ALA:O       | 2:H:103:LEU:HG     | 2.21                     | 0.40              |
| 2:H:249:ALA:O      | 2:H:250:PHE:C      | 2.64                     | 0.40              |
| 3:I:455:PHE:O      | 3:I:456:GLU:CD     | 2.65                     | 0.40              |
| 4:J:92:LEU:HA      | 4:J:104:TRP:CD1    | 2.56                     | 0.40              |
| 4:J:127:LEU:O      | 4:J:129:GLN:N      | 2.54                     | 0.40              |
| 4:J:335:PRO:O      | 4:J:337:GLU:N      | 2.54                     | 0.40              |
| 8:U:1:UNK:C        | 8:U:3:UNK:N        | 2.85                     | 0.40              |
| 8:U:27:UNK:C       | 8:U:28:UNK:O       | 2.70                     | 0.40              |
| 10:X:507:UNK:O     | 10:X:508:UNK:C     | 2.69                     | 0.40              |
| 10:Y:434:UNK:O     | 10:Y:435:UNK:C     | 2.70                     | 0.40              |
| 1:A:139:MET:HE3    | 1:A:139:MET:HB2    | 1.47                     | 0.40              |
| 1:A:161:TYR:CE2    | 1:A:186:PHE:CE1    | 3.05                     | 0.40              |
| 1:A:172:MET:N      | 1:A:182:PHE:CD1    | 2.83                     | 0.40              |
| 1:A:317:TRP:N      | 4:D:63:LEU:HD23    | 2.37                     | 0.40              |
| 11:A:1343:CLA:H143 | 11:A:1343:CLA:H112 | 1.93                     | 0.40              |
| 2:B:174:LEU:HD11   | 2:B:309:LEU:HD21   | 2.02                     | 0.40              |
| 2:B:280:PHE:O      | 2:B:281:GLN:C      | 2.61                     | 0.40              |
| 2:B:435:GLU:C      | 2:B:437:LEU:N      | 2.78                     | 0.40              |
| 3:C:88:LEU:C       | 3:C:90:PRO:HD2     | 2.47                     | 0.40              |
| 4:D:78:VAL:O       | 4:D:78:VAL:HG12    | 2.20                     | 0.40              |
| 4:D:85:MET:HB2     | 4:D:85:MET:HE2     | 1.62                     | 0.40              |
| 5:E:61:ARG:O       | 5:E:62:SER:HB2     | 2.22                     | 0.40              |
| 1:G:317:TRP:CE3    | 1:G:320:ILE:HD12   | 2.56                     | 0.40              |
| 2:H:37:MET:O       | 2:H:38:ALA:C       | 2.64                     | 0.40              |
| 2:H:149:LEU:O      | 2:H:150:CYS:C      | 2.64                     | 0.40              |
| 2:H:207:ILE:C      | 2:H:209:GLY:N      | 2.77                     | 0.40              |
| 2:H:464:PHE:HE1    | 4:J:144:ILE:HG23   | 1.86                     | 0.40              |
| 2:H:466:HIS:C      | 2:H:468:TRP:H      | 2.30                     | 0.40              |
| 11:H:1482:CLA:H61  | 11:H:1482:CLA:H41  | 1.91                     | 0.40              |
| 3:I:188:THR:HG22   | 3:I:300:GLU:CD     | 2.47                     | 0.40              |
| 3:I:244:CYS:HB3    | 11:I:1465:CLA:H93  | 2.02                     | 0.40              |
| 3:I:360:ASP:O      | 3:I:361:PHE:C      | 2.65                     | 0.40              |
| 4:J:136:VAL:O      | 4:J:136:VAL:CG1    | 2.69                     | 0.40              |
| 6:L:18:VAL:O       | 6:L:21:VAL:HB      | 2.21                     | 0.40              |
| 9:V:63:THR:O       | 9:V:84:GLY:HA3     | 2.22                     | 0.40              |
| 10:X:534:UNK:O     | 10:X:535:UNK:C     | 2.67                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-----------|-------------|----|
| 1   | A     | 295/360 (82%)   | 188 (64%)  | 67 (23%)  | 40 (14%)  | 0           | 1  |
| 1   | G     | 295/360 (82%)   | 184 (62%)  | 71 (24%)  | 40 (14%)  | 0           | 1  |
| 2   | B     | 399/510 (78%)   | 244 (61%)  | 94 (24%)  | 61 (15%)  | 0           | 0  |
| 2   | H     | 399/510 (78%)   | 246 (62%)  | 94 (24%)  | 59 (15%)  | 0           | 1  |
| 3   | C     | 353/473 (75%)   | 205 (58%)  | 96 (27%)  | 52 (15%)  | 0           | 1  |
| 3   | I     | 353/473 (75%)   | 206 (58%)  | 99 (28%)  | 48 (14%)  | 0           | 1  |
| 4   | D     | 348/352 (99%)   | 223 (64%)  | 76 (22%)  | 49 (14%)  | 0           | 1  |
| 4   | J     | 348/352 (99%)   | 222 (64%)  | 79 (23%)  | 47 (14%)  | 0           | 1  |
| 5   | E     | 67/84 (80%)     | 40 (60%)   | 13 (19%)  | 14 (21%)  | 0           | 0  |
| 5   | K     | 67/84 (80%)     | 43 (64%)   | 10 (15%)  | 14 (21%)  | 0           | 0  |
| 6   | F     | 35/44 (80%)     | 24 (69%)   | 4 (11%)   | 7 (20%)   | 0           | 0  |
| 6   | L     | 35/44 (80%)     | 22 (63%)   | 6 (17%)   | 7 (20%)   | 0           | 0  |
| 9   | T     | 134/163 (82%)   | 121 (90%)  | 11 (8%)   | 2 (2%)    | 8           | 37 |
| 9   | V     | 134/163 (82%)   | 124 (92%)  | 8 (6%)    | 2 (2%)    | 8           | 37 |
| All | All   | 3262/3972 (82%) | 2092 (64%) | 728 (22%) | 442 (14%) | 0           | 1  |

All (442) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 11  | ALA  |
| 1   | A     | 12  | ASN  |
| 1   | A     | 63  | ILE  |
| 1   | A     | 80  | GLY  |
| 1   | A     | 85  | SER  |
| 1   | A     | 95  | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 139 | MET  |
| 1   | A     | 141 | PRO  |
| 1   | A     | 142 | TRP  |
| 1   | A     | 172 | MET  |
| 1   | A     | 248 | ILE  |
| 1   | A     | 249 | VAL  |
| 1   | A     | 260 | PHE  |
| 1   | A     | 267 | ASN  |
| 1   | A     | 308 | ASP  |
| 1   | A     | 315 | ASN  |
| 1   | A     | 316 | THR  |
| 1   | A     | 332 | HIS  |
| 2   | B     | 46  | ASP  |
| 2   | B     | 62  | VAL  |
| 2   | B     | 93  | PHE  |
| 2   | B     | 133 | LEU  |
| 2   | B     | 134 | ASP  |
| 2   | B     | 135 | LEU  |
| 2   | B     | 163 | GLY  |
| 2   | B     | 171 | PRO  |
| 2   | B     | 175 | THR  |
| 2   | B     | 198 | VAL  |
| 2   | B     | 230 | ARG  |
| 2   | B     | 234 | ILE  |
| 2   | B     | 269 | GLY  |
| 2   | B     | 314 | TYR  |
| 2   | B     | 339 | ALA  |
| 2   | B     | 353 | GLU  |
| 2   | B     | 354 | LEU  |
| 2   | B     | 395 | GLN  |
| 2   | B     | 404 | GLY  |
| 2   | B     | 405 | GLU  |
| 2   | B     | 425 | ILE  |
| 3   | C     | 22  | PHE  |
| 3   | C     | 25  | ASN  |
| 3   | C     | 26  | ARG  |
| 3   | C     | 46  | SER  |
| 3   | C     | 107 | ASP  |
| 3   | C     | 135 | ARG  |
| 3   | C     | 184 | GLY  |
| 3   | C     | 186 | TYR  |
| 3   | C     | 227 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 253 | LEU  |
| 3   | C     | 256 | PRO  |
| 3   | C     | 295 | THR  |
| 3   | C     | 364 | PRO  |
| 3   | C     | 365 | TRP  |
| 3   | C     | 382 | ASN  |
| 3   | C     | 383 | ASP  |
| 4   | D     | 5   | ILE  |
| 4   | D     | 8   | ALA  |
| 4   | D     | 10  | ALA  |
| 4   | D     | 11  | GLU  |
| 4   | D     | 15  | PHE  |
| 4   | D     | 16  | ASP  |
| 4   | D     | 40  | CYS  |
| 4   | D     | 58  | TRP  |
| 4   | D     | 73  | PHE  |
| 4   | D     | 96  | GLU  |
| 4   | D     | 166 | SER  |
| 4   | D     | 218 | VAL  |
| 4   | D     | 222 | LEU  |
| 4   | D     | 230 | SER  |
| 4   | D     | 239 | GLN  |
| 4   | D     | 241 | GLU  |
| 4   | D     | 297 | ASP  |
| 4   | D     | 330 | ALA  |
| 4   | D     | 331 | PRO  |
| 4   | D     | 346 | LEU  |
| 4   | D     | 347 | PRO  |
| 5   | E     | 9   | PRO  |
| 5   | E     | 10  | PHE  |
| 5   | E     | 17  | VAL  |
| 5   | E     | 57  | ALA  |
| 5   | E     | 59  | GLU  |
| 5   | E     | 60  | GLN  |
| 5   | E     | 62  | SER  |
| 6   | F     | 13  | TYR  |
| 6   | F     | 14  | PRO  |
| 6   | F     | 15  | ILE  |
| 1   | G     | 11  | ALA  |
| 1   | G     | 12  | ASN  |
| 1   | G     | 63  | ILE  |
| 1   | G     | 80  | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 85  | SER  |
| 1   | G     | 95  | PRO  |
| 1   | G     | 139 | MET  |
| 1   | G     | 141 | PRO  |
| 1   | G     | 142 | TRP  |
| 1   | G     | 182 | PHE  |
| 1   | G     | 248 | ILE  |
| 1   | G     | 249 | VAL  |
| 1   | G     | 260 | PHE  |
| 1   | G     | 267 | ASN  |
| 1   | G     | 315 | ASN  |
| 1   | G     | 316 | THR  |
| 1   | G     | 332 | HIS  |
| 2   | H     | 46  | ASP  |
| 2   | H     | 62  | VAL  |
| 2   | H     | 93  | PHE  |
| 2   | H     | 133 | LEU  |
| 2   | H     | 134 | ASP  |
| 2   | H     | 135 | LEU  |
| 2   | H     | 163 | GLY  |
| 2   | H     | 171 | PRO  |
| 2   | H     | 175 | THR  |
| 2   | H     | 198 | VAL  |
| 2   | H     | 230 | ARG  |
| 2   | H     | 234 | ILE  |
| 2   | H     | 262 | THR  |
| 2   | H     | 314 | TYR  |
| 2   | H     | 339 | ALA  |
| 2   | H     | 353 | GLU  |
| 2   | H     | 354 | LEU  |
| 2   | H     | 395 | GLN  |
| 2   | H     | 404 | GLY  |
| 2   | H     | 405 | GLU  |
| 2   | H     | 406 | LEU  |
| 2   | H     | 425 | ILE  |
| 3   | I     | 22  | PHE  |
| 3   | I     | 25  | ASN  |
| 3   | I     | 26  | ARG  |
| 3   | I     | 46  | SER  |
| 3   | I     | 135 | ARG  |
| 3   | I     | 184 | GLY  |
| 3   | I     | 186 | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | I     | 227 | VAL  |
| 3   | I     | 253 | LEU  |
| 3   | I     | 256 | PRO  |
| 3   | I     | 295 | THR  |
| 3   | I     | 364 | PRO  |
| 3   | I     | 365 | TRP  |
| 3   | I     | 383 | ASP  |
| 4   | J     | 5   | ILE  |
| 4   | J     | 8   | ALA  |
| 4   | J     | 10  | ALA  |
| 4   | J     | 11  | GLU  |
| 4   | J     | 16  | ASP  |
| 4   | J     | 40  | CYS  |
| 4   | J     | 58  | TRP  |
| 4   | J     | 73  | PHE  |
| 4   | J     | 96  | GLU  |
| 4   | J     | 166 | SER  |
| 4   | J     | 218 | VAL  |
| 4   | J     | 222 | LEU  |
| 4   | J     | 230 | SER  |
| 4   | J     | 239 | GLN  |
| 4   | J     | 241 | GLU  |
| 4   | J     | 330 | ALA  |
| 4   | J     | 331 | PRO  |
| 4   | J     | 346 | LEU  |
| 4   | J     | 347 | PRO  |
| 5   | K     | 9   | PRO  |
| 5   | K     | 10  | PHE  |
| 5   | K     | 17  | VAL  |
| 5   | K     | 57  | ALA  |
| 5   | K     | 59  | GLU  |
| 5   | K     | 60  | GLN  |
| 5   | K     | 62  | SER  |
| 6   | L     | 13  | TYR  |
| 6   | L     | 14  | PRO  |
| 6   | L     | 15  | ILE  |
| 1   | A     | 35  | VAL  |
| 1   | A     | 90  | GLY  |
| 1   | A     | 108 | ASN  |
| 1   | A     | 116 | ILE  |
| 1   | A     | 182 | PHE  |
| 1   | A     | 185 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 192 | ILE  |
| 1   | A     | 289 | GLY  |
| 2   | B     | 76  | SER  |
| 2   | B     | 139 | PHE  |
| 2   | B     | 164 | PRO  |
| 2   | B     | 165 | GLY  |
| 2   | B     | 196 | GLY  |
| 2   | B     | 231 | MET  |
| 2   | B     | 259 | GLY  |
| 2   | B     | 262 | THR  |
| 2   | B     | 279 | TYR  |
| 2   | B     | 294 | SER  |
| 2   | B     | 331 | ASN  |
| 2   | B     | 337 | ALA  |
| 2   | B     | 406 | LEU  |
| 2   | B     | 408 | GLY  |
| 2   | B     | 409 | GLN  |
| 2   | B     | 426 | PHE  |
| 2   | B     | 437 | LEU  |
| 2   | B     | 439 | SER  |
| 2   | B     | 445 | THR  |
| 3   | C     | 80  | PRO  |
| 3   | C     | 103 | GLY  |
| 3   | C     | 117 | VAL  |
| 3   | C     | 121 | SER  |
| 3   | C     | 243 | ILE  |
| 3   | C     | 299 | SER  |
| 3   | C     | 305 | THR  |
| 3   | C     | 306 | GLY  |
| 3   | C     | 361 | PHE  |
| 3   | C     | 362 | ARG  |
| 4   | D     | 28  | VAL  |
| 4   | D     | 92  | LEU  |
| 4   | D     | 165 | SER  |
| 4   | D     | 168 | PHE  |
| 4   | D     | 259 | ILE  |
| 4   | D     | 299 | ILE  |
| 4   | D     | 348 | ARG  |
| 5   | E     | 40  | THR  |
| 6   | F     | 23  | VAL  |
| 6   | F     | 34  | LEU  |
| 1   | G     | 32  | TRP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 35  | VAL  |
| 1   | G     | 90  | GLY  |
| 1   | G     | 99  | ALA  |
| 1   | G     | 115 | ILE  |
| 1   | G     | 116 | ILE  |
| 1   | G     | 130 | GLN  |
| 1   | G     | 181 | ASN  |
| 1   | G     | 192 | ILE  |
| 1   | G     | 289 | GLY  |
| 2   | H     | 48  | SER  |
| 2   | H     | 76  | SER  |
| 2   | H     | 155 | ALA  |
| 2   | H     | 162 | PHE  |
| 2   | H     | 164 | PRO  |
| 2   | H     | 196 | GLY  |
| 2   | H     | 231 | MET  |
| 2   | H     | 259 | GLY  |
| 2   | H     | 271 | THR  |
| 2   | H     | 279 | TYR  |
| 2   | H     | 294 | SER  |
| 2   | H     | 331 | ASN  |
| 2   | H     | 337 | ALA  |
| 2   | H     | 391 | SER  |
| 2   | H     | 408 | GLY  |
| 2   | H     | 409 | GLN  |
| 2   | H     | 426 | PHE  |
| 2   | H     | 437 | LEU  |
| 2   | H     | 439 | SER  |
| 2   | H     | 445 | THR  |
| 3   | I     | 80  | PRO  |
| 3   | I     | 103 | GLY  |
| 3   | I     | 117 | VAL  |
| 3   | I     | 121 | SER  |
| 3   | I     | 243 | ILE  |
| 3   | I     | 252 | ILE  |
| 3   | I     | 299 | SER  |
| 3   | I     | 306 | GLY  |
| 3   | I     | 361 | PHE  |
| 3   | I     | 362 | ARG  |
| 3   | I     | 382 | ASN  |
| 4   | J     | 15  | PHE  |
| 4   | J     | 28  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | J     | 92  | LEU  |
| 4   | J     | 165 | SER  |
| 4   | J     | 168 | PHE  |
| 4   | J     | 259 | ILE  |
| 4   | J     | 297 | ASP  |
| 4   | J     | 299 | ILE  |
| 4   | J     | 343 | GLU  |
| 4   | J     | 348 | ARG  |
| 5   | K     | 48  | GLY  |
| 6   | L     | 34  | LEU  |
| 1   | A     | 32  | TRP  |
| 1   | A     | 99  | ALA  |
| 1   | A     | 115 | ILE  |
| 1   | A     | 130 | GLN  |
| 1   | A     | 133 | LEU  |
| 1   | A     | 167 | SER  |
| 1   | A     | 181 | ASN  |
| 2   | B     | 155 | ALA  |
| 2   | B     | 162 | PHE  |
| 2   | B     | 220 | ARG  |
| 2   | B     | 271 | THR  |
| 2   | B     | 342 | GLY  |
| 2   | B     | 352 | GLU  |
| 2   | B     | 373 | LYS  |
| 2   | B     | 374 | ASN  |
| 2   | B     | 391 | SER  |
| 3   | C     | 36  | TRP  |
| 3   | C     | 57  | ALA  |
| 3   | C     | 106 | VAL  |
| 3   | C     | 153 | ASP  |
| 3   | C     | 257 | PHE  |
| 3   | C     | 293 | ASN  |
| 3   | C     | 298 | PRO  |
| 3   | C     | 375 | LEU  |
| 3   | C     | 441 | HIS  |
| 4   | D     | 41  | ALA  |
| 4   | D     | 94  | GLY  |
| 4   | D     | 225 | ASP  |
| 4   | D     | 228 | GLY  |
| 4   | D     | 336 | HIS  |
| 4   | D     | 343 | GLU  |
| 5   | E     | 83  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | F     | 27  | ALA  |
| 1   | G     | 92  | HIS  |
| 1   | G     | 108 | ASN  |
| 1   | G     | 133 | LEU  |
| 1   | G     | 167 | SER  |
| 1   | G     | 172 | MET  |
| 1   | G     | 193 | LEU  |
| 1   | G     | 308 | ASP  |
| 2   | H     | 139 | PHE  |
| 2   | H     | 220 | ARG  |
| 2   | H     | 342 | GLY  |
| 2   | H     | 352 | GLU  |
| 2   | H     | 373 | LYS  |
| 3   | I     | 98  | GLY  |
| 3   | I     | 257 | PHE  |
| 3   | I     | 298 | PRO  |
| 3   | I     | 305 | THR  |
| 3   | I     | 375 | LEU  |
| 4   | J     | 13  | GLY  |
| 4   | J     | 41  | ALA  |
| 4   | J     | 47  | GLY  |
| 4   | J     | 94  | GLY  |
| 5   | K     | 40  | THR  |
| 9   | T     | 133 | GLY  |
| 9   | V     | 133 | GLY  |
| 1   | A     | 193 | LEU  |
| 1   | A     | 295 | PHE  |
| 1   | A     | 317 | TRP  |
| 2   | B     | 48  | SER  |
| 2   | B     | 177 | SER  |
| 2   | B     | 319 | PRO  |
| 2   | B     | 360 | PRO  |
| 2   | B     | 396 | GLY  |
| 2   | B     | 473 | THR  |
| 3   | C     | 29  | GLU  |
| 3   | C     | 285 | ILE  |
| 3   | C     | 286 | ALA  |
| 3   | C     | 294 | ASN  |
| 4   | D     | 17  | ILE  |
| 4   | D     | 29  | PHE  |
| 4   | D     | 47  | GLY  |
| 4   | D     | 79  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 333 | ASP  |
| 5   | E     | 82  | GLN  |
| 1   | G     | 185 | VAL  |
| 2   | H     | 28  | ALA  |
| 2   | H     | 165 | GLY  |
| 2   | H     | 177 | SER  |
| 2   | H     | 319 | PRO  |
| 2   | H     | 360 | PRO  |
| 2   | H     | 374 | ASN  |
| 2   | H     | 396 | GLY  |
| 3   | I     | 57  | ALA  |
| 3   | I     | 153 | ASP  |
| 3   | I     | 441 | HIS  |
| 4   | J     | 17  | ILE  |
| 4   | J     | 29  | PHE  |
| 4   | J     | 228 | GLY  |
| 4   | J     | 264 | LYS  |
| 5   | K     | 82  | GLN  |
| 5   | K     | 83  | LEU  |
| 9   | T     | 131 | GLY  |
| 9   | V     | 131 | GLY  |
| 1   | A     | 135 | TYR  |
| 1   | A     | 296 | ASN  |
| 2   | B     | 28  | ALA  |
| 3   | C     | 78  | GLU  |
| 3   | C     | 252 | ILE  |
| 3   | C     | 337 | LEU  |
| 3   | C     | 386 | PRO  |
| 4   | D     | 13  | GLY  |
| 4   | D     | 219 | GLU  |
| 4   | D     | 240 | ALA  |
| 4   | D     | 264 | LYS  |
| 5   | E     | 63  | ILE  |
| 1   | G     | 295 | PHE  |
| 1   | G     | 317 | TRP  |
| 2   | H     | 415 | PRO  |
| 3   | I     | 29  | GLU  |
| 3   | I     | 36  | TRP  |
| 3   | I     | 93  | ALA  |
| 3   | I     | 102 | GLY  |
| 3   | I     | 272 | LEU  |
| 3   | I     | 286 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | I     | 294 | ASN  |
| 3   | I     | 386 | PRO  |
| 4   | J     | 30  | VAL  |
| 4   | J     | 79  | SER  |
| 4   | J     | 89  | LEU  |
| 4   | J     | 112 | THR  |
| 4   | J     | 159 | ILE  |
| 4   | J     | 229 | ALA  |
| 4   | J     | 252 | PHE  |
| 5   | K     | 56  | TYR  |
| 5   | K     | 63  | ILE  |
| 6   | L     | 27  | ALA  |
| 2   | B     | 64  | PRO  |
| 2   | B     | 136 | PRO  |
| 2   | B     | 415 | PRO  |
| 3   | C     | 126 | GLY  |
| 3   | C     | 272 | LEU  |
| 4   | D     | 30  | VAL  |
| 4   | D     | 111 | TRP  |
| 4   | D     | 229 | ALA  |
| 5   | E     | 52  | PRO  |
| 5   | E     | 64  | PRO  |
| 1   | G     | 247 | ASN  |
| 2   | H     | 64  | PRO  |
| 3   | I     | 285 | ILE  |
| 3   | I     | 293 | ASN  |
| 4   | J     | 214 | HIS  |
| 4   | J     | 263 | ASN  |
| 5   | K     | 52  | PRO  |
| 6   | L     | 23  | VAL  |
| 1   | A     | 38  | ILE  |
| 4   | D     | 274 | VAL  |
| 2   | H     | 399 | VAL  |
| 6   | L     | 11  | VAL  |
| 3   | C     | 128 | GLY  |
| 4   | D     | 159 | ILE  |
| 6   | F     | 11  | VAL  |
| 1   | G     | 38  | ILE  |
| 2   | H     | 136 | PRO  |
| 2   | H     | 467 | ILE  |
| 3   | I     | 101 | PRO  |
| 2   | B     | 467 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 115 | GLY  |
| 5   | E     | 48  | GLY  |
| 1   | G     | 96  | ILE  |
| 3   | I     | 115 | GLY  |
| 3   | I     | 126 | GLY  |
| 4   | J     | 160 | TYR  |
| 1   | A     | 176 | ILE  |
| 3   | C     | 85  | GLY  |
| 3   | C     | 98  | GLY  |
| 3   | C     | 105 | VAL  |
| 3   | C     | 304 | PRO  |
| 3   | C     | 368 | PRO  |
| 4   | D     | 160 | TYR  |
| 3   | I     | 47  | GLY  |
| 3   | I     | 85  | GLY  |
| 2   | B     | 399 | 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     | 217/291 (75%) | 202 (93%) | 15 (7%)  | 14          | 45 |
| 1   | G     | 217/291 (75%) | 201 (93%) | 16 (7%)  | 13          | 43 |
| 2   | B     | 256/407 (63%) | 230 (90%) | 26 (10%) | 7           | 29 |
| 2   | H     | 256/407 (63%) | 227 (89%) | 29 (11%) | 5           | 24 |
| 3   | C     | 243/374 (65%) | 213 (88%) | 30 (12%) | 4           | 22 |
| 3   | I     | 243/374 (65%) | 210 (86%) | 33 (14%) | 3           | 18 |
| 4   | D     | 239/283 (84%) | 224 (94%) | 15 (6%)  | 16          | 48 |
| 4   | J     | 239/283 (84%) | 225 (94%) | 14 (6%)  | 18          | 50 |
| 5   | E     | 49/73 (67%)   | 43 (88%)  | 6 (12%)  | 5           | 22 |
| 5   | K     | 49/73 (67%)   | 43 (88%)  | 6 (12%)  | 5           | 22 |
| 6   | F     | 31/38 (82%)   | 27 (87%)  | 4 (13%)  | 4           | 20 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 6   | L     | 31/38 (82%)     | 26 (84%)   | 5 (16%)  | 2           | 13 |
| 9   | T     | 117/138 (85%)   | 116 (99%)  | 1 (1%)   | 70          | 81 |
| 9   | V     | 117/138 (85%)   | 116 (99%)  | 1 (1%)   | 70          | 81 |
| All | All   | 2304/3208 (72%) | 2103 (91%) | 201 (9%) | 9           | 36 |

All (201) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 32  | TRP  |
| 1   | A     | 75  | ASN  |
| 1   | A     | 84  | PRO  |
| 1   | A     | 87  | ASN  |
| 1   | A     | 96  | ILE  |
| 1   | A     | 116 | ILE  |
| 1   | A     | 131 | TRP  |
| 1   | A     | 139 | MET  |
| 1   | A     | 143 | ILE  |
| 1   | A     | 206 | PHE  |
| 1   | A     | 210 | LEU  |
| 1   | A     | 284 | TRP  |
| 1   | A     | 296 | ASN  |
| 1   | A     | 298 | ASN  |
| 1   | A     | 308 | ASP  |
| 2   | B     | 47  | PRO  |
| 2   | B     | 48  | SER  |
| 2   | B     | 49  | ASP  |
| 2   | B     | 55  | MET  |
| 2   | B     | 64  | PRO  |
| 2   | B     | 102 | VAL  |
| 2   | B     | 112 | CYS  |
| 2   | B     | 114 | HIS  |
| 2   | B     | 136 | PRO  |
| 2   | B     | 164 | PRO  |
| 2   | B     | 188 | ASP  |
| 2   | B     | 207 | ILE  |
| 2   | B     | 221 | PRO  |
| 2   | B     | 233 | ASN  |
| 2   | B     | 245 | VAL  |
| 2   | B     | 251 | VAL  |
| 2   | B     | 270 | PRO  |
| 2   | B     | 354 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 359 | MET  |
| 2   | B     | 405 | GLU  |
| 2   | B     | 407 | ASN  |
| 2   | B     | 410 | THR  |
| 2   | B     | 412 | THR  |
| 2   | B     | 413 | ASP  |
| 2   | B     | 415 | PRO  |
| 2   | B     | 447 | PRO  |
| 3   | C     | 77  | PRO  |
| 3   | C     | 78  | GLU  |
| 3   | C     | 95  | LEU  |
| 3   | C     | 110 | PRO  |
| 3   | C     | 124 | VAL  |
| 3   | C     | 137 | PRO  |
| 3   | C     | 157 | MET  |
| 3   | C     | 161 | LEU  |
| 3   | C     | 167 | VAL  |
| 3   | C     | 168 | LEU  |
| 3   | C     | 178 | LYS  |
| 3   | C     | 230 | LEU  |
| 3   | C     | 251 | HIS  |
| 3   | C     | 256 | PRO  |
| 3   | C     | 257 | PHE  |
| 3   | C     | 266 | TRP  |
| 3   | C     | 269 | GLU  |
| 3   | C     | 276 | LEU  |
| 3   | C     | 298 | PRO  |
| 3   | C     | 305 | THR  |
| 3   | C     | 318 | LEU  |
| 3   | C     | 364 | PRO  |
| 3   | C     | 366 | LEU  |
| 3   | C     | 368 | PRO  |
| 3   | C     | 419 | PHE  |
| 3   | C     | 424 | SER  |
| 3   | C     | 428 | THR  |
| 3   | C     | 429 | SER  |
| 3   | C     | 444 | HIS  |
| 3   | C     | 449 | ARG  |
| 4   | D     | 37  | LEU  |
| 4   | D     | 81  | PRO  |
| 4   | D     | 85  | MET  |
| 4   | D     | 93  | TRP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 95  | PRO  |
| 4   | D     | 180 | ARG  |
| 4   | D     | 191 | TRP  |
| 4   | D     | 235 | PHE  |
| 4   | D     | 244 | TYR  |
| 4   | D     | 256 | ILE  |
| 4   | D     | 329 | MET  |
| 4   | D     | 331 | PRO  |
| 4   | D     | 335 | PRO  |
| 4   | D     | 337 | GLU  |
| 4   | D     | 342 | PRO  |
| 5   | E     | 8   | ARG  |
| 5   | E     | 9   | PRO  |
| 5   | E     | 19  | TYR  |
| 5   | E     | 28  | PRO  |
| 5   | E     | 52  | PRO  |
| 5   | E     | 64  | PRO  |
| 6   | F     | 11  | VAL  |
| 6   | F     | 14  | PRO  |
| 6   | F     | 29  | PRO  |
| 6   | F     | 44  | GLN  |
| 1   | G     | 32  | TRP  |
| 1   | G     | 75  | ASN  |
| 1   | G     | 84  | PRO  |
| 1   | G     | 96  | ILE  |
| 1   | G     | 111 | PRO  |
| 1   | G     | 116 | ILE  |
| 1   | G     | 131 | TRP  |
| 1   | G     | 139 | MET  |
| 1   | G     | 143 | ILE  |
| 1   | G     | 173 | PRO  |
| 1   | G     | 206 | PHE  |
| 1   | G     | 210 | LEU  |
| 1   | G     | 284 | TRP  |
| 1   | G     | 296 | ASN  |
| 1   | G     | 298 | ASN  |
| 1   | G     | 308 | ASP  |
| 2   | H     | 47  | PRO  |
| 2   | H     | 48  | SER  |
| 2   | H     | 49  | ASP  |
| 2   | H     | 55  | MET  |
| 2   | H     | 64  | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | H     | 102 | VAL  |
| 2   | H     | 112 | CYS  |
| 2   | H     | 114 | HIS  |
| 2   | H     | 136 | PRO  |
| 2   | H     | 138 | MET  |
| 2   | H     | 164 | PRO  |
| 2   | H     | 188 | ASP  |
| 2   | H     | 191 | ASN  |
| 2   | H     | 207 | ILE  |
| 2   | H     | 233 | ASN  |
| 2   | H     | 245 | VAL  |
| 2   | H     | 251 | VAL  |
| 2   | H     | 264 | PRO  |
| 2   | H     | 265 | ILE  |
| 2   | H     | 270 | PRO  |
| 2   | H     | 354 | LEU  |
| 2   | H     | 360 | PRO  |
| 2   | H     | 405 | GLU  |
| 2   | H     | 407 | ASN  |
| 2   | H     | 410 | THR  |
| 2   | H     | 412 | THR  |
| 2   | H     | 413 | ASP  |
| 2   | H     | 415 | PRO  |
| 2   | H     | 447 | PRO  |
| 3   | I     | 74  | HIS  |
| 3   | I     | 77  | PRO  |
| 3   | I     | 78  | GLU  |
| 3   | I     | 81  | MET  |
| 3   | I     | 95  | LEU  |
| 3   | I     | 108 | THR  |
| 3   | I     | 122 | SER  |
| 3   | I     | 137 | PRO  |
| 3   | I     | 138 | GLU  |
| 3   | I     | 157 | MET  |
| 3   | I     | 158 | THR  |
| 3   | I     | 161 | LEU  |
| 3   | I     | 167 | VAL  |
| 3   | I     | 168 | LEU  |
| 3   | I     | 178 | LYS  |
| 3   | I     | 230 | LEU  |
| 3   | I     | 251 | HIS  |
| 3   | I     | 256 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | I     | 257 | PHE  |
| 3   | I     | 266 | TRP  |
| 3   | I     | 269 | GLU  |
| 3   | I     | 276 | LEU  |
| 3   | I     | 298 | PRO  |
| 3   | I     | 305 | THR  |
| 3   | I     | 318 | LEU  |
| 3   | I     | 366 | LEU  |
| 3   | I     | 368 | PRO  |
| 3   | I     | 419 | PHE  |
| 3   | I     | 424 | SER  |
| 3   | I     | 428 | THR  |
| 3   | I     | 429 | SER  |
| 3   | I     | 444 | HIS  |
| 3   | I     | 449 | ARG  |
| 4   | J     | 37  | LEU  |
| 4   | J     | 63  | LEU  |
| 4   | J     | 81  | PRO  |
| 4   | J     | 93  | TRP  |
| 4   | J     | 95  | PRO  |
| 4   | J     | 165 | SER  |
| 4   | J     | 171 | PRO  |
| 4   | J     | 180 | ARG  |
| 4   | J     | 191 | TRP  |
| 4   | J     | 235 | PHE  |
| 4   | J     | 244 | TYR  |
| 4   | J     | 331 | PRO  |
| 4   | J     | 337 | GLU  |
| 4   | J     | 342 | PRO  |
| 5   | K     | 8   | ARG  |
| 5   | K     | 9   | PRO  |
| 5   | K     | 19  | TYR  |
| 5   | K     | 28  | PRO  |
| 5   | K     | 52  | PRO  |
| 5   | K     | 64  | PRO  |
| 6   | L     | 10  | PRO  |
| 6   | L     | 11  | VAL  |
| 6   | L     | 14  | PRO  |
| 6   | L     | 29  | PRO  |
| 6   | L     | 44  | GLN  |
| 9   | T     | 50  | PRO  |
| 9   | V     | 50  | PRO  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 75  | ASN  |
| 1   | A     | 87  | ASN  |
| 1   | A     | 92  | HIS  |
| 1   | A     | 108 | ASN  |
| 1   | A     | 118 | HIS  |
| 1   | A     | 191 | ASN  |
| 1   | A     | 296 | ASN  |
| 1   | A     | 303 | ASN  |
| 1   | A     | 322 | ASN  |
| 1   | A     | 332 | HIS  |
| 2   | B     | 157 | HIS  |
| 2   | B     | 233 | ASN  |
| 2   | B     | 274 | GLN  |
| 2   | B     | 289 | GLN  |
| 3   | C     | 74  | HIS  |
| 3   | C     | 91  | HIS  |
| 3   | C     | 155 | ASN  |
| 3   | C     | 229 | ASN  |
| 3   | C     | 322 | GLN  |
| 3   | C     | 398 | HIS  |
| 4   | D     | 72  | ASN  |
| 4   | D     | 87  | HIS  |
| 4   | D     | 117 | HIS  |
| 4   | D     | 129 | GLN  |
| 4   | D     | 164 | GLN  |
| 4   | D     | 220 | ASN  |
| 4   | D     | 224 | GLN  |
| 4   | D     | 255 | GLN  |
| 4   | D     | 336 | HIS  |
| 5   | E     | 58  | GLN  |
| 6   | F     | 41  | GLN  |
| 6   | F     | 44  | GLN  |
| 1   | G     | 75  | ASN  |
| 1   | G     | 87  | ASN  |
| 1   | G     | 108 | ASN  |
| 1   | G     | 118 | HIS  |
| 1   | G     | 187 | GLN  |
| 1   | G     | 191 | ASN  |
| 1   | G     | 267 | ASN  |
| 1   | G     | 296 | ASN  |
| 1   | G     | 303 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 322 | ASN  |
| 2   | H     | 157 | HIS  |
| 2   | H     | 233 | ASN  |
| 2   | H     | 289 | GLN  |
| 3   | I     | 56  | HIS  |
| 3   | I     | 74  | HIS  |
| 3   | I     | 91  | HIS  |
| 3   | I     | 132 | HIS  |
| 3   | I     | 155 | ASN  |
| 3   | I     | 229 | ASN  |
| 3   | I     | 322 | GLN  |
| 3   | I     | 398 | HIS  |
| 4   | J     | 61  | HIS  |
| 4   | J     | 72  | ASN  |
| 4   | J     | 87  | HIS  |
| 4   | J     | 117 | HIS  |
| 4   | J     | 129 | GLN  |
| 4   | J     | 164 | GLN  |
| 4   | J     | 220 | ASN  |
| 4   | J     | 224 | GLN  |
| 4   | J     | 255 | GLN  |
| 4   | J     | 332 | GLN  |
| 4   | J     | 336 | HIS  |
| 5   | K     | 58  | GLN  |
| 6   | L     | 41  | GLN  |
| 9   | T     | 106 | ASN  |
| 9   | T     | 118 | HIS  |
| 9   | V     | 106 | ASN  |
| 9   | V     | 118 | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 92 ligands modelled in this entry, 10 are monoatomic - leaving 82 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 |
| 11  | CLA  | B     | 1486 | 2    | 45,49,73     | 1.60 | 7 (15%)  | 54,84,113   | 2.10 | 7 (12%)  |
| 11  | CLA  | I     | 1459 | 3    | 49,53,73     | 1.53 | 7 (14%)  | 58,89,113   | 2.05 | 10 (17%) |
| 11  | CLA  | G     | 1342 | 1    | 69,73,73     | 1.48 | 11 (15%) | 82,113,113  | 1.69 | 10 (12%) |
| 11  | CLA  | H     | 1485 | 2    | 51,55,73     | 1.32 | 10 (19%) | 60,91,113   | 1.73 | 6 (10%)  |
| 11  | CLA  | H     | 1495 | -    | 59,63,73     | 1.54 | 10 (16%) | 70,101,113  | 2.09 | 11 (15%) |
| 11  | CLA  | D     | 1353 | 4    | 54,58,73     | 1.53 | 10 (18%) | 64,95,113   | 1.85 | 8 (12%)  |
| 11  | CLA  | G     | 1343 | -    | 65,69,73     | 1.44 | 10 (15%) | 77,108,113  | 1.91 | 10 (12%) |
| 11  | CLA  | C     | 1461 | 3    | 27,35,73     | 2.57 | 13 (48%) | 32,60,113   | 2.33 | 4 (12%)  |
| 11  | CLA  | I     | 1468 | 3    | 27,35,73     | 2.24 | 9 (33%)  | 32,60,113   | 2.35 | 5 (15%)  |
| 11  | CLA  | B     | 1488 | -    | 69,73,73     | 1.47 | 11 (15%) | 82,113,113  | 1.76 | 11 (13%) |
| 11  | CLA  | C     | 1465 | -    | 69,73,73     | 1.22 | 6 (8%)   | 82,113,113  | 1.75 | 12 (14%) |
| 18  | HEC  | T     | 1138 | 9    | 46,50,50     | 2.11 | 15 (32%) | 58,82,82    | 2.19 | 14 (24%) |
| 11  | CLA  | H     | 1482 | -    | 69,73,73     | 1.56 | 10 (14%) | 82,113,113  | 1.93 | 10 (12%) |
| 11  | CLA  | I     | 1470 | -    | 45,49,73     | 1.54 | 9 (20%)  | 54,84,113   | 2.03 | 8 (14%)  |
| 11  | CLA  | B     | 1496 | -    | 69,73,73     | 1.23 | 7 (10%)  | 82,113,113  | 1.79 | 11 (13%) |
| 11  | CLA  | C     | 1467 | 3    | 51,55,73     | 1.58 | 5 (9%)   | 60,91,113   | 1.96 | 9 (15%)  |
| 11  | CLA  | C     | 1469 | 3    | 45,49,73     | 1.48 | 7 (15%)  | 54,84,113   | 2.20 | 8 (14%)  |
| 12  | PHO  | J     | 1352 | -    | 48,59,69     | 1.75 | 6 (12%)  | 43,87,99    | 2.34 | 13 (30%) |
| 11  | CLA  | C     | 1466 | 3    | 54,58,73     | 1.60 | 9 (16%)  | 64,95,113   | 2.01 | 11 (17%) |
| 11  | CLA  | I     | 1471 | -    | 45,49,73     | 1.63 | 6 (13%)  | 54,84,113   | 2.12 | 8 (14%)  |
| 11  | CLA  | I     | 1460 | 3    | 51,55,73     | 1.56 | 8 (15%)  | 60,91,113   | 1.91 | 7 (11%)  |
| 11  | CLA  | H     | 1486 | 2    | 45,49,73     | 1.55 | 8 (17%)  | 54,84,113   | 1.99 | 6 (11%)  |
| 11  | CLA  | B     | 1494 | -    | 69,73,73     | 1.29 | 11 (15%) | 82,113,113  | 1.74 | 10 (12%) |
| 12  | PHO  | D     | 1352 | -    | 48,59,69     | 1.75 | 9 (18%)  | 43,87,99    | 2.47 | 15 (34%) |
| 15  | PL9  | D     | 1354 | -    | 6,6,55       | 2.06 | 2 (33%)  | 6,6,69      | 1.06 | 0        |
| 11  | CLA  | H     | 1497 | 2    | 45,49,73     | 1.60 | 13 (28%) | 54,84,113   | 2.14 | 8 (14%)  |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 11  | CLA  | I     | 1466 | 3    | 54,58,73     | 1.59 | 8 (14%)  | 64,95,113   | 2.01 | 11 (17%) |
| 11  | CLA  | J     | 1353 | 4    | 54,58,73     | 1.51 | 8 (14%)  | 64,95,113   | 1.79 | 7 (10%)  |
| 11  | CLA  | H     | 1494 | -    | 69,73,73     | 1.39 | 11 (15%) | 82,113,113  | 1.86 | 11 (13%) |
| 11  | CLA  | B     | 1489 | 2    | 54,58,73     | 1.34 | 5 (9%)   | 64,95,113   | 2.02 | 10 (15%) |
| 11  | CLA  | B     | 1493 | -    | 49,53,73     | 1.62 | 5 (10%)  | 58,89,113   | 2.08 | 9 (15%)  |
| 11  | CLA  | H     | 1490 | 2    | 49,53,73     | 2.08 | 11 (22%) | 58,89,113   | 2.03 | 7 (12%)  |
| 11  | CLA  | H     | 1483 | 2    | 64,68,73     | 1.37 | 8 (12%)  | 76,107,113  | 1.64 | 9 (11%)  |
| 11  | CLA  | H     | 1488 | -    | 69,73,73     | 1.51 | 12 (17%) | 82,113,113  | 1.75 | 9 (10%)  |
| 11  | CLA  | B     | 1492 | 2    | 69,73,73     | 1.27 | 9 (13%)  | 82,113,113  | 1.95 | 13 (15%) |
| 11  | CLA  | H     | 1484 | -    | 49,53,73     | 1.29 | 6 (12%)  | 58,89,113   | 1.83 | 6 (10%)  |
| 11  | CLA  | C     | 1470 | -    | 45,49,73     | 1.54 | 6 (13%)  | 54,84,113   | 2.13 | 7 (12%)  |
| 11  | CLA  | A     | 1344 | -    | 49,53,73     | 1.60 | 7 (14%)  | 58,89,113   | 1.99 | 9 (15%)  |
| 11  | CLA  | C     | 1460 | 3    | 51,55,73     | 1.57 | 6 (11%)  | 60,91,113   | 1.99 | 9 (15%)  |
| 11  | CLA  | H     | 1496 | -    | 69,73,73     | 1.26 | 10 (14%) | 82,113,113  | 1.90 | 12 (14%) |
| 11  | CLA  | A     | 1346 | -    | 55,59,73     | 1.60 | 9 (16%)  | 64,96,113   | 1.90 | 8 (12%)  |
| 16  | HEM  | E     | 1085 | 6,5  | 32,32,50     | 2.38 | 13 (40%) | 30,54,82    | 1.61 | 4 (13%)  |
| 11  | CLA  | C     | 1464 | 3    | 60,64,73     | 1.37 | 7 (11%)  | 71,102,113  | 1.90 | 13 (18%) |
| 11  | CLA  | B     | 1483 | 2    | 64,68,73     | 1.45 | 8 (12%)  | 76,107,113  | 1.70 | 9 (11%)  |
| 11  | CLA  | C     | 1462 | -    | 60,64,73     | 1.61 | 14 (23%) | 71,102,113  | 1.76 | 12 (16%) |
| 11  | CLA  | I     | 1462 | -    | 60,64,73     | 1.69 | 14 (23%) | 71,102,113  | 1.77 | 12 (16%) |
| 11  | CLA  | C     | 1471 | -    | 45,49,73     | 1.60 | 8 (17%)  | 54,84,113   | 2.09 | 5 (9%)   |
| 11  | CLA  | C     | 1463 | 3    | 59,63,73     | 1.72 | 9 (15%)  | 70,101,113  | 1.96 | 9 (12%)  |
| 11  | CLA  | I     | 1463 | 3    | 59,63,73     | 1.76 | 7 (11%)  | 70,101,113  | 2.01 | 9 (12%)  |
| 15  | PL9  | J     | 1354 | -    | 6,6,55       | 1.96 | 2 (33%)  | 6,6,69      | 1.09 | 0        |
| 18  | HEC  | V     | 1138 | 9    | 46,50,50     | 2.10 | 15 (32%) | 58,82,82    | 2.21 | 12 (20%) |
| 11  | CLA  | C     | 1468 | 3    | 27,35,73     | 2.22 | 9 (33%)  | 32,60,113   | 2.43 | 5 (15%)  |
| 17  | BCR  | F     | 1046 | -    | 41,41,41     | 1.71 | 8 (19%)  | 56,56,56    | 2.21 | 24 (42%) |
| 16  | HEM  | L     | 1046 | 6,5  | 32,32,50     | 2.31 | 13 (40%) | 30,54,82    | 1.60 | 5 (16%)  |
| 11  | CLA  | G     | 1344 | -    | 49,53,73     | 1.52 | 6 (12%)  | 58,89,113   | 1.98 | 9 (15%)  |
| 11  | CLA  | B     | 1487 | -    | 69,73,73     | 1.62 | 12 (17%) | 82,113,113  | 1.70 | 12 (14%) |
| 11  | CLA  | J     | 1351 | 4    | 69,73,73     | 2.17 | 11 (15%) | 82,113,113  | 2.05 | 13 (15%) |
| 11  | CLA  | B     | 1495 | -    | 59,63,73     | 1.49 | 10 (16%) | 70,101,113  | 2.03 | 12 (17%) |
| 11  | CLA  | I     | 1467 | 3    | 51,55,73     | 1.37 | 4 (7%)   | 60,91,113   | 1.94 | 8 (13%)  |
| 11  | CLA  | B     | 1491 | -    | 27,35,73     | 2.11 | 7 (25%)  | 32,60,113   | 2.38 | 4 (12%)  |
| 17  | BCR  | L     | 1047 | -    | 41,41,41     | 1.66 | 7 (17%)  | 56,56,56    | 2.21 | 22 (39%) |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 11  | CLA  | B     | 1485 | 2    | 51,55,73     | 1.33 | 6 (11%)  | 60,91,113   | 1.78 | 7 (11%)  |
| 11  | CLA  | A     | 1343 | -    | 65,69,73     | 1.29 | 6 (9%)   | 77,108,113  | 1.84 | 11 (14%) |
| 11  | CLA  | A     | 1342 | 1    | 69,73,73     | 1.35 | 7 (10%)  | 82,113,113  | 1.81 | 12 (14%) |
| 11  | CLA  | I     | 1461 | 3    | 27,35,73     | 2.48 | 13 (48%) | 32,60,113   | 2.29 | 4 (12%)  |
| 11  | CLA  | H     | 1492 | 2    | 69,73,73     | 1.22 | 5 (7%)   | 82,113,113  | 1.94 | 12 (14%) |
| 11  | CLA  | B     | 1490 | 2    | 49,53,73     | 2.10 | 11 (22%) | 58,89,113   | 1.94 | 6 (10%)  |
| 11  | CLA  | I     | 1464 | 3    | 60,64,73     | 1.39 | 9 (15%)  | 71,102,113  | 1.84 | 12 (16%) |
| 11  | CLA  | H     | 1493 | -    | 49,53,73     | 1.63 | 6 (12%)  | 58,89,113   | 2.11 | 10 (17%) |
| 11  | CLA  | B     | 1497 | 2    | 45,49,73     | 1.50 | 9 (20%)  | 54,84,113   | 2.07 | 8 (14%)  |
| 12  | PHO  | G     | 1345 | -    | 58,69,69     | 1.55 | 8 (13%)  | 55,99,99    | 2.12 | 15 (27%) |
| 11  | CLA  | B     | 1482 | -    | 69,73,73     | 1.42 | 12 (17%) | 82,113,113  | 1.91 | 9 (10%)  |
| 11  | CLA  | G     | 1346 | -    | 55,59,73     | 1.60 | 8 (14%)  | 64,96,113   | 1.85 | 7 (10%)  |
| 11  | CLA  | I     | 1465 | -    | 69,73,73     | 1.23 | 8 (11%)  | 82,113,113  | 1.76 | 12 (14%) |
| 11  | CLA  | D     | 1351 | 4    | 69,73,73     | 1.65 | 10 (14%) | 82,113,113  | 1.98 | 13 (15%) |
| 11  | CLA  | C     | 1459 | 3    | 49,53,73     | 1.51 | 10 (20%) | 58,89,113   | 1.89 | 10 (17%) |
| 11  | CLA  | B     | 1484 | -    | 49,53,73     | 1.36 | 6 (12%)  | 58,89,113   | 1.90 | 6 (10%)  |
| 11  | CLA  | I     | 1469 | 3    | 45,49,73     | 1.62 | 7 (15%)  | 54,84,113   | 2.25 | 8 (14%)  |
| 11  | CLA  | H     | 1487 | -    | 69,73,73     | 1.63 | 12 (17%) | 82,113,113  | 1.70 | 11 (13%) |
| 11  | CLA  | H     | 1489 | 2    | 54,58,73     | 1.44 | 4 (7%)   | 64,95,113   | 2.11 | 8 (12%)  |
| 12  | PHO  | A     | 1345 | -    | 58,69,69     | 1.55 | 6 (10%)  | 55,99,99    | 2.14 | 16 (29%) |
| 11  | CLA  | H     | 1491 | -    | 27,35,73     | 2.17 | 9 (33%)  | 32,60,113   | 2.26 | 4 (12%)  |

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 |
|-----|------|-------|------|------|-----------|---------------|-------|
| 11  | CLA  | B     | 1486 | 2    | 1/1/10/20 | 4/10/86/115   | -     |
| 11  | CLA  | I     | 1459 | 3    | 1/1/11/20 | 9/15/91/115   | -     |
| 11  | CLA  | G     | 1342 | 1    | 1/1/15/20 | 5/39/115/115  | -     |
| 11  | CLA  | H     | 1485 | 2    | 1/1/11/20 | 9/18/94/115   | -     |
| 11  | CLA  | H     | 1495 | -    | 1/1/13/20 | 11/27/103/115 | -     |
| 11  | CLA  | D     | 1353 | 4    | 1/1/12/20 | 5/21/97/115   | -     |
| 11  | CLA  | G     | 1343 | -    | 1/1/14/20 | 17/35/111/115 | -     |
| 11  | CLA  | C     | 1461 | 3    | 1/1/5/20  | -             | -     |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 11  | CLA  | I     | 1468 | 3    | 1/1/5/20  | -             | -       |
| 11  | CLA  | B     | 1488 | -    | 1/1/15/20 | 16/39/115/115 | -       |
| 11  | CLA  | C     | 1465 | -    | 1/1/15/20 | 17/39/115/115 | -       |
| 18  | HEC  | T     | 1138 | 9    | -         | 8/14/54/54    | -       |
| 11  | CLA  | H     | 1482 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 11  | CLA  | I     | 1470 | -    | 1/1/10/20 | 4/10/86/115   | -       |
| 11  | CLA  | B     | 1496 | -    | 1/1/15/20 | 18/39/115/115 | -       |
| 11  | CLA  | C     | 1467 | 3    | 1/1/11/20 | 6/18/94/115   | -       |
| 11  | CLA  | C     | 1469 | 3    | 1/1/10/20 | 4/10/86/115   | -       |
| 12  | PHO  | J     | 1352 | -    | -         | 7/25/91/103   | 0/5/6/6 |
| 11  | CLA  | C     | 1466 | 3    | 1/1/12/20 | 9/21/97/115   | -       |
| 11  | CLA  | I     | 1471 | -    | 1/1/10/20 | 6/10/86/115   | -       |
| 11  | CLA  | I     | 1460 | 3    | 1/1/11/20 | 4/18/94/115   | -       |
| 11  | CLA  | H     | 1486 | 2    | 1/1/10/20 | 4/10/86/115   | -       |
| 11  | CLA  | B     | 1494 | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 12  | PHO  | D     | 1352 | -    | -         | 7/25/91/103   | 0/5/6/6 |
| 15  | PL9  | D     | 1354 | -    | -         | -             | 0/1/1/1 |
| 11  | CLA  | H     | 1497 | 2    | 1/1/10/20 | 4/10/86/115   | -       |
| 11  | CLA  | I     | 1466 | 3    | 1/1/12/20 | 9/21/97/115   | -       |
| 11  | CLA  | J     | 1353 | 4    | 1/1/12/20 | 5/21/97/115   | -       |
| 11  | CLA  | H     | 1494 | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 11  | CLA  | B     | 1489 | 2    | 1/1/12/20 | 3/21/97/115   | -       |
| 11  | CLA  | B     | 1493 | -    | 1/1/11/20 | 8/15/91/115   | -       |
| 11  | CLA  | H     | 1490 | 2    | 1/1/11/20 | 10/15/91/115  | -       |
| 11  | CLA  | H     | 1483 | 2    | 1/1/14/20 | 12/33/109/115 | -       |
| 11  | CLA  | H     | 1488 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 11  | CLA  | B     | 1492 | 2    | 1/1/15/20 | 15/39/115/115 | -       |
| 11  | CLA  | H     | 1484 | -    | 1/1/11/20 | 6/15/91/115   | -       |
| 11  | CLA  | C     | 1470 | -    | 1/1/10/20 | 4/10/86/115   | -       |
| 11  | CLA  | A     | 1344 | -    | 1/1/11/20 | 7/15/91/115   | -       |
| 11  | CLA  | C     | 1460 | 3    | 1/1/11/20 | 4/18/94/115   | -       |
| 11  | CLA  | H     | 1496 | -    | 1/1/15/20 | 17/39/115/115 | -       |
| 11  | CLA  | A     | 1346 | -    | 1/1/12/20 | 6/23/99/115   | -       |
| 11  | CLA  | C     | 1464 | 3    | 1/1/13/20 | 15/29/105/115 | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 11  | CLA  | B     | 1483 | 2    | 1/1/14/20 | 12/33/109/115 | -       |
| 11  | CLA  | C     | 1462 | -    | 1/1/13/20 | 8/29/105/115  | -       |
| 11  | CLA  | I     | 1462 | -    | 1/1/13/20 | 8/29/105/115  | -       |
| 11  | CLA  | C     | 1471 | -    | 1/1/10/20 | 6/10/86/115   | -       |
| 11  | CLA  | C     | 1463 | 3    | 1/1/13/20 | 11/27/103/115 | -       |
| 11  | CLA  | I     | 1463 | 3    | 2/2/13/20 | 11/27/103/115 | -       |
| 15  | PL9  | J     | 1354 | -    | -         | -             | 0/1/1/1 |
| 18  | HEC  | V     | 1138 | 9    | -         | 8/14/54/54    | -       |
| 11  | CLA  | C     | 1468 | 3    | 1/1/5/20  | -             | -       |
| 17  | BCR  | F     | 1046 | -    | -         | 3/29/63/63    | 0/2/2/2 |
| 11  | CLA  | G     | 1344 | -    | 1/1/11/20 | 7/15/91/115   | -       |
| 11  | CLA  | B     | 1487 | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 11  | CLA  | J     | 1351 | 4    | 1/1/15/20 | 12/39/115/115 | -       |
| 11  | CLA  | B     | 1495 | -    | 1/1/13/20 | 11/27/103/115 | -       |
| 11  | CLA  | I     | 1467 | 3    | 1/1/11/20 | 7/18/94/115   | -       |
| 11  | CLA  | B     | 1491 | -    | 1/1/5/20  | -             | -       |
| 17  | BCR  | L     | 1047 | -    | -         | 3/29/63/63    | 0/2/2/2 |
| 11  | CLA  | B     | 1485 | 2    | 1/1/11/20 | 9/18/94/115   | -       |
| 11  | CLA  | A     | 1343 | -    | 1/1/14/20 | 17/35/111/115 | -       |
| 11  | CLA  | A     | 1342 | 1    | 1/1/15/20 | 5/39/115/115  | -       |
| 11  | CLA  | I     | 1461 | 3    | 1/1/5/20  | -             | -       |
| 11  | CLA  | H     | 1492 | 2    | 1/1/15/20 | 15/39/115/115 | -       |
| 11  | CLA  | B     | 1490 | 2    | 1/1/11/20 | 10/15/91/115  | -       |
| 11  | CLA  | I     | 1464 | 3    | 1/1/13/20 | 15/29/105/115 | -       |
| 11  | CLA  | H     | 1493 | -    | 1/1/11/20 | 7/15/91/115   | -       |
| 11  | CLA  | B     | 1497 | 2    | 1/1/10/20 | 4/10/86/115   | -       |
| 12  | PHO  | G     | 1345 | -    | -         | 13/37/103/103 | 0/5/6/6 |
| 11  | CLA  | B     | 1482 | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 11  | CLA  | G     | 1346 | -    | 1/1/12/20 | 5/23/99/115   | -       |
| 11  | CLA  | I     | 1465 | -    | 1/1/15/20 | 16/39/115/115 | -       |
| 11  | CLA  | D     | 1351 | 4    | 1/1/15/20 | 11/39/115/115 | -       |
| 11  | CLA  | C     | 1459 | 3    | 1/1/11/20 | 9/15/91/115   | -       |
| 11  | CLA  | B     | 1484 | -    | 1/1/11/20 | 6/15/91/115   | -       |
| 11  | CLA  | I     | 1469 | 3    | 1/1/10/20 | 4/10/86/115   | -       |
| 11  | CLA  | H     | 1487 | -    | 1/1/15/20 | 10/39/115/115 | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 11  | CLA  | H     | 1489 | 2    | 1/1/12/20 | 3/21/97/115   | -       |
| 12  | PHO  | A     | 1345 | -    | -         | 10/37/103/103 | 0/5/6/6 |
| 11  | CLA  | H     | 1491 | -    | 1/1/5/20  | -             | -       |

All (706) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 11  | J     | 1351 | CLA  | MG-NA   | 13.61 | 2.38        | 2.06     |
| 11  | H     | 1490 | CLA  | MG-NA   | 9.48  | 2.28        | 2.06     |
| 11  | B     | 1490 | CLA  | MG-NA   | 9.35  | 2.28        | 2.06     |
| 11  | I     | 1463 | CLA  | MG-NA   | 9.33  | 2.28        | 2.06     |
| 11  | C     | 1461 | CLA  | MG-NA   | 8.23  | 2.25        | 2.06     |
| 11  | C     | 1463 | CLA  | MG-NA   | 7.88  | 2.25        | 2.06     |
| 11  | C     | 1467 | CLA  | MG-NA   | 7.62  | 2.24        | 2.06     |
| 11  | I     | 1461 | CLA  | MG-NA   | 7.22  | 2.23        | 2.06     |
| 11  | I     | 1469 | CLA  | MG-NA   | 7.21  | 2.23        | 2.06     |
| 12  | A     | 1345 | PHO  | C3B-C4B | 7.17  | 1.48        | 1.41     |
| 11  | C     | 1460 | CLA  | MG-NA   | 6.91  | 2.22        | 2.06     |
| 11  | G     | 1346 | CLA  | MG-NA   | 6.78  | 2.22        | 2.06     |
| 11  | B     | 1493 | CLA  | MG-NA   | 6.68  | 2.22        | 2.06     |
| 11  | I     | 1471 | CLA  | MG-NA   | 6.47  | 2.21        | 2.06     |
| 11  | H     | 1482 | CLA  | MG-NA   | 6.44  | 2.21        | 2.06     |
| 11  | C     | 1468 | CLA  | MG-NA   | 6.42  | 2.21        | 2.06     |
| 11  | D     | 1351 | CLA  | MG-NA   | 6.26  | 2.21        | 2.06     |
| 11  | I     | 1468 | CLA  | MG-NA   | 6.17  | 2.20        | 2.06     |
| 12  | J     | 1352 | PHO  | C3B-C4B | 6.16  | 1.47        | 1.41     |
| 18  | T     | 1138 | HEC  | CBB-CAB | -6.12 | 1.26        | 1.49     |
| 11  | I     | 1466 | CLA  | MG-NA   | 6.12  | 2.20        | 2.06     |
| 11  | H     | 1493 | CLA  | MG-NA   | 6.06  | 2.20        | 2.06     |
| 18  | V     | 1138 | HEC  | CBB-CAB | -6.04 | 1.27        | 1.49     |
| 11  | C     | 1466 | CLA  | MG-NA   | 5.94  | 2.20        | 2.06     |
| 11  | I     | 1467 | CLA  | MG-NA   | 5.94  | 2.20        | 2.06     |
| 11  | C     | 1471 | CLA  | MG-NA   | 5.92  | 2.20        | 2.06     |
| 11  | I     | 1459 | CLA  | MG-NA   | 5.83  | 2.20        | 2.06     |
| 11  | A     | 1346 | CLA  | MG-NA   | 5.81  | 2.20        | 2.06     |
| 11  | H     | 1489 | CLA  | MG-NA   | 5.81  | 2.20        | 2.06     |
| 12  | G     | 1345 | PHO  | C1B-C2B | 5.76  | 1.45        | 1.39     |
| 11  | I     | 1460 | CLA  | MG-NA   | 5.72  | 2.19        | 2.06     |
| 11  | C     | 1470 | CLA  | MG-NA   | 5.70  | 2.19        | 2.06     |
| 12  | D     | 1352 | PHO  | C3B-C4B | 5.66  | 1.47        | 1.41     |
| 11  | A     | 1342 | CLA  | MG-NA   | 5.62  | 2.19        | 2.06     |
| 11  | C     | 1469 | CLA  | MG-NA   | 5.55  | 2.19        | 2.06     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 11  | J     | 1351 | CLA  | MG-ND   | 5.50  | 2.16        | 2.05     |
| 12  | G     | 1345 | PHO  | C3B-C4B | 5.46  | 1.47        | 1.41     |
| 11  | A     | 1344 | CLA  | MG-NA   | 5.45  | 2.19        | 2.06     |
| 11  | B     | 1491 | CLA  | MG-NA   | 5.43  | 2.19        | 2.06     |
| 12  | D     | 1352 | PHO  | C1B-C2B | 5.42  | 1.45        | 1.39     |
| 11  | G     | 1344 | CLA  | MG-NA   | 5.38  | 2.19        | 2.06     |
| 11  | B     | 1487 | CLA  | MG-NA   | 5.33  | 2.18        | 2.06     |
| 11  | A     | 1344 | CLA  | CAA-C2A | 5.31  | 1.63        | 1.54     |
| 17  | F     | 1046 | BCR  | C1-C6   | 5.26  | 1.60        | 1.53     |
| 16  | L     | 1046 | HEM  | C4A-NA  | -5.23 | 1.32        | 1.39     |
| 11  | B     | 1486 | CLA  | MG-NA   | 5.20  | 2.18        | 2.06     |
| 11  | H     | 1487 | CLA  | MG-NA   | 5.12  | 2.18        | 2.06     |
| 11  | B     | 1483 | CLA  | MG-NA   | 5.08  | 2.18        | 2.06     |
| 11  | H     | 1495 | CLA  | MG-NA   | 5.07  | 2.18        | 2.06     |
| 11  | H     | 1491 | CLA  | MG-NA   | 5.07  | 2.18        | 2.06     |
| 11  | I     | 1470 | CLA  | MG-NA   | 5.07  | 2.18        | 2.06     |
| 18  | V     | 1138 | HEC  | CAC-C3C | 5.01  | 1.51        | 1.35     |
| 11  | D     | 1351 | CLA  | MG-NB   | 5.01  | 2.15        | 2.05     |
| 11  | D     | 1351 | CLA  | MG-NC   | 4.97  | 2.18        | 2.06     |
| 11  | B     | 1489 | CLA  | MG-NA   | 4.91  | 2.17        | 2.06     |
| 12  | A     | 1345 | PHO  | C1B-C2B | 4.91  | 1.44        | 1.39     |
| 11  | H     | 1491 | CLA  | CAD-C3D | -4.90 | 1.41        | 1.50     |
| 16  | E     | 1085 | HEM  | C4A-NA  | -4.87 | 1.33        | 1.39     |
| 11  | G     | 1342 | CLA  | MG-NA   | 4.85  | 2.17        | 2.06     |
| 11  | I     | 1462 | CLA  | CAA-C2A | 4.83  | 1.62        | 1.54     |
| 12  | J     | 1352 | PHO  | C1B-C2B | 4.81  | 1.44        | 1.39     |
| 11  | B     | 1491 | CLA  | CAD-C3D | -4.80 | 1.41        | 1.50     |
| 11  | B     | 1487 | CLA  | CAA-C2A | 4.72  | 1.62        | 1.54     |
| 11  | C     | 1464 | CLA  | MG-NA   | 4.72  | 2.17        | 2.06     |
| 16  | L     | 1046 | HEM  | C2A-C1A | 4.69  | 1.50        | 1.40     |
| 11  | H     | 1488 | CLA  | MG-NA   | 4.69  | 2.17        | 2.06     |
| 11  | B     | 1495 | CLA  | MG-NA   | 4.69  | 2.17        | 2.06     |
| 11  | H     | 1487 | CLA  | CAA-C2A | 4.68  | 1.62        | 1.54     |
| 18  | T     | 1138 | HEC  | CAC-C3C | 4.67  | 1.50        | 1.35     |
| 11  | B     | 1487 | CLA  | CHB-C1B | -4.65 | 1.29        | 1.39     |
| 11  | G     | 1343 | CLA  | CAA-C2A | 4.62  | 1.62        | 1.54     |
| 16  | E     | 1085 | HEM  | C2A-C1A | 4.62  | 1.50        | 1.40     |
| 11  | B     | 1488 | CLA  | CAA-C2A | 4.54  | 1.62        | 1.54     |
| 11  | H     | 1492 | CLA  | MG-NA   | 4.52  | 2.17        | 2.06     |
| 11  | H     | 1487 | CLA  | CHB-C1B | -4.51 | 1.29        | 1.39     |
| 11  | C     | 1462 | CLA  | CAA-C2A | 4.49  | 1.62        | 1.54     |
| 17  | L     | 1047 | BCR  | C1-C6   | 4.41  | 1.59        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 11  | B     | 1486 | CLA  | C3A-C2A | -4.40 | 1.50        | 1.54     |
| 11  | C     | 1466 | CLA  | CAA-C2A | 4.36  | 1.62        | 1.54     |
| 11  | B     | 1488 | CLA  | MG-NA   | 4.34  | 2.16        | 2.06     |
| 11  | B     | 1482 | CLA  | CAA-C2A | 4.33  | 1.62        | 1.54     |
| 11  | D     | 1353 | CLA  | MG-NA   | 4.28  | 2.16        | 2.06     |
| 11  | C     | 1463 | CLA  | CAA-C2A | 4.27  | 1.61        | 1.54     |
| 11  | H     | 1482 | CLA  | CAA-C2A | 4.27  | 1.61        | 1.54     |
| 17  | L     | 1047 | BCR  | C30-C25 | 4.22  | 1.59        | 1.53     |
| 11  | B     | 1492 | CLA  | MG-NA   | 4.21  | 2.16        | 2.06     |
| 11  | B     | 1494 | CLA  | MG-NA   | 4.16  | 2.16        | 2.06     |
| 18  | V     | 1138 | HEC  | CAB-C3B | 4.15  | 1.48        | 1.35     |
| 11  | A     | 1343 | CLA  | CAA-C2A | 4.12  | 1.61        | 1.54     |
| 11  | H     | 1483 | CLA  | MG-NA   | 4.12  | 2.16        | 2.06     |
| 18  | T     | 1138 | HEC  | CAB-C3B | 4.09  | 1.48        | 1.35     |
| 11  | H     | 1488 | CLA  | CAA-C2A | 4.09  | 1.61        | 1.54     |
| 11  | C     | 1459 | CLA  | MG-NA   | 4.08  | 2.16        | 2.06     |
| 11  | B     | 1496 | CLA  | CAA-C2A | 4.07  | 1.61        | 1.54     |
| 11  | H     | 1494 | CLA  | MG-NA   | 4.04  | 2.15        | 2.06     |
| 11  | B     | 1491 | CLA  | C3B-C4B | 4.03  | 1.48        | 1.40     |
| 11  | C     | 1465 | CLA  | CHB-C1B | -4.02 | 1.30        | 1.39     |
| 11  | H     | 1491 | CLA  | C3B-C4B | 3.97  | 1.48        | 1.40     |
| 11  | C     | 1461 | CLA  | C3B-C4B | 3.97  | 1.48        | 1.40     |
| 17  | F     | 1046 | BCR  | C2-C1   | 3.97  | 1.63        | 1.54     |
| 11  | I     | 1462 | CLA  | CHB-C1B | -3.97 | 1.30        | 1.39     |
| 11  | H     | 1486 | CLA  | C3A-C2A | -3.94 | 1.51        | 1.54     |
| 11  | B     | 1490 | CLA  | CAA-C2A | 3.93  | 1.61        | 1.54     |
| 16  | L     | 1046 | HEM  | FE-NA   | 3.93  | 2.08        | 1.95     |
| 11  | I     | 1461 | CLA  | MG-NC   | 3.89  | 2.15        | 2.06     |
| 11  | C     | 1462 | CLA  | C1D-ND  | -3.88 | 1.32        | 1.37     |
| 11  | C     | 1468 | CLA  | C2B-C1B | 3.88  | 1.48        | 1.40     |
| 11  | H     | 1496 | CLA  | MG-NA   | 3.87  | 2.15        | 2.06     |
| 11  | I     | 1464 | CLA  | MG-NA   | 3.86  | 2.15        | 2.06     |
| 11  | I     | 1468 | CLA  | CAD-C3D | -3.85 | 1.43        | 1.50     |
| 11  | G     | 1344 | CLA  | CAA-C2A | 3.83  | 1.61        | 1.54     |
| 11  | B     | 1482 | CLA  | MG-NA   | 3.81  | 2.15        | 2.06     |
| 11  | B     | 1497 | CLA  | MG-NA   | 3.81  | 2.15        | 2.06     |
| 16  | E     | 1085 | HEM  | C3A-C2A | 3.81  | 1.52        | 1.39     |
| 11  | B     | 1485 | CLA  | CHB-C1B | -3.80 | 1.30        | 1.39     |
| 11  | J     | 1353 | CLA  | MG-NA   | 3.79  | 2.15        | 2.06     |
| 11  | I     | 1465 | CLA  | CHB-C1B | -3.75 | 1.31        | 1.39     |
| 11  | H     | 1484 | CLA  | CAA-C2A | 3.72  | 1.60        | 1.54     |
| 16  | E     | 1085 | HEM  | FE-NA   | 3.71  | 2.07        | 1.95     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 11  | B     | 1488 | CLA  | CHB-C1B | -3.70 | 1.31        | 1.39     |
| 11  | C     | 1468 | CLA  | CAD-C3D | -3.64 | 1.43        | 1.50     |
| 17  | L     | 1047 | BCR  | C29-C30 | 3.64  | 1.62        | 1.54     |
| 11  | B     | 1491 | CLA  | C2B-C1B | 3.64  | 1.48        | 1.40     |
| 11  | G     | 1343 | CLA  | C1D-ND  | -3.64 | 1.33        | 1.37     |
| 11  | I     | 1468 | CLA  | MG-NC   | 3.63  | 2.14        | 2.06     |
| 11  | H     | 1486 | CLA  | MG-NA   | 3.61  | 2.14        | 2.06     |
| 11  | B     | 1490 | CLA  | O1A-CGA | 3.61  | 1.33        | 1.22     |
| 11  | G     | 1342 | CLA  | CHB-C1B | -3.61 | 1.31        | 1.39     |
| 11  | D     | 1353 | CLA  | CAA-C2A | 3.60  | 1.60        | 1.54     |
| 17  | F     | 1046 | BCR  | C30-C25 | 3.60  | 1.58        | 1.53     |
| 11  | I     | 1460 | CLA  | CAA-C2A | 3.59  | 1.60        | 1.54     |
| 18  | V     | 1138 | HEC  | CHB-C1B | -3.59 | 1.31        | 1.39     |
| 17  | F     | 1046 | BCR  | C29-C30 | 3.58  | 1.62        | 1.54     |
| 16  | E     | 1085 | HEM  | C4D-ND  | -3.57 | 1.32        | 1.40     |
| 11  | C     | 1461 | CLA  | CAD-C3D | -3.55 | 1.44        | 1.50     |
| 11  | H     | 1483 | CLA  | CHB-C1B | -3.54 | 1.31        | 1.39     |
| 17  | L     | 1047 | BCR  | C2-C1   | 3.54  | 1.62        | 1.54     |
| 11  | H     | 1489 | CLA  | C1D-ND  | -3.53 | 1.33        | 1.37     |
| 11  | C     | 1461 | CLA  | C2B-C1B | 3.53  | 1.47        | 1.40     |
| 16  | L     | 1046 | HEM  | C3D-C2D | 3.52  | 1.43        | 1.35     |
| 11  | B     | 1487 | CLA  | C5-C3   | 3.50  | 1.58        | 1.51     |
| 11  | I     | 1461 | CLA  | CAD-C3D | -3.49 | 1.44        | 1.50     |
| 16  | L     | 1046 | HEM  | FE-NC   | 3.49  | 2.06        | 1.95     |
| 11  | A     | 1346 | CLA  | CAA-C2A | 3.49  | 1.60        | 1.54     |
| 11  | C     | 1460 | CLA  | CAA-C2A | 3.46  | 1.60        | 1.54     |
| 11  | I     | 1461 | CLA  | C3B-C4B | 3.46  | 1.47        | 1.40     |
| 11  | B     | 1496 | CLA  | MG-NC   | 3.46  | 2.14        | 2.06     |
| 18  | T     | 1138 | HEC  | CHB-C1B | -3.45 | 1.31        | 1.39     |
| 11  | D     | 1351 | CLA  | CHB-C1B | -3.45 | 1.31        | 1.39     |
| 11  | H     | 1493 | CLA  | CAA-C2A | 3.45  | 1.60        | 1.54     |
| 16  | E     | 1085 | HEM  | C1D-ND  | -3.45 | 1.33        | 1.38     |
| 11  | H     | 1488 | CLA  | CHB-C1B | -3.44 | 1.31        | 1.39     |
| 11  | A     | 1342 | CLA  | CHB-C1B | -3.43 | 1.31        | 1.39     |
| 11  | I     | 1466 | CLA  | CAA-C2A | 3.42  | 1.60        | 1.54     |
| 11  | I     | 1462 | CLA  | C1-C2   | 3.42  | 1.58        | 1.49     |
| 12  | G     | 1345 | PHO  | C1D-C2D | 3.41  | 1.43        | 1.39     |
| 11  | H     | 1492 | CLA  | CHB-C1B | -3.40 | 1.31        | 1.39     |
| 11  | I     | 1462 | CLA  | C2-C3   | 3.39  | 1.40        | 1.33     |
| 16  | E     | 1085 | HEM  | C3A-C4A | 3.39  | 1.47        | 1.40     |
| 11  | H     | 1486 | CLA  | C1D-ND  | -3.39 | 1.33        | 1.37     |
| 16  | E     | 1085 | HEM  | FE-NB   | 3.38  | 2.05        | 1.94     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 18  | T     | 1138 | HEC  | C2A-C3A | 3.37  | 1.44        | 1.36     |
| 11  | H     | 1482 | CLA  | C4-C3   | 3.37  | 1.58        | 1.50     |
| 11  | I     | 1462 | CLA  | C5-C3   | 3.37  | 1.58        | 1.51     |
| 11  | I     | 1463 | CLA  | CAA-C2A | 3.36  | 1.60        | 1.54     |
| 11  | C     | 1471 | CLA  | MG-NC   | 3.35  | 2.14        | 2.06     |
| 11  | G     | 1346 | CLA  | C4C-C3C | 3.35  | 1.50        | 1.45     |
| 16  | L     | 1046 | HEM  | C3A-C2A | 3.35  | 1.50        | 1.39     |
| 11  | H     | 1490 | CLA  | CAA-C2A | 3.34  | 1.60        | 1.54     |
| 11  | I     | 1465 | CLA  | MG-NC   | 3.34  | 2.14        | 2.06     |
| 11  | C     | 1468 | CLA  | C3B-C4B | 3.33  | 1.47        | 1.40     |
| 11  | H     | 1491 | CLA  | C2B-C1B | 3.33  | 1.47        | 1.40     |
| 11  | G     | 1344 | CLA  | CHB-C1B | -3.33 | 1.32        | 1.39     |
| 11  | G     | 1342 | CLA  | MG-NB   | 3.29  | 2.12        | 2.05     |
| 11  | B     | 1497 | CLA  | C1D-ND  | -3.29 | 1.33        | 1.37     |
| 11  | C     | 1459 | CLA  | MG-NC   | 3.29  | 2.14        | 2.06     |
| 11  | H     | 1485 | CLA  | CHB-C1B | -3.29 | 1.32        | 1.39     |
| 11  | B     | 1490 | CLA  | MG-NC   | 3.28  | 2.14        | 2.06     |
| 11  | H     | 1494 | CLA  | CAA-C2A | 3.28  | 1.60        | 1.54     |
| 11  | G     | 1343 | CLA  | CHB-C1B | -3.27 | 1.32        | 1.39     |
| 17  | F     | 1046 | BCR  | C23-C22 | -3.27 | 1.38        | 1.46     |
| 11  | H     | 1487 | CLA  | C4C-C3C | 3.26  | 1.50        | 1.45     |
| 11  | J     | 1353 | CLA  | CAA-C2A | 3.26  | 1.60        | 1.54     |
| 11  | B     | 1484 | CLA  | CAA-C2A | 3.26  | 1.60        | 1.54     |
| 11  | J     | 1351 | CLA  | C1D-ND  | -3.26 | 1.33        | 1.37     |
| 11  | B     | 1495 | CLA  | CHB-C1B | -3.26 | 1.32        | 1.39     |
| 16  | L     | 1046 | HEM  | CHB-C1B | -3.24 | 1.32        | 1.38     |
| 11  | H     | 1493 | CLA  | CHB-C1B | -3.23 | 1.32        | 1.39     |
| 11  | C     | 1462 | CLA  | CHB-C1B | -3.23 | 1.32        | 1.39     |
| 11  | H     | 1495 | CLA  | C4-C3   | 3.23  | 1.58        | 1.50     |
| 11  | H     | 1484 | CLA  | C1D-C2D | -3.22 | 1.39        | 1.45     |
| 11  | H     | 1496 | CLA  | CAA-C2A | 3.22  | 1.60        | 1.54     |
| 11  | H     | 1495 | CLA  | CHB-C1B | -3.21 | 1.32        | 1.39     |
| 11  | A     | 1343 | CLA  | CHB-C1B | -3.20 | 1.32        | 1.39     |
| 11  | H     | 1490 | CLA  | O1A-CGA | 3.20  | 1.32        | 1.22     |
| 11  | B     | 1489 | CLA  | CAA-C2A | 3.19  | 1.59        | 1.54     |
| 16  | E     | 1085 | HEM  | CHB-C1B | -3.19 | 1.32        | 1.38     |
| 11  | C     | 1461 | CLA  | C3C-C4C | 3.18  | 1.50        | 1.43     |
| 11  | I     | 1468 | CLA  | C2B-C1B | 3.18  | 1.47        | 1.40     |
| 11  | I     | 1471 | CLA  | CHB-C4A | 3.18  | 1.45        | 1.37     |
| 11  | B     | 1484 | CLA  | CHB-C1B | -3.18 | 1.32        | 1.39     |
| 11  | H     | 1497 | CLA  | MG-NC   | 3.17  | 2.13        | 2.06     |
| 11  | I     | 1461 | CLA  | C2B-C1B | 3.17  | 1.47        | 1.40     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 11  | I     | 1468 | CLA  | C3B-C4B | 3.17  | 1.47        | 1.40     |
| 12  | J     | 1352 | PHO  | C3A-C2A | -3.17 | 1.52        | 1.54     |
| 11  | I     | 1471 | CLA  | MG-NC   | 3.16  | 2.13        | 2.06     |
| 11  | H     | 1488 | CLA  | C5-C3   | 3.15  | 1.57        | 1.51     |
| 16  | E     | 1085 | HEM  | FE-NC   | 3.14  | 2.05        | 1.95     |
| 11  | A     | 1344 | CLA  | CHB-C1B | -3.13 | 1.32        | 1.39     |
| 18  | V     | 1138 | HEC  | C2A-C3A | 3.13  | 1.43        | 1.36     |
| 11  | H     | 1494 | CLA  | C4-C3   | 3.13  | 1.58        | 1.50     |
| 11  | B     | 1484 | CLA  | C1D-C2D | -3.12 | 1.39        | 1.45     |
| 11  | A     | 1346 | CLA  | MG-NC   | 3.12  | 2.13        | 2.06     |
| 11  | H     | 1487 | CLA  | C5-C3   | 3.10  | 1.57        | 1.51     |
| 16  | L     | 1046 | HEM  | FE-NB   | 3.10  | 2.04        | 1.94     |
| 11  | C     | 1462 | CLA  | C2-C3   | 3.10  | 1.40        | 1.33     |
| 12  | G     | 1345 | PHO  | C3A-C2A | -3.09 | 1.52        | 1.54     |
| 11  | H     | 1493 | CLA  | C1D-ND  | -3.08 | 1.33        | 1.37     |
| 17  | F     | 1046 | BCR  | C19-C18 | -3.08 | 1.39        | 1.46     |
| 16  | E     | 1085 | HEM  | C1C-NC  | -3.08 | 1.35        | 1.39     |
| 15  | D     | 1354 | PL9  | C3-C2   | 3.08  | 1.42        | 1.32     |
| 11  | I     | 1464 | CLA  | MG-NC   | 3.07  | 2.13        | 2.06     |
| 18  | T     | 1138 | HEC  | CBA-CGA | -3.07 | 1.43        | 1.50     |
| 17  | L     | 1047 | BCR  | C23-C22 | -3.07 | 1.39        | 1.46     |
| 15  | D     | 1354 | PL9  | C6-C5   | 3.07  | 1.42        | 1.32     |
| 11  | G     | 1343 | CLA  | C5-C3   | 3.06  | 1.57        | 1.51     |
| 12  | J     | 1352 | PHO  | C4D-CHA | 3.06  | 1.44        | 1.39     |
| 11  | I     | 1470 | CLA  | MG-NC   | 3.06  | 2.13        | 2.06     |
| 11  | H     | 1497 | CLA  | OBD-CAD | 3.05  | 1.27        | 1.22     |
| 11  | I     | 1468 | CLA  | CHB-C4A | 3.05  | 1.44        | 1.36     |
| 11  | H     | 1495 | CLA  | C1D-C2D | -3.05 | 1.39        | 1.45     |
| 11  | C     | 1462 | CLA  | C1-C2   | 3.05  | 1.57        | 1.49     |
| 11  | A     | 1343 | CLA  | C1B-NB  | -3.04 | 1.33        | 1.37     |
| 12  | A     | 1345 | PHO  | C3D-CAD | -3.03 | 1.42        | 1.47     |
| 11  | C     | 1463 | CLA  | C4-C3   | 3.03  | 1.58        | 1.50     |
| 11  | H     | 1497 | CLA  | C1D-ND  | -3.02 | 1.33        | 1.37     |
| 11  | B     | 1492 | CLA  | MG-NC   | 3.01  | 2.13        | 2.06     |
| 11  | I     | 1461 | CLA  | C3C-C4C | 3.01  | 1.50        | 1.43     |
| 11  | B     | 1492 | CLA  | CHB-C1B | -3.01 | 1.32        | 1.39     |
| 11  | H     | 1494 | CLA  | MG-NC   | 3.01  | 2.13        | 2.06     |
| 11  | H     | 1497 | CLA  | CHB-C1B | -3.00 | 1.32        | 1.39     |
| 11  | I     | 1462 | CLA  | CHC-C1C | 3.00  | 1.44        | 1.38     |
| 11  | H     | 1488 | CLA  | MG-NC   | 2.99  | 2.13        | 2.06     |
| 11  | H     | 1490 | CLA  | C1B-C2B | 2.99  | 1.50        | 1.43     |
| 16  | L     | 1046 | HEM  | C3A-C4A | 2.99  | 1.46        | 1.40     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 11  | H     | 1492 | CLA  | MG-NC   | 2.98  | 2.13        | 2.06     |
| 11  | J     | 1351 | CLA  | CHB-C1B | -2.98 | 1.32        | 1.39     |
| 11  | B     | 1495 | CLA  | C1D-ND  | -2.98 | 1.34        | 1.37     |
| 11  | B     | 1485 | CLA  | MG-NC   | 2.97  | 2.13        | 2.06     |
| 11  | I     | 1466 | CLA  | CHB-C1B | -2.97 | 1.32        | 1.39     |
| 11  | H     | 1490 | CLA  | MG-NC   | 2.96  | 2.13        | 2.06     |
| 11  | C     | 1468 | CLA  | CHB-C4A | 2.95  | 1.44        | 1.36     |
| 11  | G     | 1343 | CLA  | C1B-NB  | -2.94 | 1.34        | 1.37     |
| 11  | I     | 1469 | CLA  | MG-NB   | 2.94  | 2.11        | 2.05     |
| 18  | T     | 1138 | HEC  | CBD-CAD | 2.94  | 1.62        | 1.51     |
| 11  | B     | 1487 | CLA  | C1-C2   | 2.94  | 1.57        | 1.49     |
| 11  | C     | 1462 | CLA  | MG-NB   | 2.93  | 2.11        | 2.05     |
| 11  | A     | 1343 | CLA  | C1D-ND  | -2.92 | 1.34        | 1.37     |
| 11  | B     | 1490 | CLA  | C4C-C3C | 2.92  | 1.50        | 1.45     |
| 11  | D     | 1351 | CLA  | C1D-ND  | -2.92 | 1.34        | 1.37     |
| 11  | G     | 1342 | CLA  | MG-NC   | 2.92  | 2.13        | 2.06     |
| 11  | B     | 1483 | CLA  | CHB-C1B | -2.91 | 1.32        | 1.39     |
| 11  | I     | 1462 | CLA  | C1D-ND  | -2.91 | 1.34        | 1.37     |
| 11  | C     | 1464 | CLA  | CHB-C1B | -2.91 | 1.32        | 1.39     |
| 12  | D     | 1352 | PHO  | C3D-CAD | -2.91 | 1.42        | 1.47     |
| 11  | H     | 1494 | CLA  | CHC-C1C | 2.91  | 1.44        | 1.38     |
| 11  | C     | 1462 | CLA  | C4-C3   | 2.90  | 1.57        | 1.50     |
| 11  | H     | 1484 | CLA  | MG-NC   | 2.89  | 2.13        | 2.06     |
| 11  | I     | 1462 | CLA  | MG-NC   | 2.89  | 2.13        | 2.06     |
| 11  | C     | 1461 | CLA  | MG-NC   | 2.88  | 2.13        | 2.06     |
| 12  | G     | 1345 | PHO  | C3D-CAD | -2.87 | 1.42        | 1.47     |
| 11  | G     | 1342 | CLA  | C1B-NB  | -2.87 | 1.34        | 1.37     |
| 11  | G     | 1342 | CLA  | CBA-CGA | -2.87 | 1.42        | 1.50     |
| 11  | I     | 1462 | CLA  | C4-C3   | 2.87  | 1.57        | 1.50     |
| 11  | I     | 1462 | CLA  | MG-NB   | 2.87  | 2.11        | 2.05     |
| 12  | D     | 1352 | PHO  | C4D-CHA | 2.87  | 1.43        | 1.39     |
| 11  | G     | 1346 | CLA  | CAA-C2A | 2.86  | 1.59        | 1.54     |
| 11  | H     | 1482 | CLA  | C1-C2   | 2.85  | 1.57        | 1.49     |
| 11  | B     | 1490 | CLA  | CHB-C4A | 2.85  | 1.44        | 1.37     |
| 11  | H     | 1497 | CLA  | MG-NA   | 2.84  | 2.13        | 2.06     |
| 11  | B     | 1484 | CLA  | MG-NA   | 2.84  | 2.13        | 2.06     |
| 11  | B     | 1482 | CLA  | C5-C3   | 2.84  | 1.57        | 1.51     |
| 11  | C     | 1462 | CLA  | C5-C3   | 2.83  | 1.57        | 1.51     |
| 11  | B     | 1492 | CLA  | C4-C3   | 2.82  | 1.57        | 1.50     |
| 11  | H     | 1487 | CLA  | C1-C2   | 2.82  | 1.57        | 1.49     |
| 11  | C     | 1462 | CLA  | MG-NA   | 2.82  | 2.13        | 2.06     |
| 11  | H     | 1490 | CLA  | CMB-C2B | 2.81  | 1.56        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 16  | L     | 1046 | HEM  | C1C-NC  | -2.81 | 1.35        | 1.39     |
| 11  | B     | 1490 | CLA  | C1B-C2B | 2.81  | 1.49        | 1.43     |
| 11  | C     | 1464 | CLA  | C4-C3   | 2.81  | 1.57        | 1.50     |
| 11  | H     | 1494 | CLA  | C1D-C2D | -2.81 | 1.39        | 1.45     |
| 11  | C     | 1466 | CLA  | CHB-C1B | -2.81 | 1.33        | 1.39     |
| 11  | A     | 1342 | CLA  | C1D-ND  | -2.80 | 1.34        | 1.37     |
| 11  | J     | 1351 | CLA  | C3B-C4B | 2.80  | 1.50        | 1.42     |
| 11  | H     | 1483 | CLA  | MG-NC   | 2.80  | 2.12        | 2.06     |
| 11  | I     | 1470 | CLA  | CAA-C2A | 2.80  | 1.59        | 1.53     |
| 11  | B     | 1495 | CLA  | C1D-C2D | -2.80 | 1.39        | 1.45     |
| 11  | D     | 1353 | CLA  | C1D-C2D | -2.79 | 1.39        | 1.45     |
| 17  | L     | 1047 | BCR  | C26-C25 | 2.79  | 1.39        | 1.34     |
| 11  | C     | 1465 | CLA  | MG-NC   | 2.79  | 2.12        | 2.06     |
| 11  | A     | 1342 | CLA  | C1D-C2D | -2.78 | 1.39        | 1.45     |
| 11  | I     | 1464 | CLA  | CAA-C2A | 2.78  | 1.59        | 1.54     |
| 11  | A     | 1346 | CLA  | C4-C3   | 2.77  | 1.57        | 1.50     |
| 11  | H     | 1493 | CLA  | C4C-C3C | 2.77  | 1.49        | 1.45     |
| 11  | D     | 1351 | CLA  | CHC-C1C | 2.76  | 1.44        | 1.38     |
| 18  | T     | 1138 | HEC  | C1A-NA  | 2.76  | 1.44        | 1.39     |
| 11  | I     | 1464 | CLA  | C4-C3   | 2.75  | 1.57        | 1.50     |
| 11  | C     | 1470 | CLA  | MG-NC   | 2.75  | 2.12        | 2.06     |
| 11  | I     | 1471 | CLA  | C4C-C3C | 2.75  | 1.49        | 1.45     |
| 11  | H     | 1497 | CLA  | CBD-CGD | 2.75  | 1.60        | 1.52     |
| 11  | B     | 1487 | CLA  | C4C-C3C | 2.74  | 1.49        | 1.45     |
| 11  | I     | 1466 | CLA  | MG-NC   | 2.74  | 2.12        | 2.06     |
| 11  | C     | 1469 | CLA  | CHB-C4A | 2.74  | 1.44        | 1.37     |
| 11  | B     | 1494 | CLA  | MG-NC   | 2.74  | 2.12        | 2.06     |
| 16  | L     | 1046 | HEM  | C4D-ND  | -2.73 | 1.34        | 1.40     |
| 18  | T     | 1138 | HEC  | CMA-C3A | 2.73  | 1.56        | 1.50     |
| 11  | H     | 1485 | CLA  | C1D-ND  | -2.72 | 1.34        | 1.37     |
| 11  | B     | 1493 | CLA  | CAA-C2A | 2.72  | 1.59        | 1.54     |
| 11  | C     | 1459 | CLA  | CBA-CGA | -2.72 | 1.44        | 1.50     |
| 11  | H     | 1491 | CLA  | C3C-C4C | 2.71  | 1.49        | 1.43     |
| 11  | B     | 1497 | CLA  | CAA-C2A | 2.71  | 1.58        | 1.53     |
| 11  | H     | 1482 | CLA  | C5-C3   | 2.71  | 1.56        | 1.51     |
| 17  | L     | 1047 | BCR  | C19-C18 | -2.70 | 1.40        | 1.46     |
| 11  | H     | 1495 | CLA  | C1D-ND  | -2.70 | 1.34        | 1.37     |
| 11  | C     | 1470 | CLA  | C1D-ND  | -2.70 | 1.34        | 1.37     |
| 11  | B     | 1494 | CLA  | C4-C3   | 2.70  | 1.57        | 1.50     |
| 11  | C     | 1463 | CLA  | C1D-ND  | -2.70 | 1.34        | 1.37     |
| 11  | H     | 1490 | CLA  | C4C-C3C | 2.70  | 1.49        | 1.45     |
| 11  | H     | 1488 | CLA  | C1D-C2D | -2.70 | 1.40        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 11  | B     | 1488 | CLA  | MG-NC   | 2.69  | 2.12        | 2.06     |
| 11  | H     | 1496 | CLA  | CHB-C4A | 2.69  | 1.44        | 1.37     |
| 11  | H     | 1489 | CLA  | C4-C3   | 2.69  | 1.57        | 1.50     |
| 11  | A     | 1346 | CLA  | CHB-C1B | -2.69 | 1.33        | 1.39     |
| 11  | H     | 1488 | CLA  | CHC-C1C | 2.69  | 1.43        | 1.38     |
| 11  | I     | 1461 | CLA  | C2C-C1C | 2.69  | 1.49        | 1.43     |
| 12  | J     | 1352 | PHO  | C3D-CAD | -2.69 | 1.42        | 1.47     |
| 11  | I     | 1464 | CLA  | CHB-C1B | -2.69 | 1.33        | 1.39     |
| 11  | B     | 1488 | CLA  | CHC-C1C | 2.68  | 1.43        | 1.38     |
| 15  | J     | 1354 | PL9  | C6-C5   | 2.67  | 1.41        | 1.32     |
| 11  | D     | 1351 | CLA  | C1C-C2C | 2.67  | 1.49        | 1.44     |
| 11  | G     | 1342 | CLA  | C1D-ND  | -2.67 | 1.34        | 1.37     |
| 11  | G     | 1344 | CLA  | C1D-ND  | -2.67 | 1.34        | 1.37     |
| 11  | B     | 1483 | CLA  | MG-NC   | 2.67  | 2.12        | 2.06     |
| 11  | B     | 1496 | CLA  | C1D-C2D | -2.66 | 1.40        | 1.45     |
| 11  | J     | 1351 | CLA  | CHC-C1C | 2.66  | 1.43        | 1.38     |
| 11  | I     | 1471 | CLA  | MG-NB   | 2.66  | 2.11        | 2.05     |
| 11  | H     | 1494 | CLA  | C1D-ND  | -2.65 | 1.34        | 1.37     |
| 11  | I     | 1459 | CLA  | CHB-C1B | -2.65 | 1.33        | 1.39     |
| 11  | J     | 1353 | CLA  | MG-NC   | 2.65  | 2.12        | 2.06     |
| 11  | C     | 1468 | CLA  | MG-NC   | 2.65  | 2.12        | 2.06     |
| 11  | B     | 1486 | CLA  | C1D-C2D | -2.64 | 1.40        | 1.45     |
| 11  | C     | 1461 | CLA  | CHC-C1C | 2.63  | 1.43        | 1.38     |
| 11  | A     | 1342 | CLA  | O1D-CGD | -2.63 | 1.14        | 1.21     |
| 11  | H     | 1483 | CLA  | CAA-CBA | -2.63 | 1.45        | 1.52     |
| 11  | C     | 1461 | CLA  | C2C-C1C | 2.62  | 1.49        | 1.43     |
| 11  | B     | 1495 | CLA  | C4-C3   | 2.62  | 1.57        | 1.50     |
| 11  | J     | 1351 | CLA  | C1D-C2D | -2.62 | 1.40        | 1.45     |
| 11  | G     | 1343 | CLA  | C3D-C4D | -2.62 | 1.38        | 1.44     |
| 12  | D     | 1352 | PHO  | C3A-C2A | -2.62 | 1.52        | 1.54     |
| 11  | C     | 1471 | CLA  | CAA-C2A | 2.62  | 1.58        | 1.53     |
| 11  | B     | 1482 | CLA  | MG-NC   | 2.62  | 2.12        | 2.06     |
| 11  | B     | 1488 | CLA  | C1-C2   | 2.61  | 1.56        | 1.49     |
| 18  | V     | 1138 | HEC  | C1C-NC  | -2.61 | 1.34        | 1.39     |
| 11  | B     | 1490 | CLA  | C1C-C2C | 2.61  | 1.49        | 1.44     |
| 11  | B     | 1484 | CLA  | C1D-ND  | -2.61 | 1.34        | 1.37     |
| 11  | B     | 1482 | CLA  | C4-C3   | 2.61  | 1.57        | 1.50     |
| 11  | C     | 1464 | CLA  | MG-NC   | 2.61  | 2.12        | 2.06     |
| 11  | C     | 1465 | CLA  | MG-NA   | 2.61  | 2.12        | 2.06     |
| 11  | H     | 1484 | CLA  | CHB-C1B | -2.60 | 1.33        | 1.39     |
| 11  | B     | 1490 | CLA  | CMB-C2B | 2.60  | 1.56        | 1.50     |
| 11  | G     | 1342 | CLA  | CAA-CBA | -2.60 | 1.45        | 1.52     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 11  | D     | 1353 | CLA  | CHB-C1B | -2.60 | 1.33        | 1.39     |
| 11  | I     | 1469 | CLA  | CHB-C4A | 2.59  | 1.44        | 1.37     |
| 18  | V     | 1138 | HEC  | CMB-C2B | 2.59  | 1.56        | 1.50     |
| 11  | G     | 1344 | CLA  | C1D-C2D | -2.59 | 1.40        | 1.45     |
| 11  | C     | 1462 | CLA  | CHC-C1C | 2.59  | 1.43        | 1.38     |
| 18  | V     | 1138 | HEC  | CBD-CAD | 2.59  | 1.60        | 1.51     |
| 11  | H     | 1486 | CLA  | C1D-C2D | -2.58 | 1.40        | 1.45     |
| 11  | J     | 1353 | CLA  | CHB-C1B | -2.58 | 1.33        | 1.39     |
| 11  | C     | 1469 | CLA  | MG-NC   | 2.58  | 2.12        | 2.06     |
| 11  | I     | 1460 | CLA  | CHB-C1B | -2.58 | 1.33        | 1.39     |
| 11  | B     | 1494 | CLA  | CHC-C1C | 2.58  | 1.43        | 1.38     |
| 11  | B     | 1497 | CLA  | C1C-C2C | 2.58  | 1.49        | 1.44     |
| 18  | V     | 1138 | HEC  | CMA-C3A | 2.57  | 1.56        | 1.50     |
| 11  | C     | 1470 | CLA  | CAA-C2A | 2.57  | 1.58        | 1.53     |
| 11  | I     | 1466 | CLA  | C1D-C2D | -2.57 | 1.40        | 1.45     |
| 11  | I     | 1460 | CLA  | CHC-C1C | 2.57  | 1.43        | 1.38     |
| 11  | C     | 1471 | CLA  | C1B-C2B | 2.57  | 1.49        | 1.43     |
| 11  | C     | 1464 | CLA  | CBA-CGA | -2.56 | 1.43        | 1.50     |
| 11  | B     | 1482 | CLA  | C4C-C3C | 2.56  | 1.49        | 1.45     |
| 11  | C     | 1466 | CLA  | C1D-ND  | -2.56 | 1.34        | 1.37     |
| 11  | B     | 1487 | CLA  | CHC-C1C | 2.55  | 1.43        | 1.38     |
| 11  | C     | 1470 | CLA  | C1D-C2D | -2.55 | 1.40        | 1.45     |
| 11  | H     | 1496 | CLA  | MG-NC   | 2.55  | 2.12        | 2.06     |
| 11  | B     | 1497 | CLA  | CBD-CGD | 2.55  | 1.60        | 1.52     |
| 18  | V     | 1138 | HEC  | CBA-CGA | -2.55 | 1.44        | 1.50     |
| 11  | B     | 1493 | CLA  | CHD-C1D | 2.55  | 1.43        | 1.38     |
| 11  | H     | 1487 | CLA  | C3B-C4B | 2.54  | 1.50        | 1.42     |
| 11  | B     | 1494 | CLA  | CAA-C2A | 2.54  | 1.58        | 1.54     |
| 11  | H     | 1486 | CLA  | MG-NB   | 2.53  | 2.10        | 2.05     |
| 11  | C     | 1463 | CLA  | C5-C3   | 2.53  | 1.56        | 1.51     |
| 11  | C     | 1466 | CLA  | MG-NC   | 2.53  | 2.12        | 2.06     |
| 11  | I     | 1463 | CLA  | C4-C3   | 2.53  | 1.56        | 1.50     |
| 11  | I     | 1459 | CLA  | C1D-ND  | -2.53 | 1.34        | 1.37     |
| 11  | I     | 1466 | CLA  | C3B-C4B | 2.52  | 1.50        | 1.42     |
| 11  | C     | 1465 | CLA  | CAA-C2A | 2.52  | 1.58        | 1.54     |
| 11  | I     | 1459 | CLA  | MG-NC   | 2.51  | 2.12        | 2.06     |
| 11  | B     | 1496 | CLA  | CHB-C1B | -2.51 | 1.33        | 1.39     |
| 11  | B     | 1485 | CLA  | C1D-ND  | -2.51 | 1.34        | 1.37     |
| 11  | H     | 1488 | CLA  | CMD-C2D | 2.51  | 1.55        | 1.50     |
| 11  | J     | 1353 | CLA  | C1-C2   | 2.51  | 1.56        | 1.49     |
| 11  | H     | 1482 | CLA  | C4C-C3C | 2.51  | 1.49        | 1.45     |
| 16  | L     | 1046 | HEM  | FE-ND   | 2.50  | 2.02        | 1.94     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 11  | H     | 1483 | CLA  | C1D-C2D | -2.50 | 1.40        | 1.45     |
| 18  | T     | 1138 | HEC  | CAA-C2A | 2.50  | 1.57        | 1.51     |
| 11  | C     | 1459 | CLA  | CAA-CBA | -2.50 | 1.45        | 1.52     |
| 11  | G     | 1346 | CLA  | C4-C3   | 2.50  | 1.56        | 1.50     |
| 11  | I     | 1465 | CLA  | CAA-C2A | 2.49  | 1.58        | 1.54     |
| 11  | C     | 1470 | CLA  | CHB-C4A | 2.49  | 1.43        | 1.37     |
| 11  | B     | 1484 | CLA  | MG-NC   | 2.49  | 2.12        | 2.06     |
| 11  | B     | 1494 | CLA  | CHB-C4A | 2.49  | 1.43        | 1.37     |
| 11  | I     | 1460 | CLA  | CMB-C2B | 2.49  | 1.55        | 1.50     |
| 11  | C     | 1471 | CLA  | CHB-C4A | 2.48  | 1.43        | 1.37     |
| 12  | A     | 1345 | PHO  | CAA-CBA | -2.48 | 1.45        | 1.52     |
| 11  | H     | 1488 | CLA  | C4-C3   | 2.48  | 1.56        | 1.50     |
| 11  | C     | 1469 | CLA  | MG-NB   | 2.48  | 2.10        | 2.05     |
| 11  | B     | 1486 | CLA  | CHB-C4A | 2.48  | 1.43        | 1.37     |
| 12  | J     | 1352 | PHO  | C4A-C3A | -2.48 | 1.47        | 1.51     |
| 18  | T     | 1138 | HEC  | C1C-C2C | 2.47  | 1.48        | 1.43     |
| 11  | B     | 1487 | CLA  | MG-NC   | 2.47  | 2.12        | 2.06     |
| 11  | B     | 1495 | CLA  | CAA-CBA | -2.47 | 1.45        | 1.52     |
| 11  | C     | 1459 | CLA  | CAA-C2A | 2.47  | 1.58        | 1.54     |
| 11  | C     | 1467 | CLA  | C1D-C2D | -2.47 | 1.40        | 1.45     |
| 11  | H     | 1497 | CLA  | CAA-C2A | 2.47  | 1.58        | 1.53     |
| 11  | B     | 1496 | CLA  | CHB-C4A | 2.47  | 1.43        | 1.37     |
| 11  | H     | 1496 | CLA  | C4-C3   | 2.47  | 1.56        | 1.50     |
| 11  | B     | 1485 | CLA  | C1B-NB  | -2.46 | 1.34        | 1.37     |
| 11  | I     | 1468 | CLA  | CHC-C1C | 2.46  | 1.43        | 1.38     |
| 11  | B     | 1497 | CLA  | C1D-C2D | -2.45 | 1.40        | 1.45     |
| 11  | B     | 1490 | CLA  | O2A-CGA | -2.45 | 1.22        | 1.30     |
| 11  | H     | 1491 | CLA  | C4D-C3D | -2.45 | 1.41        | 1.46     |
| 11  | H     | 1490 | CLA  | O2A-CGA | -2.45 | 1.22        | 1.30     |
| 11  | B     | 1487 | CLA  | C6-C5   | 2.44  | 1.61        | 1.52     |
| 11  | I     | 1463 | CLA  | C5-C3   | 2.44  | 1.56        | 1.51     |
| 11  | B     | 1497 | CLA  | MG-NC   | 2.44  | 2.12        | 2.06     |
| 11  | C     | 1463 | CLA  | CHB-C1B | -2.44 | 1.33        | 1.39     |
| 11  | A     | 1344 | CLA  | MG-NC   | 2.44  | 2.12        | 2.06     |
| 11  | H     | 1488 | CLA  | C1C-C2C | 2.44  | 1.49        | 1.44     |
| 11  | H     | 1490 | CLA  | CHB-C4A | 2.44  | 1.43        | 1.37     |
| 11  | C     | 1461 | CLA  | CHB-C4A | 2.44  | 1.42        | 1.36     |
| 11  | D     | 1353 | CLA  | O2A-CGA | 2.43  | 1.40        | 1.33     |
| 11  | B     | 1483 | CLA  | C1D-C2D | -2.43 | 1.40        | 1.45     |
| 16  | L     | 1046 | HEM  | C1B-NB  | -2.43 | 1.35        | 1.40     |
| 12  | D     | 1352 | PHO  | C4A-C3A | -2.43 | 1.47        | 1.51     |
| 11  | H     | 1497 | CLA  | C1C-C2C | 2.43  | 1.49        | 1.44     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 11  | B     | 1493 | CLA  | CHB-C1B | -2.42 | 1.34        | 1.39     |
| 11  | D     | 1351 | CLA  | C3B-C4B | 2.42  | 1.49        | 1.42     |
| 11  | H     | 1492 | CLA  | C4-C3   | 2.42  | 1.56        | 1.50     |
| 11  | J     | 1351 | CLA  | C1C-C2C | 2.42  | 1.49        | 1.44     |
| 11  | B     | 1493 | CLA  | C1D-ND  | -2.42 | 1.34        | 1.37     |
| 11  | C     | 1469 | CLA  | CAA-C2A | 2.42  | 1.58        | 1.53     |
| 12  | D     | 1352 | PHO  | C4-C3   | 2.42  | 1.56        | 1.50     |
| 11  | C     | 1459 | CLA  | C4C-C3C | 2.41  | 1.49        | 1.45     |
| 11  | B     | 1488 | CLA  | C1D-C2D | -2.41 | 1.40        | 1.45     |
| 11  | I     | 1461 | CLA  | CHB-C4A | 2.41  | 1.42        | 1.36     |
| 11  | J     | 1351 | CLA  | C4-C3   | 2.40  | 1.56        | 1.50     |
| 11  | I     | 1469 | CLA  | C1B-C2B | 2.40  | 1.48        | 1.43     |
| 11  | C     | 1466 | CLA  | CMD-C2D | 2.40  | 1.55        | 1.50     |
| 11  | I     | 1470 | CLA  | CMB-C2B | 2.40  | 1.55        | 1.50     |
| 11  | G     | 1344 | CLA  | C3B-C4B | 2.40  | 1.49        | 1.42     |
| 11  | I     | 1461 | CLA  | C2D-C3D | 2.40  | 1.43        | 1.36     |
| 12  | A     | 1345 | PHO  | C3A-C2A | -2.40 | 1.52        | 1.54     |
| 11  | B     | 1488 | CLA  | C1D-ND  | -2.39 | 1.34        | 1.37     |
| 11  | I     | 1466 | CLA  | C1D-ND  | -2.39 | 1.34        | 1.37     |
| 11  | B     | 1489 | CLA  | C1C-NC  | -2.39 | 1.34        | 1.37     |
| 18  | V     | 1138 | HEC  | CAA-C2A | 2.38  | 1.57        | 1.51     |
| 11  | I     | 1461 | CLA  | CHD-C1D | 2.38  | 1.44        | 1.38     |
| 11  | H     | 1485 | CLA  | MG-NB   | 2.38  | 2.10        | 2.05     |
| 11  | I     | 1463 | CLA  | C1D-C2D | -2.38 | 1.40        | 1.45     |
| 11  | I     | 1462 | CLA  | C1C-C2C | 2.38  | 1.49        | 1.44     |
| 11  | C     | 1461 | CLA  | C4D-C3D | -2.38 | 1.41        | 1.46     |
| 11  | H     | 1497 | CLA  | CMA-C3A | 2.38  | 1.58        | 1.53     |
| 15  | J     | 1354 | PL9  | C3-C2   | 2.38  | 1.40        | 1.32     |
| 11  | B     | 1491 | CLA  | C4D-C3D | -2.38 | 1.41        | 1.46     |
| 11  | H     | 1487 | CLA  | C6-C5   | 2.38  | 1.60        | 1.52     |
| 11  | H     | 1487 | CLA  | CHD-C1D | 2.38  | 1.43        | 1.38     |
| 11  | H     | 1495 | CLA  | C1B-NB  | -2.37 | 1.34        | 1.37     |
| 11  | I     | 1462 | CLA  | MG-NA   | 2.37  | 2.11        | 2.06     |
| 11  | B     | 1497 | CLA  | CHB-C1B | -2.36 | 1.34        | 1.39     |
| 11  | J     | 1353 | CLA  | CMB-C2B | 2.36  | 1.55        | 1.50     |
| 11  | I     | 1467 | CLA  | CHB-C1B | -2.36 | 1.34        | 1.39     |
| 11  | H     | 1491 | CLA  | C2C-C1C | 2.36  | 1.48        | 1.43     |
| 11  | C     | 1462 | CLA  | MG-NC   | 2.36  | 2.11        | 2.06     |
| 11  | C     | 1468 | CLA  | C4D-C3D | -2.36 | 1.41        | 1.46     |
| 11  | C     | 1465 | CLA  | OBD-CAD | 2.36  | 1.26        | 1.22     |
| 11  | I     | 1460 | CLA  | O2A-CGA | 2.35  | 1.40        | 1.33     |
| 11  | C     | 1469 | CLA  | C1B-C2B | 2.35  | 1.48        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 11  | I     | 1460 | CLA  | MG-NC   | 2.35  | 2.11        | 2.06     |
| 12  | G     | 1345 | PHO  | CAA-CBA | -2.35 | 1.45        | 1.52     |
| 11  | H     | 1489 | CLA  | CAA-C2A | 2.35  | 1.58        | 1.54     |
| 11  | G     | 1342 | CLA  | CHC-C1C | 2.34  | 1.43        | 1.38     |
| 11  | H     | 1488 | CLA  | C1-C2   | 2.34  | 1.55        | 1.49     |
| 11  | I     | 1463 | CLA  | MG-NC   | 2.34  | 2.11        | 2.06     |
| 11  | H     | 1497 | CLA  | C3A-C2A | 2.34  | 1.56        | 1.54     |
| 11  | H     | 1485 | CLA  | CAA-CBA | -2.34 | 1.45        | 1.52     |
| 11  | H     | 1482 | CLA  | CHB-C4A | 2.34  | 1.43        | 1.37     |
| 11  | C     | 1468 | CLA  | CHC-C1C | 2.34  | 1.43        | 1.38     |
| 11  | B     | 1482 | CLA  | CMD-C2D | 2.34  | 1.55        | 1.50     |
| 11  | I     | 1465 | CLA  | MG-NB   | 2.34  | 2.10        | 2.05     |
| 18  | V     | 1138 | HEC  | C4D-ND  | -2.33 | 1.35        | 1.39     |
| 11  | A     | 1346 | CLA  | C1D-ND  | -2.33 | 1.34        | 1.37     |
| 11  | H     | 1485 | CLA  | C1B-NB  | -2.33 | 1.34        | 1.37     |
| 11  | B     | 1492 | CLA  | C5-C3   | 2.32  | 1.56        | 1.51     |
| 11  | D     | 1353 | CLA  | MG-NC   | 2.32  | 2.11        | 2.06     |
| 11  | H     | 1496 | CLA  | C1D-C2D | -2.32 | 1.40        | 1.45     |
| 11  | H     | 1494 | CLA  | C1B-NB  | -2.32 | 1.34        | 1.37     |
| 11  | A     | 1346 | CLA  | C1D-C2D | -2.32 | 1.40        | 1.45     |
| 11  | I     | 1470 | CLA  | CHB-C4A | 2.32  | 1.43        | 1.37     |
| 11  | H     | 1491 | CLA  | CHB-C1B | -2.32 | 1.33        | 1.39     |
| 11  | C     | 1463 | CLA  | C1C-C2C | 2.31  | 1.49        | 1.44     |
| 11  | H     | 1487 | CLA  | CHC-C1C | 2.31  | 1.43        | 1.38     |
| 12  | A     | 1345 | PHO  | C4A-C3A | -2.31 | 1.47        | 1.51     |
| 11  | H     | 1490 | CLA  | C1C-C2C | 2.31  | 1.49        | 1.44     |
| 11  | C     | 1461 | CLA  | CHB-C1B | -2.31 | 1.33        | 1.39     |
| 11  | H     | 1485 | CLA  | C1C-C2C | 2.31  | 1.49        | 1.44     |
| 11  | B     | 1486 | CLA  | MG-NC   | 2.31  | 2.11        | 2.06     |
| 11  | B     | 1490 | CLA  | CMD-C2D | 2.30  | 1.55        | 1.50     |
| 11  | B     | 1482 | CLA  | C1-C2   | 2.30  | 1.55        | 1.49     |
| 18  | T     | 1138 | HEC  | CMB-C2B | 2.30  | 1.55        | 1.50     |
| 11  | C     | 1466 | CLA  | C1C-NC  | -2.30 | 1.34        | 1.37     |
| 11  | I     | 1470 | CLA  | C1D-C2D | -2.30 | 1.40        | 1.45     |
| 11  | I     | 1464 | CLA  | C1C-C2C | 2.29  | 1.49        | 1.44     |
| 11  | H     | 1496 | CLA  | C5-C3   | 2.29  | 1.56        | 1.51     |
| 16  | E     | 1085 | HEM  | C3D-C2D | 2.29  | 1.40        | 1.35     |
| 11  | C     | 1466 | CLA  | CMB-C2B | 2.29  | 1.55        | 1.50     |
| 11  | H     | 1485 | CLA  | C1D-C2D | -2.28 | 1.40        | 1.45     |
| 11  | I     | 1461 | CLA  | CHC-C1C | 2.28  | 1.43        | 1.38     |
| 11  | I     | 1468 | CLA  | C4D-C3D | -2.28 | 1.41        | 1.46     |
| 11  | I     | 1464 | CLA  | C1D-C2D | -2.27 | 1.40        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 11  | B     | 1488 | CLA  | C5-C3   | 2.27  | 1.56        | 1.51     |
| 11  | H     | 1491 | CLA  | MG-NC   | 2.27  | 2.11        | 2.06     |
| 11  | H     | 1495 | CLA  | CAA-CBA | -2.27 | 1.46        | 1.52     |
| 12  | D     | 1352 | PHO  | CHA-CBD | 2.27  | 1.54        | 1.51     |
| 18  | T     | 1138 | HEC  | C1D-ND  | -2.27 | 1.35        | 1.39     |
| 11  | D     | 1353 | CLA  | C4-C3   | 2.27  | 1.56        | 1.50     |
| 11  | D     | 1351 | CLA  | CAA-C2A | 2.27  | 1.58        | 1.54     |
| 16  | E     | 1085 | HEM  | C3B-C4B | 2.27  | 1.48        | 1.43     |
| 11  | B     | 1488 | CLA  | C1C-C2C | 2.26  | 1.49        | 1.44     |
| 11  | H     | 1497 | CLA  | C1D-C2D | -2.26 | 1.40        | 1.45     |
| 11  | B     | 1482 | CLA  | C1B-C2B | 2.26  | 1.48        | 1.43     |
| 18  | T     | 1138 | HEC  | C1B-C2B | 2.26  | 1.48        | 1.43     |
| 11  | H     | 1496 | CLA  | C1D-ND  | -2.26 | 1.34        | 1.37     |
| 11  | I     | 1463 | CLA  | C1D-ND  | -2.26 | 1.34        | 1.37     |
| 11  | H     | 1486 | CLA  | MG-NC   | 2.26  | 2.11        | 2.06     |
| 11  | B     | 1482 | CLA  | CHB-C1B | -2.25 | 1.34        | 1.39     |
| 11  | H     | 1494 | CLA  | CHB-C1B | -2.25 | 1.34        | 1.39     |
| 11  | C     | 1463 | CLA  | C1D-C2D | -2.25 | 1.40        | 1.45     |
| 11  | B     | 1486 | CLA  | CHB-C1B | -2.25 | 1.34        | 1.39     |
| 11  | A     | 1342 | CLA  | CAA-CBA | -2.25 | 1.46        | 1.52     |
| 11  | G     | 1346 | CLA  | CBD-CGD | 2.25  | 1.59        | 1.52     |
| 11  | J     | 1353 | CLA  | CMD-C2D | 2.24  | 1.55        | 1.50     |
| 11  | B     | 1494 | CLA  | CHB-C1B | -2.24 | 1.34        | 1.39     |
| 11  | B     | 1483 | CLA  | CHB-C4A | 2.24  | 1.43        | 1.37     |
| 11  | H     | 1484 | CLA  | C1D-ND  | -2.24 | 1.34        | 1.37     |
| 11  | C     | 1459 | CLA  | CHC-C1C | 2.23  | 1.43        | 1.38     |
| 11  | H     | 1495 | CLA  | O2A-CGA | 2.23  | 1.39        | 1.33     |
| 11  | H     | 1490 | CLA  | CHD-C1D | 2.23  | 1.42        | 1.38     |
| 11  | B     | 1497 | CLA  | CMB-C2B | 2.23  | 1.55        | 1.50     |
| 11  | H     | 1496 | CLA  | MG-NB   | 2.23  | 2.10        | 2.05     |
| 11  | I     | 1459 | CLA  | CAA-C2A | 2.23  | 1.58        | 1.54     |
| 11  | H     | 1497 | CLA  | CMB-C2B | 2.23  | 1.55        | 1.50     |
| 11  | I     | 1465 | CLA  | MG-NA   | 2.22  | 2.11        | 2.06     |
| 17  | F     | 1046 | BCR  | C29-C28 | -2.21 | 1.47        | 1.52     |
| 11  | I     | 1460 | CLA  | C1C-C2C | 2.21  | 1.49        | 1.44     |
| 11  | H     | 1495 | CLA  | C5-C3   | 2.21  | 1.55        | 1.51     |
| 11  | H     | 1496 | CLA  | CHB-C1B | -2.21 | 1.34        | 1.39     |
| 11  | B     | 1485 | CLA  | CAA-CBA | -2.21 | 1.46        | 1.52     |
| 11  | H     | 1482 | CLA  | C1C-C2C | 2.21  | 1.49        | 1.44     |
| 11  | B     | 1482 | CLA  | C1C-C2C | 2.20  | 1.49        | 1.44     |
| 11  | H     | 1487 | CLA  | C1C-C2C | 2.20  | 1.49        | 1.44     |
| 11  | C     | 1469 | CLA  | C1D-C2D | -2.20 | 1.41        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 18  | T     | 1138 | HEC  | C1C-NC  | -2.20 | 1.35        | 1.39     |
| 11  | I     | 1461 | CLA  | C4D-C3D | -2.20 | 1.41        | 1.46     |
| 11  | B     | 1494 | CLA  | C1B-NB  | -2.19 | 1.35        | 1.37     |
| 11  | I     | 1465 | CLA  | C1D-ND  | -2.18 | 1.35        | 1.37     |
| 11  | I     | 1465 | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 11  | G     | 1346 | CLA  | CHB-C1B | -2.18 | 1.34        | 1.39     |
| 11  | I     | 1461 | CLA  | CHB-C1B | -2.18 | 1.34        | 1.39     |
| 18  | V     | 1138 | HEC  | C1C-C2C | 2.18  | 1.48        | 1.43     |
| 11  | H     | 1485 | CLA  | MG-NC   | 2.17  | 2.11        | 2.06     |
| 11  | I     | 1464 | CLA  | CHC-C1C | 2.17  | 1.42        | 1.38     |
| 18  | V     | 1138 | HEC  | C1D-ND  | -2.17 | 1.35        | 1.39     |
| 11  | C     | 1466 | CLA  | C1D-C2D | -2.17 | 1.41        | 1.45     |
| 11  | B     | 1487 | CLA  | C3B-C4B | 2.17  | 1.49        | 1.42     |
| 11  | H     | 1494 | CLA  | CHB-C4A | 2.17  | 1.43        | 1.37     |
| 11  | I     | 1466 | CLA  | CMB-C2B | 2.17  | 1.55        | 1.50     |
| 11  | C     | 1462 | CLA  | C3B-C4B | 2.17  | 1.49        | 1.42     |
| 11  | H     | 1488 | CLA  | C1D-ND  | -2.17 | 1.35        | 1.37     |
| 11  | H     | 1492 | CLA  | C1D-ND  | -2.16 | 1.35        | 1.37     |
| 11  | C     | 1468 | CLA  | C2C-C1C | 2.16  | 1.48        | 1.43     |
| 11  | B     | 1495 | CLA  | MG-NC   | 2.16  | 2.11        | 2.06     |
| 11  | J     | 1353 | CLA  | C4C-C3C | 2.16  | 1.48        | 1.45     |
| 11  | G     | 1343 | CLA  | C1-C2   | 2.16  | 1.55        | 1.49     |
| 11  | H     | 1487 | CLA  | C1D-ND  | -2.16 | 1.35        | 1.37     |
| 17  | F     | 1046 | BCR  | C26-C25 | 2.16  | 1.38        | 1.34     |
| 12  | G     | 1345 | PHO  | C1D-ND  | -2.15 | 1.34        | 1.38     |
| 11  | H     | 1486 | CLA  | CHB-C1B | -2.15 | 1.34        | 1.39     |
| 11  | C     | 1464 | CLA  | C4C-C3C | 2.15  | 1.48        | 1.45     |
| 11  | C     | 1467 | CLA  | CHB-C4A | 2.15  | 1.43        | 1.37     |
| 11  | B     | 1487 | CLA  | C1C-C2C | 2.15  | 1.48        | 1.44     |
| 11  | C     | 1460 | CLA  | CMD-C2D | 2.14  | 1.55        | 1.50     |
| 11  | B     | 1485 | CLA  | C1D-C2D | -2.14 | 1.41        | 1.45     |
| 11  | B     | 1495 | CLA  | CAA-C2A | 2.14  | 1.58        | 1.54     |
| 11  | A     | 1343 | CLA  | C3D-C4D | -2.14 | 1.39        | 1.44     |
| 11  | I     | 1468 | CLA  | C2C-C1C | 2.14  | 1.48        | 1.43     |
| 11  | A     | 1344 | CLA  | CMB-C2B | 2.13  | 1.55        | 1.50     |
| 11  | H     | 1483 | CLA  | C4C-C3C | 2.13  | 1.48        | 1.45     |
| 11  | B     | 1482 | CLA  | CMB-C2B | 2.13  | 1.55        | 1.50     |
| 11  | B     | 1488 | CLA  | CMD-C2D | 2.13  | 1.55        | 1.50     |
| 11  | I     | 1469 | CLA  | C1D-ND  | -2.13 | 1.35        | 1.37     |
| 11  | B     | 1487 | CLA  | CHD-C1D | 2.13  | 1.42        | 1.38     |
| 11  | H     | 1493 | CLA  | MG-NC   | 2.13  | 2.11        | 2.06     |
| 11  | J     | 1351 | CLA  | CBA-CGA | -2.13 | 1.44        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 11  | I     | 1470 | CLA  | C1B-C2B | 2.13  | 1.48        | 1.43     |
| 11  | D     | 1351 | CLA  | C4-C3   | 2.13  | 1.55        | 1.50     |
| 11  | A     | 1344 | CLA  | C1D-C2D | -2.13 | 1.41        | 1.45     |
| 11  | I     | 1469 | CLA  | CAA-C2A | 2.13  | 1.57        | 1.53     |
| 11  | I     | 1471 | CLA  | C1B-C2B | 2.12  | 1.48        | 1.43     |
| 11  | B     | 1489 | CLA  | C4-C3   | 2.12  | 1.56        | 1.50     |
| 11  | C     | 1471 | CLA  | C4C-C3C | 2.12  | 1.48        | 1.45     |
| 11  | C     | 1471 | CLA  | CMB-C2B | 2.12  | 1.55        | 1.50     |
| 11  | C     | 1471 | CLA  | C1D-C2D | -2.12 | 1.41        | 1.45     |
| 11  | C     | 1459 | CLA  | CMB-C2B | 2.12  | 1.55        | 1.50     |
| 11  | H     | 1483 | CLA  | CBA-CGA | -2.12 | 1.44        | 1.50     |
| 11  | G     | 1346 | CLA  | C1D-ND  | -2.12 | 1.35        | 1.37     |
| 11  | H     | 1482 | CLA  | CMB-C2B | 2.12  | 1.55        | 1.50     |
| 11  | B     | 1483 | CLA  | CHC-C1C | 2.12  | 1.42        | 1.38     |
| 11  | A     | 1343 | CLA  | CHB-C4A | 2.12  | 1.43        | 1.37     |
| 11  | G     | 1343 | CLA  | C1B-C2B | 2.11  | 1.48        | 1.43     |
| 11  | B     | 1492 | CLA  | CHD-C1D | 2.11  | 1.42        | 1.38     |
| 11  | H     | 1486 | CLA  | C1B-C2B | 2.11  | 1.48        | 1.43     |
| 11  | H     | 1485 | CLA  | CAA-C2A | 2.11  | 1.57        | 1.54     |
| 11  | C     | 1462 | CLA  | C1C-C2C | 2.11  | 1.48        | 1.44     |
| 11  | I     | 1469 | CLA  | C1D-C2D | -2.11 | 1.41        | 1.45     |
| 11  | C     | 1467 | CLA  | C1C-NC  | -2.10 | 1.34        | 1.37     |
| 18  | V     | 1138 | HEC  | CHA-C4D | 2.10  | 1.44        | 1.39     |
| 11  | G     | 1343 | CLA  | C1D-C2D | -2.10 | 1.41        | 1.45     |
| 11  | I     | 1465 | CLA  | CMD-C2D | 2.10  | 1.55        | 1.50     |
| 11  | D     | 1353 | CLA  | CMB-C2B | 2.10  | 1.55        | 1.50     |
| 11  | A     | 1344 | CLA  | CHC-C1C | 2.10  | 1.42        | 1.38     |
| 11  | B     | 1489 | CLA  | CHB-C1B | -2.10 | 1.34        | 1.39     |
| 11  | I     | 1470 | CLA  | C1D-ND  | -2.10 | 1.35        | 1.37     |
| 11  | J     | 1351 | CLA  | C3D-C4D | -2.09 | 1.39        | 1.44     |
| 12  | D     | 1352 | PHO  | OBD-CAD | 2.09  | 1.25        | 1.22     |
| 11  | B     | 1491 | CLA  | C2C-C1C | 2.09  | 1.48        | 1.43     |
| 11  | H     | 1485 | CLA  | CHC-C1C | 2.09  | 1.42        | 1.38     |
| 11  | C     | 1464 | CLA  | C3B-C4B | 2.08  | 1.48        | 1.42     |
| 11  | I     | 1459 | CLA  | MG-NB   | 2.08  | 2.09        | 2.05     |
| 11  | I     | 1470 | CLA  | MG-ND   | -2.08 | 2.01        | 2.05     |
| 11  | H     | 1494 | CLA  | CAA-CBA | -2.08 | 1.46        | 1.52     |
| 11  | B     | 1496 | CLA  | C4-C3   | 2.07  | 1.55        | 1.50     |
| 11  | G     | 1342 | CLA  | C4-C3   | 2.07  | 1.55        | 1.50     |
| 11  | B     | 1492 | CLA  | CMB-C2B | 2.07  | 1.55        | 1.50     |
| 11  | C     | 1460 | CLA  | CHB-C1B | -2.07 | 1.34        | 1.39     |
| 11  | H     | 1482 | CLA  | C1D-C2D | -2.07 | 1.41        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 11  | C     | 1467 | CLA  | CAA-CBA | -2.07 | 1.46        | 1.52     |
| 11  | H     | 1483 | CLA  | CHB-C4A | 2.07  | 1.42        | 1.37     |
| 11  | B     | 1496 | CLA  | C1B-C2B | 2.07  | 1.48        | 1.43     |
| 11  | D     | 1353 | CLA  | C1-C2   | 2.07  | 1.55        | 1.49     |
| 12  | G     | 1345 | PHO  | C4A-C3A | -2.07 | 1.47        | 1.51     |
| 11  | A     | 1346 | CLA  | C4C-C3C | 2.06  | 1.48        | 1.45     |
| 11  | C     | 1461 | CLA  | MG-NB   | 2.06  | 2.09        | 2.05     |
| 11  | C     | 1459 | CLA  | CHB-C1B | -2.06 | 1.34        | 1.39     |
| 11  | B     | 1494 | CLA  | C1D-C2D | -2.06 | 1.41        | 1.45     |
| 11  | B     | 1483 | CLA  | CAA-CBA | -2.06 | 1.46        | 1.52     |
| 11  | I     | 1467 | CLA  | C3B-C4B | 2.06  | 1.48        | 1.42     |
| 11  | G     | 1346 | CLA  | C1D-C2D | -2.06 | 1.41        | 1.45     |
| 11  | A     | 1346 | CLA  | CHD-C1D | 2.06  | 1.42        | 1.38     |
| 11  | A     | 1342 | CLA  | CBA-CGA | -2.05 | 1.44        | 1.50     |
| 11  | H     | 1497 | CLA  | C3B-C4B | 2.05  | 1.48        | 1.42     |
| 11  | D     | 1353 | CLA  | C2-C3   | 2.05  | 1.38        | 1.32     |
| 11  | G     | 1342 | CLA  | C1D-C2D | -2.05 | 1.41        | 1.45     |
| 11  | I     | 1459 | CLA  | CHC-C1C | 2.05  | 1.42        | 1.38     |
| 11  | H     | 1484 | CLA  | C3B-C4B | 2.04  | 1.48        | 1.42     |
| 11  | C     | 1463 | CLA  | MG-NC   | 2.04  | 2.11        | 2.06     |
| 11  | G     | 1343 | CLA  | MG-NC   | 2.04  | 2.11        | 2.06     |
| 11  | B     | 1483 | CLA  | CHD-C1D | 2.03  | 1.42        | 1.38     |
| 11  | C     | 1459 | CLA  | MG-NB   | 2.03  | 2.09        | 2.05     |
| 11  | C     | 1465 | CLA  | C1D-C2D | -2.02 | 1.41        | 1.45     |
| 11  | I     | 1467 | CLA  | CHB-C4A | 2.02  | 1.42        | 1.37     |
| 11  | B     | 1494 | CLA  | C4C-C3C | 2.02  | 1.48        | 1.45     |
| 11  | B     | 1492 | CLA  | CAA-CBA | -2.02 | 1.46        | 1.52     |
| 11  | B     | 1495 | CLA  | C1-C2   | 2.02  | 1.54        | 1.49     |
| 11  | C     | 1460 | CLA  | C3B-C4B | 2.02  | 1.48        | 1.42     |
| 11  | B     | 1492 | CLA  | MG-NB   | 2.01  | 2.09        | 2.05     |
| 11  | C     | 1461 | CLA  | C2D-C3D | 2.01  | 1.42        | 1.36     |
| 11  | H     | 1495 | CLA  | C1C-C2C | 2.01  | 1.48        | 1.44     |
| 11  | B     | 1495 | CLA  | O2A-CGA | 2.01  | 1.39        | 1.33     |
| 11  | I     | 1462 | CLA  | C1D-C2D | -2.01 | 1.41        | 1.45     |
| 11  | B     | 1494 | CLA  | C5-C3   | 2.01  | 1.55        | 1.51     |
| 11  | B     | 1486 | CLA  | C1D-ND  | -2.01 | 1.35        | 1.37     |
| 11  | C     | 1460 | CLA  | MG-NC   | 2.01  | 2.11        | 2.06     |
| 11  | I     | 1464 | CLA  | C4C-C3C | 2.00  | 1.48        | 1.45     |
| 11  | I     | 1462 | CLA  | C3B-C4B | 2.00  | 1.48        | 1.42     |
| 11  | B     | 1491 | CLA  | CHC-C1C | 2.00  | 1.42        | 1.38     |
| 11  | C     | 1462 | CLA  | CMB-C2B | 2.00  | 1.54        | 1.50     |

All (769) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 11  | I     | 1469 | CLA  | C4A-NA-C1A  | 13.40  | 112.79      | 106.68   |
| 11  | C     | 1469 | CLA  | C4A-NA-C1A  | 13.11  | 112.66      | 106.68   |
| 11  | H     | 1495 | CLA  | C4A-NA-C1A  | 12.76  | 112.50      | 106.68   |
| 11  | I     | 1463 | CLA  | C4A-NA-C1A  | 12.62  | 112.44      | 106.68   |
| 11  | H     | 1496 | CLA  | C4A-NA-C1A  | 12.56  | 112.41      | 106.68   |
| 11  | H     | 1489 | CLA  | C4A-NA-C1A  | 12.52  | 112.39      | 106.68   |
| 11  | H     | 1482 | CLA  | C4A-NA-C1A  | 12.46  | 112.36      | 106.68   |
| 11  | C     | 1470 | CLA  | C4A-NA-C1A  | 12.44  | 112.35      | 106.68   |
| 11  | C     | 1471 | CLA  | C4A-NA-C1A  | 12.36  | 112.32      | 106.68   |
| 11  | B     | 1492 | CLA  | C4A-NA-C1A  | 12.35  | 112.31      | 106.68   |
| 11  | I     | 1471 | CLA  | C4A-NA-C1A  | 12.15  | 112.22      | 106.68   |
| 11  | B     | 1482 | CLA  | C4A-NA-C1A  | 12.12  | 112.21      | 106.68   |
| 11  | H     | 1497 | CLA  | C4A-NA-C1A  | 12.12  | 112.21      | 106.68   |
| 11  | C     | 1463 | CLA  | C4A-NA-C1A  | 12.05  | 112.18      | 106.68   |
| 11  | H     | 1492 | CLA  | C4A-NA-C1A  | 12.05  | 112.17      | 106.68   |
| 11  | H     | 1494 | CLA  | C4A-NA-C1A  | 12.05  | 112.17      | 106.68   |
| 11  | A     | 1344 | CLA  | C4A-NA-C1A  | 12.00  | 112.15      | 106.68   |
| 11  | B     | 1495 | CLA  | C4A-NA-C1A  | 12.00  | 112.15      | 106.68   |
| 11  | C     | 1467 | CLA  | C4A-NA-C1A  | 11.98  | 112.15      | 106.68   |
| 11  | C     | 1460 | CLA  | C4A-NA-C1A  | 11.98  | 112.14      | 106.68   |
| 11  | I     | 1459 | CLA  | C4A-NA-C1A  | 11.96  | 112.14      | 106.68   |
| 11  | H     | 1490 | CLA  | C4A-NA-C1A  | 11.94  | 112.13      | 106.68   |
| 11  | B     | 1486 | CLA  | C4A-NA-C1A  | 11.93  | 112.12      | 106.68   |
| 11  | C     | 1466 | CLA  | C4A-NA-C1A  | 11.80  | 112.06      | 106.68   |
| 11  | H     | 1493 | CLA  | C4A-NA-C1A  | 11.79  | 112.06      | 106.68   |
| 11  | I     | 1467 | CLA  | C4A-NA-C1A  | 11.79  | 112.06      | 106.68   |
| 11  | G     | 1344 | CLA  | C4A-NA-C1A  | 11.78  | 112.05      | 106.68   |
| 11  | I     | 1466 | CLA  | C4A-NA-C1A  | 11.78  | 112.05      | 106.68   |
| 11  | B     | 1489 | CLA  | C4A-NA-C1A  | 11.75  | 112.04      | 106.68   |
| 11  | I     | 1460 | CLA  | C4A-NA-C1A  | 11.71  | 112.02      | 106.68   |
| 11  | J     | 1351 | CLA  | C4A-NA-C1A  | 11.68  | 112.01      | 106.68   |
| 11  | B     | 1493 | CLA  | C4A-NA-C1A  | 11.66  | 112.00      | 106.68   |
| 11  | B     | 1497 | CLA  | C4A-NA-C1A  | 11.55  | 111.95      | 106.68   |
| 11  | B     | 1491 | CLA  | C4A-NA-C1A  | 11.51  | 111.93      | 106.68   |
| 11  | D     | 1353 | CLA  | C4A-NA-C1A  | 11.51  | 111.93      | 106.68   |
| 11  | I     | 1470 | CLA  | C4A-NA-C1A  | 11.49  | 111.92      | 106.68   |
| 11  | A     | 1346 | CLA  | C4A-NA-C1A  | 11.49  | 111.92      | 106.68   |
| 11  | C     | 1468 | CLA  | C4A-NA-C1A  | 11.37  | 111.86      | 106.68   |
| 11  | A     | 1342 | CLA  | C4A-NA-C1A  | 11.23  | 111.80      | 106.68   |
| 12  | D     | 1352 | PHO  | C4D-CHA-CBD | -11.22 | 103.07      | 108.45   |
| 11  | B     | 1484 | CLA  | C4A-NA-C1A  | 11.22  | 111.80      | 106.68   |
| 11  | I     | 1468 | CLA  | C4A-NA-C1A  | 11.16  | 111.77      | 106.68   |
| 11  | H     | 1488 | CLA  | C4A-NA-C1A  | 11.14  | 111.76      | 106.68   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 11  | B     | 1490 | CLA  | C4A-NA-C1A  | 11.10 | 111.74      | 106.68   |
| 11  | H     | 1486 | CLA  | C4A-NA-C1A  | 11.07 | 111.73      | 106.68   |
| 11  | B     | 1496 | CLA  | C4A-NA-C1A  | 11.07 | 111.73      | 106.68   |
| 11  | C     | 1461 | CLA  | C4A-NA-C1A  | 11.02 | 111.71      | 106.68   |
| 11  | B     | 1488 | CLA  | C4A-NA-C1A  | 10.94 | 111.67      | 106.68   |
| 11  | J     | 1353 | CLA  | C4A-NA-C1A  | 10.93 | 111.67      | 106.68   |
| 11  | D     | 1351 | CLA  | C4A-NA-C1A  | 10.87 | 111.64      | 106.68   |
| 11  | C     | 1464 | CLA  | C4A-NA-C1A  | 10.85 | 111.63      | 106.68   |
| 11  | B     | 1494 | CLA  | C4A-NA-C1A  | 10.83 | 111.62      | 106.68   |
| 11  | B     | 1483 | CLA  | C4A-NA-C1A  | 10.82 | 111.61      | 106.68   |
| 11  | B     | 1485 | CLA  | C4A-NA-C1A  | 10.74 | 111.58      | 106.68   |
| 11  | G     | 1346 | CLA  | C4A-NA-C1A  | 10.74 | 111.58      | 106.68   |
| 11  | C     | 1465 | CLA  | C4A-NA-C1A  | 10.64 | 111.53      | 106.68   |
| 11  | C     | 1459 | CLA  | C4A-NA-C1A  | 10.64 | 111.53      | 106.68   |
| 11  | H     | 1491 | CLA  | C4A-NA-C1A  | 10.63 | 111.53      | 106.68   |
| 11  | I     | 1464 | CLA  | C4A-NA-C1A  | 10.55 | 111.49      | 106.68   |
| 11  | H     | 1484 | CLA  | C4A-NA-C1A  | 10.49 | 111.47      | 106.68   |
| 11  | H     | 1485 | CLA  | C4A-NA-C1A  | 10.44 | 111.44      | 106.68   |
| 11  | I     | 1461 | CLA  | C4A-NA-C1A  | 10.42 | 111.43      | 106.68   |
| 11  | I     | 1465 | CLA  | C4A-NA-C1A  | 10.38 | 111.42      | 106.68   |
| 11  | G     | 1342 | CLA  | C4A-NA-C1A  | 10.19 | 111.33      | 106.68   |
| 11  | H     | 1483 | CLA  | C4A-NA-C1A  | 10.01 | 111.25      | 106.68   |
| 12  | J     | 1352 | PHO  | C4D-CHA-CBD | -9.95 | 103.68      | 108.45   |
| 11  | G     | 1343 | CLA  | C4A-NA-C1A  | 9.88  | 111.19      | 106.68   |
| 11  | A     | 1343 | CLA  | C4A-NA-C1A  | 9.83  | 111.16      | 106.68   |
| 11  | C     | 1462 | CLA  | C4A-NA-C1A  | 9.82  | 111.16      | 106.68   |
| 11  | B     | 1487 | CLA  | C4A-NA-C1A  | 9.66  | 111.09      | 106.68   |
| 11  | I     | 1462 | CLA  | C4A-NA-C1A  | 9.65  | 111.08      | 106.68   |
| 11  | H     | 1487 | CLA  | C4A-NA-C1A  | 9.63  | 111.07      | 106.68   |
| 12  | A     | 1345 | PHO  | C4D-CHA-CBD | -9.34 | 103.97      | 108.45   |
| 12  | G     | 1345 | PHO  | C4D-CHA-CBD | -9.11 | 104.08      | 108.45   |
| 18  | V     | 1138 | HEC  | CBC-CAC-C3C | -8.37 | 110.70      | 127.43   |
| 18  | T     | 1138 | HEC  | CBC-CAC-C3C | -8.31 | 110.82      | 127.43   |
| 11  | G     | 1343 | CLA  | C1-C2-C3    | 8.09  | 139.45      | 126.20   |
| 11  | D     | 1351 | CLA  | C1-C2-C3    | 7.51  | 138.50      | 126.20   |
| 11  | J     | 1351 | CLA  | C1-C2-C3    | 7.25  | 138.08      | 126.20   |
| 11  | A     | 1343 | CLA  | C1-C2-C3    | 7.00  | 137.67      | 126.20   |
| 18  | V     | 1138 | HEC  | CAD-C3D-C2D | 6.90  | 142.56      | 127.07   |
| 18  | T     | 1138 | HEC  | CAD-C3D-C2D | 6.64  | 141.97      | 127.07   |
| 18  | V     | 1138 | HEC  | CAD-C3D-C4D | -6.12 | 112.98      | 124.94   |
| 18  | T     | 1138 | HEC  | CAD-C3D-C4D | -5.86 | 113.48      | 124.94   |
| 17  | F     | 1046 | BCR  | C38-C26-C25 | 5.68  | 130.68      | 124.48   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12  | G     | 1345 | PHO  | C1-C2-C3    | 5.29  | 134.87      | 126.20   |
| 17  | L     | 1047 | BCR  | C38-C26-C25 | 5.25  | 130.21      | 124.48   |
| 12  | A     | 1345 | PHO  | C1-C2-C3    | 5.17  | 134.66      | 126.20   |
| 18  | T     | 1138 | HEC  | C2A-C1A-NA  | -5.07 | 105.43      | 110.32   |
| 11  | B     | 1495 | CLA  | CAA-C2A-C3A | -5.02 | 99.44       | 113.00   |
| 11  | H     | 1482 | CLA  | CAA-C2A-C3A | -4.87 | 99.83       | 113.00   |
| 11  | H     | 1495 | CLA  | CAA-C2A-C3A | -4.87 | 99.84       | 113.00   |
| 18  | V     | 1138 | HEC  | C2A-C1A-NA  | -4.79 | 105.70      | 110.32   |
| 11  | B     | 1492 | CLA  | C7-C6-C5    | -4.77 | 100.56      | 113.26   |
| 11  | B     | 1489 | CLA  | C1-C2-C3    | 4.71  | 134.38      | 126.76   |
| 11  | B     | 1482 | CLA  | CAA-C2A-C3A | -4.69 | 100.33      | 113.00   |
| 11  | B     | 1486 | CLA  | CAA-C2A-C3A | -4.65 | 105.58      | 116.23   |
| 16  | E     | 1085 | HEM  | C4A-NA-C1A  | 4.60  | 109.97      | 106.25   |
| 16  | L     | 1046 | HEM  | C4A-NA-C1A  | 4.57  | 109.94      | 106.25   |
| 11  | H     | 1489 | CLA  | C1-C2-C3    | 4.52  | 134.07      | 126.76   |
| 11  | B     | 1494 | CLA  | C1-C2-C3    | 4.50  | 133.57      | 126.20   |
| 11  | B     | 1482 | CLA  | CED-O2D-CGD | 4.43  | 125.96      | 115.92   |
| 11  | H     | 1492 | CLA  | C1-C2-C3    | 4.41  | 133.43      | 126.20   |
| 11  | H     | 1492 | CLA  | C7-C6-C5    | -4.41 | 101.52      | 113.26   |
| 11  | B     | 1495 | CLA  | O2A-CGA-CBA | 4.41  | 125.27      | 111.83   |
| 17  | L     | 1047 | BCR  | C7-C8-C9    | 4.36  | 132.68      | 126.23   |
| 12  | G     | 1345 | PHO  | O2D-CGD-CBD | 4.35  | 115.72      | 110.95   |
| 11  | I     | 1471 | CLA  | CAA-C2A-C3A | -4.34 | 106.27      | 116.23   |
| 11  | B     | 1493 | CLA  | CAA-C2A-C3A | -4.34 | 101.27      | 113.00   |
| 11  | I     | 1465 | CLA  | C7-C6-C5    | -4.31 | 101.77      | 113.26   |
| 11  | H     | 1486 | CLA  | CAA-C2A-C3A | -4.29 | 106.39      | 116.23   |
| 11  | C     | 1465 | CLA  | C7-C6-C5    | -4.26 | 101.91      | 113.26   |
| 11  | H     | 1493 | CLA  | CAA-C2A-C3A | -4.26 | 101.50      | 113.00   |
| 18  | T     | 1138 | HEC  | CBD-CAD-C3D | -4.23 | 100.84      | 112.53   |
| 11  | J     | 1351 | CLA  | C3B-C4B-NB  | -4.16 | 106.81      | 110.53   |
| 11  | H     | 1494 | CLA  | C1-C2-C3    | 4.15  | 132.99      | 126.20   |
| 11  | I     | 1470 | CLA  | CMA-C3A-C2A | -4.12 | 106.79      | 116.23   |
| 11  | H     | 1495 | CLA  | O2A-CGA-CBA | 4.07  | 124.24      | 111.83   |
| 12  | A     | 1345 | PHO  | O2D-CGD-CBD | 4.05  | 115.40      | 110.95   |
| 18  | V     | 1138 | HEC  | CBD-CAD-C3D | -4.05 | 101.35      | 112.53   |
| 11  | H     | 1482 | CLA  | CED-O2D-CGD | 4.04  | 125.07      | 115.92   |
| 11  | B     | 1492 | CLA  | C1-C2-C3    | 4.02  | 132.78      | 126.20   |
| 11  | I     | 1461 | CLA  | C1B-NB-C4B  | 3.99  | 109.11      | 106.31   |
| 11  | H     | 1494 | CLA  | C7-C6-C5    | -3.98 | 102.65      | 113.26   |
| 11  | C     | 1466 | CLA  | CAA-C2A-C3A | -3.98 | 102.24      | 113.00   |
| 11  | D     | 1351 | CLA  | C3B-C4B-NB  | -3.98 | 106.98      | 110.53   |
| 17  | L     | 1047 | BCR  | C2-C1-C6    | 3.95  | 116.18      | 110.44   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 11  | B     | 1486 | CLA  | CMA-C3A-C2A | -3.91 | 107.27      | 116.23   |
| 11  | B     | 1494 | CLA  | C7-C6-C5    | -3.90 | 102.86      | 113.26   |
| 11  | I     | 1466 | CLA  | CAA-C2A-C3A | -3.90 | 102.46      | 113.00   |
| 11  | H     | 1487 | CLA  | O2A-CGA-CBA | 3.89  | 123.71      | 111.83   |
| 17  | F     | 1046 | BCR  | C7-C8-C9    | 3.86  | 131.95      | 126.23   |
| 17  | L     | 1047 | BCR  | C29-C30-C25 | 3.86  | 116.04      | 110.44   |
| 16  | E     | 1085 | HEM  | C3A-C2A-C1A | -3.85 | 102.52      | 106.81   |
| 11  | C     | 1471 | CLA  | CAA-C2A-C3A | -3.85 | 107.41      | 116.23   |
| 11  | I     | 1471 | CLA  | CMA-C3A-C2A | -3.84 | 107.42      | 116.23   |
| 17  | F     | 1046 | BCR  | C2-C1-C6    | 3.83  | 116.01      | 110.44   |
| 11  | I     | 1469 | CLA  | CAA-C2A-C3A | -3.83 | 107.45      | 116.23   |
| 17  | F     | 1046 | BCR  | C29-C30-C25 | 3.82  | 115.99      | 110.44   |
| 17  | L     | 1047 | BCR  | C33-C5-C6   | 3.82  | 128.65      | 124.48   |
| 11  | I     | 1468 | CLA  | C1B-NB-C4B  | 3.80  | 108.97      | 106.31   |
| 11  | C     | 1468 | CLA  | C1B-NB-C4B  | 3.79  | 108.97      | 106.31   |
| 11  | G     | 1343 | CLA  | CED-O2D-CGD | 3.79  | 124.52      | 115.92   |
| 11  | C     | 1464 | CLA  | CED-O2D-CGD | 3.79  | 124.51      | 115.92   |
| 11  | B     | 1488 | CLA  | O2D-CGD-CBD | 3.75  | 117.79      | 111.23   |
| 11  | H     | 1486 | CLA  | CMA-C3A-C2A | -3.75 | 107.64      | 116.23   |
| 11  | B     | 1482 | CLA  | O2A-CGA-CBA | 3.73  | 123.20      | 111.83   |
| 11  | H     | 1493 | CLA  | CBA-CAA-C2A | 3.73  | 124.88      | 113.79   |
| 11  | I     | 1469 | CLA  | CMA-C3A-C2A | -3.72 | 107.70      | 116.23   |
| 11  | B     | 1493 | CLA  | CBA-CAA-C2A | 3.72  | 124.86      | 113.79   |
| 11  | A     | 1342 | CLA  | C7-C6-C5    | -3.71 | 103.38      | 113.26   |
| 11  | C     | 1469 | CLA  | CMA-C3A-C2A | -3.70 | 107.73      | 116.23   |
| 11  | C     | 1470 | CLA  | CMA-C3A-C2A | -3.70 | 107.75      | 116.23   |
| 11  | C     | 1466 | CLA  | C1-C2-C3    | 3.69  | 132.73      | 126.76   |
| 11  | C     | 1459 | CLA  | CAA-C2A-C3A | -3.69 | 103.03      | 113.00   |
| 11  | C     | 1469 | CLA  | CAA-C2A-C3A | -3.68 | 107.78      | 116.23   |
| 11  | B     | 1487 | CLA  | O2A-CGA-CBA | 3.66  | 123.00      | 111.83   |
| 11  | G     | 1342 | CLA  | C7-C6-C5    | -3.64 | 103.55      | 113.26   |
| 17  | L     | 1047 | BCR  | C15-C14-C13 | 3.63  | 132.38      | 127.28   |
| 11  | I     | 1464 | CLA  | CED-O2D-CGD | 3.63  | 124.15      | 115.92   |
| 11  | H     | 1482 | CLA  | C1-C2-C3    | 3.63  | 132.14      | 126.20   |
| 11  | C     | 1461 | CLA  | C1B-NB-C4B  | 3.62  | 108.85      | 106.31   |
| 11  | A     | 1343 | CLA  | CED-O2D-CGD | 3.61  | 124.11      | 115.92   |
| 11  | C     | 1470 | CLA  | CAA-C2A-C3A | -3.59 | 108.00      | 116.23   |
| 16  | E     | 1085 | HEM  | C3D-C4D-CHA | -3.59 | 116.44      | 125.84   |
| 11  | B     | 1497 | CLA  | C2A-C3A-C4A | 3.59  | 105.79      | 101.59   |
| 11  | I     | 1459 | CLA  | CAA-C2A-C3A | -3.57 | 103.36      | 113.00   |
| 11  | H     | 1489 | CLA  | O2D-CGD-CBD | 3.56  | 117.45      | 111.23   |
| 11  | C     | 1468 | CLA  | C1C-NC-C4C  | 3.56  | 108.30      | 106.68   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12  | D     | 1352 | PHO  | O2A-CGA-CBA | 3.55  | 122.67      | 111.83   |
| 11  | B     | 1482 | CLA  | C1-C2-C3    | 3.55  | 132.01      | 126.20   |
| 17  | F     | 1046 | BCR  | C33-C5-C6   | 3.55  | 128.35      | 124.48   |
| 17  | L     | 1047 | BCR  | C12-C13-C14 | -3.54 | 113.44      | 119.01   |
| 17  | F     | 1046 | BCR  | C35-C13-C12 | 3.53  | 123.47      | 118.09   |
| 18  | V     | 1138 | HEC  | CHA-C4D-ND  | 3.53  | 130.25      | 123.86   |
| 17  | F     | 1046 | BCR  | C23-C24-C25 | 3.52  | 136.40      | 127.00   |
| 18  | T     | 1138 | HEC  | CHA-C4D-ND  | 3.51  | 130.23      | 123.86   |
| 11  | B     | 1484 | CLA  | CAA-C2A-C3A | -3.51 | 103.50      | 113.00   |
| 11  | B     | 1492 | CLA  | CED-O2D-CGD | 3.51  | 123.88      | 115.92   |
| 16  | L     | 1046 | HEM  | C3A-C2A-C1A | -3.50 | 102.91      | 106.81   |
| 11  | I     | 1470 | CLA  | CAA-C2A-C3A | -3.50 | 108.19      | 116.23   |
| 11  | H     | 1497 | CLA  | CAA-C2A-C3A | -3.49 | 108.22      | 116.23   |
| 11  | H     | 1484 | CLA  | CAA-C2A-C3A | -3.48 | 103.59      | 113.00   |
| 11  | B     | 1491 | CLA  | C1C-NC-C4C  | 3.48  | 108.27      | 106.68   |
| 11  | I     | 1463 | CLA  | CED-O2D-CGD | 3.48  | 123.81      | 115.92   |
| 11  | H     | 1490 | CLA  | CED-O2D-CGD | 3.47  | 123.80      | 115.92   |
| 11  | B     | 1497 | CLA  | CAA-C2A-C3A | -3.46 | 108.28      | 116.23   |
| 11  | C     | 1471 | CLA  | CMA-C3A-C2A | -3.46 | 108.30      | 116.23   |
| 11  | B     | 1496 | CLA  | C7-C6-C5    | -3.44 | 104.09      | 113.26   |
| 16  | L     | 1046 | HEM  | C3D-C4D-CHA | -3.44 | 116.83      | 125.84   |
| 11  | C     | 1464 | CLA  | C7-C6-C5    | -3.43 | 104.12      | 113.26   |
| 11  | H     | 1495 | CLA  | O2D-CGD-CBD | 3.41  | 117.20      | 111.23   |
| 11  | I     | 1464 | CLA  | C7-C6-C5    | -3.41 | 104.16      | 113.26   |
| 11  | G     | 1343 | CLA  | O2A-CGA-CBA | 3.41  | 122.23      | 111.83   |
| 11  | I     | 1462 | CLA  | C3B-C4B-NB  | -3.41 | 107.49      | 110.53   |
| 11  | H     | 1496 | CLA  | C7-C6-C5    | -3.41 | 104.19      | 113.26   |
| 11  | B     | 1490 | CLA  | CED-O2D-CGD | 3.40  | 123.63      | 115.92   |
| 11  | C     | 1462 | CLA  | CED-O2D-CGD | 3.40  | 123.62      | 115.92   |
| 17  | F     | 1046 | BCR  | C38-C26-C27 | -3.40 | 106.36      | 113.60   |
| 12  | A     | 1345 | PHO  | OBD-CAD-CBD | -3.39 | 120.85      | 125.82   |
| 12  | G     | 1345 | PHO  | C7-C6-C5    | -3.38 | 104.25      | 113.26   |
| 11  | B     | 1489 | CLA  | O2D-CGD-CBD | 3.37  | 117.13      | 111.23   |
| 11  | C     | 1460 | CLA  | O2A-CGA-CBA | 3.37  | 122.12      | 111.83   |
| 18  | V     | 1138 | HEC  | C4A-NA-C1A  | 3.37  | 111.32      | 105.82   |
| 11  | B     | 1483 | CLA  | CAA-C2A-C3A | -3.37 | 103.89      | 113.00   |
| 11  | H     | 1488 | CLA  | O2D-CGD-CBD | 3.37  | 117.12      | 111.23   |
| 12  | D     | 1352 | PHO  | C2D-C1D-ND  | 3.37  | 111.86      | 109.43   |
| 11  | A     | 1342 | CLA  | CED-O2D-CGD | 3.36  | 123.54      | 115.92   |
| 11  | H     | 1492 | CLA  | C6-C5-C3    | 3.35  | 121.64      | 113.47   |
| 11  | I     | 1465 | CLA  | C1-C2-C3    | 3.35  | 131.68      | 126.20   |
| 11  | I     | 1462 | CLA  | CAA-C2A-C3A | -3.34 | 103.97      | 113.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | F     | 1046 | BCR  | C15-C14-C13 | 3.34  | 131.96      | 127.28   |
| 12  | D     | 1352 | PHO  | CAA-C2A-C3A | -3.34 | 103.98      | 113.00   |
| 11  | B     | 1496 | CLA  | C1-C2-C3    | 3.33  | 131.66      | 126.20   |
| 12  | J     | 1352 | PHO  | C4A-C3A-C2A | 3.33  | 106.01      | 102.84   |
| 17  | F     | 1046 | BCR  | C30-C25-C26 | -3.33 | 118.09      | 122.64   |
| 12  | J     | 1352 | PHO  | C7-C6-C5    | -3.33 | 104.39      | 113.26   |
| 11  | H     | 1482 | CLA  | O2A-CGA-CBA | 3.31  | 121.94      | 111.83   |
| 11  | H     | 1492 | CLA  | CED-O2D-CGD | 3.31  | 123.43      | 115.92   |
| 12  | A     | 1345 | PHO  | CED-O2D-CGD | 3.31  | 123.43      | 115.92   |
| 11  | B     | 1496 | CLA  | C6-C5-C3    | 3.31  | 121.52      | 113.47   |
| 17  | F     | 1046 | BCR  | C12-C13-C14 | -3.31 | 113.81      | 119.01   |
| 11  | H     | 1497 | CLA  | C2A-C3A-C4A | 3.29  | 105.45      | 101.59   |
| 11  | H     | 1488 | CLA  | C3B-C4B-NB  | -3.28 | 107.60      | 110.53   |
| 17  | L     | 1047 | BCR  | C35-C13-C12 | 3.28  | 123.10      | 118.09   |
| 11  | I     | 1466 | CLA  | C1-C2-C3    | 3.28  | 132.07      | 126.76   |
| 11  | H     | 1497 | CLA  | CED-O2D-CGD | 3.28  | 123.35      | 115.92   |
| 12  | J     | 1352 | PHO  | CAA-C2A-C3A | -3.28 | 104.14      | 113.00   |
| 12  | G     | 1345 | PHO  | CED-O2D-CGD | 3.28  | 123.34      | 115.92   |
| 11  | I     | 1464 | CLA  | O2D-CGD-CBD | 3.27  | 116.95      | 111.23   |
| 11  | B     | 1492 | CLA  | C6-C5-C3    | 3.27  | 121.44      | 113.47   |
| 11  | I     | 1462 | CLA  | O2A-CGA-CBA | 3.27  | 121.81      | 111.83   |
| 11  | B     | 1487 | CLA  | C1-C2-C3    | 3.27  | 131.55      | 126.20   |
| 11  | B     | 1488 | CLA  | C3B-C4B-NB  | -3.26 | 107.62      | 110.53   |
| 11  | I     | 1463 | CLA  | C7-C6-C5    | -3.26 | 104.57      | 113.26   |
| 12  | D     | 1352 | PHO  | O2D-CGD-CBD | 3.26  | 114.53      | 110.95   |
| 11  | C     | 1463 | CLA  | C7-C6-C5    | -3.26 | 104.58      | 113.26   |
| 11  | C     | 1464 | CLA  | C1-C2-C3    | -3.25 | 120.87      | 126.20   |
| 11  | H     | 1489 | CLA  | O2A-CGA-CBA | 3.24  | 121.70      | 111.83   |
| 11  | H     | 1491 | CLA  | C1B-NB-C4B  | 3.23  | 108.58      | 106.31   |
| 12  | D     | 1352 | PHO  | C7-C6-C5    | -3.22 | 104.68      | 113.26   |
| 17  | L     | 1047 | BCR  | C30-C25-C26 | -3.22 | 118.24      | 122.64   |
| 11  | I     | 1466 | CLA  | CED-O2D-CGD | 3.22  | 123.22      | 115.92   |
| 12  | J     | 1352 | PHO  | C2D-C1D-ND  | 3.22  | 111.75      | 109.43   |
| 12  | J     | 1352 | PHO  | CED-O2D-CGD | 3.21  | 123.19      | 115.92   |
| 18  | T     | 1138 | HEC  | C4A-NA-C1A  | 3.21  | 111.05      | 105.82   |
| 11  | I     | 1465 | CLA  | C3B-C4B-NB  | -3.21 | 107.67      | 110.53   |
| 17  | L     | 1047 | BCR  | C38-C26-C27 | -3.21 | 106.76      | 113.60   |
| 12  | D     | 1352 | PHO  | C4A-C3A-C2A | 3.21  | 105.89      | 102.84   |
| 11  | H     | 1491 | CLA  | C1C-NC-C4C  | 3.20  | 108.14      | 106.68   |
| 11  | I     | 1463 | CLA  | O2A-CGA-CBA | 3.20  | 121.60      | 111.83   |
| 11  | C     | 1463 | CLA  | CED-O2D-CGD | 3.20  | 123.17      | 115.92   |
| 11  | J     | 1351 | CLA  | O2A-CGA-CBA | 3.19  | 121.56      | 111.83   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 11  | I     | 1460 | CLA  | CED-O2D-CGD | 3.19  | 123.15      | 115.92   |
| 11  | B     | 1487 | CLA  | C3B-C4B-NB  | -3.18 | 107.69      | 110.53   |
| 12  | J     | 1352 | PHO  | O2A-CGA-CBA | 3.17  | 121.51      | 111.83   |
| 11  | H     | 1483 | CLA  | CAA-C2A-C3A | -3.17 | 104.44      | 113.00   |
| 12  | A     | 1345 | PHO  | C7-C6-C5    | -3.16 | 104.83      | 113.26   |
| 11  | I     | 1460 | CLA  | O2A-CGA-CBA | 3.16  | 121.47      | 111.83   |
| 11  | H     | 1496 | CLA  | C1-C2-C3    | 3.16  | 131.38      | 126.20   |
| 11  | B     | 1486 | CLA  | C2A-C3A-C4A | 3.16  | 105.29      | 101.59   |
| 11  | G     | 1346 | CLA  | C1-C2-C3    | 3.15  | 131.37      | 126.20   |
| 11  | H     | 1484 | CLA  | CED-O2D-CGD | 3.15  | 123.06      | 115.92   |
| 11  | A     | 1343 | CLA  | O2A-CGA-CBA | 3.14  | 121.41      | 111.83   |
| 12  | A     | 1345 | PHO  | C2D-C1D-ND  | 3.14  | 111.70      | 109.43   |
| 11  | H     | 1487 | CLA  | C1-C2-C3    | 3.12  | 131.31      | 126.20   |
| 11  | B     | 1488 | CLA  | CAA-C2A-C3A | -3.12 | 104.56      | 113.00   |
| 11  | H     | 1487 | CLA  | O2D-CGD-CBD | 3.12  | 116.69      | 111.23   |
| 11  | I     | 1462 | CLA  | CED-O2D-CGD | 3.12  | 122.99      | 115.92   |
| 12  | J     | 1352 | PHO  | OBD-CAD-CBD | -3.12 | 121.25      | 125.82   |
| 11  | G     | 1344 | CLA  | CAA-C2A-C3A | -3.11 | 104.58      | 113.00   |
| 17  | L     | 1047 | BCR  | C23-C24-C25 | 3.11  | 135.31      | 127.00   |
| 11  | H     | 1497 | CLA  | C3B-C4B-NB  | -3.11 | 107.76      | 110.53   |
| 11  | B     | 1489 | CLA  | O2A-CGA-CBA | 3.10  | 121.30      | 111.83   |
| 11  | I     | 1461 | CLA  | C1C-NC-C4C  | 3.10  | 108.09      | 106.68   |
| 11  | C     | 1463 | CLA  | C6-C5-C3    | 3.10  | 121.02      | 113.47   |
| 11  | C     | 1463 | CLA  | O2A-CGA-CBA | 3.10  | 121.28      | 111.83   |
| 11  | G     | 1342 | CLA  | O2A-CGA-CBA | 3.09  | 121.25      | 111.83   |
| 11  | I     | 1463 | CLA  | C6-C5-C3    | 3.08  | 120.98      | 113.47   |
| 11  | C     | 1460 | CLA  | CED-O2D-CGD | 3.08  | 122.91      | 115.92   |
| 11  | A     | 1346 | CLA  | O2A-CGA-CBA | 3.08  | 121.22      | 111.83   |
| 11  | C     | 1462 | CLA  | CAA-C2A-C3A | -3.07 | 104.69      | 113.00   |
| 11  | H     | 1495 | CLA  | C2A-C1A-CHA | 3.07  | 129.20      | 123.87   |
| 11  | I     | 1469 | CLA  | C2A-C3A-C4A | 3.05  | 105.17      | 101.59   |
| 11  | B     | 1485 | CLA  | CED-O2D-CGD | 3.04  | 122.82      | 115.92   |
| 12  | G     | 1345 | PHO  | OBD-CAD-CBD | -3.03 | 121.38      | 125.82   |
| 11  | B     | 1497 | CLA  | O2D-CGD-CBD | 3.00  | 116.48      | 111.23   |
| 11  | D     | 1351 | CLA  | O2A-CGA-CBA | 3.00  | 120.99      | 111.83   |
| 11  | A     | 1343 | CLA  | CAA-C2A-C3A | -3.00 | 104.90      | 113.00   |
| 11  | C     | 1471 | CLA  | C2A-C3A-C4A | 2.99  | 105.10      | 101.59   |
| 11  | B     | 1495 | CLA  | C2A-C1A-CHA | 2.99  | 129.06      | 123.87   |
| 11  | C     | 1468 | CLA  | C2A-C1A-CHA | 2.99  | 127.34      | 122.71   |
| 11  | G     | 1346 | CLA  | O2A-CGA-CBA | 2.98  | 120.93      | 111.83   |
| 17  | L     | 1047 | BCR  | C34-C9-C8   | 2.98  | 122.64      | 118.09   |
| 11  | J     | 1353 | CLA  | O2A-CGA-CBA | 2.98  | 120.92      | 111.83   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 11  | G     | 1342 | CLA  | CED-O2D-CGD | 2.98  | 122.67      | 115.92   |
| 11  | A     | 1342 | CLA  | C3B-C4B-NB  | -2.97 | 107.88      | 110.53   |
| 11  | C     | 1462 | CLA  | C3B-C4B-NB  | -2.97 | 107.88      | 110.53   |
| 11  | C     | 1465 | CLA  | C3B-C4B-NB  | -2.97 | 107.88      | 110.53   |
| 11  | B     | 1497 | CLA  | C3B-C4B-NB  | -2.97 | 107.88      | 110.53   |
| 17  | F     | 1046 | BCR  | C1-C6-C5    | -2.96 | 118.58      | 122.64   |
| 11  | I     | 1464 | CLA  | C1-C2-C3    | -2.96 | 121.34      | 126.20   |
| 11  | H     | 1496 | CLA  | CED-O2D-CGD | 2.96  | 122.63      | 115.92   |
| 11  | B     | 1495 | CLA  | C3B-C4B-NB  | -2.96 | 107.89      | 110.53   |
| 11  | D     | 1353 | CLA  | O2A-CGA-CBA | 2.96  | 120.86      | 111.83   |
| 17  | F     | 1046 | BCR  | C1-C6-C7    | 2.95  | 123.67      | 115.65   |
| 11  | A     | 1344 | CLA  | CAA-C2A-C3A | -2.95 | 105.04      | 113.00   |
| 17  | L     | 1047 | BCR  | C1-C6-C5    | -2.94 | 118.61      | 122.64   |
| 11  | I     | 1464 | CLA  | O2A-CGA-CBA | 2.94  | 120.80      | 111.83   |
| 11  | C     | 1470 | CLA  | CED-O2D-CGD | 2.93  | 122.57      | 115.92   |
| 17  | L     | 1047 | BCR  | C1-C6-C7    | 2.93  | 123.58      | 115.65   |
| 11  | C     | 1464 | CLA  | O2D-CGD-CBD | 2.92  | 116.34      | 111.23   |
| 11  | J     | 1351 | CLA  | CED-O2D-CGD | 2.92  | 122.54      | 115.92   |
| 11  | H     | 1494 | CLA  | O2A-CGA-CBA | 2.92  | 120.74      | 111.83   |
| 11  | C     | 1465 | CLA  | O2D-CGD-CBD | 2.92  | 116.33      | 111.23   |
| 11  | H     | 1497 | CLA  | O2D-CGD-CBD | 2.92  | 116.33      | 111.23   |
| 11  | C     | 1464 | CLA  | O2A-CGA-CBA | 2.91  | 120.72      | 111.83   |
| 11  | D     | 1353 | CLA  | CAA-C2A-C3A | -2.91 | 105.13      | 113.00   |
| 11  | C     | 1462 | CLA  | O2A-CGA-CBA | 2.91  | 120.72      | 111.83   |
| 11  | B     | 1491 | CLA  | C1B-NB-C4B  | 2.91  | 108.35      | 106.31   |
| 11  | C     | 1461 | CLA  | C1C-NC-C4C  | 2.91  | 108.01      | 106.68   |
| 11  | C     | 1469 | CLA  | C2A-C3A-C4A | 2.91  | 105.00      | 101.59   |
| 11  | I     | 1464 | CLA  | O2A-C1-C2   | 2.91  | 119.29      | 108.11   |
| 11  | C     | 1466 | CLA  | CED-O2D-CGD | 2.90  | 122.50      | 115.92   |
| 11  | H     | 1488 | CLA  | CAA-C2A-C3A | -2.90 | 105.15      | 113.00   |
| 11  | G     | 1346 | CLA  | O2D-CGD-CBD | 2.90  | 116.30      | 111.23   |
| 12  | D     | 1352 | PHO  | OBD-CAD-CBD | -2.90 | 121.57      | 125.82   |
| 11  | A     | 1342 | CLA  | O2A-CGA-CBA | 2.89  | 120.65      | 111.83   |
| 11  | I     | 1470 | CLA  | C2A-C3A-C4A | 2.89  | 104.98      | 101.59   |
| 11  | H     | 1486 | CLA  | C2A-C3A-C4A | 2.89  | 104.98      | 101.59   |
| 11  | B     | 1484 | CLA  | CED-O2D-CGD | 2.89  | 122.47      | 115.92   |
| 11  | I     | 1465 | CLA  | O2D-CGD-CBD | 2.88  | 116.27      | 111.23   |
| 11  | I     | 1468 | CLA  | C2A-C1A-CHA | 2.88  | 127.17      | 122.71   |
| 11  | H     | 1492 | CLA  | C3B-C4B-NB  | -2.87 | 107.97      | 110.53   |
| 11  | B     | 1496 | CLA  | C2A-C3A-C4A | 2.87  | 106.50      | 101.87   |
| 11  | C     | 1466 | CLA  | O2A-CGA-CBA | 2.86  | 120.54      | 111.83   |
| 12  | J     | 1352 | PHO  | O2D-CGD-CBD | 2.85  | 114.08      | 110.95   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 11  | C     | 1462 | CLA  | C7-C6-C5    | -2.85 | 105.66      | 113.26   |
| 11  | I     | 1465 | CLA  | O2A-CGA-CBA | 2.85  | 120.53      | 111.83   |
| 11  | C     | 1470 | CLA  | C2A-C3A-C4A | 2.85  | 104.93      | 101.59   |
| 11  | J     | 1353 | CLA  | C1-C2-C3    | 2.85  | 131.38      | 126.76   |
| 11  | B     | 1496 | CLA  | O2A-CGA-CBA | 2.84  | 120.50      | 111.83   |
| 11  | B     | 1488 | CLA  | O2A-CGA-CBA | 2.84  | 120.50      | 111.83   |
| 11  | J     | 1351 | CLA  | CAA-C2A-C3A | -2.83 | 105.36      | 113.00   |
| 11  | I     | 1465 | CLA  | CED-O2D-CGD | 2.83  | 122.32      | 115.92   |
| 11  | H     | 1493 | CLA  | CED-O2D-CGD | 2.82  | 122.32      | 115.92   |
| 11  | I     | 1466 | CLA  | C3B-C4B-NB  | -2.82 | 108.02      | 110.53   |
| 11  | J     | 1351 | CLA  | C2A-C1A-CHA | 2.82  | 128.75      | 123.87   |
| 17  | L     | 1047 | BCR  | C19-C18-C17 | -2.82 | 114.58      | 119.01   |
| 11  | G     | 1346 | CLA  | CAA-C2A-C3A | -2.81 | 105.40      | 113.00   |
| 17  | L     | 1047 | BCR  | C33-C5-C4   | -2.81 | 107.60      | 113.60   |
| 11  | I     | 1461 | CLA  | C2A-C1A-CHA | 2.81  | 127.07      | 122.71   |
| 11  | B     | 1487 | CLA  | CED-O2D-CGD | 2.81  | 122.29      | 115.92   |
| 11  | H     | 1483 | CLA  | CED-O2D-CGD | 2.80  | 122.28      | 115.92   |
| 11  | H     | 1486 | CLA  | CED-O2D-CGD | 2.80  | 122.28      | 115.92   |
| 11  | B     | 1482 | CLA  | CBA-CAA-C2A | 2.80  | 122.14      | 113.79   |
| 11  | A     | 1346 | CLA  | C1-C2-C3    | 2.80  | 130.79      | 126.20   |
| 11  | H     | 1483 | CLA  | O2A-CGA-CBA | 2.80  | 120.38      | 111.83   |
| 11  | B     | 1485 | CLA  | C2A-C3A-C4A | 2.80  | 106.40      | 101.87   |
| 11  | I     | 1466 | CLA  | O2A-CGA-CBA | 2.80  | 120.38      | 111.83   |
| 11  | H     | 1487 | CLA  | C3B-C4B-NB  | -2.79 | 108.04      | 110.53   |
| 11  | C     | 1464 | CLA  | O2A-C1-C2   | 2.79  | 118.84      | 108.11   |
| 12  | G     | 1345 | PHO  | C2D-C1D-ND  | 2.79  | 111.44      | 109.43   |
| 17  | L     | 1047 | BCR  | C8-C9-C10   | -2.79 | 114.63      | 119.01   |
| 11  | H     | 1495 | CLA  | C3B-C4B-NB  | -2.79 | 108.04      | 110.53   |
| 11  | J     | 1351 | CLA  | O2A-C1-C2   | 2.78  | 118.82      | 108.11   |
| 17  | F     | 1046 | BCR  | C36-C18-C19 | 2.78  | 122.34      | 118.09   |
| 11  | B     | 1490 | CLA  | CAA-C2A-C3A | -2.78 | 105.48      | 113.00   |
| 11  | H     | 1490 | CLA  | CAA-C2A-C3A | -2.78 | 105.48      | 113.00   |
| 11  | H     | 1491 | CLA  | C2A-C1A-CHA | 2.78  | 127.02      | 122.71   |
| 11  | I     | 1459 | CLA  | C3B-C4B-NB  | -2.78 | 108.05      | 110.53   |
| 11  | B     | 1491 | CLA  | C2A-C1A-CHA | 2.78  | 127.02      | 122.71   |
| 11  | A     | 1342 | CLA  | CAA-C2A-C3A | -2.77 | 105.51      | 113.00   |
| 11  | H     | 1496 | CLA  | C6-C5-C3    | 2.77  | 120.21      | 113.47   |
| 11  | C     | 1461 | CLA  | C2A-C1A-CHA | 2.77  | 127.00      | 122.71   |
| 12  | G     | 1345 | PHO  | O1D-CGD-CBD | -2.76 | 120.53      | 124.72   |
| 11  | I     | 1465 | CLA  | C12-C11-C10 | -2.75 | 100.93      | 113.28   |
| 11  | B     | 1485 | CLA  | CAA-C2A-C3A | -2.75 | 105.56      | 113.00   |
| 11  | B     | 1494 | CLA  | CED-O2D-CGD | 2.74  | 122.14      | 115.92   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 11  | C     | 1467 | CLA  | C2A-C1A-CHA | 2.74  | 128.62      | 123.87   |
| 11  | H     | 1495 | CLA  | CED-O2D-CGD | 2.74  | 122.13      | 115.92   |
| 11  | C     | 1465 | CLA  | C1-C2-C3    | 2.74  | 130.68      | 126.20   |
| 11  | I     | 1466 | CLA  | CBA-CAA-C2A | 2.73  | 121.93      | 113.79   |
| 11  | I     | 1471 | CLA  | C2A-C3A-C4A | 2.73  | 104.79      | 101.59   |
| 11  | C     | 1465 | CLA  | O2A-CGA-CBA | 2.73  | 120.16      | 111.83   |
| 17  | F     | 1046 | BCR  | C33-C5-C4   | -2.73 | 107.77      | 113.60   |
| 11  | B     | 1482 | CLA  | C2A-C3A-C4A | 2.73  | 106.28      | 101.87   |
| 11  | I     | 1459 | CLA  | CED-O2D-CGD | 2.72  | 122.09      | 115.92   |
| 17  | F     | 1046 | BCR  | C34-C9-C8   | 2.72  | 122.25      | 118.09   |
| 11  | A     | 1343 | CLA  | C2A-C3A-C4A | 2.72  | 106.25      | 101.87   |
| 11  | H     | 1482 | CLA  | CBA-CAA-C2A | 2.71  | 121.87      | 113.79   |
| 17  | F     | 1046 | BCR  | C19-C18-C17 | -2.71 | 114.75      | 119.01   |
| 11  | B     | 1497 | CLA  | CMA-C3A-C2A | -2.71 | 110.02      | 116.23   |
| 11  | H     | 1493 | CLA  | C3B-C4B-NB  | -2.71 | 108.11      | 110.53   |
| 11  | A     | 1346 | CLA  | CED-O2D-CGD | 2.70  | 122.04      | 115.92   |
| 11  | G     | 1343 | CLA  | C2A-C3A-C4A | 2.69  | 106.22      | 101.87   |
| 11  | C     | 1465 | CLA  | C12-C11-C10 | -2.69 | 101.21      | 113.28   |
| 11  | B     | 1494 | CLA  | O2A-CGA-CBA | 2.69  | 120.05      | 111.83   |
| 11  | D     | 1351 | CLA  | O2A-C1-C2   | 2.69  | 118.47      | 108.11   |
| 11  | B     | 1487 | CLA  | C12-C11-C10 | -2.69 | 101.22      | 113.28   |
| 11  | G     | 1342 | CLA  | CAA-C2A-C3A | -2.68 | 105.75      | 113.00   |
| 11  | H     | 1496 | CLA  | C2A-C3A-C4A | 2.68  | 106.20      | 101.87   |
| 11  | C     | 1466 | CLA  | CBA-CAA-C2A | 2.68  | 121.77      | 113.79   |
| 11  | H     | 1490 | CLA  | C2A-C1A-CHA | 2.68  | 128.51      | 123.87   |
| 11  | H     | 1494 | CLA  | CED-O2D-CGD | 2.68  | 121.98      | 115.92   |
| 12  | A     | 1345 | PHO  | O1D-CGD-CBD | -2.67 | 120.67      | 124.72   |
| 11  | G     | 1343 | CLA  | CAA-C2A-C3A | -2.67 | 105.78      | 113.00   |
| 11  | I     | 1469 | CLA  | CED-O2D-CGD | 2.67  | 121.97      | 115.92   |
| 11  | B     | 1483 | CLA  | O2D-CGD-CBD | 2.66  | 115.89      | 111.23   |
| 11  | A     | 1343 | CLA  | CBA-CAA-C2A | 2.66  | 121.72      | 113.79   |
| 11  | H     | 1485 | CLA  | CED-O2D-CGD | 2.66  | 121.95      | 115.92   |
| 11  | I     | 1459 | CLA  | CMD-C2D-C1D | 2.66  | 129.41      | 124.73   |
| 11  | C     | 1463 | CLA  | C3B-C4B-NB  | -2.65 | 108.16      | 110.53   |
| 11  | C     | 1465 | CLA  | CED-O2D-CGD | 2.65  | 121.93      | 115.92   |
| 11  | B     | 1497 | CLA  | CED-O2D-CGD | 2.65  | 121.92      | 115.92   |
| 11  | I     | 1459 | CLA  | O2A-CGA-CBA | 2.65  | 122.36      | 114.00   |
| 11  | G     | 1344 | CLA  | C3B-C4B-NB  | -2.64 | 108.17      | 110.53   |
| 12  | G     | 1345 | PHO  | C4A-C3A-C2A | 2.64  | 105.35      | 102.84   |
| 11  | J     | 1353 | CLA  | CAA-C2A-C3A | -2.64 | 105.88      | 113.00   |
| 11  | I     | 1463 | CLA  | C2A-C1A-CHA | 2.64  | 128.44      | 123.87   |
| 11  | A     | 1346 | CLA  | O2D-CGD-CBD | 2.64  | 115.84      | 111.23   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 11  | H     | 1493 | CLA  | C2A-C3A-C4A | 2.63  | 106.12      | 101.87   |
| 12  | J     | 1352 | PHO  | C1-C2-C3    | 2.63  | 130.50      | 126.20   |
| 11  | B     | 1483 | CLA  | O2A-CGA-CBA | 2.63  | 119.84      | 111.83   |
| 11  | H     | 1494 | CLA  | C2A-C3A-C4A | 2.62  | 106.11      | 101.87   |
| 11  | H     | 1487 | CLA  | C12-C11-C10 | -2.61 | 101.57      | 113.28   |
| 11  | B     | 1492 | CLA  | O2A-CGA-CBA | 2.61  | 119.79      | 111.83   |
| 11  | C     | 1471 | CLA  | CED-O2D-CGD | 2.61  | 121.83      | 115.92   |
| 11  | D     | 1351 | CLA  | C12-C11-C10 | -2.60 | 101.61      | 113.28   |
| 11  | J     | 1353 | CLA  | C2A-C3A-C4A | 2.60  | 106.08      | 101.87   |
| 11  | I     | 1459 | CLA  | C2A-C3A-C4A | 2.60  | 106.07      | 101.87   |
| 12  | D     | 1352 | PHO  | CED-O2D-CGD | 2.60  | 121.82      | 115.92   |
| 11  | H     | 1492 | CLA  | C6-C7-C8    | 2.60  | 124.61      | 115.97   |
| 11  | B     | 1494 | CLA  | C6-C5-C3    | 2.60  | 119.80      | 113.47   |
| 11  | H     | 1483 | CLA  | C3B-C4B-NB  | -2.60 | 108.21      | 110.53   |
| 11  | B     | 1483 | CLA  | C7-C6-C5    | -2.59 | 106.35      | 113.26   |
| 11  | H     | 1484 | CLA  | O2A-CGA-CBA | 2.59  | 122.19      | 114.00   |
| 11  | H     | 1489 | CLA  | CMD-C2D-C1D | 2.58  | 129.28      | 124.73   |
| 11  | D     | 1351 | CLA  | C2A-C3A-C4A | 2.58  | 106.04      | 101.87   |
| 11  | A     | 1344 | CLA  | O2D-CGD-CBD | 2.58  | 115.74      | 111.23   |
| 17  | F     | 1046 | BCR  | C23-C22-C21 | -2.58 | 114.95      | 119.01   |
| 11  | B     | 1487 | CLA  | O2D-CGD-CBD | 2.58  | 115.73      | 111.23   |
| 11  | G     | 1342 | CLA  | C3B-C4B-NB  | -2.58 | 108.23      | 110.53   |
| 11  | H     | 1494 | CLA  | C3B-C4B-NB  | -2.57 | 108.23      | 110.53   |
| 11  | H     | 1492 | CLA  | O2A-CGA-CBA | 2.57  | 119.68      | 111.83   |
| 11  | H     | 1488 | CLA  | C1-O2A-CGA  | 2.57  | 122.88      | 116.65   |
| 11  | H     | 1496 | CLA  | O2A-CGA-CBA | 2.57  | 119.68      | 111.83   |
| 11  | B     | 1489 | CLA  | C3B-C4B-NB  | -2.57 | 108.23      | 110.53   |
| 11  | G     | 1343 | CLA  | CBA-CAA-C2A | 2.57  | 121.44      | 113.79   |
| 11  | H     | 1488 | CLA  | O2A-CGA-CBA | 2.57  | 119.66      | 111.83   |
| 11  | I     | 1470 | CLA  | CED-O2D-CGD | 2.56  | 121.73      | 115.92   |
| 11  | I     | 1467 | CLA  | O2A-CGA-CBA | 2.56  | 119.63      | 111.83   |
| 11  | B     | 1490 | CLA  | CMA-C3A-C2A | -2.55 | 104.11      | 113.98   |
| 11  | I     | 1468 | CLA  | C1C-NC-C4C  | 2.55  | 107.84      | 106.68   |
| 11  | C     | 1470 | CLA  | C3B-C4B-NB  | -2.55 | 108.25      | 110.53   |
| 11  | B     | 1495 | CLA  | O2D-CGD-CBD | 2.55  | 115.68      | 111.23   |
| 11  | C     | 1469 | CLA  | CED-O2D-CGD | 2.55  | 121.69      | 115.92   |
| 11  | H     | 1482 | CLA  | C2A-C3A-C4A | 2.54  | 105.98      | 101.87   |
| 11  | D     | 1353 | CLA  | C2A-C3A-C4A | 2.54  | 105.97      | 101.87   |
| 11  | C     | 1459 | CLA  | O2A-CGA-CBA | 2.54  | 122.02      | 114.00   |
| 12  | A     | 1345 | PHO  | C4A-C3A-C2A | 2.54  | 105.25      | 102.84   |
| 11  | I     | 1463 | CLA  | CAA-C2A-C3A | -2.54 | 106.15      | 113.00   |
| 11  | C     | 1467 | CLA  | O2A-CGA-CBA | 2.53  | 119.56      | 111.83   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 11  | H     | 1485 | CLA  | O2A-CGA-CBA | 2.53  | 119.56      | 111.83   |
| 11  | C     | 1462 | CLA  | O2A-C1-C2   | 2.53  | 117.84      | 108.11   |
| 11  | A     | 1344 | CLA  | CED-O2D-CGD | 2.53  | 121.65      | 115.92   |
| 11  | B     | 1490 | CLA  | C2A-C1A-CHA | 2.53  | 128.25      | 123.87   |
| 11  | B     | 1488 | CLA  | C1-C2-C3    | 2.53  | 130.33      | 126.20   |
| 16  | L     | 1046 | HEM  | C3A-C4A-NA  | 2.52  | 111.85      | 109.71   |
| 11  | B     | 1493 | CLA  | O2A-CGA-CBA | 2.52  | 121.96      | 114.00   |
| 11  | A     | 1344 | CLA  | O2A-CGA-CBA | 2.51  | 121.94      | 114.00   |
| 11  | B     | 1495 | CLA  | C2A-C3A-C4A | 2.51  | 105.93      | 101.87   |
| 12  | A     | 1345 | PHO  | OBD-CAD-C3D | 2.51  | 131.80      | 127.89   |
| 11  | A     | 1342 | CLA  | C1-C2-C3    | 2.51  | 130.30      | 126.20   |
| 11  | I     | 1463 | CLA  | C3B-C4B-NB  | -2.51 | 108.29      | 110.53   |
| 11  | B     | 1493 | CLA  | C2A-C3A-C4A | 2.50  | 105.91      | 101.87   |
| 11  | H     | 1483 | CLA  | O2D-CGD-CBD | 2.50  | 115.61      | 111.23   |
| 11  | C     | 1467 | CLA  | CED-O2D-CGD | 2.50  | 121.59      | 115.92   |
| 11  | C     | 1459 | CLA  | CED-O2D-CGD | 2.50  | 121.59      | 115.92   |
| 17  | L     | 1047 | BCR  | C16-C17-C18 | 2.49  | 130.77      | 127.28   |
| 11  | A     | 1346 | CLA  | CAA-C2A-C3A | -2.49 | 106.26      | 113.00   |
| 11  | H     | 1488 | CLA  | CMD-C2D-C1D | 2.49  | 129.12      | 124.73   |
| 11  | I     | 1467 | CLA  | CED-O2D-CGD | 2.49  | 121.57      | 115.92   |
| 11  | C     | 1460 | CLA  | C3B-C4B-NB  | -2.49 | 108.31      | 110.53   |
| 11  | C     | 1463 | CLA  | CAA-C2A-C3A | -2.48 | 106.29      | 113.00   |
| 11  | D     | 1353 | CLA  | C1-C2-C3    | 2.48  | 130.78      | 126.76   |
| 11  | I     | 1462 | CLA  | C7-C6-C5    | -2.48 | 106.65      | 113.26   |
| 11  | B     | 1486 | CLA  | O2D-CGD-CBD | 2.48  | 115.57      | 111.23   |
| 18  | V     | 1138 | HEC  | CHB-C4A-NA  | 2.48  | 127.16      | 124.45   |
| 11  | B     | 1484 | CLA  | O2A-CGA-CBA | 2.48  | 121.83      | 114.00   |
| 11  | C     | 1469 | CLA  | O2D-CGD-CBD | 2.47  | 115.56      | 111.23   |
| 11  | H     | 1485 | CLA  | C2A-C3A-C4A | 2.47  | 105.87      | 101.87   |
| 11  | B     | 1493 | CLA  | O2D-CGD-CBD | 2.47  | 115.55      | 111.23   |
| 11  | I     | 1471 | CLA  | CED-O2D-CGD | 2.47  | 121.52      | 115.92   |
| 11  | H     | 1487 | CLA  | CED-O2D-CGD | 2.45  | 121.48      | 115.92   |
| 11  | H     | 1490 | CLA  | CMA-C3A-C2A | -2.45 | 104.49      | 113.98   |
| 11  | G     | 1342 | CLA  | C2A-C3A-C4A | 2.45  | 105.83      | 101.87   |
| 11  | C     | 1466 | CLA  | O2D-CGD-CBD | 2.45  | 115.51      | 111.23   |
| 11  | A     | 1344 | CLA  | CAA-CBA-CGA | 2.45  | 119.02      | 112.49   |
| 11  | B     | 1496 | CLA  | O2D-CGD-CBD | 2.44  | 115.50      | 111.23   |
| 11  | B     | 1496 | CLA  | CED-O2D-CGD | 2.44  | 121.46      | 115.92   |
| 17  | L     | 1047 | BCR  | C36-C18-C19 | 2.44  | 121.82      | 118.09   |
| 11  | C     | 1464 | CLA  | C3B-C4B-NB  | -2.44 | 108.35      | 110.53   |
| 11  | J     | 1351 | CLA  | C12-C11-C10 | -2.44 | 102.34      | 113.28   |
| 11  | H     | 1487 | CLA  | C1-O2A-CGA  | 2.44  | 122.55      | 116.65   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 11  | B     | 1490 | CLA  | C2A-C3A-C4A | 2.44  | 105.81      | 101.87   |
| 11  | H     | 1483 | CLA  | C7-C6-C5    | -2.44 | 106.77      | 113.26   |
| 11  | C     | 1464 | CLA  | C2A-C1A-CHA | 2.44  | 128.09      | 123.87   |
| 11  | B     | 1489 | CLA  | CMD-C2D-C1D | 2.44  | 129.02      | 124.73   |
| 11  | D     | 1351 | CLA  | CED-O2D-CGD | 2.43  | 121.44      | 115.92   |
| 11  | G     | 1344 | CLA  | O2D-CGD-CBD | 2.43  | 115.47      | 111.23   |
| 11  | B     | 1494 | CLA  | C2A-C1A-CHA | 2.43  | 128.08      | 123.87   |
| 11  | H     | 1496 | CLA  | C2A-C1A-CHA | 2.43  | 128.08      | 123.87   |
| 11  | C     | 1459 | CLA  | C2A-C1A-CHA | 2.42  | 128.07      | 123.87   |
| 11  | B     | 1488 | CLA  | C1-O2A-CGA  | 2.42  | 122.51      | 116.65   |
| 11  | B     | 1484 | CLA  | C2A-C3A-C4A | 2.42  | 105.78      | 101.87   |
| 11  | B     | 1487 | CLA  | C1-O2A-CGA  | 2.42  | 122.50      | 116.65   |
| 11  | D     | 1351 | CLA  | CAA-C2A-C3A | -2.42 | 106.47      | 113.00   |
| 11  | I     | 1467 | CLA  | C2A-C1A-CHA | 2.41  | 128.06      | 123.87   |
| 11  | B     | 1482 | CLA  | C1-O2A-CGA  | 2.41  | 122.48      | 116.65   |
| 11  | C     | 1460 | CLA  | C2A-C3A-C4A | 2.41  | 105.76      | 101.87   |
| 12  | A     | 1345 | PHO  | O2A-CGA-CBA | 2.41  | 119.18      | 111.83   |
| 11  | H     | 1497 | CLA  | CMA-C3A-C2A | -2.41 | 110.71      | 116.23   |
| 11  | B     | 1494 | CLA  | C3B-C4B-NB  | -2.41 | 108.38      | 110.53   |
| 11  | I     | 1464 | CLA  | C2A-C1A-CHA | 2.40  | 128.03      | 123.87   |
| 11  | I     | 1466 | CLA  | O2D-CGD-CBD | 2.39  | 115.41      | 111.23   |
| 11  | D     | 1351 | CLA  | CBA-CAA-C2A | 2.39  | 120.91      | 113.79   |
| 11  | B     | 1485 | CLA  | O2A-CGA-CBA | 2.39  | 119.12      | 111.83   |
| 11  | H     | 1482 | CLA  | C2A-C1A-CHA | 2.39  | 128.01      | 123.87   |
| 11  | B     | 1492 | CLA  | C3B-C4B-NB  | -2.38 | 108.40      | 110.53   |
| 11  | H     | 1485 | CLA  | CAA-C2A-C3A | -2.38 | 106.56      | 113.00   |
| 11  | H     | 1490 | CLA  | C2A-C3A-C4A | 2.38  | 105.71      | 101.87   |
| 11  | B     | 1495 | CLA  | O1A-CGA-CBA | -2.38 | 114.48      | 123.78   |
| 18  | T     | 1138 | HEC  | CHA-C4D-C3D | -2.38 | 120.10      | 125.30   |
| 11  | A     | 1342 | CLA  | C16-C15-C13 | 2.37  | 123.85      | 115.97   |
| 11  | H     | 1492 | CLA  | C2A-C1A-CHA | 2.37  | 127.98      | 123.87   |
| 11  | H     | 1488 | CLA  | C1-C2-C3    | 2.37  | 130.08      | 126.20   |
| 12  | A     | 1345 | PHO  | CBC-CAC-C3C | -2.37 | 109.48      | 112.87   |
| 11  | B     | 1492 | CLA  | O2D-CGD-CBD | 2.37  | 115.37      | 111.23   |
| 11  | A     | 1344 | CLA  | C2A-C3A-C4A | 2.36  | 105.69      | 101.87   |
| 11  | I     | 1459 | CLA  | C2A-C1A-CHA | 2.36  | 127.97      | 123.87   |
| 11  | H     | 1489 | CLA  | CED-O2D-CGD | 2.36  | 121.27      | 115.92   |
| 11  | I     | 1467 | CLA  | C3B-C4B-NB  | -2.36 | 108.42      | 110.53   |
| 11  | H     | 1494 | CLA  | C2A-C1A-CHA | 2.36  | 127.96      | 123.87   |
| 11  | B     | 1489 | CLA  | CED-O2D-CGD | 2.36  | 121.26      | 115.92   |
| 17  | F     | 1046 | BCR  | C8-C9-C10   | -2.36 | 115.30      | 119.01   |
| 11  | C     | 1459 | CLA  | C3B-C4B-NB  | -2.35 | 108.43      | 110.53   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12  | G     | 1345 | PHO  | O2A-CGA-CBA | 2.35  | 119.01      | 111.83   |
| 11  | I     | 1464 | CLA  | C3B-C4B-NB  | -2.35 | 108.43      | 110.53   |
| 17  | L     | 1047 | BCR  | C23-C22-C21 | -2.35 | 115.31      | 119.01   |
| 11  | H     | 1486 | CLA  | O2D-CGD-CBD | 2.35  | 115.34      | 111.23   |
| 11  | I     | 1462 | CLA  | O2A-C1-C2   | 2.35  | 117.15      | 108.11   |
| 11  | I     | 1469 | CLA  | C2A-C1A-CHA | 2.35  | 127.93      | 123.86   |
| 11  | G     | 1342 | CLA  | C16-C15-C13 | 2.35  | 123.76      | 115.97   |
| 11  | A     | 1342 | CLA  | CBA-CAA-C2A | 2.35  | 120.77      | 113.79   |
| 12  | D     | 1352 | PHO  | C1-C2-C3    | 2.35  | 130.04      | 126.20   |
| 11  | B     | 1488 | CLA  | CMD-C2D-C1D | 2.34  | 128.86      | 124.73   |
| 11  | G     | 1344 | CLA  | O2A-CGA-CBA | 2.34  | 121.41      | 114.00   |
| 11  | B     | 1492 | CLA  | C6-C7-C8    | 2.34  | 123.75      | 115.97   |
| 11  | C     | 1459 | CLA  | O2D-CGD-CBD | 2.34  | 115.32      | 111.23   |
| 11  | H     | 1492 | CLA  | CAA-C2A-C3A | -2.34 | 106.68      | 113.00   |
| 11  | H     | 1496 | CLA  | C1-O2A-CGA  | 2.34  | 122.31      | 116.65   |
| 11  | B     | 1486 | CLA  | CED-O2D-CGD | 2.32  | 121.18      | 115.92   |
| 11  | G     | 1346 | CLA  | CMA-C3A-C2A | -2.32 | 105.01      | 113.98   |
| 17  | F     | 1046 | BCR  | C37-C22-C23 | 2.32  | 121.63      | 118.09   |
| 11  | J     | 1351 | CLA  | C2A-C3A-C4A | 2.31  | 105.61      | 101.87   |
| 11  | B     | 1495 | CLA  | CED-O2D-CGD | 2.31  | 121.16      | 115.92   |
| 12  | A     | 1345 | PHO  | C4D-ND-C1D  | -2.31 | 106.10      | 108.87   |
| 11  | H     | 1496 | CLA  | O2D-CGD-CBD | 2.31  | 115.27      | 111.23   |
| 12  | G     | 1345 | PHO  | C4D-ND-C1D  | -2.31 | 106.11      | 108.87   |
| 11  | I     | 1464 | CLA  | C2A-C3A-C4A | 2.30  | 105.59      | 101.87   |
| 11  | I     | 1462 | CLA  | C6-C5-C3    | 2.30  | 119.08      | 113.47   |
| 12  | G     | 1345 | PHO  | C3D-C4D-ND  | 2.30  | 110.66      | 107.71   |
| 11  | I     | 1466 | CLA  | C2A-C3A-C4A | 2.30  | 105.58      | 101.87   |
| 11  | I     | 1462 | CLA  | C6-C7-C8    | 2.30  | 123.60      | 115.97   |
| 12  | J     | 1352 | PHO  | CMA-C3A-C4A | -2.30 | 109.66      | 114.61   |
| 11  | I     | 1471 | CLA  | CMD-C2D-C1D | 2.29  | 128.77      | 124.73   |
| 11  | I     | 1468 | CLA  | C2A-C3A-C4A | 2.29  | 106.21      | 103.58   |
| 18  | T     | 1138 | HEC  | CAA-C2A-C1A | 2.29  | 129.51      | 124.85   |
| 11  | B     | 1494 | CLA  | C2A-C3A-C4A | 2.29  | 105.57      | 101.87   |
| 11  | I     | 1466 | CLA  | C2A-C1A-CHA | 2.29  | 127.84      | 123.87   |
| 11  | H     | 1494 | CLA  | C6-C5-C3    | 2.29  | 119.05      | 113.47   |
| 12  | A     | 1345 | PHO  | C3D-C4D-ND  | 2.29  | 110.64      | 107.71   |
| 11  | H     | 1487 | CLA  | CAA-C2A-C3A | -2.29 | 106.82      | 113.00   |
| 11  | D     | 1351 | CLA  | C2A-C1A-CHA | 2.29  | 127.83      | 123.87   |
| 11  | H     | 1493 | CLA  | O2A-CGA-CBA | 2.28  | 121.22      | 114.00   |
| 11  | G     | 1344 | CLA  | CED-O2D-CGD | 2.28  | 121.09      | 115.92   |
| 11  | H     | 1493 | CLA  | CMD-C2D-C1D | 2.28  | 128.75      | 124.73   |
| 11  | B     | 1489 | CLA  | C1-O2A-CGA  | 2.28  | 122.17      | 116.65   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 11  | C     | 1464 | CLA  | CMD-C2D-C1D | 2.28  | 128.74      | 124.73   |
| 16  | E     | 1085 | HEM  | C3A-C4A-NA  | 2.28  | 111.64      | 109.71   |
| 11  | H     | 1497 | CLA  | CMD-C2D-C1D | 2.27  | 128.73      | 124.73   |
| 18  | T     | 1138 | HEC  | CHA-C1A-C2A | 2.27  | 128.46      | 124.86   |
| 12  | G     | 1345 | PHO  | CMA-C3A-C4A | -2.27 | 109.71      | 114.61   |
| 11  | C     | 1463 | CLA  | C2A-C1A-CHA | 2.27  | 127.81      | 123.87   |
| 11  | B     | 1494 | CLA  | C1-O2A-CGA  | 2.27  | 122.14      | 116.65   |
| 11  | C     | 1464 | CLA  | CAA-C2A-C3A | -2.27 | 106.88      | 113.00   |
| 11  | I     | 1465 | CLA  | C1-O2A-CGA  | 2.26  | 122.13      | 116.65   |
| 11  | A     | 1342 | CLA  | C2A-C3A-C4A | 2.26  | 105.53      | 101.87   |
| 11  | A     | 1342 | CLA  | C2A-C1A-CHA | 2.26  | 127.79      | 123.87   |
| 11  | H     | 1494 | CLA  | C1-O2A-CGA  | 2.26  | 122.12      | 116.65   |
| 17  | F     | 1046 | BCR  | C16-C17-C18 | 2.26  | 130.45      | 127.28   |
| 12  | J     | 1352 | PHO  | C6-C5-C3    | 2.26  | 118.97      | 113.47   |
| 11  | H     | 1485 | CLA  | CMD-C2D-C1D | 2.26  | 128.70      | 124.73   |
| 11  | J     | 1351 | CLA  | C5-C3-C2    | -2.25 | 116.11      | 121.17   |
| 11  | B     | 1492 | CLA  | C2A-C3A-C4A | 2.25  | 105.51      | 101.87   |
| 11  | B     | 1492 | CLA  | CMD-C2D-C1D | 2.25  | 128.70      | 124.73   |
| 11  | I     | 1463 | CLA  | O2D-CGD-CBD | 2.25  | 115.17      | 111.23   |
| 11  | C     | 1460 | CLA  | O2D-CGD-CBD | 2.25  | 115.17      | 111.23   |
| 11  | C     | 1470 | CLA  | C2A-C1A-CHA | 2.25  | 127.76      | 123.86   |
| 11  | C     | 1466 | CLA  | C3B-C4B-NB  | -2.25 | 108.52      | 110.53   |
| 11  | I     | 1462 | CLA  | C2A-C3A-C4A | 2.25  | 105.50      | 101.87   |
| 11  | H     | 1492 | CLA  | CMD-C2D-C1D | 2.25  | 128.68      | 124.73   |
| 11  | I     | 1462 | CLA  | CMD-C2D-C1D | 2.24  | 128.68      | 124.73   |
| 11  | H     | 1495 | CLA  | C2A-C3A-C4A | 2.24  | 105.49      | 101.87   |
| 18  | V     | 1138 | HEC  | O2A-CGA-CBA | 2.24  | 121.09      | 114.00   |
| 11  | B     | 1482 | CLA  | C2A-C1A-CHA | 2.24  | 127.76      | 123.87   |
| 11  | J     | 1353 | CLA  | CED-O2D-CGD | 2.24  | 121.00      | 115.92   |
| 18  | T     | 1138 | HEC  | CAD-CBD-CGD | 2.24  | 119.60      | 113.67   |
| 11  | C     | 1469 | CLA  | C2B-C1B-NB  | -2.24 | 108.01      | 110.33   |
| 12  | D     | 1352 | PHO  | OBD-CAD-C3D | 2.24  | 131.38      | 127.89   |
| 11  | C     | 1466 | CLA  | C2A-C3A-C4A | 2.24  | 105.48      | 101.87   |
| 11  | C     | 1466 | CLA  | C2A-C1A-CHA | 2.23  | 127.74      | 123.87   |
| 11  | I     | 1469 | CLA  | C2B-C1B-NB  | -2.23 | 108.01      | 110.33   |
| 11  | H     | 1483 | CLA  | C2A-C3A-C4A | 2.23  | 105.47      | 101.87   |
| 11  | I     | 1467 | CLA  | C2A-C3A-C4A | 2.23  | 105.47      | 101.87   |
| 11  | C     | 1462 | CLA  | CMD-C2D-C1D | 2.22  | 128.65      | 124.73   |
| 11  | B     | 1496 | CLA  | C2A-C1A-CHA | 2.22  | 127.72      | 123.87   |
| 11  | B     | 1489 | CLA  | C2A-C3A-C4A | 2.22  | 105.45      | 101.87   |
| 11  | I     | 1470 | CLA  | O2D-CGD-CBD | 2.22  | 115.11      | 111.23   |
| 11  | I     | 1465 | CLA  | C2A-C3A-C4A | 2.22  | 105.45      | 101.87   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 11  | B     | 1487 | CLA  | CMD-C2D-C1D | 2.21  | 128.63      | 124.73   |
| 12  | D     | 1352 | PHO  | CMA-C3A-C4A | -2.21 | 109.84      | 114.61   |
| 11  | G     | 1342 | CLA  | CMD-C2D-C1D | 2.21  | 128.62      | 124.73   |
| 11  | C     | 1459 | CLA  | CBA-CAA-C2A | 2.21  | 120.36      | 113.79   |
| 11  | C     | 1462 | CLA  | C2A-C3A-C4A | 2.21  | 105.44      | 101.87   |
| 11  | I     | 1460 | CLA  | C3B-C4B-NB  | -2.20 | 108.56      | 110.53   |
| 11  | I     | 1465 | CLA  | CAA-C2A-C3A | -2.20 | 107.04      | 113.00   |
| 18  | T     | 1138 | HEC  | CHB-C4A-NA  | 2.20  | 126.85      | 124.45   |
| 11  | C     | 1468 | CLA  | C2A-C3A-C4A | 2.20  | 106.10      | 103.58   |
| 11  | H     | 1494 | CLA  | O2D-CGD-CBD | 2.20  | 115.08      | 111.23   |
| 11  | D     | 1353 | CLA  | CED-O2D-CGD | 2.20  | 120.91      | 115.92   |
| 11  | H     | 1489 | CLA  | CAA-C2A-C3A | -2.20 | 107.05      | 113.00   |
| 18  | V     | 1138 | HEC  | CHA-C1A-C2A | 2.20  | 128.34      | 124.86   |
| 11  | B     | 1487 | CLA  | CAA-C2A-C3A | -2.20 | 107.06      | 113.00   |
| 11  | I     | 1459 | CLA  | O2D-CGD-CBD | 2.20  | 115.07      | 111.23   |
| 11  | A     | 1343 | CLA  | CMD-C2D-C1D | 2.20  | 128.59      | 124.73   |
| 12  | A     | 1345 | PHO  | C5-C3-C2    | -2.20 | 116.24      | 121.17   |
| 11  | I     | 1466 | CLA  | CMD-C2D-C1D | 2.19  | 128.59      | 124.73   |
| 11  | C     | 1462 | CLA  | C6-C5-C3    | 2.19  | 118.81      | 113.47   |
| 11  | A     | 1346 | CLA  | CMA-C3A-C2A | -2.19 | 105.50      | 113.98   |
| 11  | B     | 1492 | CLA  | C2A-C1A-CHA | 2.19  | 127.67      | 123.87   |
| 11  | H     | 1490 | CLA  | O2D-CGD-CBD | 2.19  | 115.06      | 111.23   |
| 11  | B     | 1483 | CLA  | C3B-C4B-NB  | -2.19 | 108.57      | 110.53   |
| 11  | I     | 1460 | CLA  | CBA-CAA-C2A | 2.19  | 120.31      | 113.79   |
| 11  | I     | 1459 | CLA  | CBA-CAA-C2A | 2.19  | 120.30      | 113.79   |
| 12  | G     | 1345 | PHO  | OBD-CAD-C3D | 2.18  | 131.30      | 127.89   |
| 11  | B     | 1496 | CLA  | C3B-C4B-NB  | -2.18 | 108.58      | 110.53   |
| 18  | T     | 1138 | HEC  | CAA-C2A-C3A | -2.18 | 123.78      | 127.87   |
| 11  | B     | 1496 | CLA  | CBA-CAA-C2A | 2.18  | 120.28      | 113.79   |
| 11  | C     | 1462 | CLA  | C6-C7-C8    | 2.18  | 123.21      | 115.97   |
| 11  | J     | 1351 | CLA  | C7-C6-C5    | -2.18 | 107.46      | 113.26   |
| 11  | H     | 1482 | CLA  | C1-O2A-CGA  | 2.18  | 121.92      | 116.65   |
| 18  | V     | 1138 | HEC  | CAA-C2A-C1A | 2.18  | 129.28      | 124.85   |
| 11  | D     | 1351 | CLA  | CMD-C2D-C1D | 2.17  | 128.55      | 124.73   |
| 11  | I     | 1462 | CLA  | C1-O2A-CGA  | 2.17  | 121.91      | 116.65   |
| 11  | H     | 1484 | CLA  | C2A-C3A-C4A | 2.17  | 105.38      | 101.87   |
| 11  | B     | 1495 | CLA  | O2A-C1-C2   | 2.17  | 116.46      | 108.11   |
| 11  | D     | 1351 | CLA  | C5-C3-C2    | -2.17 | 116.30      | 121.17   |
| 17  | F     | 1046 | BCR  | C11-C10-C9  | 2.17  | 130.32      | 127.28   |
| 11  | C     | 1462 | CLA  | C1-O2A-CGA  | 2.17  | 121.89      | 116.65   |
| 11  | C     | 1460 | CLA  | CBA-CAA-C2A | 2.17  | 120.24      | 113.79   |
| 12  | J     | 1352 | PHO  | C4D-ND-C1D  | -2.16 | 106.28      | 108.87   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 11  | G     | 1342 | CLA  | CBA-CAA-C2A | 2.16  | 120.23      | 113.79   |
| 12  | D     | 1352 | PHO  | C4D-ND-C1D  | -2.16 | 106.28      | 108.87   |
| 11  | B     | 1483 | CLA  | C2A-C3A-C4A | 2.16  | 105.36      | 101.87   |
| 11  | B     | 1493 | CLA  | CED-O2D-CGD | 2.16  | 120.81      | 115.92   |
| 11  | C     | 1469 | CLA  | C2A-C1A-CHA | 2.16  | 127.60      | 123.86   |
| 11  | I     | 1460 | CLA  | C2A-C3A-C4A | 2.15  | 105.35      | 101.87   |
| 11  | B     | 1492 | CLA  | CAA-C2A-C3A | -2.15 | 107.19      | 113.00   |
| 11  | G     | 1343 | CLA  | CMD-C2D-C1D | 2.15  | 128.51      | 124.73   |
| 18  | V     | 1138 | HEC  | CHA-C4D-C3D | -2.15 | 120.59      | 125.30   |
| 11  | G     | 1343 | CLA  | C12-C11-C10 | -2.15 | 103.66      | 113.28   |
| 11  | B     | 1483 | CLA  | CED-O2D-CGD | 2.15  | 120.78      | 115.92   |
| 11  | C     | 1465 | CLA  | C6-C5-C3    | 2.15  | 118.69      | 113.47   |
| 11  | B     | 1487 | CLA  | C4D-CHA-C1A | 2.14  | 123.80      | 121.24   |
| 11  | C     | 1459 | CLA  | CMD-C2D-C1D | 2.14  | 128.50      | 124.73   |
| 11  | A     | 1346 | CLA  | C2A-C3A-C4A | 2.14  | 105.33      | 101.87   |
| 11  | I     | 1467 | CLA  | CAA-C2A-C3A | -2.14 | 107.22      | 113.00   |
| 11  | G     | 1344 | CLA  | C2A-C3A-C4A | 2.14  | 105.33      | 101.87   |
| 16  | L     | 1046 | HEM  | C3D-C4D-ND  | 2.14  | 110.92      | 109.42   |
| 11  | I     | 1471 | CLA  | C2A-C1A-CHA | 2.13  | 127.56      | 123.86   |
| 17  | L     | 1047 | BCR  | C32-C1-C2   | -2.13 | 100.77      | 108.95   |
| 11  | H     | 1495 | CLA  | C7-C6-C5    | -2.13 | 107.59      | 113.26   |
| 11  | A     | 1343 | CLA  | C12-C11-C10 | -2.13 | 103.74      | 113.28   |
| 11  | B     | 1483 | CLA  | C2A-C1A-CHA | 2.13  | 127.56      | 123.87   |
| 11  | C     | 1467 | CLA  | CAA-C2A-C3A | -2.12 | 107.26      | 113.00   |
| 11  | D     | 1353 | CLA  | C2A-C1A-CHA | 2.12  | 127.55      | 123.87   |
| 11  | I     | 1470 | CLA  | C2A-C1A-CHA | 2.12  | 127.54      | 123.86   |
| 11  | G     | 1346 | CLA  | CED-O2D-CGD | 2.12  | 120.72      | 115.92   |
| 11  | C     | 1466 | CLA  | CMD-C2D-C1D | 2.12  | 128.46      | 124.73   |
| 11  | A     | 1344 | CLA  | C3B-C4B-NB  | -2.12 | 108.64      | 110.53   |
| 11  | C     | 1465 | CLA  | C2A-C3A-C4A | 2.11  | 105.28      | 101.87   |
| 11  | A     | 1343 | CLA  | CMA-C3A-C2A | -2.11 | 105.81      | 113.98   |
| 12  | G     | 1345 | PHO  | C5-C3-C2    | -2.11 | 116.42      | 121.17   |
| 11  | A     | 1343 | CLA  | O2A-C1-C2   | -2.11 | 99.98       | 108.11   |
| 11  | G     | 1344 | CLA  | CAA-CBA-CGA | 2.11  | 118.12      | 112.49   |
| 11  | C     | 1465 | CLA  | C2A-C1A-CHA | 2.10  | 127.52      | 123.87   |
| 11  | I     | 1465 | CLA  | C2A-C1A-CHA | 2.10  | 127.52      | 123.87   |
| 11  | B     | 1488 | CLA  | O1D-CGD-CBD | -2.10 | 120.37      | 124.52   |
| 11  | H     | 1489 | CLA  | C3B-C4B-NB  | -2.10 | 108.65      | 110.53   |
| 11  | B     | 1493 | CLA  | C3B-C4B-NB  | -2.10 | 108.66      | 110.53   |
| 11  | H     | 1493 | CLA  | O2D-CGD-CBD | 2.10  | 114.90      | 111.23   |
| 11  | H     | 1487 | CLA  | CBA-CAA-C2A | 2.10  | 120.03      | 113.79   |
| 11  | C     | 1467 | CLA  | CMA-C3A-C2A | -2.10 | 105.88      | 113.98   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 11  | J     | 1351 | CLA  | CBA-CAA-C2A | 2.10  | 120.03      | 113.79   |
| 11  | B     | 1489 | CLA  | CAA-C2A-C3A | -2.10 | 107.33      | 113.00   |
| 12  | D     | 1352 | PHO  | C6-C5-C3    | 2.09  | 118.56      | 113.47   |
| 11  | B     | 1488 | CLA  | CGD-CBD-CAD | -2.09 | 104.09      | 110.85   |
| 11  | A     | 1342 | CLA  | O2D-CGD-CBD | 2.09  | 114.88      | 111.23   |
| 11  | H     | 1496 | CLA  | CBA-CAA-C2A | 2.09  | 120.00      | 113.79   |
| 11  | B     | 1488 | CLA  | CAA-CBA-CGA | 2.08  | 119.13      | 113.21   |
| 17  | L     | 1047 | BCR  | C37-C22-C23 | 2.08  | 121.27      | 118.09   |
| 11  | I     | 1464 | CLA  | CAA-C2A-C3A | -2.08 | 107.38      | 113.00   |
| 11  | B     | 1495 | CLA  | C7-C6-C5    | -2.08 | 107.72      | 113.26   |
| 11  | C     | 1467 | CLA  | C3B-C4B-NB  | -2.08 | 108.68      | 110.53   |
| 11  | C     | 1460 | CLA  | CMD-C2D-C1D | 2.07  | 128.37      | 124.73   |
| 11  | B     | 1484 | CLA  | C2A-C1A-CHA | 2.06  | 127.45      | 123.87   |
| 11  | C     | 1467 | CLA  | C2A-C3A-C4A | 2.06  | 105.20      | 101.87   |
| 11  | B     | 1495 | CLA  | CBA-CAA-C2A | 2.06  | 119.92      | 113.79   |
| 11  | C     | 1464 | CLA  | CBA-CAA-C2A | 2.06  | 119.92      | 113.79   |
| 11  | G     | 1344 | CLA  | C2A-C1A-CHA | 2.06  | 127.44      | 123.87   |
| 17  | F     | 1046 | BCR  | C20-C21-C22 | 2.06  | 130.16      | 127.28   |
| 11  | H     | 1492 | CLA  | C2A-C3A-C4A | 2.06  | 105.19      | 101.87   |
| 11  | I     | 1460 | CLA  | C2A-C1A-CHA | 2.06  | 127.44      | 123.87   |
| 11  | C     | 1465 | CLA  | C1-O2A-CGA  | 2.06  | 121.63      | 116.65   |
| 11  | H     | 1483 | CLA  | C2A-C1A-CHA | 2.05  | 127.43      | 123.87   |
| 11  | B     | 1485 | CLA  | CMD-C2D-C1D | 2.05  | 128.35      | 124.73   |
| 11  | B     | 1487 | CLA  | C2A-C3A-C4A | 2.05  | 105.18      | 101.87   |
| 11  | C     | 1463 | CLA  | O2D-CGD-CBD | 2.05  | 114.82      | 111.23   |
| 11  | C     | 1464 | CLA  | C2A-C3A-C4A | 2.05  | 105.18      | 101.87   |
| 11  | B     | 1493 | CLA  | C4D-CHA-C1A | 2.05  | 123.69      | 121.24   |
| 11  | B     | 1486 | CLA  | C2A-C1A-CHA | 2.04  | 127.40      | 123.86   |
| 11  | H     | 1495 | CLA  | O2A-C1-C2   | 2.04  | 115.97      | 108.11   |
| 11  | A     | 1344 | CLA  | C2A-C1A-CHA | 2.04  | 127.41      | 123.87   |
| 11  | I     | 1464 | CLA  | CBA-CAA-C2A | 2.04  | 119.86      | 113.79   |
| 12  | A     | 1345 | PHO  | CMA-C3A-C4A | -2.03 | 110.23      | 114.61   |
| 11  | I     | 1469 | CLA  | O2D-CGD-CBD | 2.03  | 114.78      | 111.23   |
| 11  | I     | 1471 | CLA  | C3B-C4B-NB  | -2.03 | 108.72      | 110.53   |
| 11  | H     | 1487 | CLA  | CMD-C2D-C1D | 2.03  | 128.31      | 124.73   |
| 12  | D     | 1352 | PHO  | O2A-CGA-O1A | -2.03 | 118.55      | 123.63   |
| 11  | J     | 1353 | CLA  | C2A-C1A-CHA | 2.03  | 127.39      | 123.87   |
| 11  | B     | 1485 | CLA  | C3B-C4B-NB  | -2.03 | 108.72      | 110.53   |
| 18  | T     | 1138 | HEC  | O2A-CGA-CBA | 2.03  | 120.40      | 114.00   |
| 11  | I     | 1470 | CLA  | C3B-C4B-NB  | -2.03 | 108.72      | 110.53   |
| 11  | H     | 1493 | CLA  | C4D-CHA-C1A | 2.03  | 123.66      | 121.24   |
| 11  | D     | 1353 | CLA  | O2D-CGD-CBD | 2.03  | 114.77      | 111.23   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | F     | 1046 | BCR  | C3-C4-C5    | 2.02  | 117.66      | 114.06   |
| 11  | H     | 1488 | CLA  | CAA-CBA-CGA | 2.02  | 118.94      | 113.21   |
| 11  | I     | 1467 | CLA  | CMA-C3A-C2A | -2.02 | 106.19      | 113.98   |
| 11  | H     | 1496 | CLA  | C3B-C4B-NB  | -2.02 | 108.73      | 110.53   |
| 11  | H     | 1482 | CLA  | C2D-C1D-ND  | 2.01  | 112.12      | 110.13   |
| 11  | G     | 1343 | CLA  | CMA-C3A-C2A | -2.01 | 106.21      | 113.98   |
| 11  | B     | 1497 | CLA  | CMD-C2D-C1D | 2.00  | 128.26      | 124.73   |
| 11  | C     | 1467 | CLA  | C4D-CHA-C1A | 2.00  | 123.63      | 121.24   |
| 11  | H     | 1484 | CLA  | C2A-C1A-CHA | 2.00  | 127.34      | 123.87   |
| 11  | C     | 1460 | CLA  | C2A-C1A-CHA | 2.00  | 127.34      | 123.87   |
| 11  | C     | 1459 | CLA  | C2A-C3A-C4A | 2.00  | 105.10      | 101.87   |
| 11  | H     | 1495 | CLA  | O1A-CGA-CBA | -2.00 | 115.96      | 123.78   |

All (71) chirality outliers are listed below:

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 11  | A     | 1342 | CLA  | ND   |
| 11  | A     | 1343 | CLA  | ND   |
| 11  | A     | 1344 | CLA  | ND   |
| 11  | A     | 1346 | CLA  | ND   |
| 11  | B     | 1482 | CLA  | ND   |
| 11  | B     | 1483 | CLA  | ND   |
| 11  | B     | 1484 | CLA  | ND   |
| 11  | B     | 1485 | CLA  | ND   |
| 11  | B     | 1486 | CLA  | ND   |
| 11  | B     | 1487 | CLA  | ND   |
| 11  | B     | 1488 | CLA  | ND   |
| 11  | B     | 1489 | CLA  | ND   |
| 11  | B     | 1490 | CLA  | ND   |
| 11  | B     | 1491 | CLA  | ND   |
| 11  | B     | 1492 | CLA  | ND   |
| 11  | B     | 1493 | CLA  | ND   |
| 11  | B     | 1494 | CLA  | ND   |
| 11  | B     | 1495 | CLA  | ND   |
| 11  | B     | 1496 | CLA  | ND   |
| 11  | B     | 1497 | CLA  | ND   |
| 11  | C     | 1459 | CLA  | ND   |
| 11  | C     | 1460 | CLA  | ND   |
| 11  | C     | 1461 | CLA  | ND   |
| 11  | C     | 1462 | CLA  | ND   |
| 11  | C     | 1463 | CLA  | ND   |
| 11  | C     | 1464 | CLA  | ND   |

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| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 11  | C     | 1465 | CLA  | ND   |
| 11  | C     | 1466 | CLA  | ND   |
| 11  | C     | 1467 | CLA  | ND   |
| 11  | C     | 1468 | CLA  | ND   |
| 11  | C     | 1469 | CLA  | ND   |
| 11  | C     | 1470 | CLA  | ND   |
| 11  | C     | 1471 | CLA  | ND   |
| 11  | D     | 1351 | CLA  | ND   |
| 11  | D     | 1353 | CLA  | ND   |
| 11  | G     | 1342 | CLA  | ND   |
| 11  | G     | 1343 | CLA  | ND   |
| 11  | G     | 1344 | CLA  | ND   |
| 11  | G     | 1346 | CLA  | ND   |
| 11  | H     | 1482 | CLA  | ND   |
| 11  | H     | 1483 | CLA  | ND   |
| 11  | H     | 1484 | CLA  | ND   |
| 11  | H     | 1485 | CLA  | ND   |
| 11  | H     | 1486 | CLA  | ND   |
| 11  | H     | 1487 | CLA  | ND   |
| 11  | H     | 1488 | CLA  | ND   |
| 11  | H     | 1489 | CLA  | ND   |
| 11  | H     | 1490 | CLA  | ND   |
| 11  | H     | 1491 | CLA  | ND   |
| 11  | H     | 1492 | CLA  | ND   |
| 11  | H     | 1493 | CLA  | ND   |
| 11  | H     | 1494 | CLA  | ND   |
| 11  | H     | 1495 | CLA  | ND   |
| 11  | H     | 1496 | CLA  | ND   |
| 11  | H     | 1497 | CLA  | ND   |
| 11  | I     | 1459 | CLA  | ND   |
| 11  | I     | 1460 | CLA  | ND   |
| 11  | I     | 1461 | CLA  | ND   |
| 11  | I     | 1462 | CLA  | ND   |
| 11  | I     | 1463 | CLA  | C8   |
| 11  | I     | 1463 | CLA  | ND   |
| 11  | I     | 1464 | CLA  | ND   |
| 11  | I     | 1465 | CLA  | ND   |
| 11  | I     | 1466 | CLA  | ND   |
| 11  | I     | 1467 | CLA  | ND   |
| 11  | I     | 1468 | CLA  | ND   |
| 11  | I     | 1469 | CLA  | ND   |
| 11  | I     | 1470 | CLA  | ND   |

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| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 11  | I     | 1471 | CLA  | ND   |
| 11  | J     | 1351 | CLA  | ND   |
| 11  | J     | 1353 | CLA  | ND   |

All (641) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 11  | A     | 1343 | CLA  | C1A-C2A-CAA-CBA |
| 11  | A     | 1343 | CLA  | C2B-C3B-CAB-CBB |
| 11  | A     | 1343 | CLA  | C4B-C3B-CAB-CBB |
| 11  | A     | 1343 | CLA  | CBD-CGD-O2D-CED |
| 11  | A     | 1344 | CLA  | C2B-C3B-CAB-CBB |
| 11  | A     | 1344 | CLA  | C4B-C3B-CAB-CBB |
| 11  | A     | 1344 | CLA  | CAD-CBD-CGD-O2D |
| 11  | A     | 1346 | CLA  | C2-C3-C5-C6     |
| 11  | A     | 1346 | CLA  | C4-C3-C5-C6     |
| 11  | B     | 1482 | CLA  | C2B-C3B-CAB-CBB |
| 11  | B     | 1482 | CLA  | C4B-C3B-CAB-CBB |
| 11  | B     | 1482 | CLA  | C4-C3-C5-C6     |
| 11  | B     | 1483 | CLA  | C2B-C3B-CAB-CBB |
| 11  | B     | 1483 | CLA  | C4B-C3B-CAB-CBB |
| 11  | B     | 1483 | CLA  | C4-C3-C5-C6     |
| 11  | B     | 1484 | CLA  | C2B-C3B-CAB-CBB |
| 11  | B     | 1484 | CLA  | C4B-C3B-CAB-CBB |
| 11  | B     | 1485 | CLA  | C1A-C2A-CAA-CBA |
| 11  | B     | 1485 | CLA  | C2B-C3B-CAB-CBB |
| 11  | B     | 1485 | CLA  | C4B-C3B-CAB-CBB |
| 11  | B     | 1485 | CLA  | CBD-CGD-O2D-CED |
| 11  | B     | 1486 | CLA  | CBD-CGD-O2D-CED |
| 11  | B     | 1487 | CLA  | C2B-C3B-CAB-CBB |
| 11  | B     | 1487 | CLA  | C4B-C3B-CAB-CBB |
| 11  | B     | 1487 | CLA  | O2A-C1-C2-C3    |
| 11  | B     | 1488 | CLA  | C3A-C2A-CAA-CBA |
| 11  | B     | 1489 | CLA  | CBD-CGD-O2D-CED |
| 11  | B     | 1492 | CLA  | C2B-C3B-CAB-CBB |
| 11  | B     | 1492 | CLA  | C4B-C3B-CAB-CBB |
| 11  | B     | 1492 | CLA  | C6-C7-C8-C9     |
| 11  | B     | 1492 | CLA  | C11-C12-C13-C15 |
| 11  | B     | 1494 | CLA  | C2B-C3B-CAB-CBB |
| 11  | B     | 1494 | CLA  | C4B-C3B-CAB-CBB |
| 11  | B     | 1495 | CLA  | C4B-C3B-CAB-CBB |
| 11  | B     | 1495 | CLA  | CHA-CBD-CGD-O1D |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 11  | B     | 1495 | CLA  | CHA-CBD-CGD-O2D |
| 11  | B     | 1495 | CLA  | CBD-CGD-O2D-CED |
| 11  | B     | 1496 | CLA  | C4B-C3B-CAB-CBB |
| 11  | B     | 1497 | CLA  | CHA-CBD-CGD-O1D |
| 11  | B     | 1497 | CLA  | CHA-CBD-CGD-O2D |
| 11  | B     | 1497 | CLA  | CBD-CGD-O2D-CED |
| 11  | C     | 1459 | CLA  | C1A-C2A-CAA-CBA |
| 11  | C     | 1462 | CLA  | C1A-C2A-CAA-CBA |
| 11  | C     | 1463 | CLA  | C2B-C3B-CAB-CBB |
| 11  | C     | 1463 | CLA  | C4B-C3B-CAB-CBB |
| 11  | C     | 1463 | CLA  | CHA-CBD-CGD-O1D |
| 11  | C     | 1463 | CLA  | CHA-CBD-CGD-O2D |
| 11  | C     | 1463 | CLA  | CBD-CGD-O2D-CED |
| 11  | C     | 1464 | CLA  | C1A-C2A-CAA-CBA |
| 11  | C     | 1464 | CLA  | C3A-C2A-CAA-CBA |
| 11  | C     | 1464 | CLA  | C2B-C3B-CAB-CBB |
| 11  | C     | 1464 | CLA  | C4B-C3B-CAB-CBB |
| 11  | C     | 1465 | CLA  | C2B-C3B-CAB-CBB |
| 11  | C     | 1465 | CLA  | C4B-C3B-CAB-CBB |
| 11  | C     | 1466 | CLA  | C1A-C2A-CAA-CBA |
| 11  | C     | 1466 | CLA  | CHA-CBD-CGD-O1D |
| 11  | C     | 1466 | CLA  | CHA-CBD-CGD-O2D |
| 11  | C     | 1466 | CLA  | O2A-C1-C2-C3    |
| 11  | C     | 1470 | CLA  | C2B-C3B-CAB-CBB |
| 11  | C     | 1470 | CLA  | C4B-C3B-CAB-CBB |
| 11  | C     | 1470 | CLA  | CBD-CGD-O2D-CED |
| 11  | G     | 1343 | CLA  | C1A-C2A-CAA-CBA |
| 11  | G     | 1343 | CLA  | C2B-C3B-CAB-CBB |
| 11  | G     | 1343 | CLA  | C4B-C3B-CAB-CBB |
| 11  | G     | 1343 | CLA  | CBD-CGD-O2D-CED |
| 11  | G     | 1344 | CLA  | C4B-C3B-CAB-CBB |
| 11  | G     | 1344 | CLA  | CAD-CBD-CGD-O2D |
| 11  | G     | 1346 | CLA  | C2-C3-C5-C6     |
| 11  | G     | 1346 | CLA  | C4-C3-C5-C6     |
| 11  | H     | 1482 | CLA  | C2B-C3B-CAB-CBB |
| 11  | H     | 1482 | CLA  | C4B-C3B-CAB-CBB |
| 11  | H     | 1482 | CLA  | C4-C3-C5-C6     |
| 11  | H     | 1483 | CLA  | C2B-C3B-CAB-CBB |
| 11  | H     | 1483 | CLA  | C4B-C3B-CAB-CBB |
| 11  | H     | 1484 | CLA  | C2B-C3B-CAB-CBB |
| 11  | H     | 1484 | CLA  | C4B-C3B-CAB-CBB |
| 11  | H     | 1485 | CLA  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 11  | H     | 1485 | CLA  | C2B-C3B-CAB-CBB |
| 11  | H     | 1485 | CLA  | C4B-C3B-CAB-CBB |
| 11  | H     | 1485 | CLA  | CBD-CGD-O2D-CED |
| 11  | H     | 1486 | CLA  | CBD-CGD-O2D-CED |
| 11  | H     | 1487 | CLA  | C2B-C3B-CAB-CBB |
| 11  | H     | 1487 | CLA  | C4B-C3B-CAB-CBB |
| 11  | H     | 1487 | CLA  | O2A-C1-C2-C3    |
| 11  | H     | 1489 | CLA  | CBD-CGD-O2D-CED |
| 11  | H     | 1490 | CLA  | CBD-CGD-O2D-CED |
| 11  | H     | 1492 | CLA  | C2B-C3B-CAB-CBB |
| 11  | H     | 1492 | CLA  | C4B-C3B-CAB-CBB |
| 11  | H     | 1492 | CLA  | CBD-CGD-O2D-CED |
| 11  | H     | 1492 | CLA  | C6-C7-C8-C9     |
| 11  | H     | 1492 | CLA  | C11-C12-C13-C15 |
| 11  | H     | 1494 | CLA  | C2B-C3B-CAB-CBB |
| 11  | H     | 1494 | CLA  | C4B-C3B-CAB-CBB |
| 11  | H     | 1495 | CLA  | C4B-C3B-CAB-CBB |
| 11  | H     | 1495 | CLA  | CHA-CBD-CGD-O1D |
| 11  | H     | 1495 | CLA  | CHA-CBD-CGD-O2D |
| 11  | H     | 1495 | CLA  | CBD-CGD-O2D-CED |
| 11  | H     | 1496 | CLA  | C4B-C3B-CAB-CBB |
| 11  | H     | 1496 | CLA  | C6-C7-C8-C9     |
| 11  | H     | 1497 | CLA  | CHA-CBD-CGD-O1D |
| 11  | H     | 1497 | CLA  | CHA-CBD-CGD-O2D |
| 11  | H     | 1497 | CLA  | CBD-CGD-O2D-CED |
| 11  | I     | 1459 | CLA  | C1A-C2A-CAA-CBA |
| 11  | I     | 1462 | CLA  | C1A-C2A-CAA-CBA |
| 11  | I     | 1463 | CLA  | C2B-C3B-CAB-CBB |
| 11  | I     | 1463 | CLA  | C4B-C3B-CAB-CBB |
| 11  | I     | 1463 | CLA  | CHA-CBD-CGD-O2D |
| 11  | I     | 1464 | CLA  | C1A-C2A-CAA-CBA |
| 11  | I     | 1464 | CLA  | C3A-C2A-CAA-CBA |
| 11  | I     | 1464 | CLA  | C2B-C3B-CAB-CBB |
| 11  | I     | 1464 | CLA  | C4B-C3B-CAB-CBB |
| 11  | I     | 1465 | CLA  | C2B-C3B-CAB-CBB |
| 11  | I     | 1465 | CLA  | C4B-C3B-CAB-CBB |
| 11  | I     | 1466 | CLA  | C1A-C2A-CAA-CBA |
| 11  | I     | 1466 | CLA  | CHA-CBD-CGD-O1D |
| 11  | I     | 1466 | CLA  | CHA-CBD-CGD-O2D |
| 11  | I     | 1466 | CLA  | O2A-C1-C2-C3    |
| 11  | I     | 1467 | CLA  | CAD-CBD-CGD-O2D |
| 11  | I     | 1470 | CLA  | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 11  | I     | 1470 | CLA  | C4B-C3B-CAB-CBB |
| 11  | I     | 1470 | CLA  | CBD-CGD-O2D-CED |
| 17  | F     | 1046 | BCR  | C6-C7-C8-C9     |
| 17  | L     | 1047 | BCR  | C6-C7-C8-C9     |
| 18  | T     | 1138 | HEC  | C2B-C3B-CAB-CBB |
| 18  | T     | 1138 | HEC  | C4B-C3B-CAB-CBB |
| 18  | T     | 1138 | HEC  | C2C-C3C-CAC-CBC |
| 18  | V     | 1138 | HEC  | C4B-C3B-CAB-CBB |
| 18  | V     | 1138 | HEC  | C2C-C3C-CAC-CBC |
| 11  | B     | 1494 | CLA  | O1D-CGD-O2D-CED |
| 11  | C     | 1467 | CLA  | O1D-CGD-O2D-CED |
| 11  | C     | 1471 | CLA  | O1D-CGD-O2D-CED |
| 11  | H     | 1494 | CLA  | O1D-CGD-O2D-CED |
| 11  | I     | 1467 | CLA  | O1D-CGD-O2D-CED |
| 11  | A     | 1343 | CLA  | O1D-CGD-O2D-CED |
| 11  | A     | 1344 | CLA  | O1D-CGD-O2D-CED |
| 11  | G     | 1343 | CLA  | O1D-CGD-O2D-CED |
| 11  | G     | 1344 | CLA  | O1D-CGD-O2D-CED |
| 11  | H     | 1485 | CLA  | O1D-CGD-O2D-CED |
| 11  | I     | 1471 | CLA  | O1D-CGD-O2D-CED |
| 11  | A     | 1344 | CLA  | CBD-CGD-O2D-CED |
| 11  | B     | 1484 | CLA  | CBD-CGD-O2D-CED |
| 11  | B     | 1490 | CLA  | CBD-CGD-O2D-CED |
| 11  | B     | 1492 | CLA  | CBD-CGD-O2D-CED |
| 11  | B     | 1493 | CLA  | CBD-CGD-O2D-CED |
| 11  | B     | 1494 | CLA  | CBD-CGD-O2D-CED |
| 11  | C     | 1459 | CLA  | CBD-CGD-O2D-CED |
| 11  | C     | 1460 | CLA  | CBD-CGD-O2D-CED |
| 11  | C     | 1464 | CLA  | CBD-CGD-O2D-CED |
| 11  | C     | 1465 | CLA  | CBD-CGD-O2D-CED |
| 11  | C     | 1467 | CLA  | CBD-CGD-O2D-CED |
| 11  | C     | 1469 | CLA  | CBD-CGD-O2D-CED |
| 11  | C     | 1471 | CLA  | CBD-CGD-O2D-CED |
| 11  | G     | 1344 | CLA  | CBD-CGD-O2D-CED |
| 11  | H     | 1484 | CLA  | CBD-CGD-O2D-CED |
| 11  | H     | 1493 | CLA  | CBD-CGD-O2D-CED |
| 11  | H     | 1494 | CLA  | CBD-CGD-O2D-CED |
| 11  | I     | 1459 | CLA  | CBD-CGD-O2D-CED |
| 11  | I     | 1460 | CLA  | CBD-CGD-O2D-CED |
| 11  | I     | 1463 | CLA  | CBD-CGD-O2D-CED |
| 11  | I     | 1464 | CLA  | CBD-CGD-O2D-CED |
| 11  | I     | 1465 | CLA  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 11  | I     | 1466 | CLA  | CBD-CGD-O2D-CED |
| 11  | I     | 1467 | CLA  | CBD-CGD-O2D-CED |
| 11  | I     | 1469 | CLA  | CBD-CGD-O2D-CED |
| 11  | I     | 1471 | CLA  | CBD-CGD-O2D-CED |
| 12  | D     | 1352 | PHO  | CBD-CGD-O2D-CED |
| 12  | J     | 1352 | PHO  | CBD-CGD-O2D-CED |
| 11  | B     | 1485 | CLA  | O1D-CGD-O2D-CED |
| 11  | C     | 1460 | CLA  | O1D-CGD-O2D-CED |
| 11  | C     | 1464 | CLA  | O1D-CGD-O2D-CED |
| 11  | C     | 1469 | CLA  | O1D-CGD-O2D-CED |
| 11  | I     | 1460 | CLA  | O1D-CGD-O2D-CED |
| 11  | I     | 1464 | CLA  | O1D-CGD-O2D-CED |
| 11  | I     | 1469 | CLA  | O1D-CGD-O2D-CED |
| 11  | C     | 1466 | CLA  | CBD-CGD-O2D-CED |
| 11  | B     | 1497 | CLA  | O1D-CGD-O2D-CED |
| 11  | H     | 1486 | CLA  | O1D-CGD-O2D-CED |
| 11  | B     | 1486 | CLA  | O1D-CGD-O2D-CED |
| 11  | B     | 1489 | CLA  | O1D-CGD-O2D-CED |
| 11  | H     | 1489 | CLA  | O1D-CGD-O2D-CED |
| 11  | H     | 1492 | CLA  | O1D-CGD-O2D-CED |
| 11  | H     | 1497 | CLA  | O1D-CGD-O2D-CED |
| 11  | B     | 1496 | CLA  | CBD-CGD-O2D-CED |
| 11  | C     | 1462 | CLA  | CBD-CGD-O2D-CED |
| 11  | D     | 1351 | CLA  | CBD-CGD-O2D-CED |
| 11  | D     | 1353 | CLA  | CBD-CGD-O2D-CED |
| 11  | H     | 1496 | CLA  | CBD-CGD-O2D-CED |
| 11  | I     | 1462 | CLA  | CBD-CGD-O2D-CED |
| 11  | J     | 1351 | CLA  | CBD-CGD-O2D-CED |
| 11  | J     | 1353 | CLA  | CBD-CGD-O2D-CED |
| 11  | B     | 1495 | CLA  | O1D-CGD-O2D-CED |
| 11  | C     | 1459 | CLA  | O1D-CGD-O2D-CED |
| 11  | C     | 1463 | CLA  | O1D-CGD-O2D-CED |
| 11  | C     | 1470 | CLA  | O1D-CGD-O2D-CED |
| 11  | H     | 1490 | CLA  | O1D-CGD-O2D-CED |
| 11  | H     | 1495 | CLA  | O1D-CGD-O2D-CED |
| 11  | I     | 1465 | CLA  | O1D-CGD-O2D-CED |
| 11  | I     | 1470 | CLA  | O1D-CGD-O2D-CED |
| 11  | C     | 1463 | CLA  | C4-C3-C5-C6     |
| 11  | I     | 1463 | CLA  | C4-C3-C5-C6     |
| 11  | B     | 1482 | CLA  | C2-C3-C5-C6     |
| 11  | B     | 1483 | CLA  | C2-C3-C5-C6     |
| 11  | C     | 1463 | CLA  | C2-C3-C5-C6     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 11  | H     | 1482 | CLA  | C2-C3-C5-C6     |
| 11  | I     | 1463 | CLA  | C2-C3-C5-C6     |
| 11  | B     | 1492 | CLA  | O1D-CGD-O2D-CED |
| 11  | H     | 1484 | CLA  | O1D-CGD-O2D-CED |
| 11  | I     | 1459 | CLA  | O1D-CGD-O2D-CED |
| 11  | I     | 1463 | CLA  | O1D-CGD-O2D-CED |
| 12  | J     | 1352 | PHO  | O1D-CGD-O2D-CED |
| 11  | B     | 1490 | CLA  | C2A-CAA-CBA-CGA |
| 11  | B     | 1484 | CLA  | O1D-CGD-O2D-CED |
| 11  | B     | 1493 | CLA  | O1D-CGD-O2D-CED |
| 11  | C     | 1465 | CLA  | O1D-CGD-O2D-CED |
| 12  | D     | 1352 | PHO  | O1D-CGD-O2D-CED |
| 11  | B     | 1490 | CLA  | O1D-CGD-O2D-CED |
| 11  | H     | 1493 | CLA  | O1D-CGD-O2D-CED |
| 11  | I     | 1466 | CLA  | O1D-CGD-O2D-CED |
| 11  | B     | 1486 | CLA  | C2C-C3C-CAC-CBC |
| 11  | C     | 1466 | CLA  | O1D-CGD-O2D-CED |
| 11  | H     | 1483 | CLA  | C4-C3-C5-C6     |
| 11  | H     | 1487 | CLA  | C4-C3-C5-C6     |
| 12  | D     | 1352 | PHO  | C4-C3-C5-C6     |
| 11  | B     | 1487 | CLA  | C2-C3-C5-C6     |
| 11  | H     | 1487 | CLA  | C2-C3-C5-C6     |
| 11  | H     | 1483 | CLA  | CBD-CGD-O2D-CED |
| 11  | H     | 1490 | CLA  | C2A-CAA-CBA-CGA |
| 11  | H     | 1486 | CLA  | C2C-C3C-CAC-CBC |
| 11  | B     | 1483 | CLA  | CBD-CGD-O2D-CED |
| 11  | B     | 1496 | CLA  | O1D-CGD-O2D-CED |
| 11  | B     | 1487 | CLA  | C4-C3-C5-C6     |
| 12  | D     | 1352 | PHO  | C2-C3-C5-C6     |
| 11  | A     | 1346 | CLA  | CBD-CGD-O2D-CED |
| 11  | A     | 1343 | CLA  | C11-C12-C13-C14 |
| 11  | B     | 1488 | CLA  | C14-C13-C15-C16 |
| 11  | B     | 1496 | CLA  | C6-C7-C8-C9     |
| 11  | B     | 1496 | CLA  | C14-C13-C15-C16 |
| 11  | C     | 1462 | CLA  | C6-C7-C8-C9     |
| 11  | G     | 1343 | CLA  | C11-C12-C13-C14 |
| 11  | H     | 1488 | CLA  | C14-C13-C15-C16 |
| 11  | H     | 1496 | CLA  | C14-C13-C15-C16 |
| 11  | I     | 1462 | CLA  | C6-C7-C8-C9     |
| 11  | H     | 1496 | CLA  | O1D-CGD-O2D-CED |
| 11  | I     | 1462 | CLA  | O1D-CGD-O2D-CED |
| 11  | C     | 1462 | CLA  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 11  | D     | 1351 | CLA  | O1D-CGD-O2D-CED |
| 11  | J     | 1351 | CLA  | O1D-CGD-O2D-CED |
| 11  | J     | 1353 | CLA  | O1D-CGD-O2D-CED |
| 11  | B     | 1496 | CLA  | C15-C16-C17-C18 |
| 12  | A     | 1345 | PHO  | C10-C11-C12-C13 |
| 12  | G     | 1345 | PHO  | C15-C16-C17-C18 |
| 11  | D     | 1353 | CLA  | O1D-CGD-O2D-CED |
| 12  | A     | 1345 | PHO  | C15-C16-C17-C18 |
| 11  | B     | 1488 | CLA  | C5-C6-C7-C8     |
| 11  | B     | 1488 | CLA  | C13-C15-C16-C17 |
| 11  | H     | 1496 | CLA  | C15-C16-C17-C18 |
| 11  | B     | 1486 | CLA  | C4C-C3C-CAC-CBC |
| 11  | B     | 1492 | CLA  | C2A-CAA-CBA-CGA |
| 11  | C     | 1460 | CLA  | C2A-CAA-CBA-CGA |
| 11  | H     | 1488 | CLA  | C2A-CAA-CBA-CGA |
| 11  | H     | 1492 | CLA  | C2A-CAA-CBA-CGA |
| 11  | I     | 1460 | CLA  | C2A-CAA-CBA-CGA |
| 11  | I     | 1465 | CLA  | C10-C11-C12-C13 |
| 12  | G     | 1345 | PHO  | C10-C11-C12-C13 |
| 11  | H     | 1488 | CLA  | C5-C6-C7-C8     |
| 11  | H     | 1488 | CLA  | C13-C15-C16-C17 |
| 11  | C     | 1465 | CLA  | C10-C11-C12-C13 |
| 11  | C     | 1471 | CLA  | C2C-C3C-CAC-CBC |
| 11  | G     | 1346 | CLA  | CBD-CGD-O2D-CED |
| 11  | B     | 1488 | CLA  | C2A-CAA-CBA-CGA |
| 11  | C     | 1459 | CLA  | C2A-CAA-CBA-CGA |
| 11  | I     | 1459 | CLA  | C2A-CAA-CBA-CGA |
| 11  | A     | 1343 | CLA  | C10-C11-C12-C13 |
| 11  | I     | 1464 | CLA  | C5-C6-C7-C8     |
| 11  | H     | 1486 | CLA  | C4C-C3C-CAC-CBC |
| 11  | C     | 1464 | CLA  | C5-C6-C7-C8     |
| 11  | G     | 1343 | CLA  | C10-C11-C12-C13 |
| 11  | H     | 1483 | CLA  | C10-C11-C12-C13 |
| 11  | H     | 1495 | CLA  | C4-C3-C5-C6     |
| 11  | H     | 1483 | CLA  | C2-C3-C5-C6     |
| 11  | I     | 1471 | CLA  | C2C-C3C-CAC-CBC |
| 11  | B     | 1483 | CLA  | C10-C11-C12-C13 |
| 11  | A     | 1343 | CLA  | C2A-CAA-CBA-CGA |
| 11  | G     | 1343 | CLA  | C2A-CAA-CBA-CGA |
| 11  | I     | 1463 | CLA  | C2A-CAA-CBA-CGA |
| 11  | H     | 1483 | CLA  | O1D-CGD-O2D-CED |
| 11  | G     | 1342 | CLA  | C15-C16-C17-C18 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 12  | D     | 1352 | PHO  | C6-C7-C8-C9     |
| 12  | J     | 1352 | PHO  | C6-C7-C8-C9     |
| 11  | A     | 1342 | CLA  | C4B-C3B-CAB-CBB |
| 11  | B     | 1488 | CLA  | C4B-C3B-CAB-CBB |
| 11  | B     | 1490 | CLA  | C4B-C3B-CAB-CBB |
| 11  | C     | 1459 | CLA  | C4B-C3B-CAB-CBB |
| 11  | C     | 1471 | CLA  | C4B-C3B-CAB-CBB |
| 11  | G     | 1342 | CLA  | C4B-C3B-CAB-CBB |
| 11  | H     | 1488 | CLA  | C4B-C3B-CAB-CBB |
| 11  | H     | 1490 | CLA  | C4B-C3B-CAB-CBB |
| 11  | I     | 1469 | CLA  | C4B-C3B-CAB-CBB |
| 11  | I     | 1471 | CLA  | C4B-C3B-CAB-CBB |
| 11  | B     | 1483 | CLA  | C2A-CAA-CBA-CGA |
| 11  | C     | 1464 | CLA  | C2A-CAA-CBA-CGA |
| 11  | I     | 1464 | CLA  | C2A-CAA-CBA-CGA |
| 11  | G     | 1343 | CLA  | C11-C12-C13-C15 |
| 11  | A     | 1342 | CLA  | C15-C16-C17-C18 |
| 11  | A     | 1343 | CLA  | C3A-C2A-CAA-CBA |
| 11  | B     | 1485 | CLA  | C3A-C2A-CAA-CBA |
| 11  | B     | 1493 | CLA  | C3A-C2A-CAA-CBA |
| 11  | C     | 1462 | CLA  | C3A-C2A-CAA-CBA |
| 11  | C     | 1466 | CLA  | C3A-C2A-CAA-CBA |
| 11  | G     | 1343 | CLA  | C3A-C2A-CAA-CBA |
| 11  | H     | 1485 | CLA  | C3A-C2A-CAA-CBA |
| 11  | H     | 1488 | CLA  | C3A-C2A-CAA-CBA |
| 11  | H     | 1493 | CLA  | C3A-C2A-CAA-CBA |
| 11  | I     | 1462 | CLA  | C3A-C2A-CAA-CBA |
| 11  | I     | 1466 | CLA  | C3A-C2A-CAA-CBA |
| 11  | B     | 1483 | CLA  | O1D-CGD-O2D-CED |
| 12  | D     | 1352 | PHO  | C6-C7-C8-C10    |
| 12  | J     | 1352 | PHO  | C6-C7-C8-C10    |
| 11  | A     | 1342 | CLA  | C2B-C3B-CAB-CBB |
| 11  | B     | 1490 | CLA  | C2B-C3B-CAB-CBB |
| 11  | B     | 1495 | CLA  | C2B-C3B-CAB-CBB |
| 11  | B     | 1496 | CLA  | C2B-C3B-CAB-CBB |
| 11  | C     | 1459 | CLA  | C2B-C3B-CAB-CBB |
| 11  | C     | 1469 | CLA  | C2B-C3B-CAB-CBB |
| 11  | C     | 1471 | CLA  | C2B-C3B-CAB-CBB |
| 11  | G     | 1342 | CLA  | C2B-C3B-CAB-CBB |
| 11  | G     | 1344 | CLA  | C2B-C3B-CAB-CBB |
| 11  | H     | 1490 | CLA  | C2B-C3B-CAB-CBB |
| 11  | H     | 1495 | CLA  | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 11  | H     | 1496 | CLA  | C2B-C3B-CAB-CBB |
| 11  | I     | 1469 | CLA  | C2B-C3B-CAB-CBB |
| 11  | I     | 1471 | CLA  | C2B-C3B-CAB-CBB |
| 11  | C     | 1463 | CLA  | C2A-CAA-CBA-CGA |
| 11  | H     | 1483 | CLA  | C2A-CAA-CBA-CGA |
| 11  | H     | 1496 | CLA  | C13-C15-C16-C17 |
| 12  | J     | 1352 | PHO  | C4-C3-C5-C6     |
| 11  | H     | 1495 | CLA  | C2-C3-C5-C6     |
| 12  | J     | 1352 | PHO  | C2-C3-C5-C6     |
| 11  | A     | 1343 | CLA  | C5-C6-C7-C8     |
| 11  | B     | 1496 | CLA  | C5-C6-C7-C8     |
| 11  | A     | 1343 | CLA  | C14-C13-C15-C16 |
| 11  | G     | 1343 | CLA  | C14-C13-C15-C16 |
| 11  | B     | 1495 | CLA  | C4-C3-C5-C6     |
| 11  | H     | 1492 | CLA  | C4-C3-C5-C6     |
| 11  | H     | 1496 | CLA  | C5-C6-C7-C8     |
| 11  | I     | 1465 | CLA  | C5-C6-C7-C8     |
| 11  | C     | 1463 | CLA  | C5-C6-C7-C8     |
| 11  | B     | 1488 | CLA  | C1A-C2A-CAA-CBA |
| 11  | B     | 1493 | CLA  | C1A-C2A-CAA-CBA |
| 11  | H     | 1488 | CLA  | C1A-C2A-CAA-CBA |
| 11  | H     | 1493 | CLA  | C1A-C2A-CAA-CBA |
| 11  | G     | 1343 | CLA  | C5-C6-C7-C8     |
| 11  | A     | 1343 | CLA  | C11-C12-C13-C15 |
| 11  | B     | 1482 | CLA  | C11-C10-C8-C7   |
| 11  | B     | 1494 | CLA  | C6-C7-C8-C10    |
| 11  | B     | 1496 | CLA  | C11-C10-C8-C7   |
| 11  | D     | 1351 | CLA  | C11-C12-C13-C15 |
| 11  | H     | 1482 | CLA  | C11-C10-C8-C7   |
| 11  | H     | 1494 | CLA  | C6-C7-C8-C10    |
| 11  | H     | 1496 | CLA  | C11-C10-C8-C7   |
| 11  | I     | 1462 | CLA  | C6-C7-C8-C10    |
| 11  | J     | 1351 | CLA  | C11-C12-C13-C15 |
| 12  | A     | 1345 | PHO  | C12-C13-C15-C16 |
| 12  | G     | 1345 | PHO  | C6-C7-C8-C10    |
| 12  | G     | 1345 | PHO  | C12-C13-C15-C16 |
| 11  | A     | 1346 | CLA  | O1D-CGD-O2D-CED |
| 11  | C     | 1465 | CLA  | C5-C6-C7-C8     |
| 11  | A     | 1342 | CLA  | C2A-CAA-CBA-CGA |
| 11  | G     | 1342 | CLA  | C2A-CAA-CBA-CGA |
| 11  | H     | 1484 | CLA  | C2A-CAA-CBA-CGA |
| 11  | B     | 1488 | CLA  | C11-C12-C13-C14 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 11  | C     | 1465 | CLA  | C6-C7-C8-C9     |
| 11  | D     | 1351 | CLA  | C11-C12-C13-C14 |
| 11  | H     | 1494 | CLA  | C6-C7-C8-C9     |
| 11  | H     | 1496 | CLA  | C11-C10-C8-C9   |
| 11  | I     | 1465 | CLA  | C6-C7-C8-C9     |
| 11  | J     | 1351 | CLA  | C11-C12-C13-C14 |
| 12  | G     | 1345 | PHO  | C14-C13-C15-C16 |
| 11  | I     | 1463 | CLA  | C5-C6-C7-C8     |
| 11  | B     | 1496 | CLA  | C13-C15-C16-C17 |
| 11  | H     | 1492 | CLA  | C2-C3-C5-C6     |
| 11  | D     | 1351 | CLA  | O2A-C1-C2-C3    |
| 11  | J     | 1351 | CLA  | O2A-C1-C2-C3    |
| 11  | B     | 1494 | CLA  | C5-C6-C7-C8     |
| 11  | D     | 1351 | CLA  | C5-C6-C7-C8     |
| 11  | A     | 1343 | CLA  | C4-C3-C5-C6     |
| 11  | G     | 1343 | CLA  | C4-C3-C5-C6     |
| 11  | H     | 1494 | CLA  | C2-C3-C5-C6     |
| 11  | B     | 1482 | CLA  | C11-C10-C8-C9   |
| 11  | B     | 1482 | CLA  | C11-C12-C13-C14 |
| 11  | B     | 1494 | CLA  | C6-C7-C8-C9     |
| 11  | B     | 1496 | CLA  | C11-C10-C8-C9   |
| 11  | C     | 1464 | CLA  | C6-C7-C8-C9     |
| 11  | G     | 1342 | CLA  | C14-C13-C15-C16 |
| 11  | H     | 1482 | CLA  | C11-C10-C8-C9   |
| 11  | H     | 1482 | CLA  | C11-C12-C13-C14 |
| 11  | H     | 1488 | CLA  | C11-C12-C13-C14 |
| 12  | A     | 1345 | PHO  | C6-C7-C8-C9     |
| 12  | G     | 1345 | PHO  | C6-C7-C8-C9     |
| 11  | J     | 1351 | CLA  | C5-C6-C7-C8     |
| 11  | C     | 1469 | CLA  | C4B-C3B-CAB-CBB |
| 11  | D     | 1353 | CLA  | C4B-C3B-CAB-CBB |
| 11  | I     | 1459 | CLA  | C4B-C3B-CAB-CBB |
| 11  | J     | 1353 | CLA  | C4B-C3B-CAB-CBB |
| 11  | H     | 1487 | CLA  | CAA-CBA-CGA-O2A |
| 11  | B     | 1484 | CLA  | C2A-CAA-CBA-CGA |
| 11  | B     | 1487 | CLA  | CAA-CBA-CGA-O2A |
| 11  | B     | 1482 | CLA  | C11-C12-C13-C15 |
| 11  | B     | 1488 | CLA  | C11-C12-C13-C15 |
| 11  | B     | 1492 | CLA  | C6-C7-C8-C10    |
| 11  | C     | 1465 | CLA  | C6-C7-C8-C10    |
| 11  | H     | 1488 | CLA  | C11-C12-C13-C15 |
| 11  | H     | 1492 | CLA  | C6-C7-C8-C10    |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 11  | I     | 1465 | CLA  | C6-C7-C8-C10    |
| 12  | A     | 1345 | PHO  | C6-C7-C8-C10    |
| 11  | B     | 1487 | CLA  | C3A-C2A-CAA-CBA |
| 11  | H     | 1487 | CLA  | C3A-C2A-CAA-CBA |
| 11  | B     | 1487 | CLA  | C5-C6-C7-C8     |
| 11  | D     | 1351 | CLA  | C13-C15-C16-C17 |
| 11  | H     | 1494 | CLA  | C4-C3-C5-C6     |
| 11  | G     | 1346 | CLA  | O1D-CGD-O2D-CED |
| 11  | I     | 1459 | CLA  | C2B-C3B-CAB-CBB |
| 17  | F     | 1046 | BCR  | C23-C24-C25-C30 |
| 17  | L     | 1047 | BCR  | C23-C24-C25-C30 |
| 11  | B     | 1492 | CLA  | C15-C16-C17-C18 |
| 11  | J     | 1351 | CLA  | C13-C15-C16-C17 |
| 11  | A     | 1343 | CLA  | C2-C3-C5-C6     |
| 11  | G     | 1343 | CLA  | C2-C3-C5-C6     |
| 11  | H     | 1482 | CLA  | CBD-CGD-O2D-CED |
| 11  | H     | 1487 | CLA  | C5-C6-C7-C8     |
| 12  | A     | 1345 | PHO  | C5-C6-C7-C8     |
| 11  | H     | 1482 | CLA  | C11-C12-C13-C15 |
| 12  | G     | 1345 | PHO  | C5-C6-C7-C8     |
| 11  | B     | 1494 | CLA  | C2-C3-C5-C6     |
| 11  | H     | 1494 | CLA  | C5-C6-C7-C8     |
| 11  | B     | 1495 | CLA  | C2-C3-C5-C6     |
| 11  | A     | 1342 | CLA  | C14-C13-C15-C16 |
| 11  | I     | 1464 | CLA  | C6-C7-C8-C9     |
| 12  | A     | 1345 | PHO  | C14-C13-C15-C16 |
| 11  | H     | 1492 | CLA  | C15-C16-C17-C18 |
| 11  | H     | 1482 | CLA  | O1D-CGD-O2D-CED |
| 11  | B     | 1494 | CLA  | C4-C3-C5-C6     |
| 11  | I     | 1464 | CLA  | C11-C10-C8-C9   |
| 12  | G     | 1345 | PHO  | C4C-C3C-CAC-CBC |
| 11  | C     | 1466 | CLA  | C4B-C3B-CAB-CBB |
| 11  | G     | 1344 | CLA  | C1A-C2A-CAA-CBA |
| 11  | I     | 1466 | CLA  | C4B-C3B-CAB-CBB |
| 11  | B     | 1492 | CLA  | C4-C3-C5-C6     |
| 11  | B     | 1488 | CLA  | C12-C13-C15-C16 |
| 11  | B     | 1496 | CLA  | C12-C13-C15-C16 |
| 11  | C     | 1462 | CLA  | C6-C7-C8-C10    |
| 11  | H     | 1488 | CLA  | C12-C13-C15-C16 |
| 11  | H     | 1496 | CLA  | C12-C13-C15-C16 |
| 18  | T     | 1138 | HEC  | C4C-C3C-CAC-CBC |
| 18  | V     | 1138 | HEC  | C4C-C3C-CAC-CBC |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 11  | H     | 1495 | CLA  | C2A-CAA-CBA-CGA |
| 11  | C     | 1471 | CLA  | C4C-C3C-CAC-CBC |
| 11  | C     | 1464 | CLA  | C11-C10-C8-C9   |
| 11  | A     | 1343 | CLA  | CAD-CBD-CGD-O2D |
| 11  | B     | 1490 | CLA  | CAD-CBD-CGD-O2D |
| 11  | C     | 1464 | CLA  | CAD-CBD-CGD-O2D |
| 11  | C     | 1467 | CLA  | CAD-CBD-CGD-O2D |
| 11  | G     | 1343 | CLA  | CAD-CBD-CGD-O2D |
| 11  | H     | 1490 | CLA  | CAD-CBD-CGD-O2D |
| 11  | H     | 1492 | CLA  | CAD-CBD-CGD-O2D |
| 11  | I     | 1464 | CLA  | CAD-CBD-CGD-O2D |
| 11  | B     | 1495 | CLA  | C2A-CAA-CBA-CGA |
| 11  | A     | 1343 | CLA  | CAD-CBD-CGD-O1D |
| 11  | A     | 1344 | CLA  | CAD-CBD-CGD-O1D |
| 11  | A     | 1346 | CLA  | CHA-CBD-CGD-O1D |
| 11  | A     | 1346 | CLA  | CHA-CBD-CGD-O2D |
| 11  | B     | 1489 | CLA  | CAD-CBD-CGD-O1D |
| 11  | B     | 1490 | CLA  | CAD-CBD-CGD-O1D |
| 11  | B     | 1492 | CLA  | CAD-CBD-CGD-O1D |
| 11  | C     | 1464 | CLA  | CAD-CBD-CGD-O1D |
| 11  | C     | 1465 | CLA  | CHA-CBD-CGD-O1D |
| 11  | C     | 1465 | CLA  | CHA-CBD-CGD-O2D |
| 11  | C     | 1467 | CLA  | CAD-CBD-CGD-O1D |
| 11  | G     | 1343 | CLA  | CAD-CBD-CGD-O1D |
| 11  | G     | 1344 | CLA  | CAD-CBD-CGD-O1D |
| 11  | H     | 1490 | CLA  | CAD-CBD-CGD-O1D |
| 11  | H     | 1492 | CLA  | CAD-CBD-CGD-O1D |
| 11  | I     | 1463 | CLA  | CHA-CBD-CGD-O1D |
| 11  | I     | 1464 | CLA  | CAD-CBD-CGD-O1D |
| 11  | I     | 1465 | CLA  | CHA-CBD-CGD-O1D |
| 11  | I     | 1465 | CLA  | CHA-CBD-CGD-O2D |
| 11  | I     | 1467 | CLA  | CAD-CBD-CGD-O1D |
| 18  | V     | 1138 | HEC  | C2B-C3B-CAB-CBB |
| 11  | B     | 1488 | CLA  | C2B-C3B-CAB-CBB |
| 11  | H     | 1488 | CLA  | C2B-C3B-CAB-CBB |
| 11  | B     | 1494 | CLA  | C13-C15-C16-C17 |
| 11  | C     | 1465 | CLA  | C13-C15-C16-C17 |
| 11  | I     | 1465 | CLA  | C13-C15-C16-C17 |
| 11  | D     | 1353 | CLA  | C2A-CAA-CBA-CGA |
| 11  | H     | 1482 | CLA  | CAA-CBA-CGA-O2A |
| 11  | H     | 1488 | CLA  | C6-C7-C8-C9     |
| 11  | C     | 1465 | CLA  | C12-C13-C15-C16 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 11  | J     | 1353 | CLA  | C2A-CAA-CBA-CGA |
| 11  | I     | 1471 | CLA  | C4C-C3C-CAC-CBC |
| 11  | H     | 1494 | CLA  | C13-C15-C16-C17 |
| 11  | B     | 1482 | CLA  | CAA-CBA-CGA-O2A |
| 11  | C     | 1465 | CLA  | C14-C13-C15-C16 |
| 11  | I     | 1465 | CLA  | C14-C13-C15-C16 |
| 11  | C     | 1459 | CLA  | C3A-C2A-CAA-CBA |
| 11  | I     | 1463 | CLA  | C2-C1-O2A-CGA   |
| 12  | G     | 1345 | PHO  | C2-C1-O2A-CGA   |
| 12  | G     | 1345 | PHO  | O1D-CGD-O2D-CED |
| 11  | C     | 1459 | CLA  | CAA-CBA-CGA-O2A |
| 11  | B     | 1488 | CLA  | C6-C7-C8-C9     |
| 11  | B     | 1492 | CLA  | C11-C12-C13-C14 |
| 11  | H     | 1492 | CLA  | C11-C12-C13-C14 |
| 11  | C     | 1459 | CLA  | CAA-CBA-CGA-O1A |
| 11  | I     | 1459 | CLA  | CAA-CBA-CGA-O2A |
| 11  | B     | 1487 | CLA  | CAA-CBA-CGA-O1A |
| 11  | A     | 1344 | CLA  | C1A-C2A-CAA-CBA |
| 11  | B     | 1490 | CLA  | C1A-C2A-CAA-CBA |
| 11  | H     | 1487 | CLA  | C1A-C2A-CAA-CBA |
| 11  | H     | 1496 | CLA  | C2C-C3C-CAC-CBC |
| 11  | C     | 1462 | CLA  | C2B-C3B-CAB-CBB |
| 11  | C     | 1466 | CLA  | C2B-C3B-CAB-CBB |
| 11  | I     | 1462 | CLA  | C2B-C3B-CAB-CBB |
| 11  | I     | 1466 | CLA  | C2B-C3B-CAB-CBB |
| 11  | J     | 1353 | CLA  | C2B-C3B-CAB-CBB |
| 11  | B     | 1490 | CLA  | CAA-CBA-CGA-O1A |
| 11  | I     | 1459 | CLA  | CAA-CBA-CGA-O1A |
| 11  | H     | 1490 | CLA  | CAA-CBA-CGA-O1A |
| 11  | B     | 1483 | CLA  | C11-C10-C8-C7   |
| 11  | I     | 1465 | CLA  | C12-C13-C15-C16 |
| 11  | A     | 1343 | CLA  | C12-C13-C15-C16 |
| 11  | G     | 1343 | CLA  | C12-C13-C15-C16 |
| 11  | J     | 1351 | CLA  | C2-C3-C5-C6     |
| 11  | B     | 1488 | CLA  | O1D-CGD-O2D-CED |
| 11  | C     | 1465 | CLA  | C11-C10-C8-C9   |
| 11  | H     | 1487 | CLA  | CAA-CBA-CGA-O1A |
| 11  | C     | 1465 | CLA  | C4-C3-C5-C6     |
| 11  | D     | 1351 | CLA  | C4-C3-C5-C6     |
| 11  | J     | 1351 | CLA  | C4-C3-C5-C6     |
| 12  | A     | 1345 | PHO  | C4-C3-C5-C6     |
| 12  | G     | 1345 | PHO  | C4-C3-C5-C6     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 11  | B     | 1492 | CLA  | C2-C3-C5-C6     |
| 11  | D     | 1351 | CLA  | C2-C3-C5-C6     |
| 12  | G     | 1345 | PHO  | C2-C3-C5-C6     |
| 11  | H     | 1490 | CLA  | CAA-CBA-CGA-O2A |
| 11  | B     | 1493 | CLA  | CAA-CBA-CGA-O1A |
| 11  | B     | 1496 | CLA  | C4-C3-C5-C6     |
| 11  | B     | 1495 | CLA  | CAA-CBA-CGA-O2A |
| 12  | A     | 1345 | PHO  | C2-C3-C5-C6     |
| 11  | B     | 1493 | CLA  | C4B-C3B-CAB-CBB |
| 11  | C     | 1462 | CLA  | C4B-C3B-CAB-CBB |
| 11  | I     | 1462 | CLA  | C4B-C3B-CAB-CBB |
| 11  | B     | 1488 | CLA  | CBD-CGD-O2D-CED |
| 11  | B     | 1490 | CLA  | CAA-CBA-CGA-O2A |
| 18  | V     | 1138 | HEC  | CAA-CBA-CGA-O1A |
| 11  | B     | 1485 | CLA  | C4C-C3C-CAC-CBC |
| 11  | B     | 1488 | CLA  | C15-C16-C17-C18 |
| 11  | B     | 1496 | CLA  | C6-C7-C8-C10    |
| 11  | C     | 1465 | CLA  | C11-C10-C8-C7   |
| 11  | B     | 1485 | CLA  | C2-C1-O2A-CGA   |
| 11  | H     | 1485 | CLA  | C2-C1-O2A-CGA   |
| 11  | I     | 1465 | CLA  | C11-C10-C8-C9   |
| 11  | B     | 1485 | CLA  | C2C-C3C-CAC-CBC |
| 11  | H     | 1495 | CLA  | CAA-CBA-CGA-O2A |
| 11  | C     | 1463 | CLA  | C2-C1-O2A-CGA   |
| 11  | H     | 1492 | CLA  | C2-C1-O2A-CGA   |
| 11  | H     | 1488 | CLA  | C10-C11-C12-C13 |
| 11  | B     | 1483 | CLA  | C3A-C2A-CAA-CBA |
| 11  | B     | 1495 | CLA  | C3A-C2A-CAA-CBA |
| 11  | I     | 1459 | CLA  | C3A-C2A-CAA-CBA |
| 11  | J     | 1351 | CLA  | C3A-C2A-CAA-CBA |
| 12  | J     | 1352 | PHO  | O2A-C1-C2-C3    |
| 18  | T     | 1138 | HEC  | CAD-CBD-CGD-O2D |
| 11  | B     | 1482 | CLA  | C5-C6-C7-C8     |
| 11  | H     | 1485 | CLA  | C2C-C3C-CAC-CBC |
| 11  | H     | 1485 | CLA  | C4C-C3C-CAC-CBC |
| 18  | T     | 1138 | HEC  | CAD-CBD-CGD-O1D |
| 18  | T     | 1138 | HEC  | CAA-CBA-CGA-O1A |
| 12  | G     | 1345 | PHO  | CBD-CGD-O2D-CED |
| 11  | I     | 1467 | CLA  | CAA-CBA-CGA-O2A |
| 18  | V     | 1138 | HEC  | CAD-CBD-CGD-O2D |
| 11  | H     | 1483 | CLA  | C11-C10-C8-C7   |
| 11  | H     | 1496 | CLA  | C6-C7-C8-C10    |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 11  | I     | 1465 | CLA  | C11-C10-C8-C7   |
| 11  | B     | 1493 | CLA  | C2B-C3B-CAB-CBB |
| 11  | D     | 1353 | CLA  | C2B-C3B-CAB-CBB |
| 17  | F     | 1046 | BCR  | C23-C24-C25-C26 |
| 17  | L     | 1047 | BCR  | C23-C24-C25-C26 |
| 11  | C     | 1467 | CLA  | CAA-CBA-CGA-O2A |
| 11  | B     | 1496 | CLA  | C2C-C3C-CAC-CBC |
| 11  | B     | 1492 | CLA  | C2-C1-O2A-CGA   |
| 11  | H     | 1496 | CLA  | C2-C1-O2A-CGA   |
| 18  | V     | 1138 | HEC  | CAD-CBD-CGD-O1D |
| 11  | B     | 1493 | CLA  | CAA-CBA-CGA-O2A |
| 11  | I     | 1464 | CLA  | CAA-CBA-CGA-O2A |
| 11  | C     | 1464 | CLA  | C11-C10-C8-C7   |
| 11  | H     | 1496 | CLA  | C4C-C3C-CAC-CBC |
| 11  | I     | 1464 | CLA  | C11-C10-C8-C7   |
| 11  | B     | 1496 | CLA  | C2-C3-C5-C6     |
| 11  | H     | 1493 | CLA  | CAA-CBA-CGA-O2A |
| 11  | C     | 1464 | CLA  | CAA-CBA-CGA-O2A |
| 11  | B     | 1483 | CLA  | C1A-C2A-CAA-CBA |
| 11  | B     | 1487 | CLA  | C1A-C2A-CAA-CBA |
| 11  | C     | 1460 | CLA  | C4B-C3B-CAB-CBB |
| 11  | C     | 1465 | CLA  | C1A-C2A-CAA-CBA |
| 11  | D     | 1351 | CLA  | C1A-C2A-CAA-CBA |
| 11  | G     | 1346 | CLA  | C1A-C2A-CAA-CBA |
| 11  | H     | 1483 | CLA  | C1A-C2A-CAA-CBA |
| 11  | H     | 1490 | CLA  | C1A-C2A-CAA-CBA |
| 11  | H     | 1493 | CLA  | C4B-C3B-CAB-CBB |
| 11  | J     | 1351 | CLA  | C1A-C2A-CAA-CBA |
| 18  | V     | 1138 | HEC  | CAA-CBA-CGA-O2A |
| 11  | H     | 1493 | CLA  | CAA-CBA-CGA-O1A |
| 18  | T     | 1138 | HEC  | CAA-CBA-CGA-O2A |
| 11  | B     | 1488 | CLA  | C10-C11-C12-C13 |
| 12  | A     | 1345 | PHO  | C2-C1-O2A-CGA   |
| 12  | D     | 1352 | PHO  | O2A-C1-C2-C3    |
| 11  | I     | 1467 | CLA  | C2A-CAA-CBA-CGA |
| 11  | B     | 1482 | CLA  | C3A-C2A-CAA-CBA |
| 11  | D     | 1351 | CLA  | C3A-C2A-CAA-CBA |
| 11  | H     | 1482 | CLA  | C3A-C2A-CAA-CBA |
| 11  | H     | 1483 | CLA  | C3A-C2A-CAA-CBA |
| 11  | H     | 1495 | CLA  | C3A-C2A-CAA-CBA |
| 11  | H     | 1496 | CLA  | C4-C3-C5-C6     |
| 11  | I     | 1465 | CLA  | C4-C3-C5-C6     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 11  | C     | 1467 | CLA  | CAA-CBA-CGA-O1A |
| 11  | H     | 1484 | CLA  | CAA-CBA-CGA-O2A |
| 11  | H     | 1494 | CLA  | C2A-CAA-CBA-CGA |
| 11  | B     | 1483 | CLA  | C11-C10-C8-C9   |
| 11  | H     | 1483 | CLA  | C11-C10-C8-C9   |
| 11  | B     | 1484 | CLA  | CAA-CBA-CGA-O2A |
| 11  | I     | 1467 | CLA  | CAA-CBA-CGA-O1A |
| 11  | H     | 1488 | CLA  | O1D-CGD-O2D-CED |
| 11  | H     | 1488 | CLA  | C15-C16-C17-C18 |
| 11  | I     | 1464 | CLA  | CAA-CBA-CGA-O1A |
| 11  | B     | 1492 | CLA  | CAD-CBD-CGD-O2D |
| 11  | H     | 1489 | CLA  | CAD-CBD-CGD-O2D |
| 11  | I     | 1460 | CLA  | CAD-CBD-CGD-O2D |
| 11  | J     | 1351 | CLA  | CAD-CBD-CGD-O2D |
| 11  | B     | 1496 | CLA  | C2-C1-O2A-CGA   |
| 11  | C     | 1464 | CLA  | CAA-CBA-CGA-O1A |
| 11  | H     | 1482 | CLA  | C5-C6-C7-C8     |
| 11  | B     | 1496 | CLA  | C4C-C3C-CAC-CBC |

There are no ring outliers.

77 monomers are involved in 435 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 11  | B     | 1486 | CLA  | 10      | 0            |
| 11  | I     | 1459 | CLA  | 3       | 0            |
| 11  | G     | 1342 | CLA  | 18      | 0            |
| 11  | H     | 1485 | CLA  | 5       | 0            |
| 11  | H     | 1495 | CLA  | 2       | 0            |
| 11  | D     | 1353 | CLA  | 6       | 0            |
| 11  | G     | 1343 | CLA  | 7       | 0            |
| 11  | B     | 1488 | CLA  | 7       | 0            |
| 11  | C     | 1465 | CLA  | 5       | 0            |
| 18  | T     | 1138 | HEC  | 2       | 0            |
| 11  | H     | 1482 | CLA  | 2       | 0            |
| 11  | I     | 1470 | CLA  | 3       | 0            |
| 11  | B     | 1496 | CLA  | 13      | 0            |
| 11  | C     | 1467 | CLA  | 7       | 0            |
| 11  | C     | 1469 | CLA  | 6       | 0            |
| 12  | J     | 1352 | PHO  | 9       | 0            |
| 11  | C     | 1466 | CLA  | 10      | 0            |
| 11  | I     | 1471 | CLA  | 5       | 0            |
| 11  | I     | 1460 | CLA  | 3       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 11  | H     | 1486 | CLA  | 12      | 0            |
| 11  | B     | 1494 | CLA  | 2       | 0            |
| 12  | D     | 1352 | PHO  | 4       | 0            |
| 15  | D     | 1354 | PL9  | 1       | 0            |
| 11  | H     | 1497 | CLA  | 8       | 0            |
| 11  | I     | 1466 | CLA  | 10      | 0            |
| 11  | J     | 1353 | CLA  | 5       | 0            |
| 11  | H     | 1494 | CLA  | 2       | 0            |
| 11  | B     | 1489 | CLA  | 4       | 0            |
| 11  | H     | 1490 | CLA  | 1       | 0            |
| 11  | H     | 1483 | CLA  | 3       | 0            |
| 11  | H     | 1488 | CLA  | 14      | 0            |
| 11  | B     | 1492 | CLA  | 5       | 0            |
| 11  | H     | 1484 | CLA  | 7       | 0            |
| 11  | C     | 1470 | CLA  | 3       | 0            |
| 11  | A     | 1344 | CLA  | 5       | 0            |
| 11  | C     | 1460 | CLA  | 4       | 0            |
| 11  | H     | 1496 | CLA  | 12      | 0            |
| 11  | A     | 1346 | CLA  | 5       | 0            |
| 16  | E     | 1085 | HEM  | 2       | 0            |
| 11  | C     | 1464 | CLA  | 8       | 0            |
| 11  | B     | 1483 | CLA  | 4       | 0            |
| 11  | C     | 1462 | CLA  | 4       | 0            |
| 11  | I     | 1462 | CLA  | 4       | 0            |
| 11  | C     | 1471 | CLA  | 5       | 0            |
| 11  | C     | 1463 | CLA  | 9       | 0            |
| 11  | I     | 1463 | CLA  | 10      | 0            |
| 15  | J     | 1354 | PL9  | 1       | 0            |
| 18  | V     | 1138 | HEC  | 2       | 0            |
| 17  | F     | 1046 | BCR  | 4       | 0            |
| 16  | L     | 1046 | HEM  | 2       | 0            |
| 11  | G     | 1344 | CLA  | 5       | 0            |
| 11  | B     | 1487 | CLA  | 7       | 0            |
| 11  | J     | 1351 | CLA  | 11      | 0            |
| 11  | B     | 1495 | CLA  | 3       | 0            |
| 11  | I     | 1467 | CLA  | 7       | 0            |
| 11  | B     | 1491 | CLA  | 3       | 0            |
| 17  | L     | 1047 | BCR  | 3       | 0            |
| 11  | B     | 1485 | CLA  | 4       | 0            |
| 11  | A     | 1343 | CLA  | 12      | 0            |
| 11  | A     | 1342 | CLA  | 17      | 0            |
| 11  | H     | 1492 | CLA  | 6       | 0            |

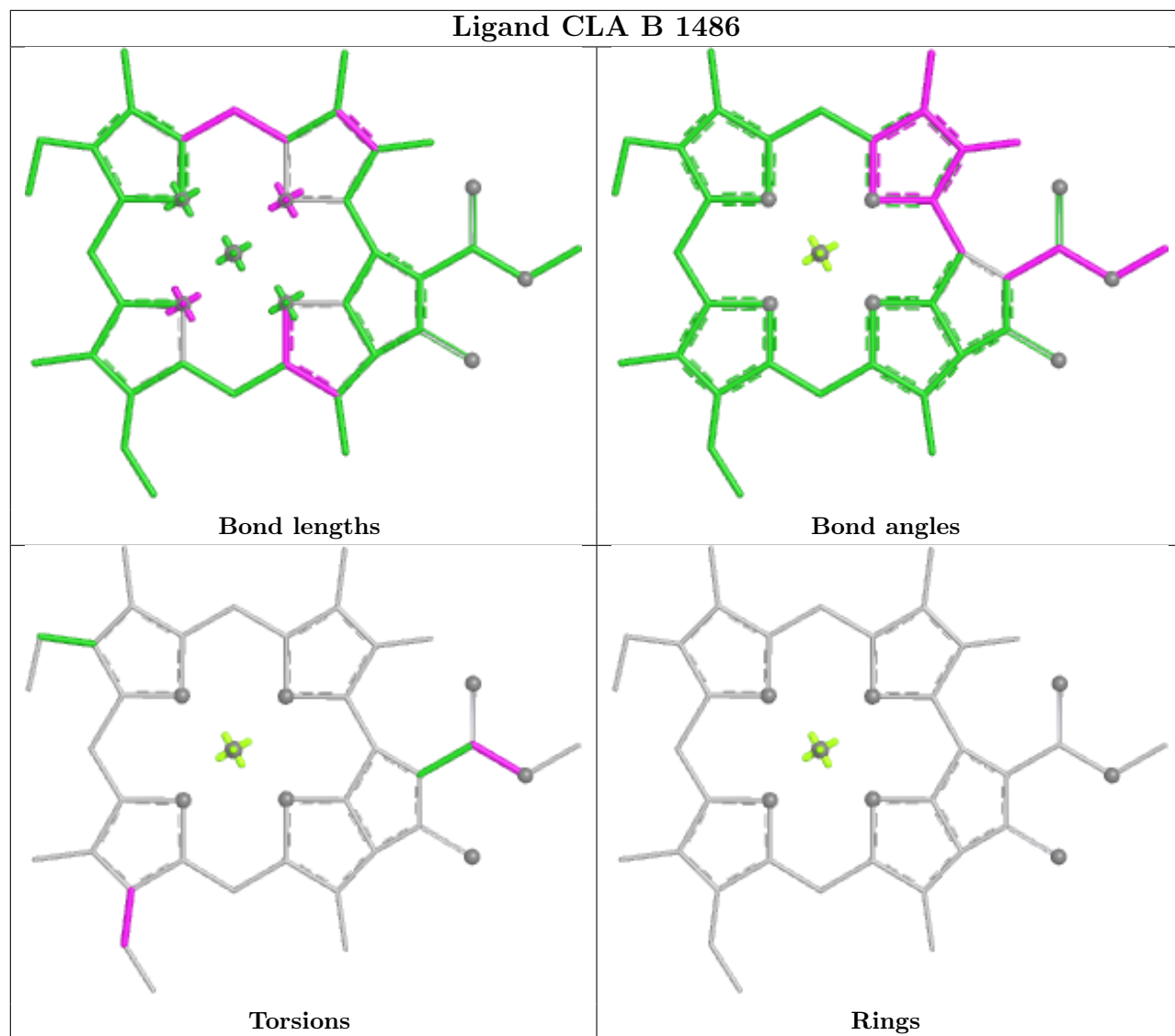
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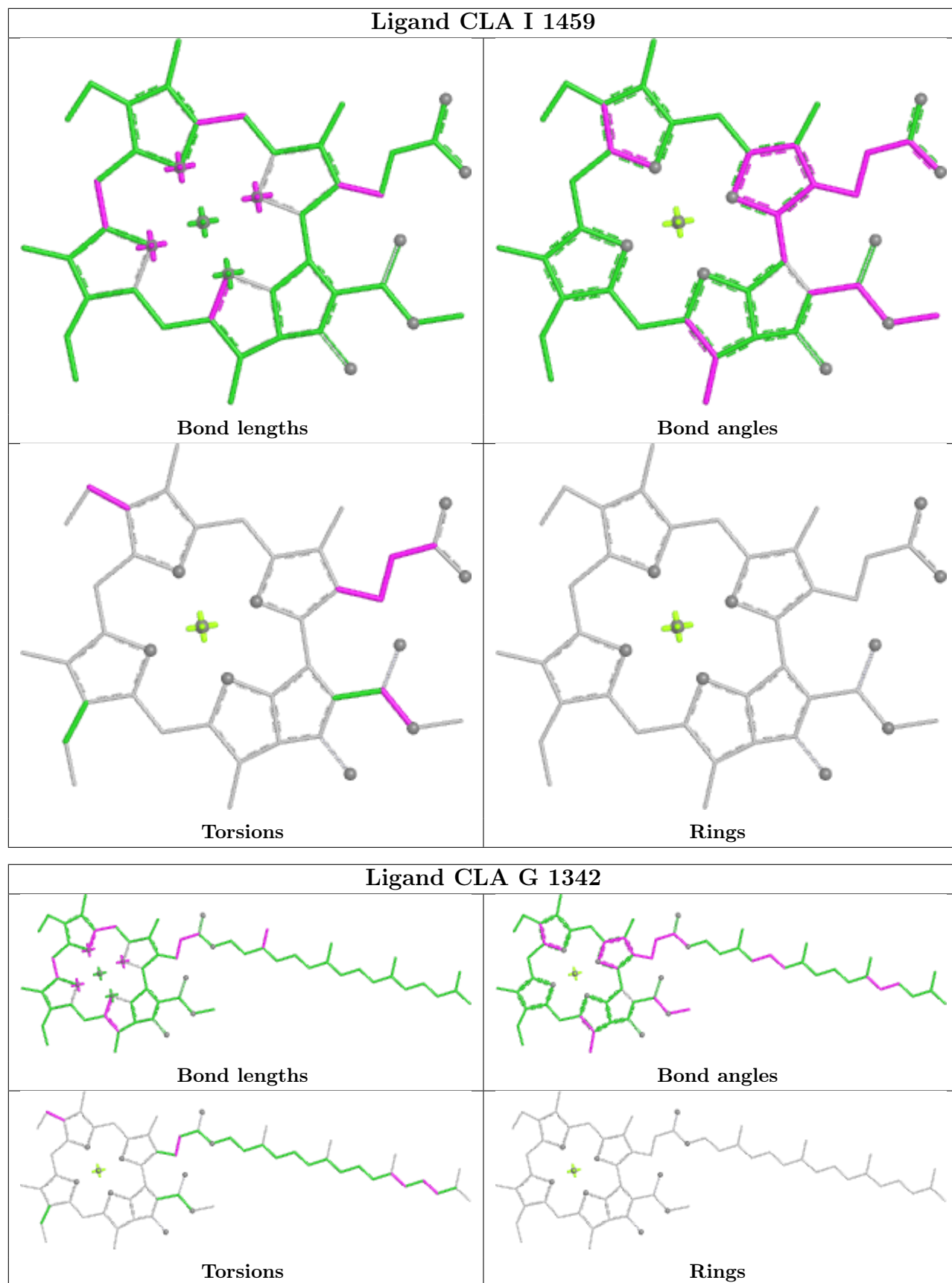
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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 11  | B     | 1490 | CLA  | 3       | 0            |
| 11  | I     | 1464 | CLA  | 9       | 0            |
| 11  | H     | 1493 | CLA  | 1       | 0            |
| 11  | B     | 1497 | CLA  | 9       | 0            |
| 12  | G     | 1345 | PHO  | 16      | 0            |
| 11  | B     | 1482 | CLA  | 1       | 0            |
| 11  | G     | 1346 | CLA  | 4       | 0            |
| 11  | I     | 1465 | CLA  | 9       | 0            |
| 11  | D     | 1351 | CLA  | 12      | 0            |
| 11  | C     | 1459 | CLA  | 4       | 0            |
| 11  | B     | 1484 | CLA  | 7       | 0            |
| 11  | I     | 1469 | CLA  | 4       | 0            |
| 11  | H     | 1487 | CLA  | 5       | 0            |
| 11  | H     | 1489 | CLA  | 4       | 0            |
| 12  | A     | 1345 | PHO  | 13      | 0            |
| 11  | H     | 1491 | CLA  | 2       | 0            |

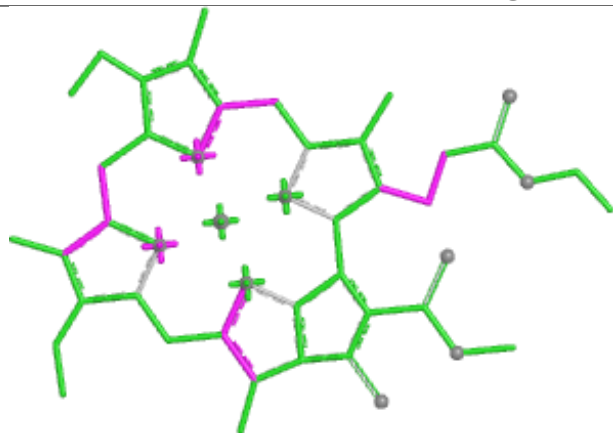
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 B 1486

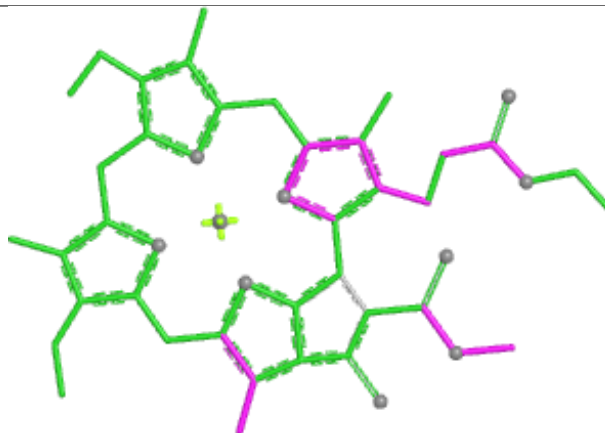




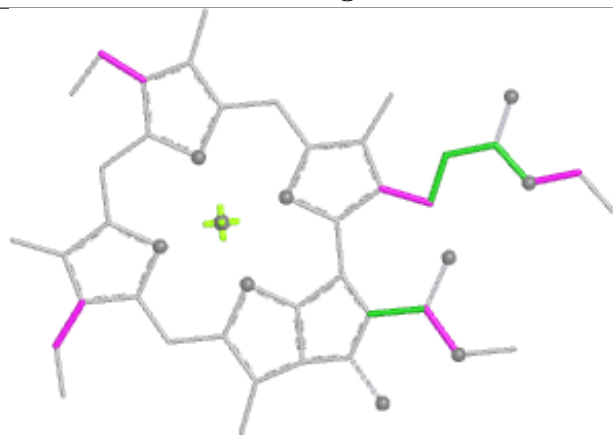
## Ligand CLA H 1485



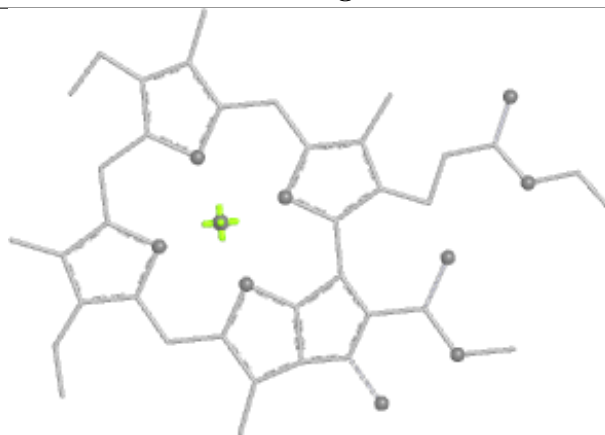
Bond lengths



Bond angles

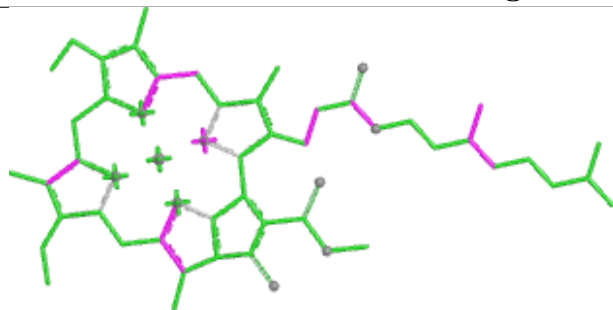


Torsions

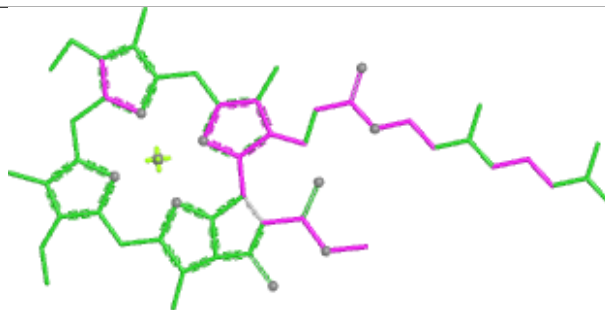


Rings

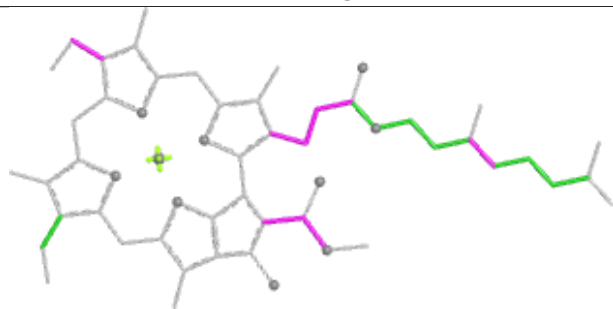
## Ligand CLA H 1495



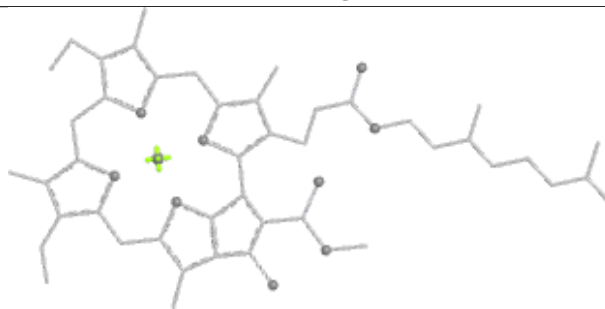
Bond lengths



Bond angles

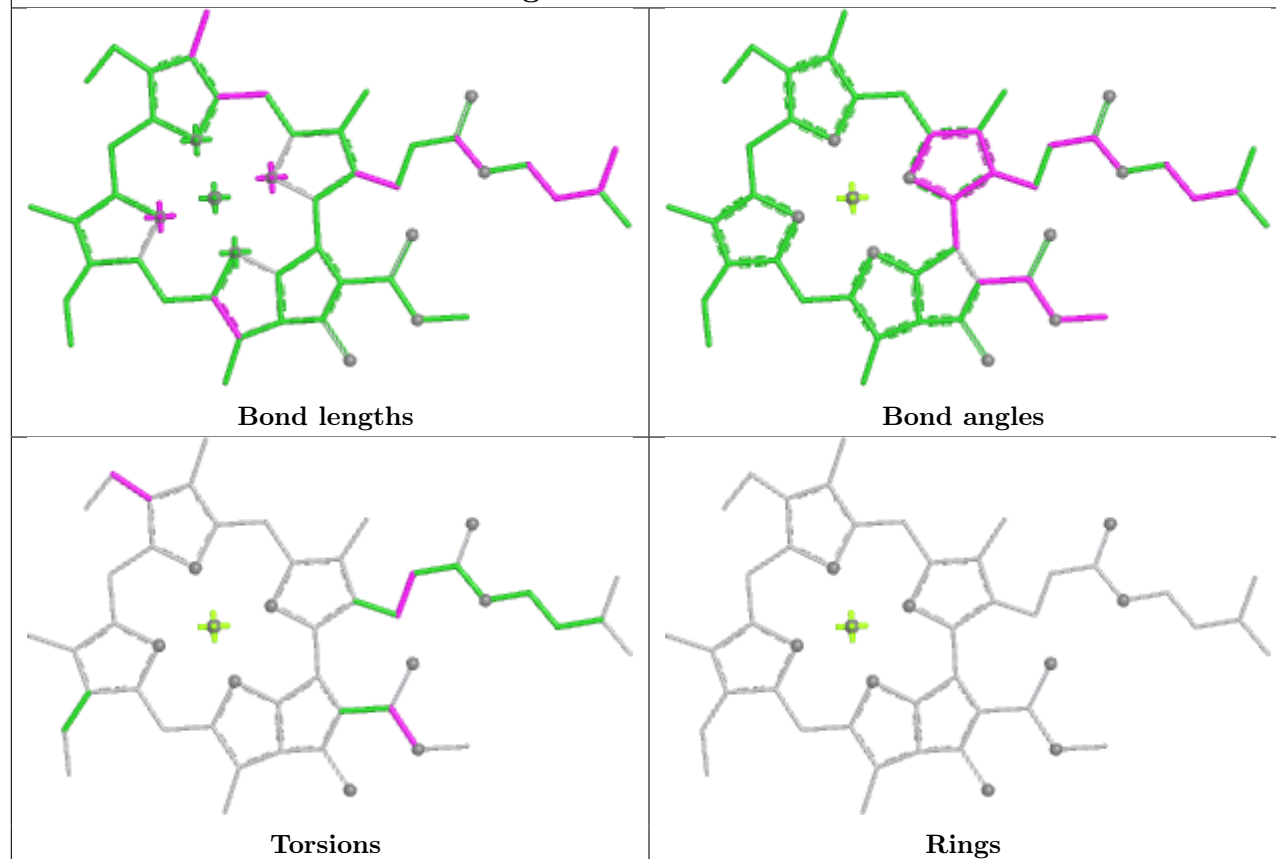


Torsions

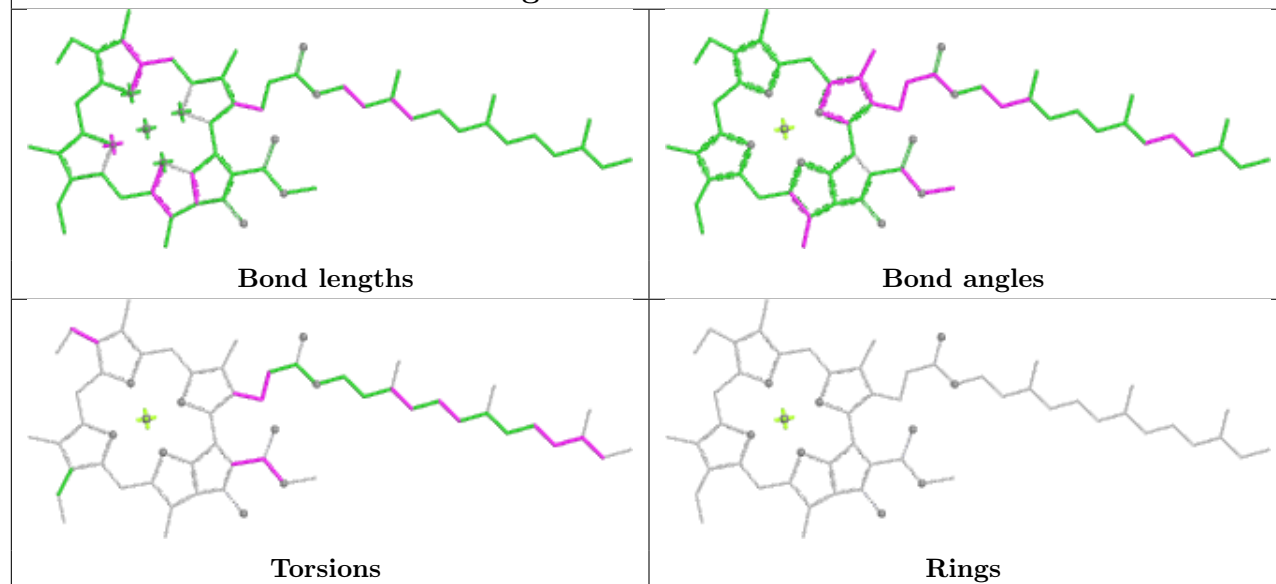


Rings

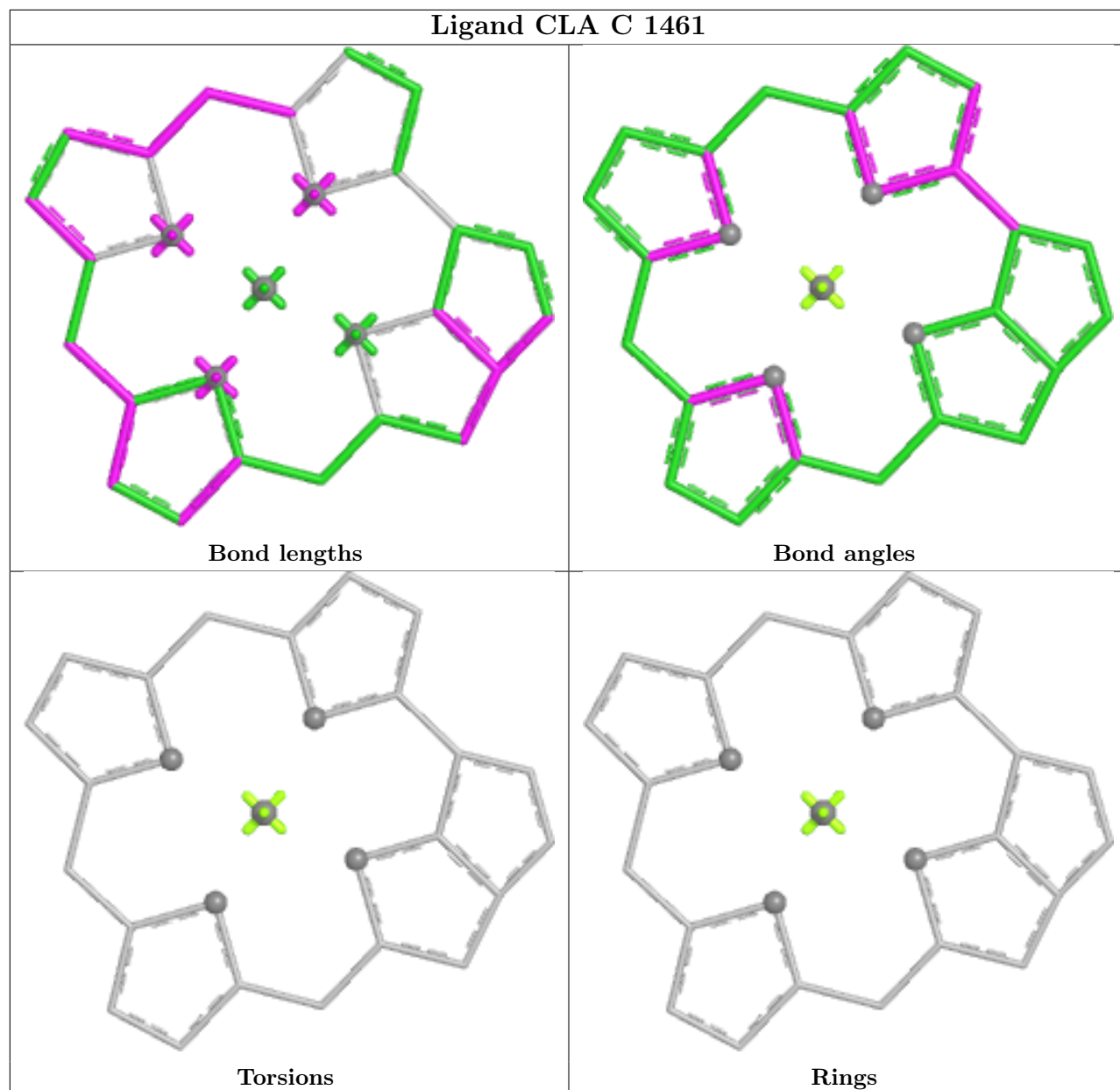
## Ligand CLA D 1353



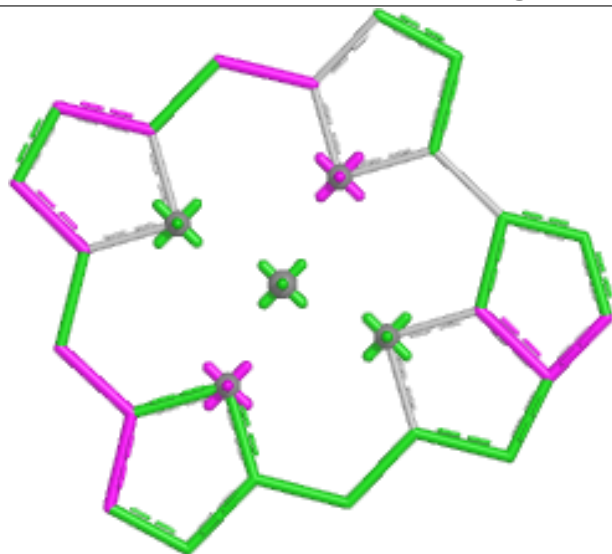
## Ligand CLA G 1343



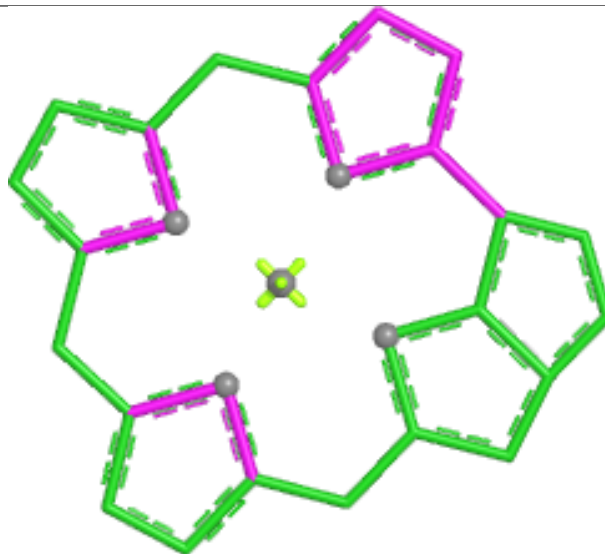
## Ligand CLA C 1461



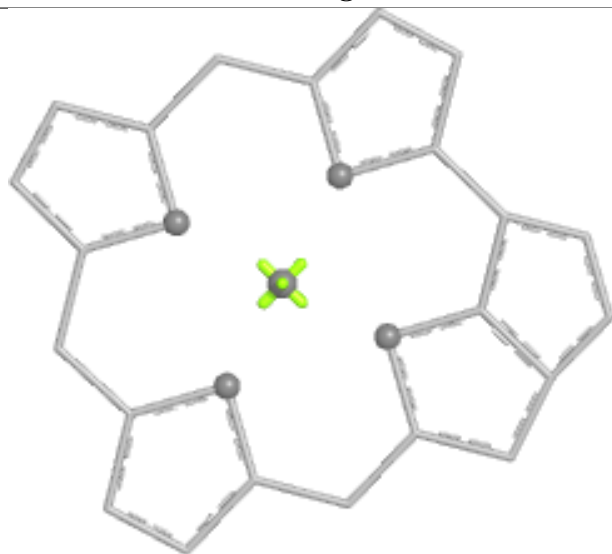
## Ligand CLA I 1468



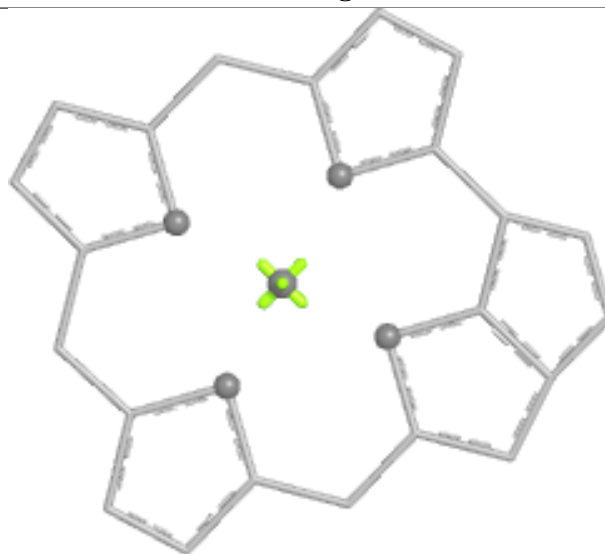
Bond lengths



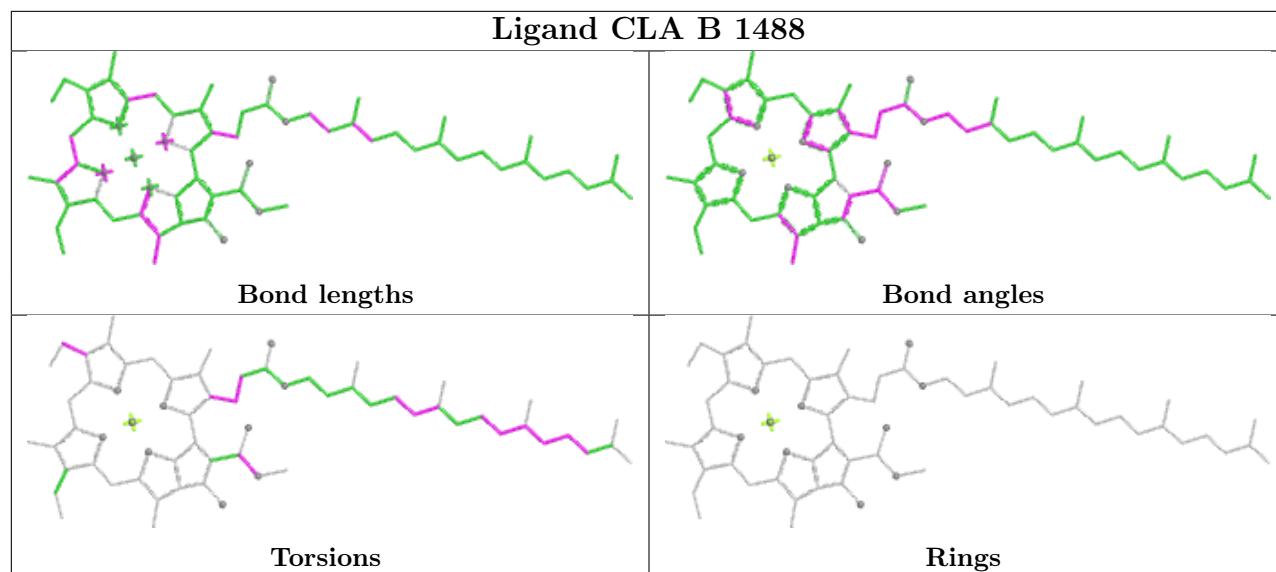
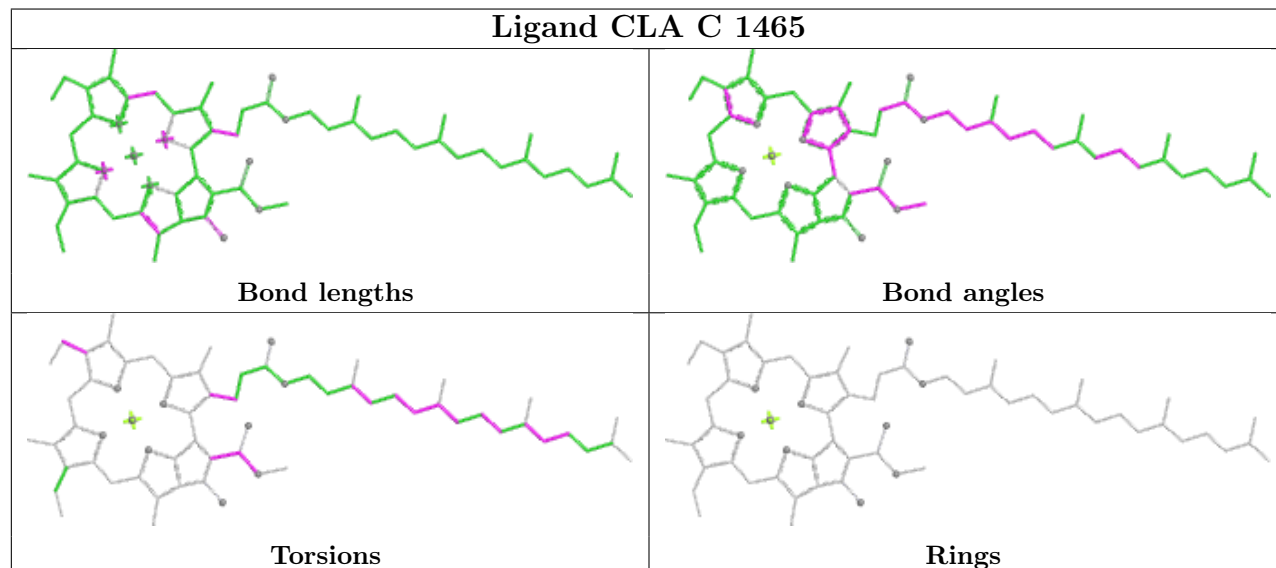
Bond angles



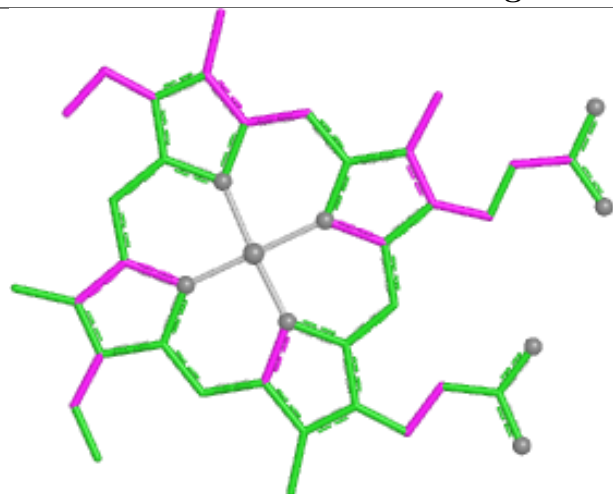
Torsions



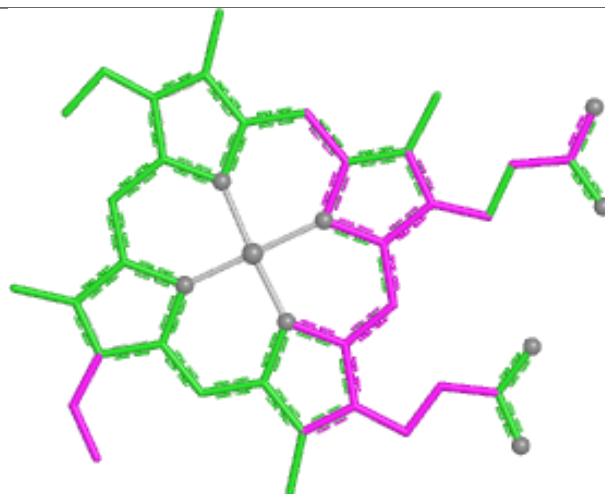
Rings

**Ligand CLA B 1488****Ligand CLA C 1465**

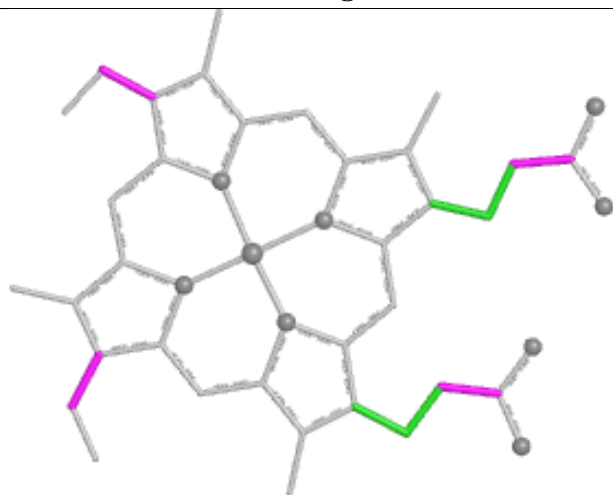
## Ligand HEC T 1138



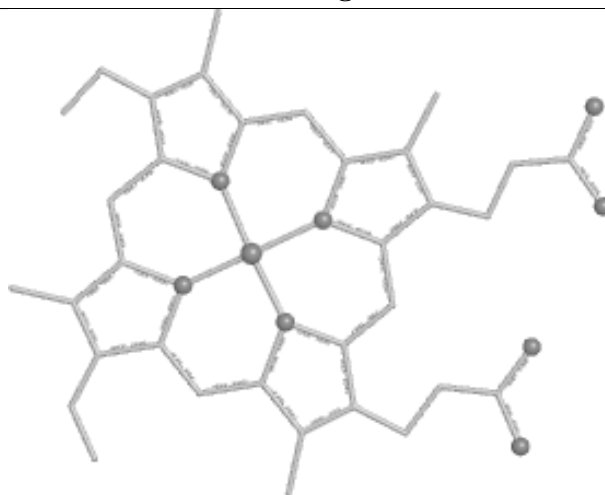
Bond lengths



Bond angles

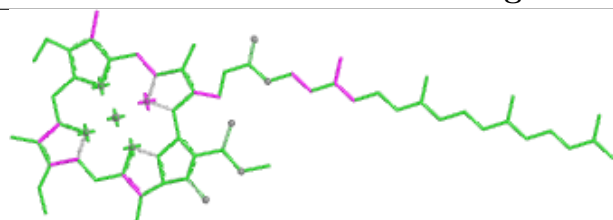


Torsions

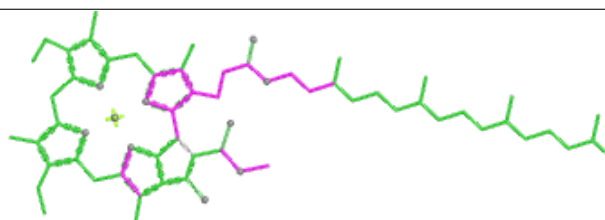


Rings

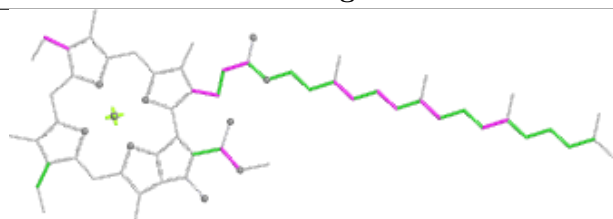
## Ligand CLA H 1482



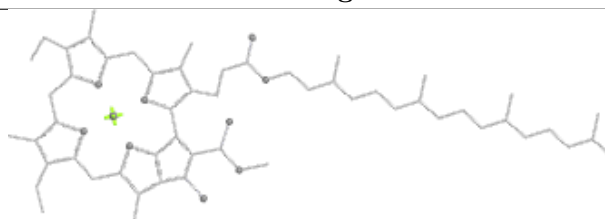
Bond lengths



Bond angles

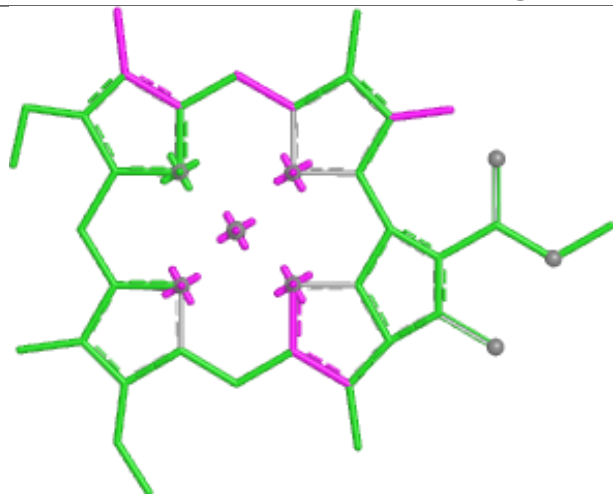


Torsions

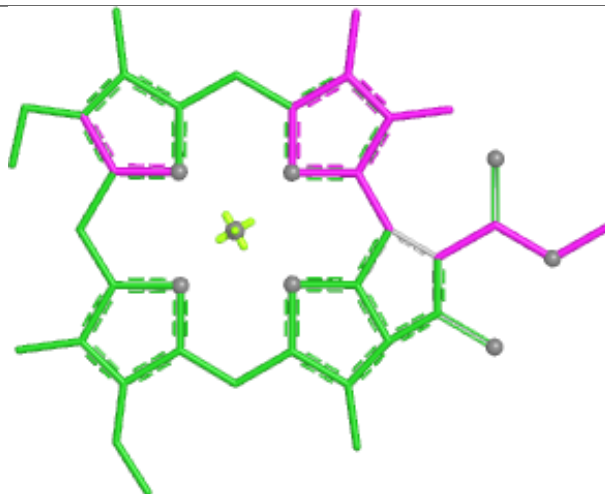


Rings

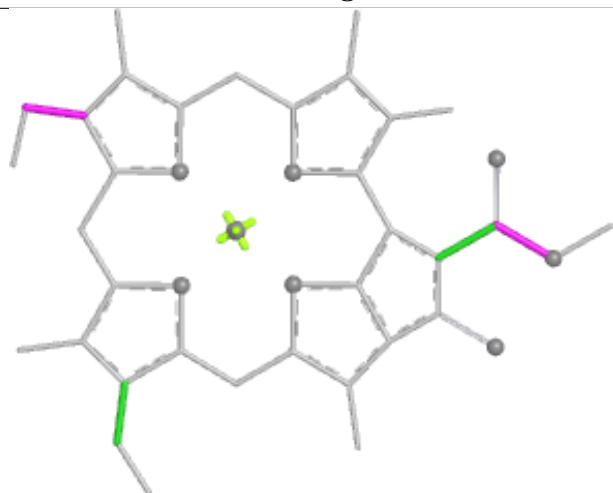
## Ligand CLA I 1470



Bond lengths



Bond angles

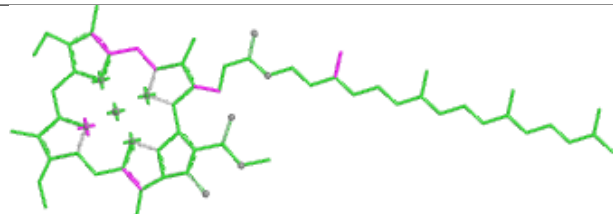


Torsions

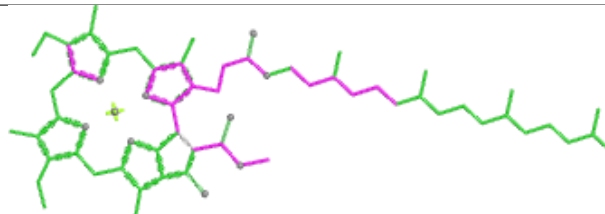


Rings

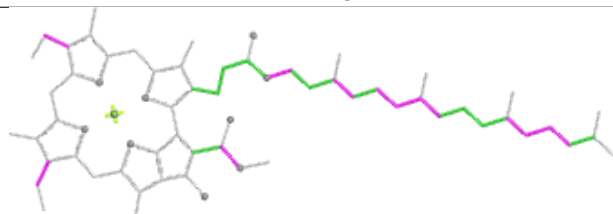
## Ligand CLA B 1496



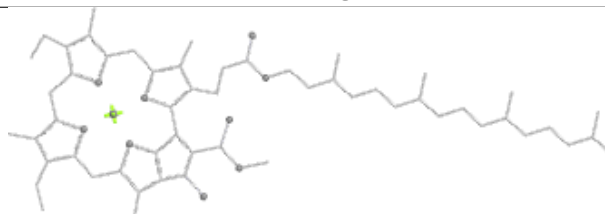
Bond lengths



Bond angles

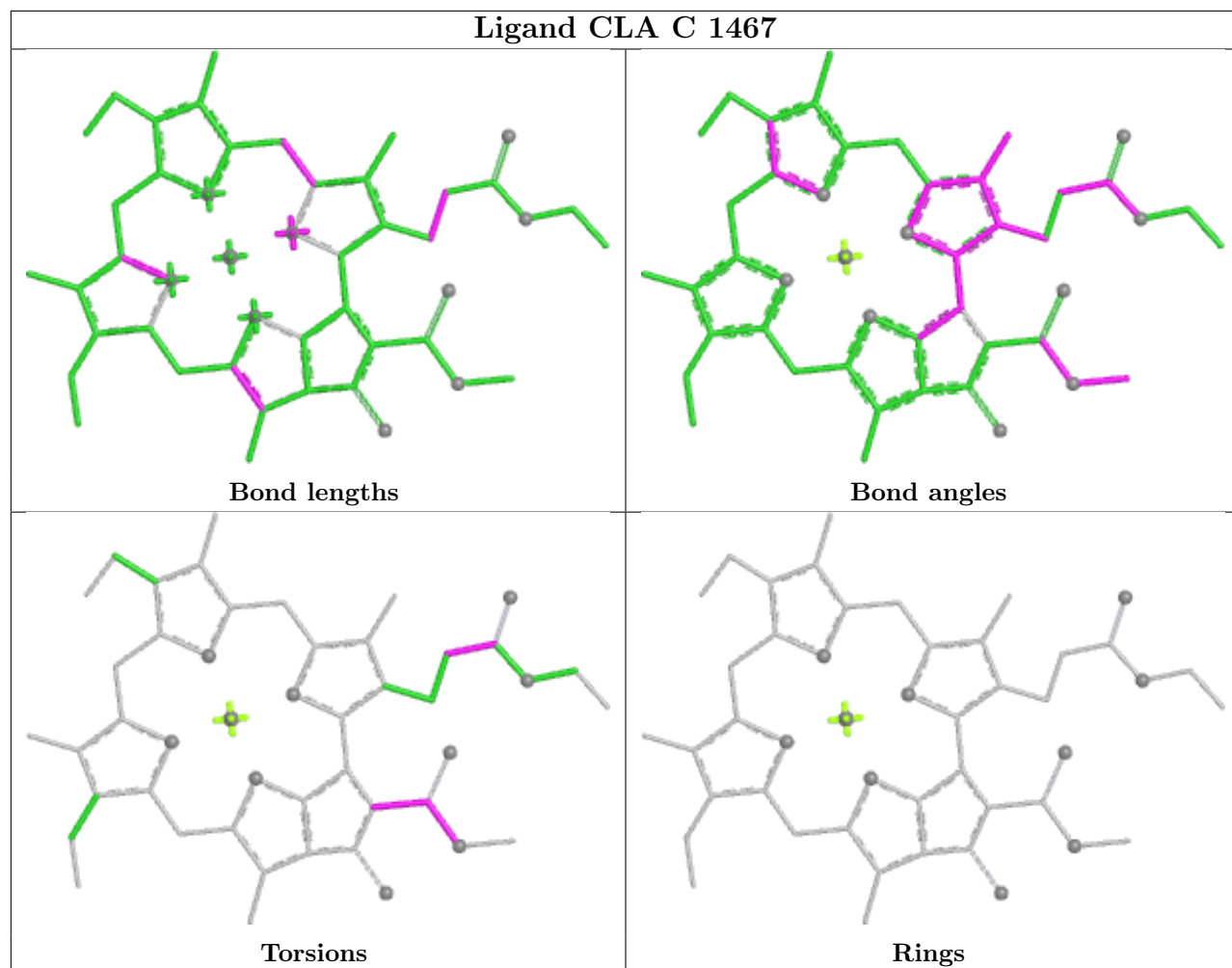


Torsions

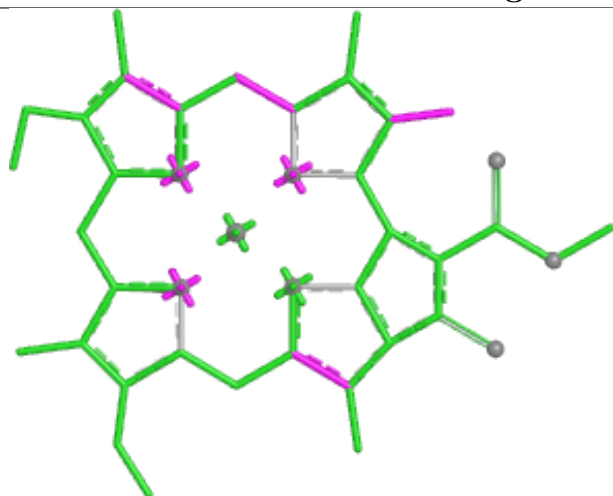


Rings

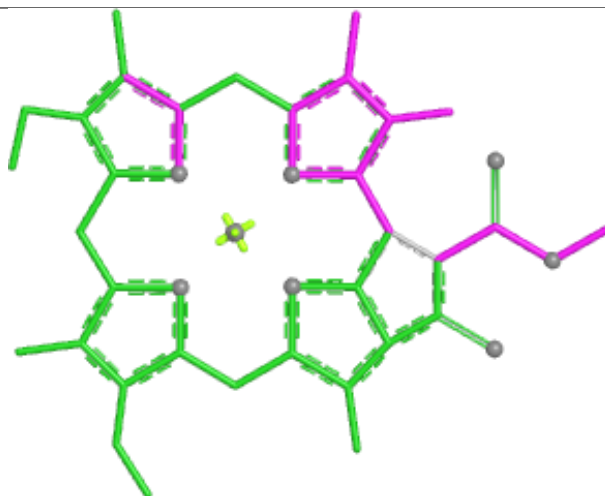
## Ligand CLA C 1467



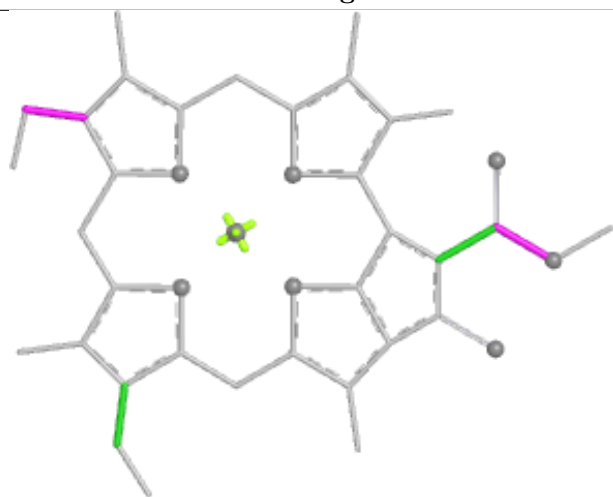
## Ligand CLA C 1469



Bond lengths



Bond angles

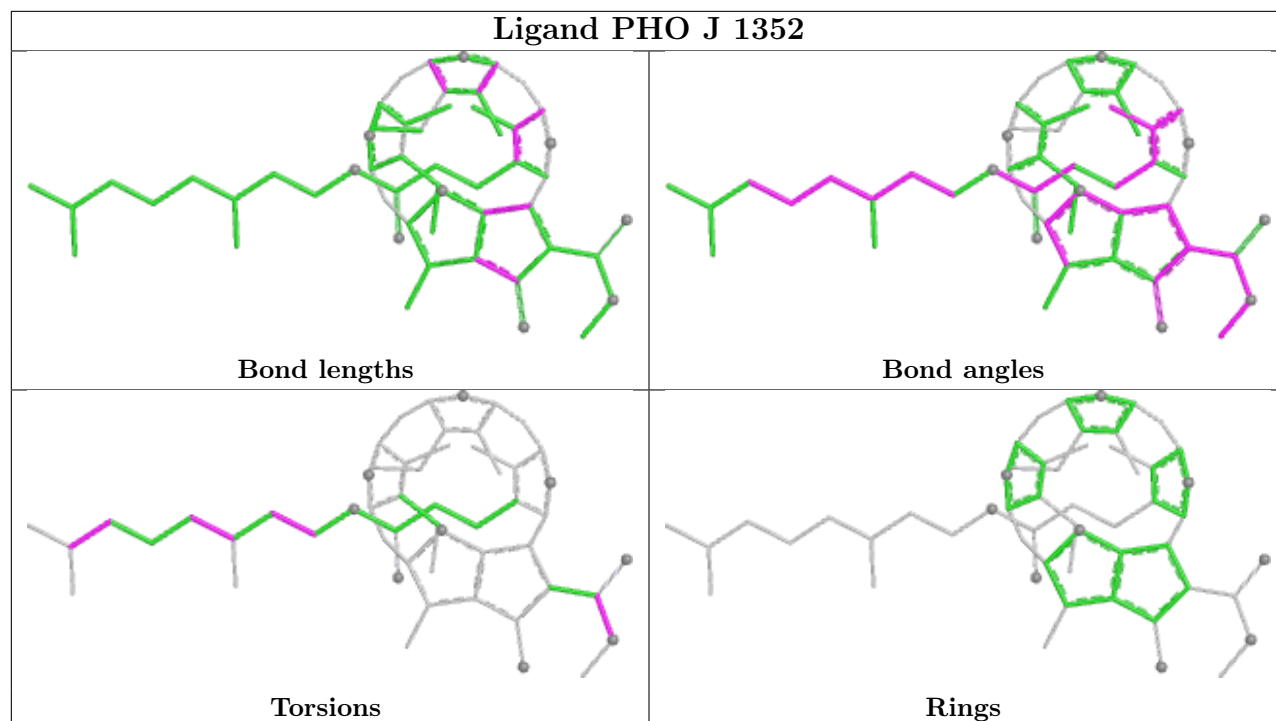


Torsions

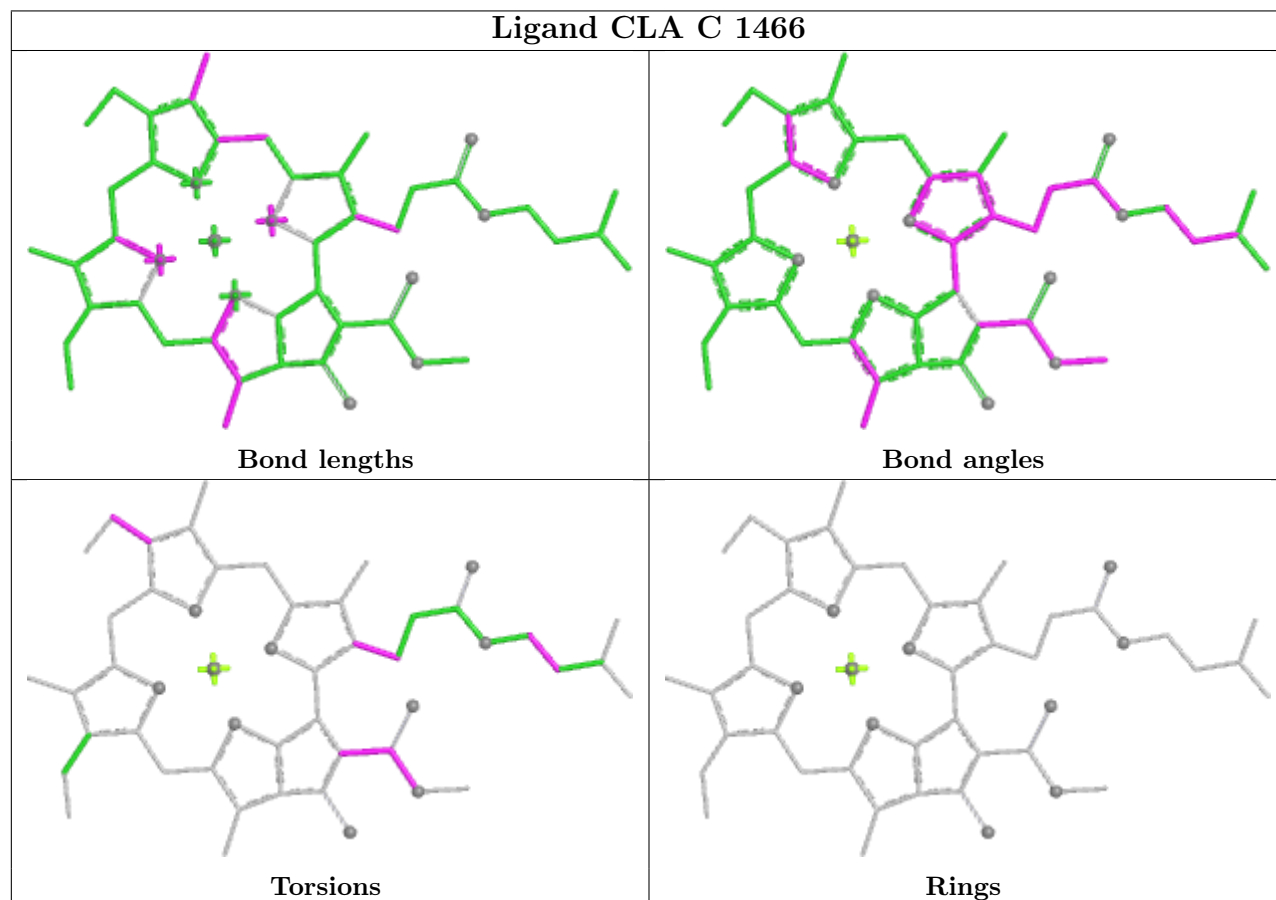


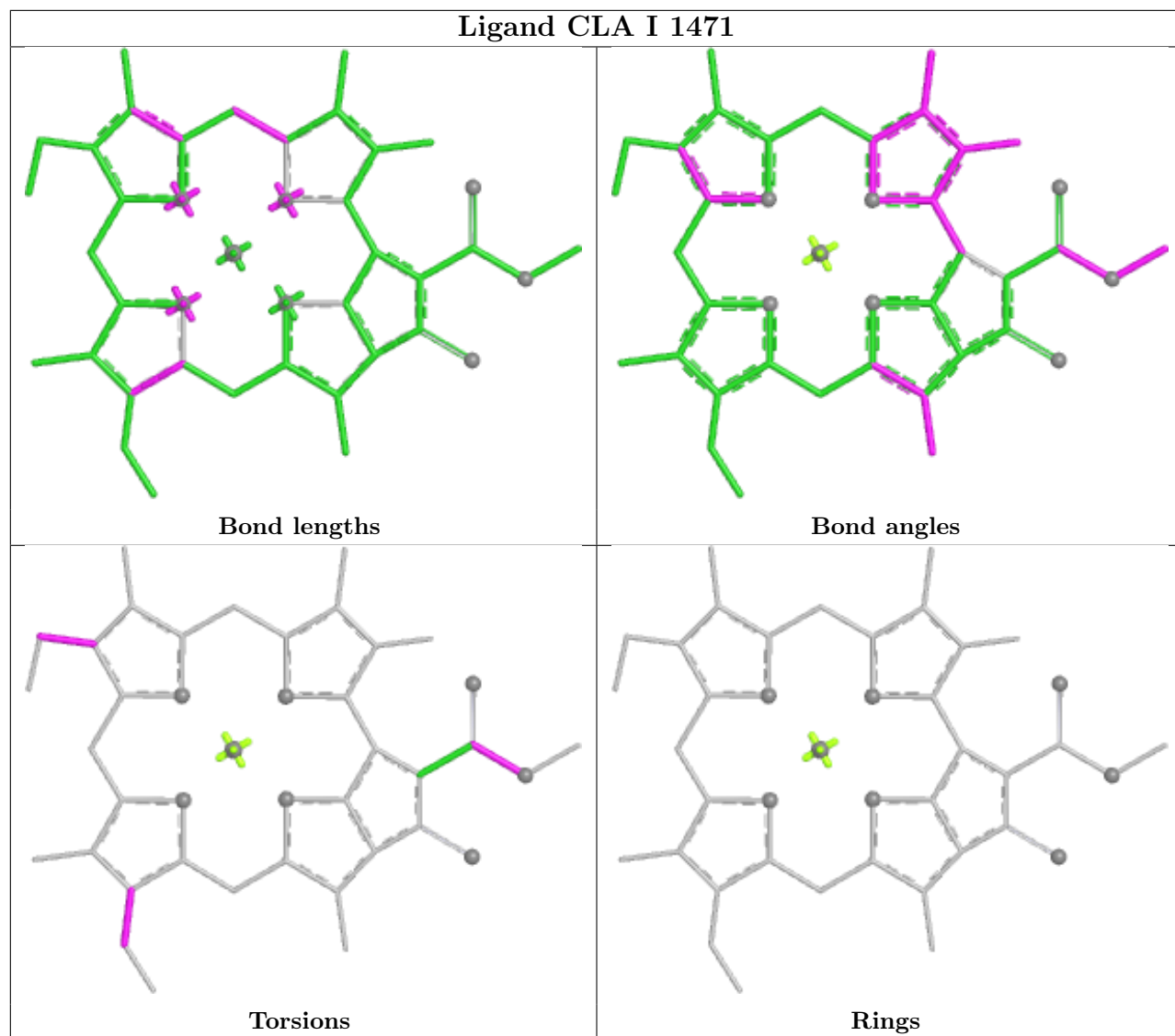
Rings

## Ligand PHO J 1352

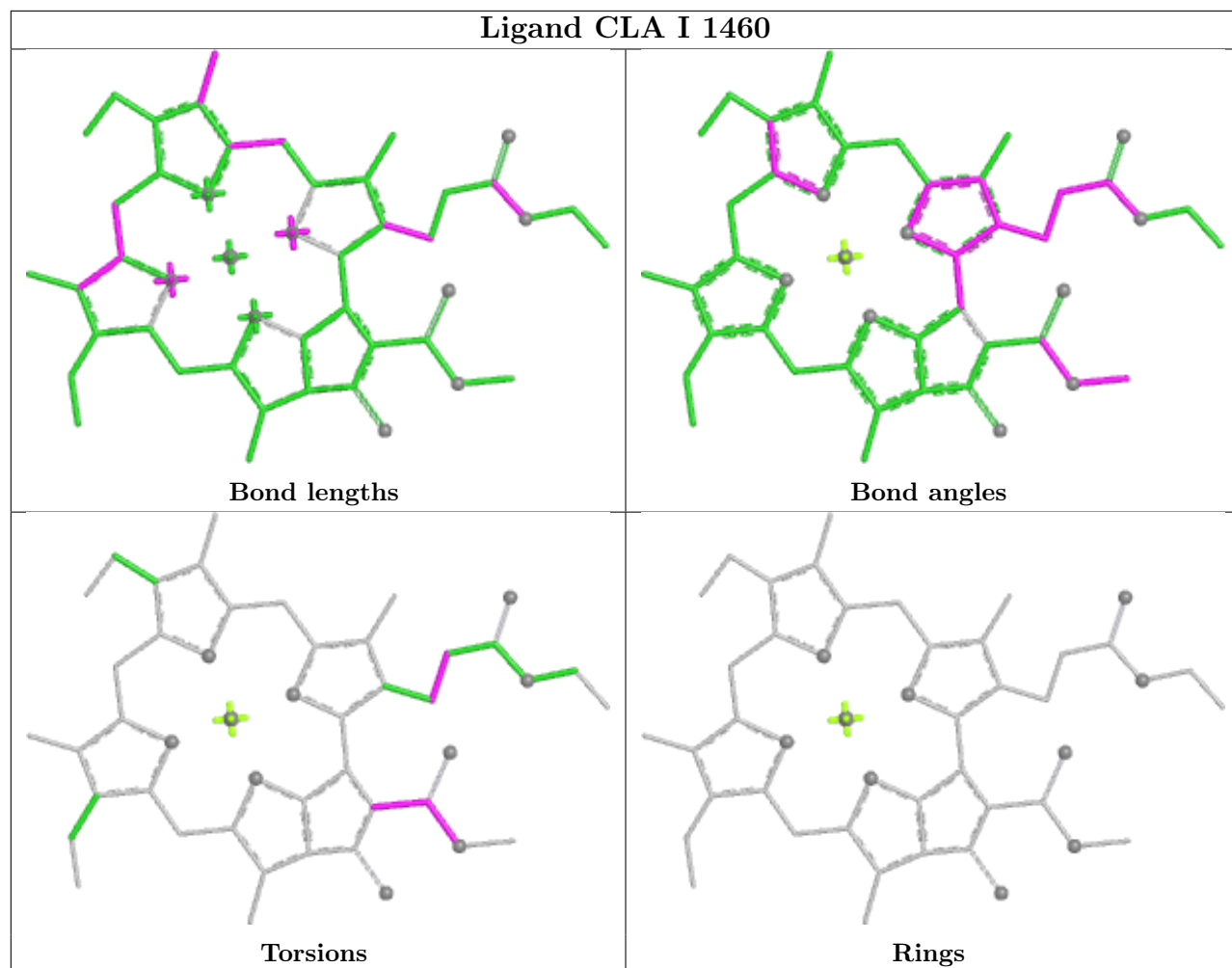


## Ligand CLA C 1466

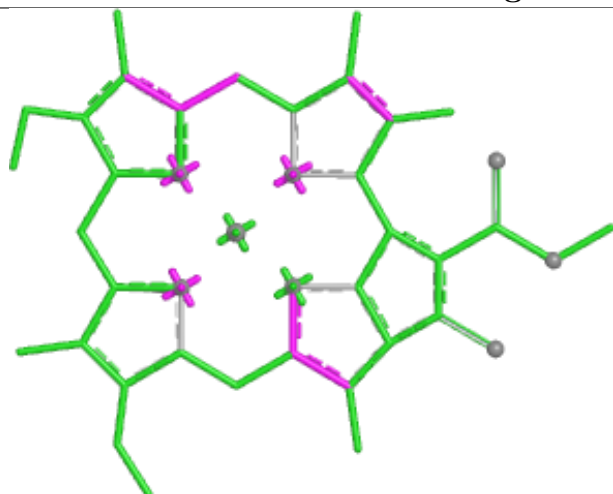




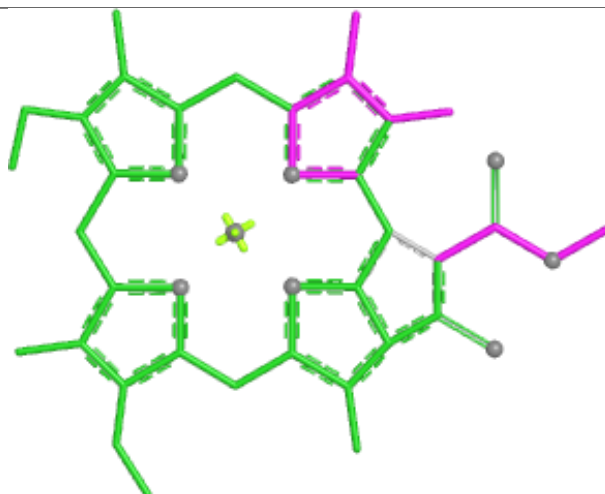
## Ligand CLA I 1460



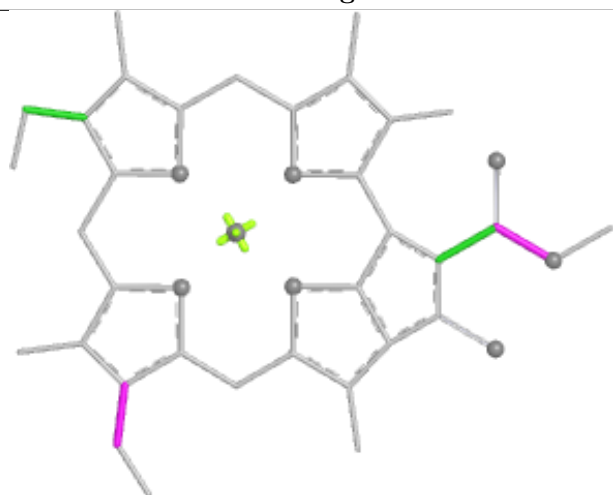
## Ligand CLA H 1486



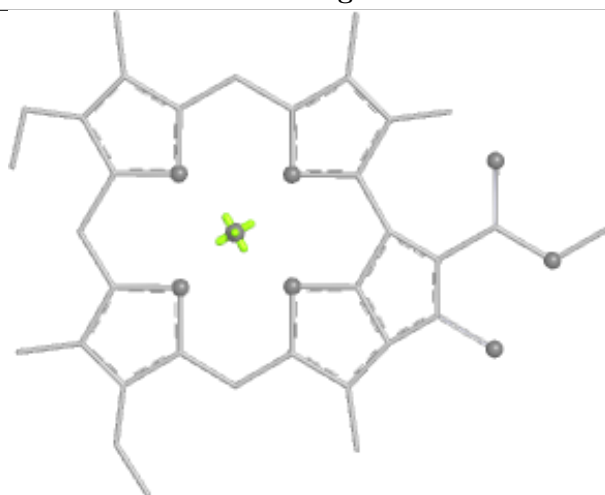
Bond lengths



Bond angles

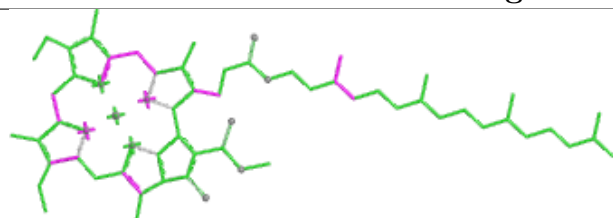


Torsions

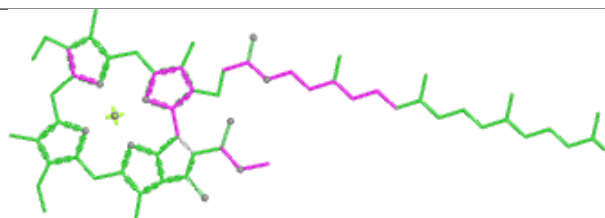


Rings

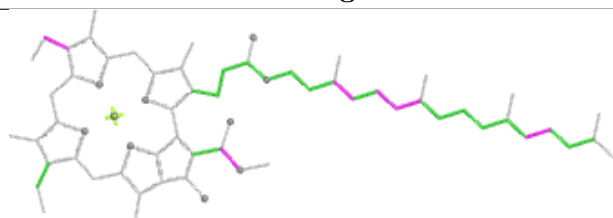
## Ligand CLA B 1494



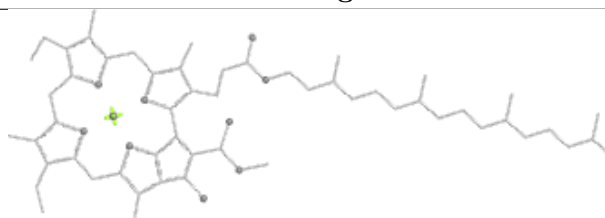
Bond lengths



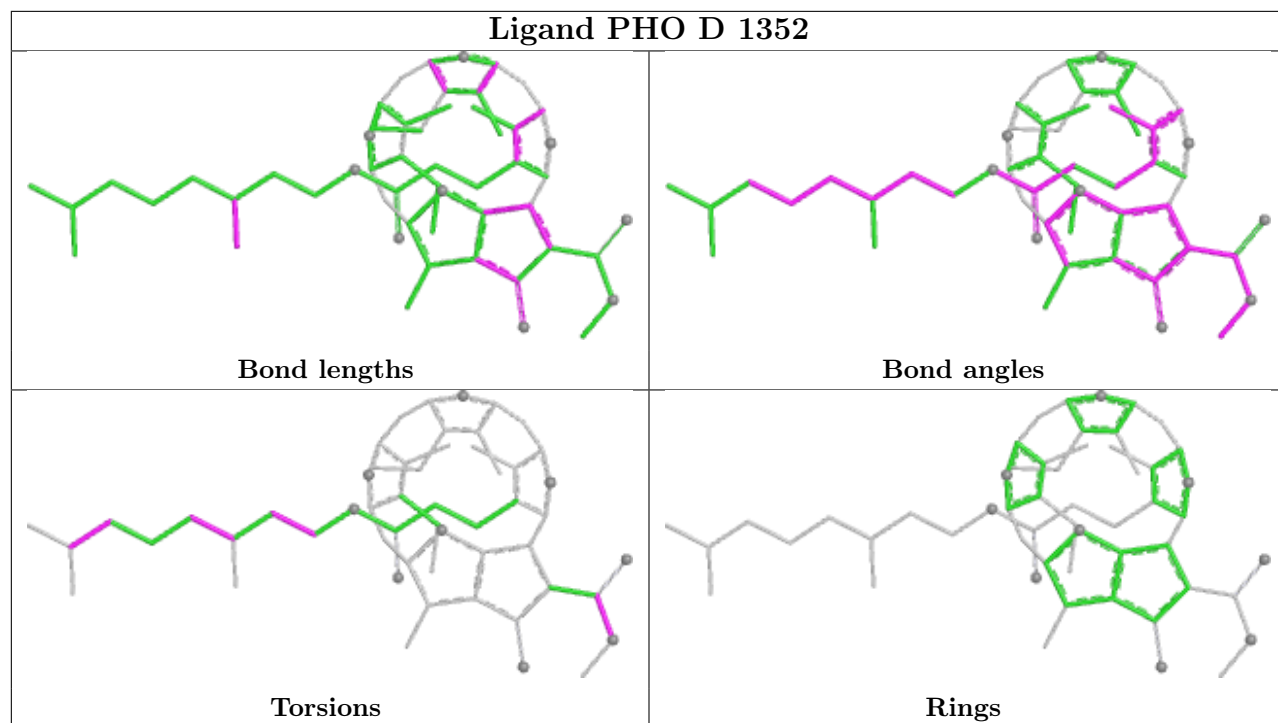
Bond angles

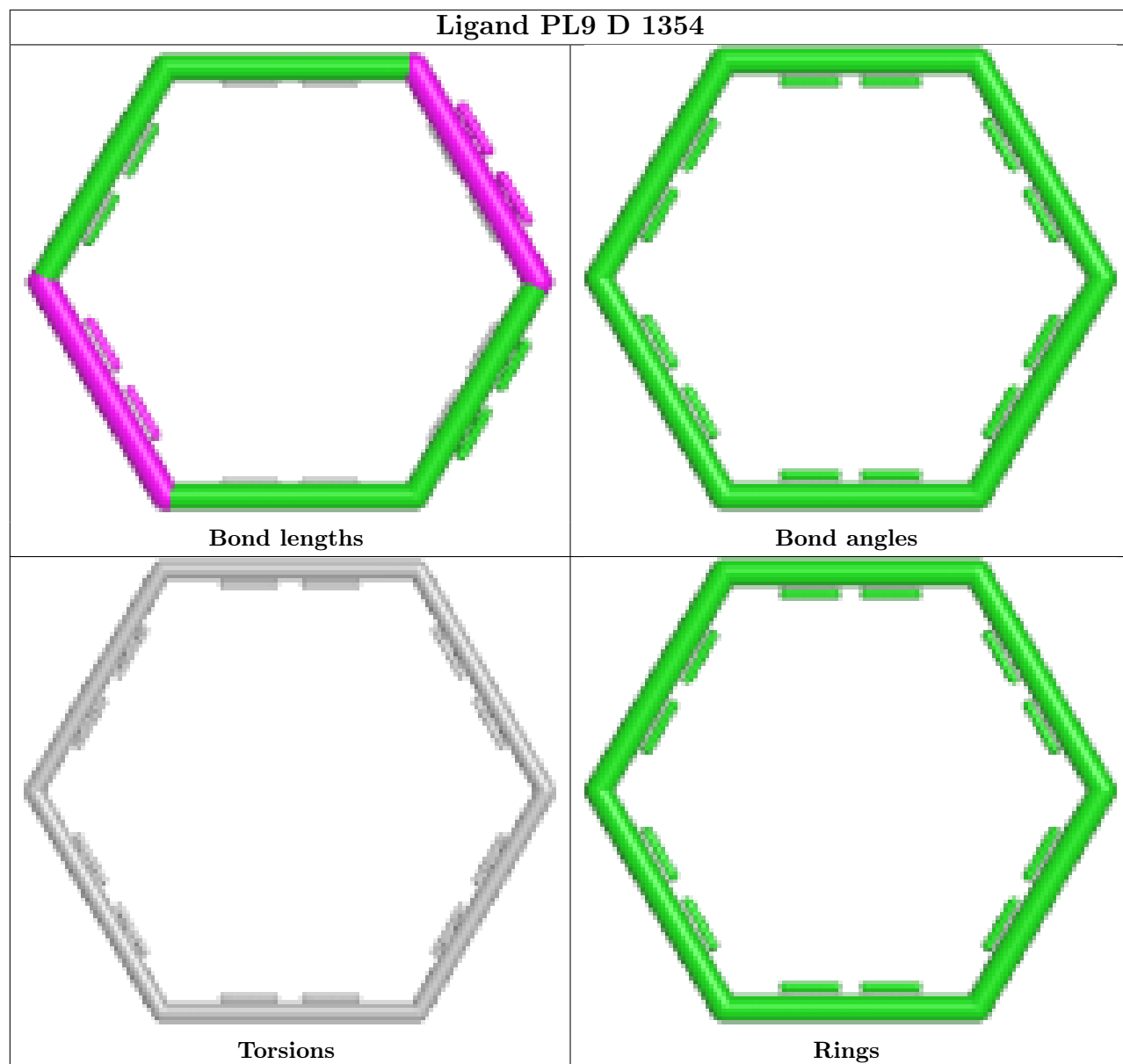


Torsions

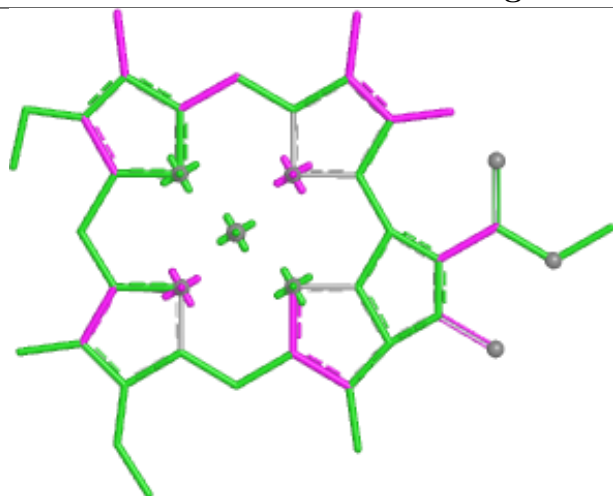


Rings

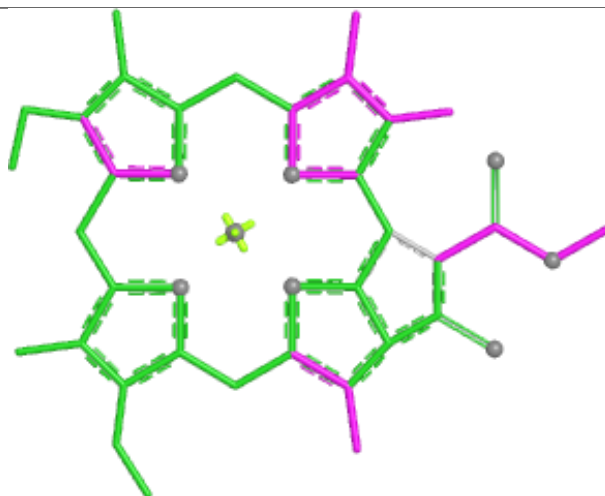




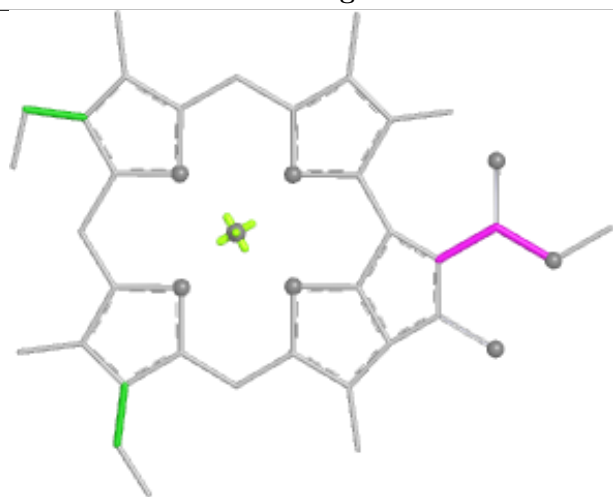
## Ligand CLA H 1497



Bond lengths



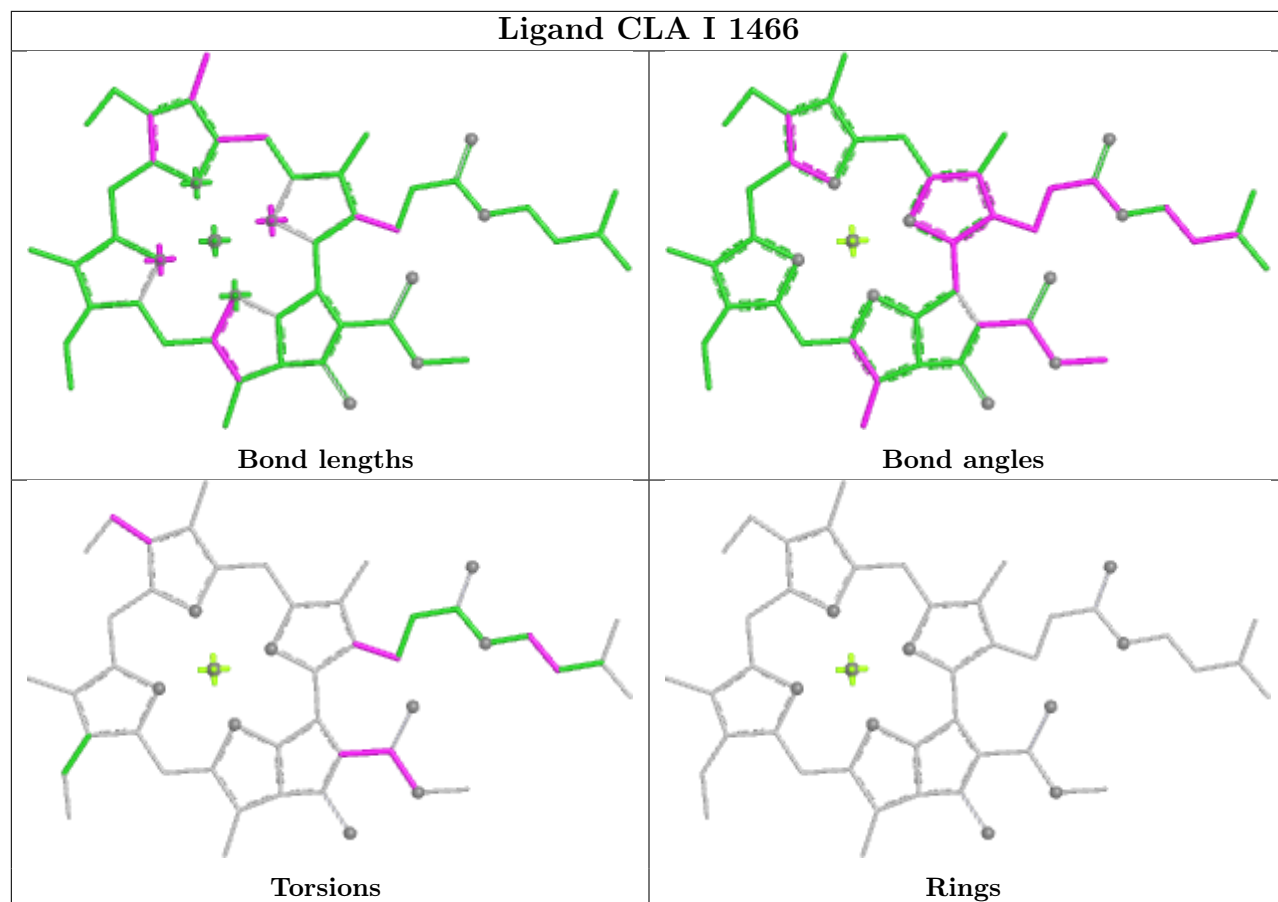
Bond angles

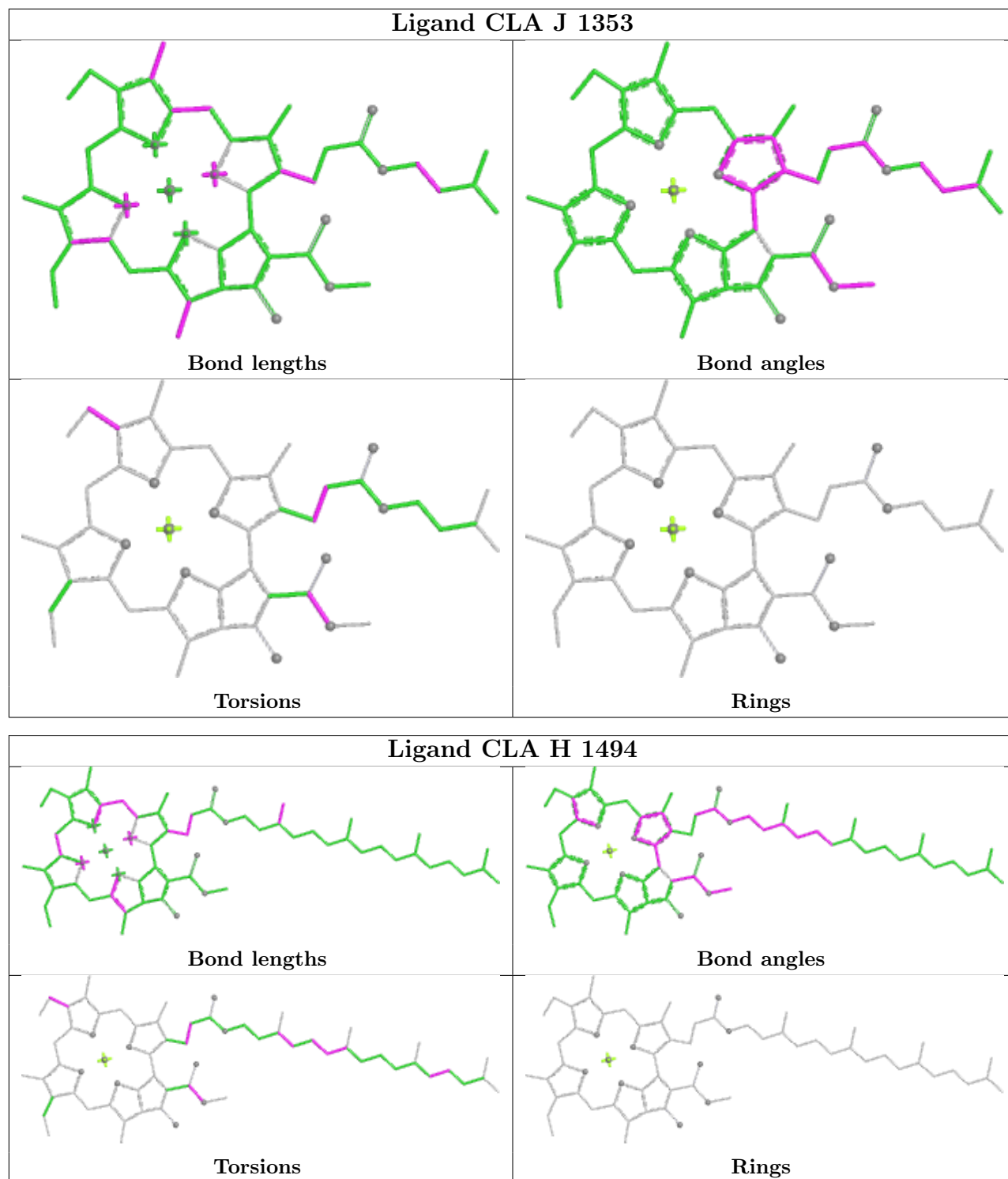


Torsions

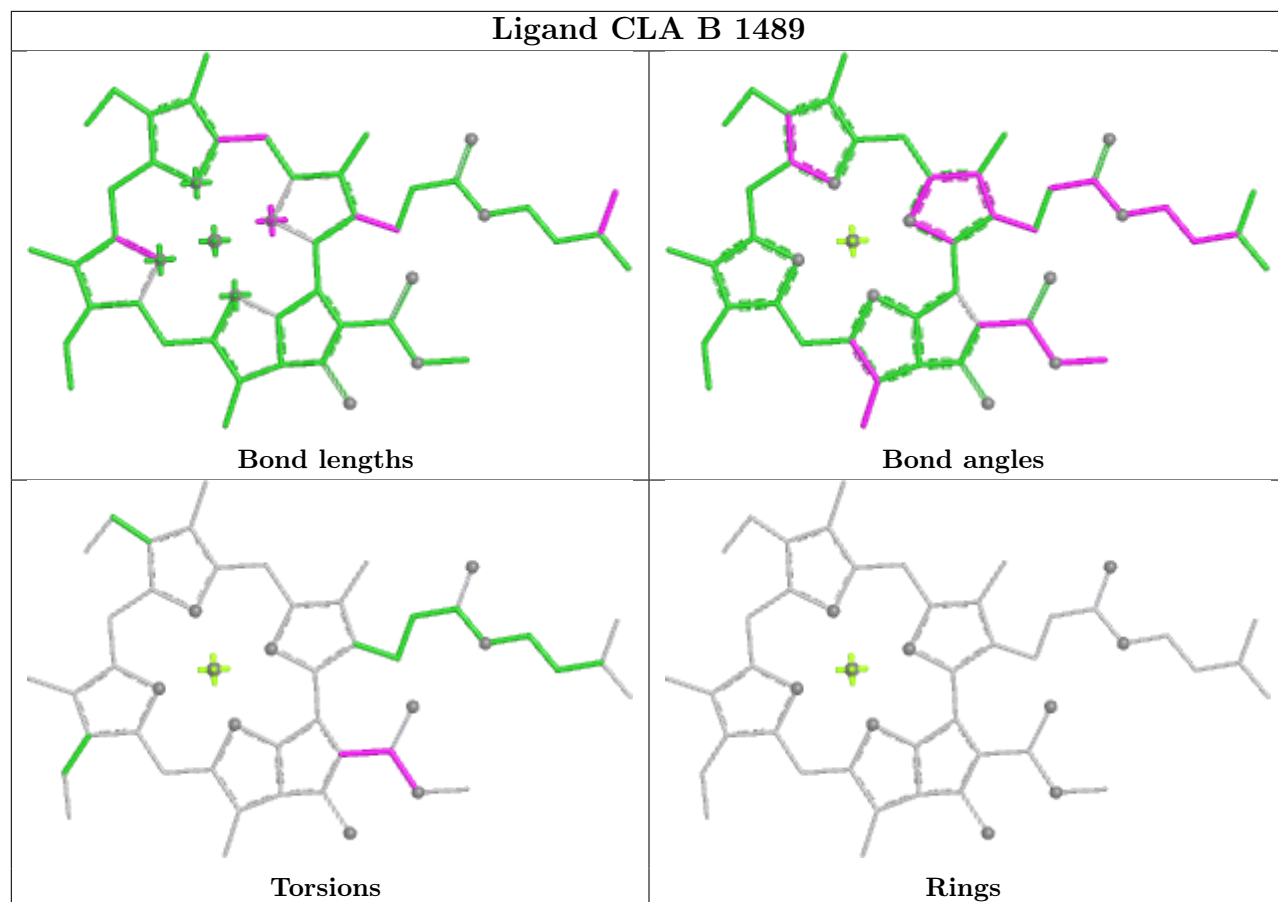


Rings

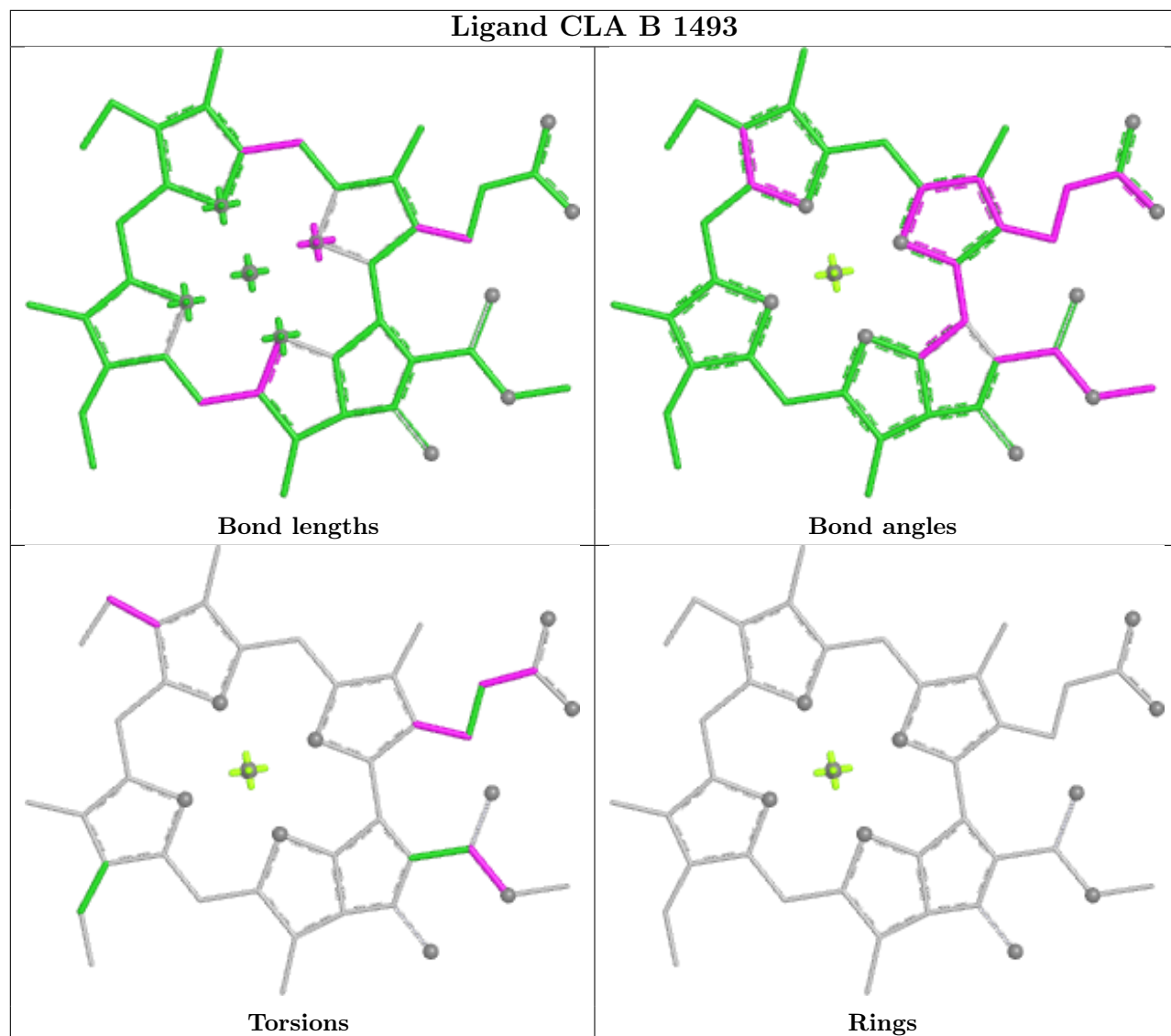




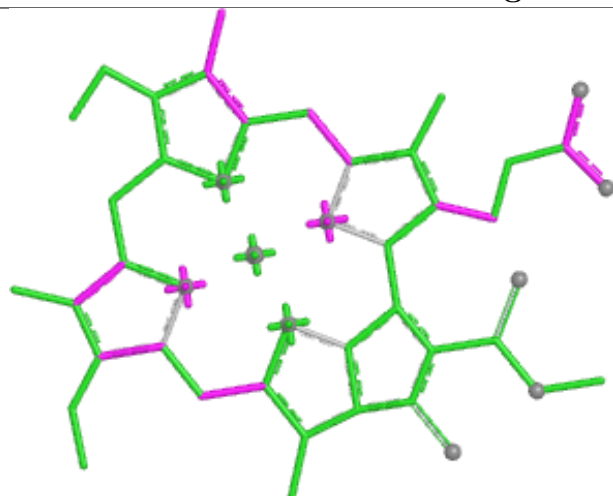
## Ligand CLA B 1489



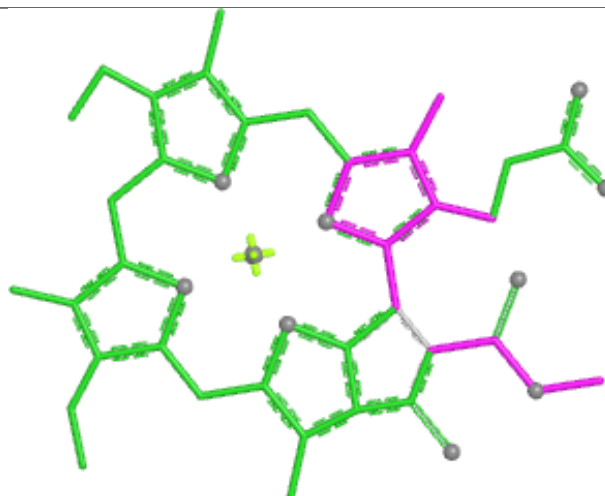
## Ligand CLA B 1493



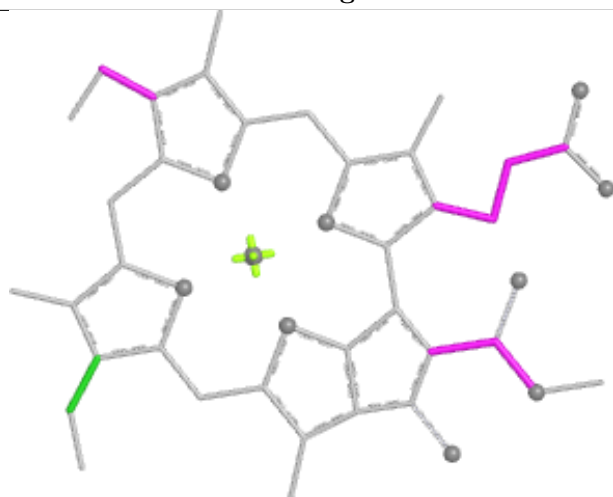
## Ligand CLA H 1490



Bond lengths



Bond angles

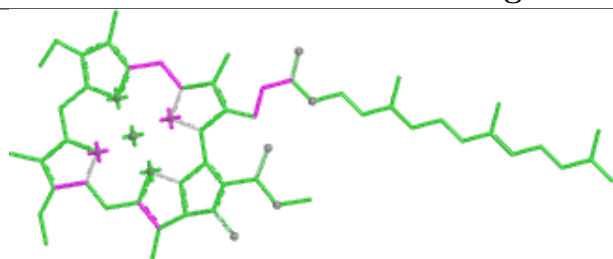


Torsions

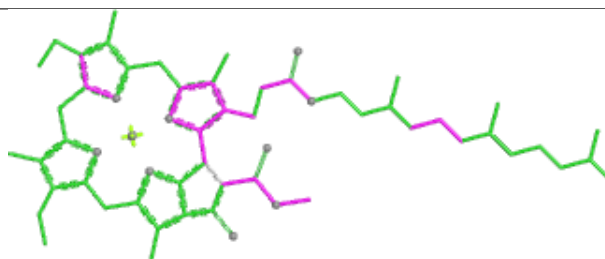


Rings

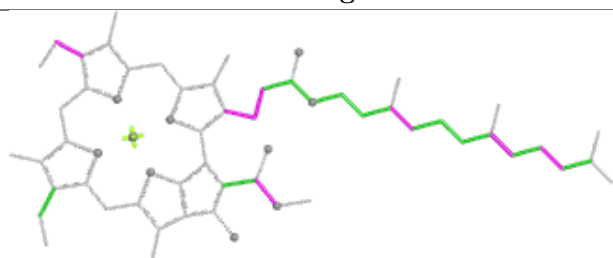
## Ligand CLA H 1483



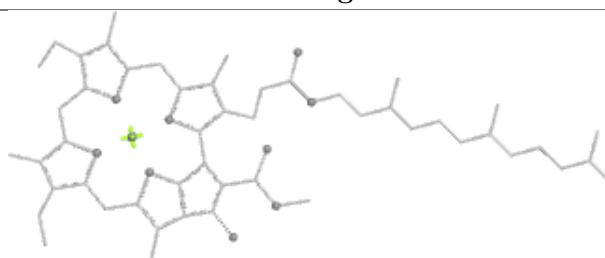
Bond lengths



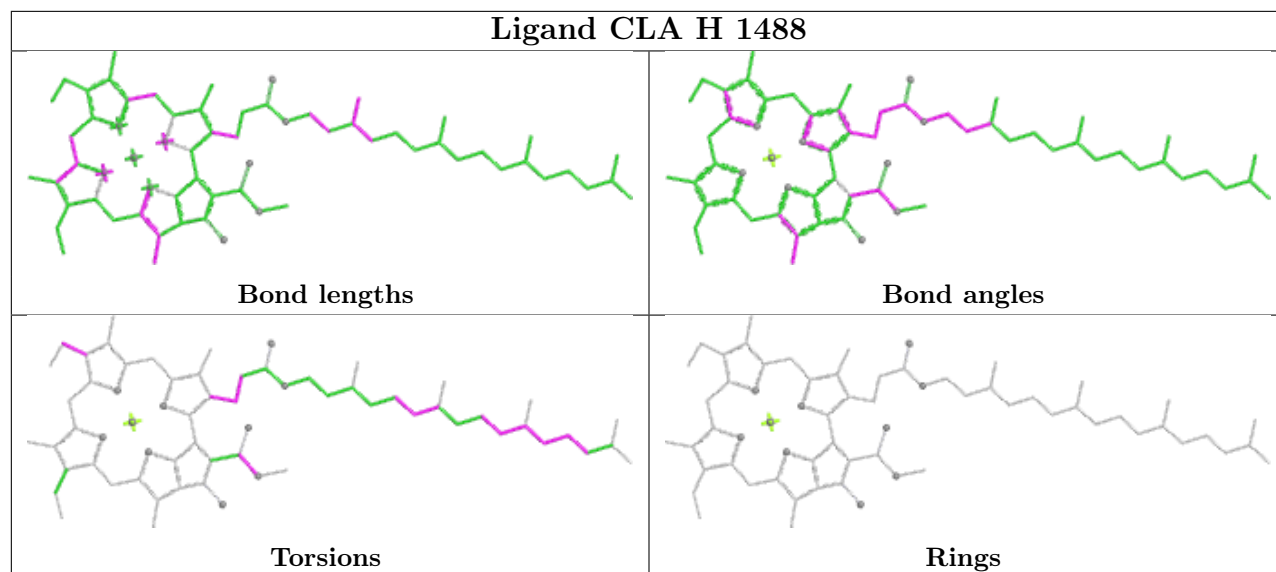
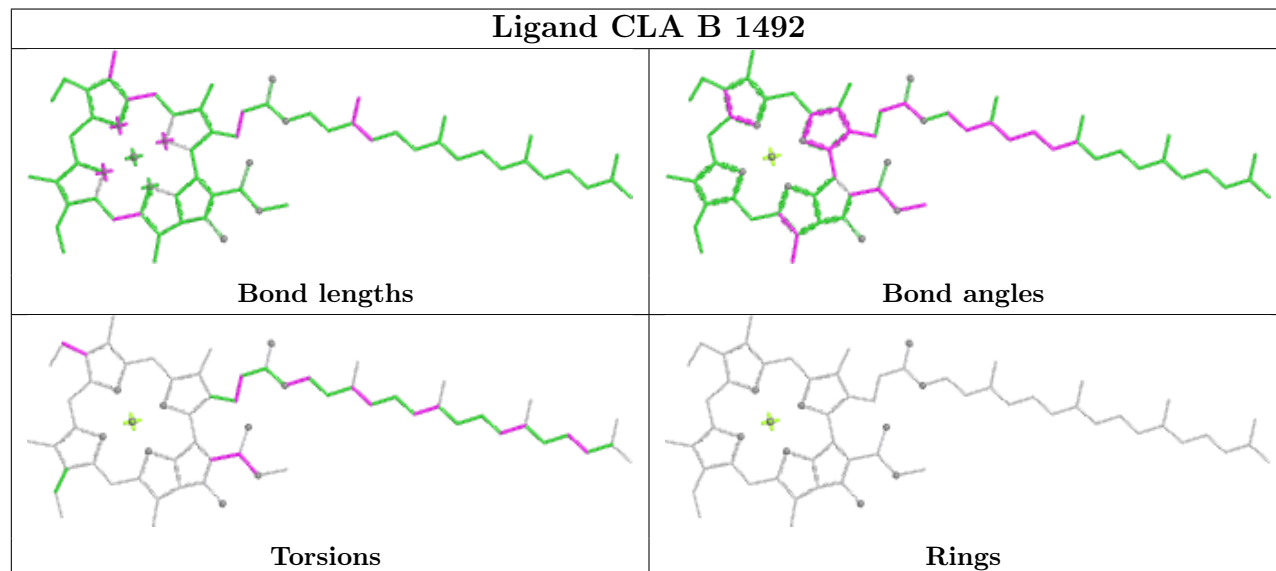
Bond angles



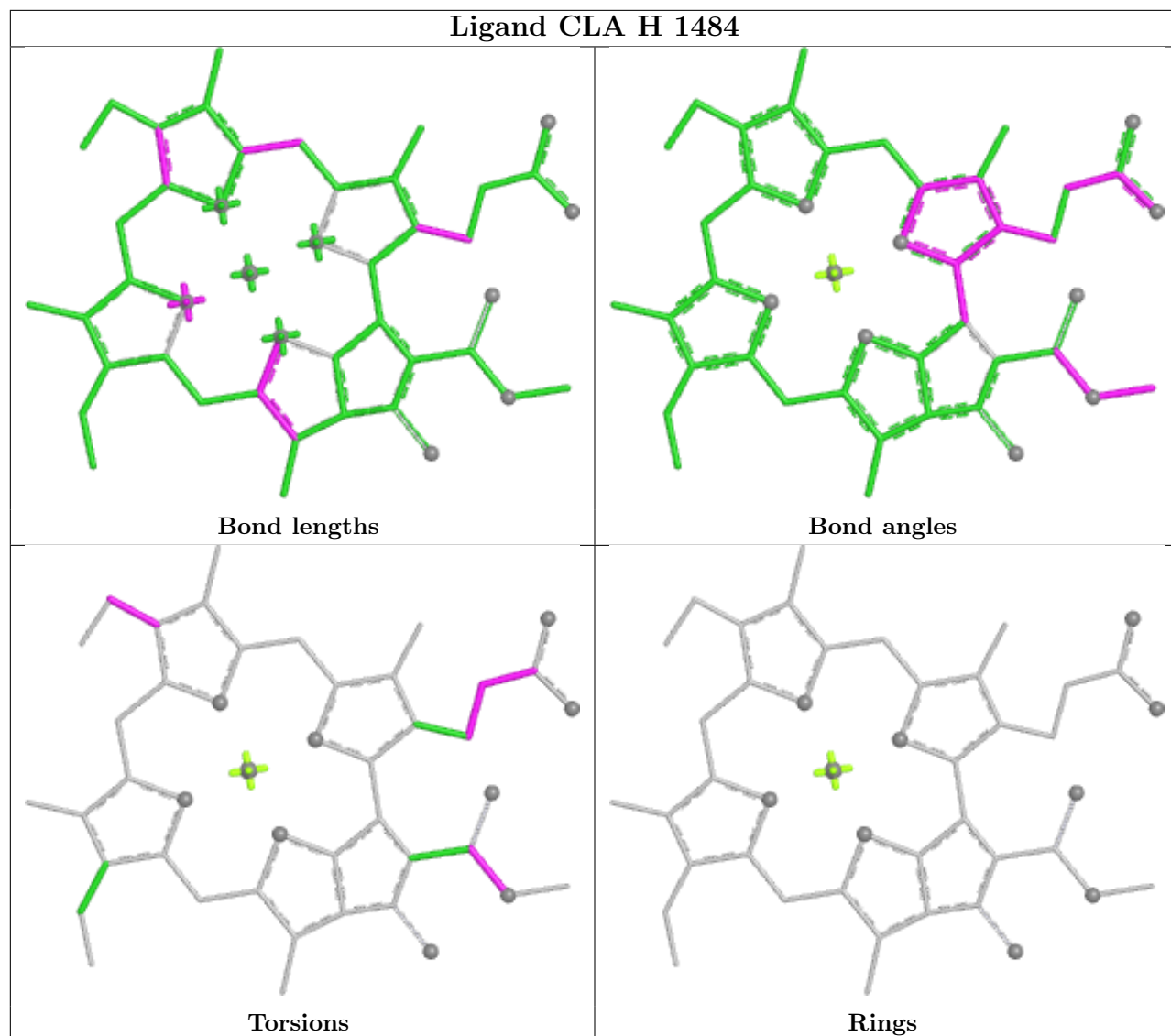
Torsions



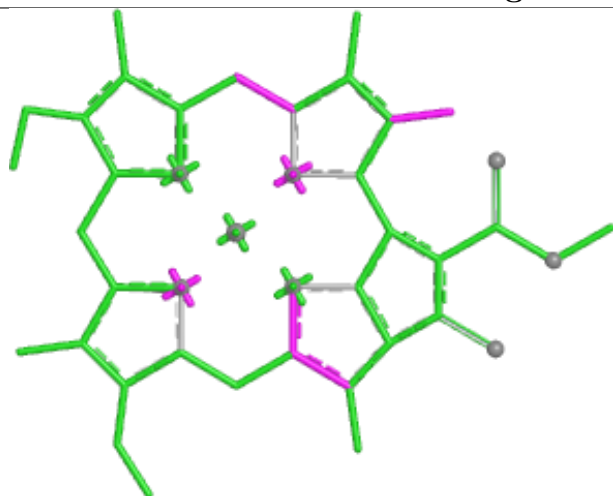
Rings

**Ligand CLA H 1488****Ligand CLA B 1492**

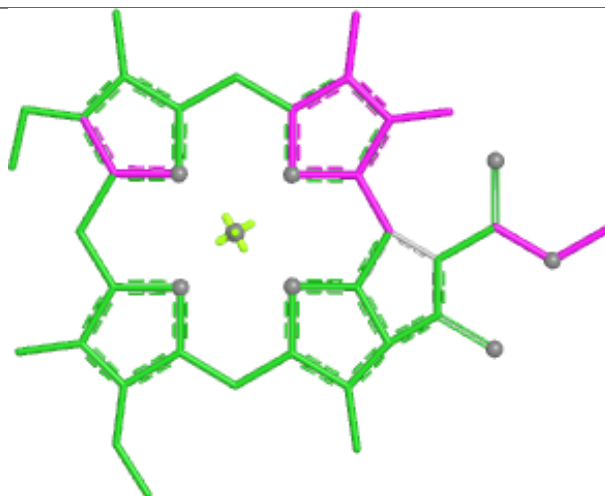
## Ligand CLA H 1484



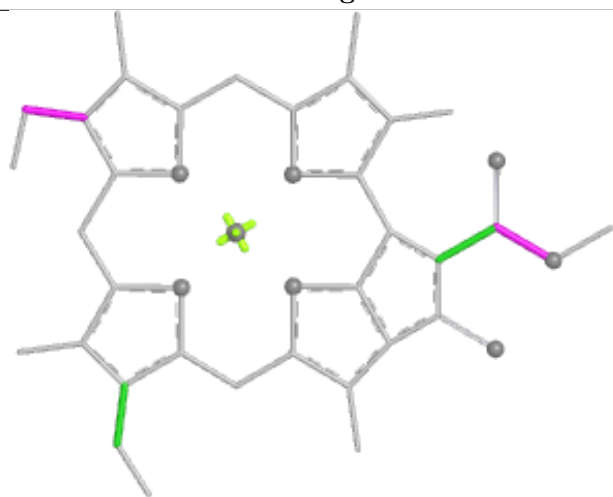
## Ligand CLA C 1470



Bond lengths



Bond angles

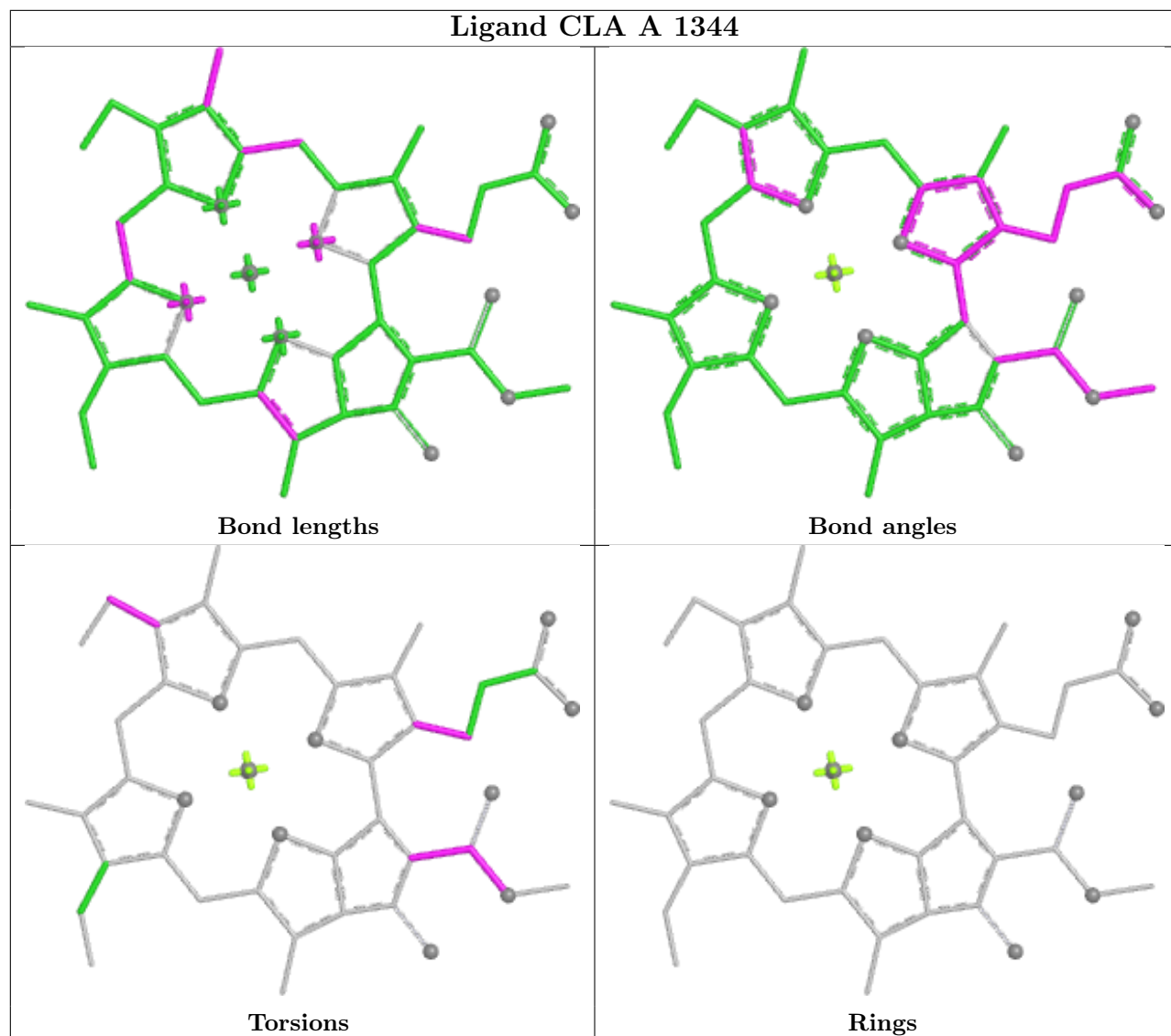


Torsions

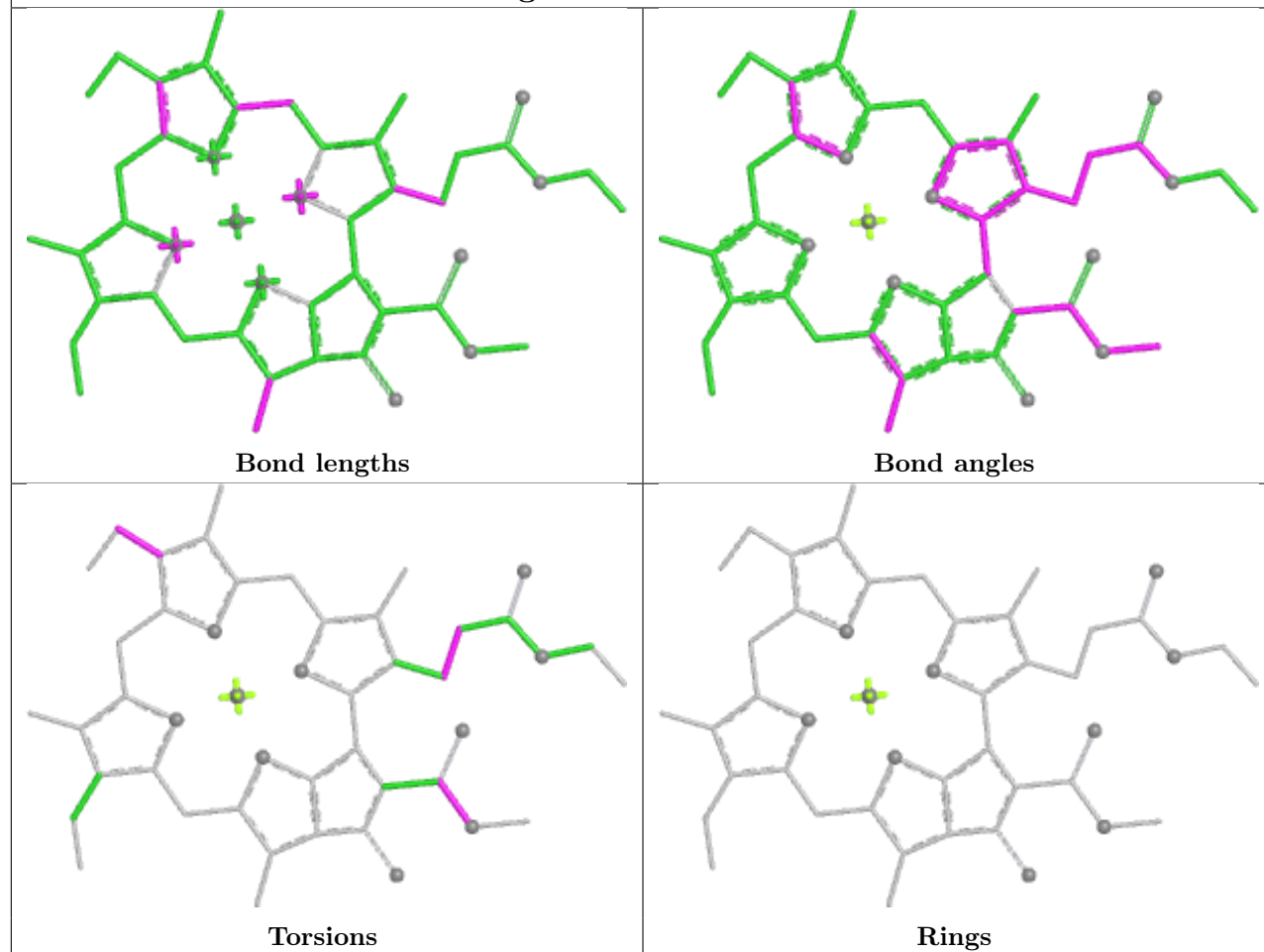


Rings

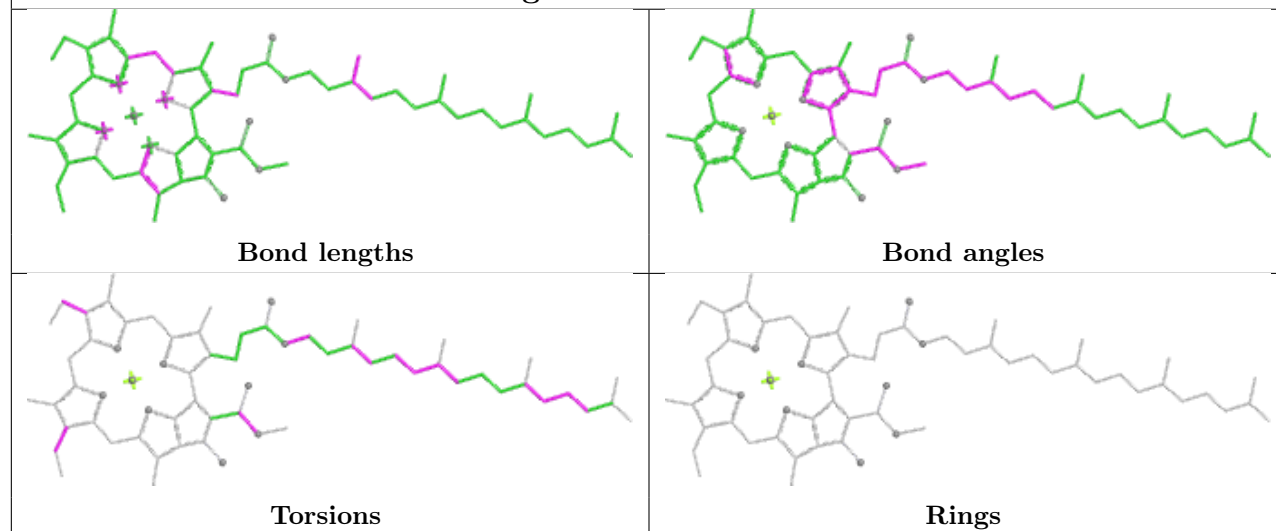
## Ligand CLA A 1344



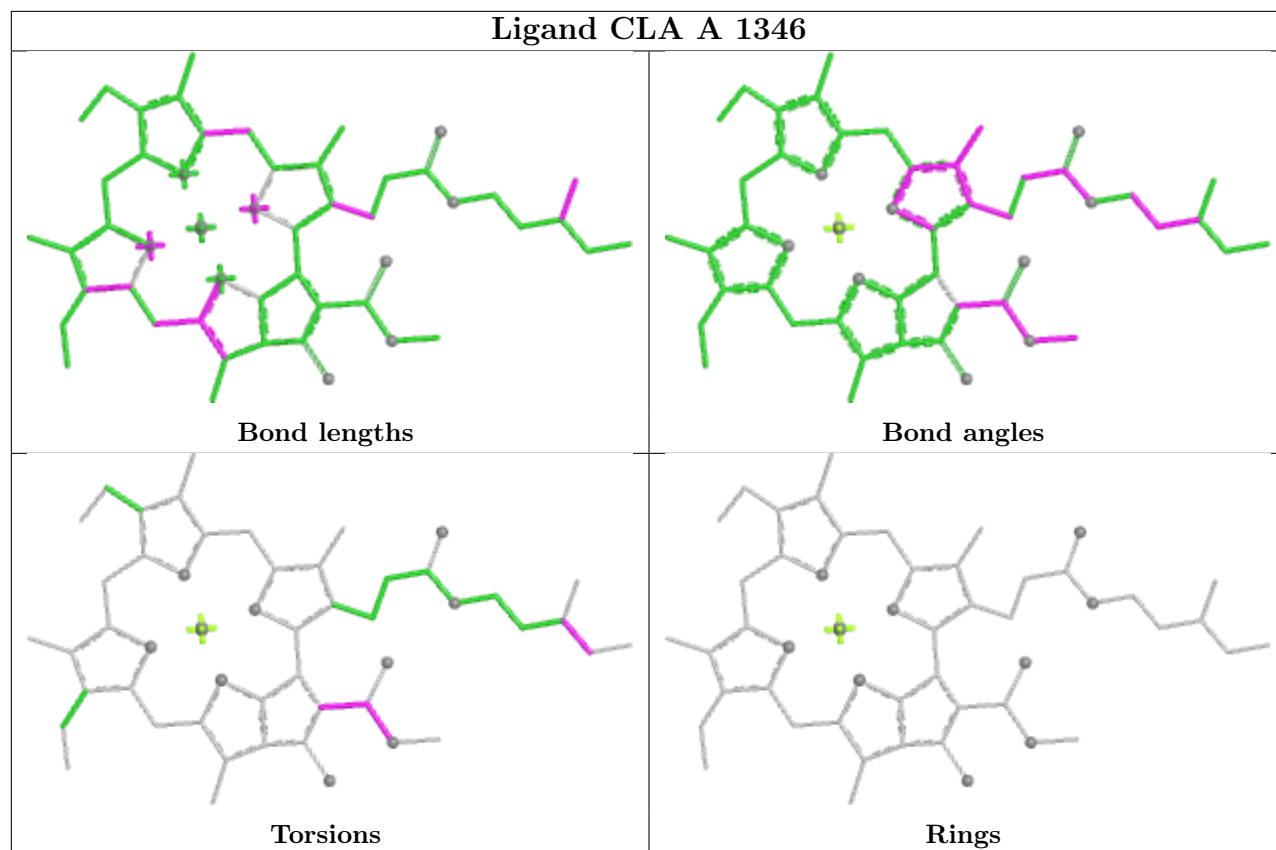
## Ligand CLA C 1460



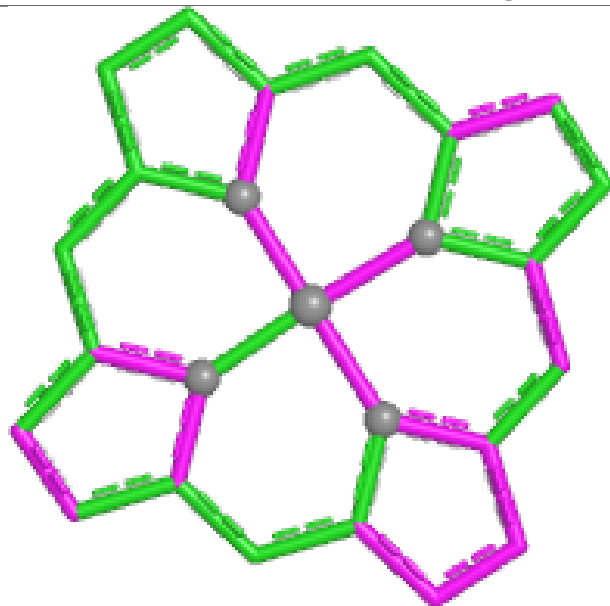
## Ligand CLA H 1496



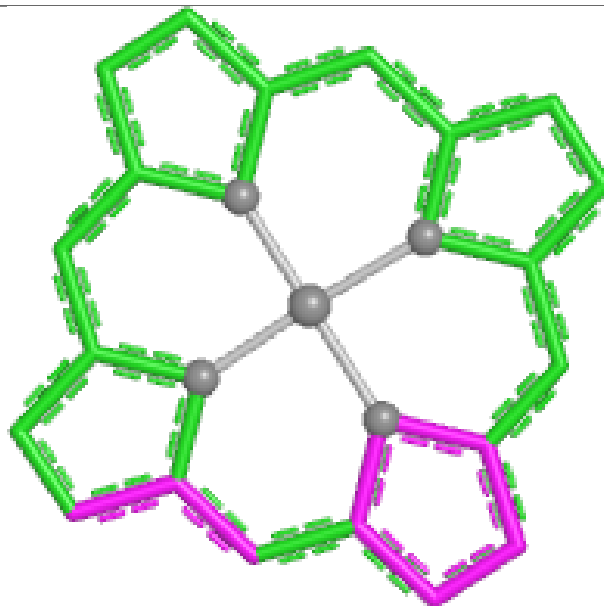
## Ligand CLA A 1346



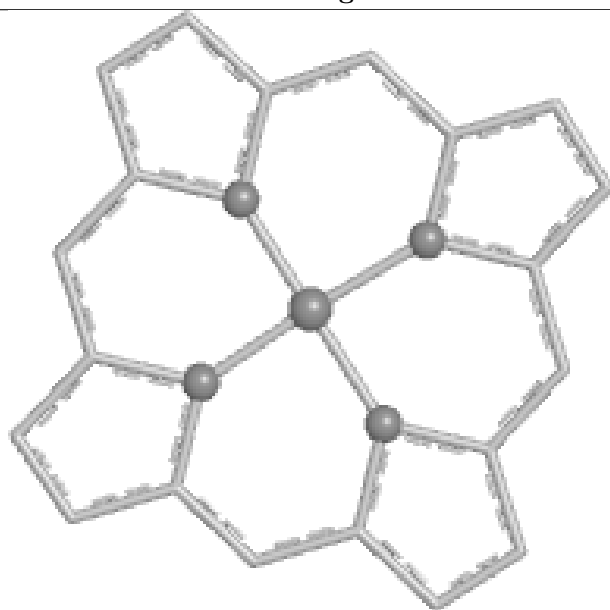
## Ligand HEM E 1085



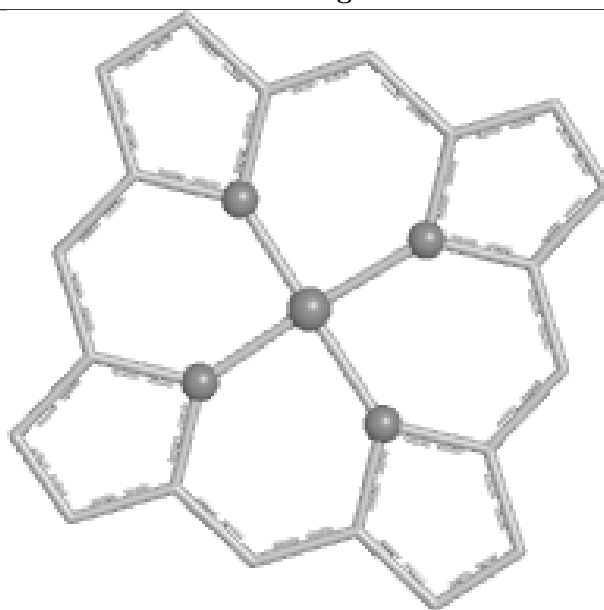
Bond lengths



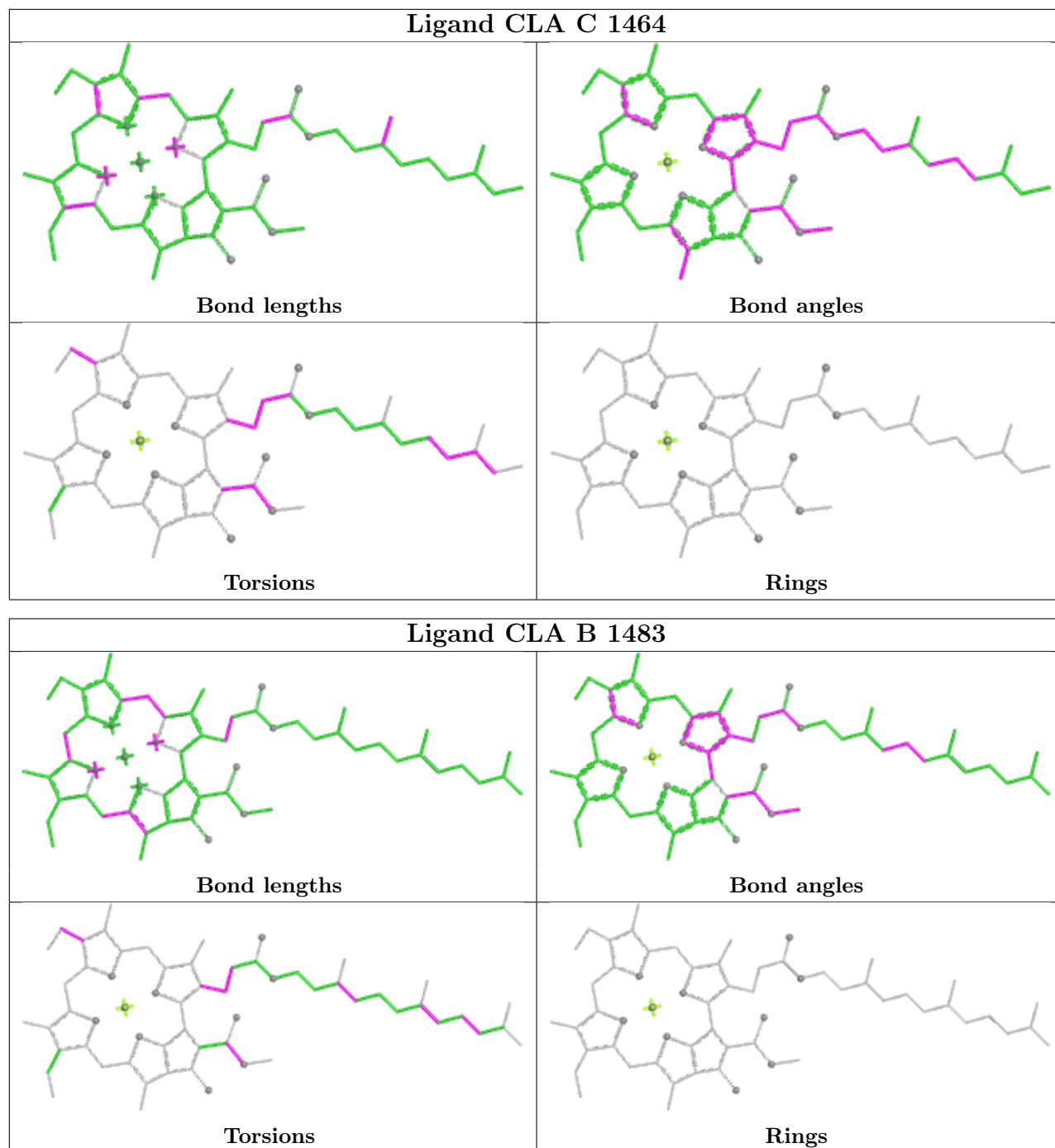
Bond angles



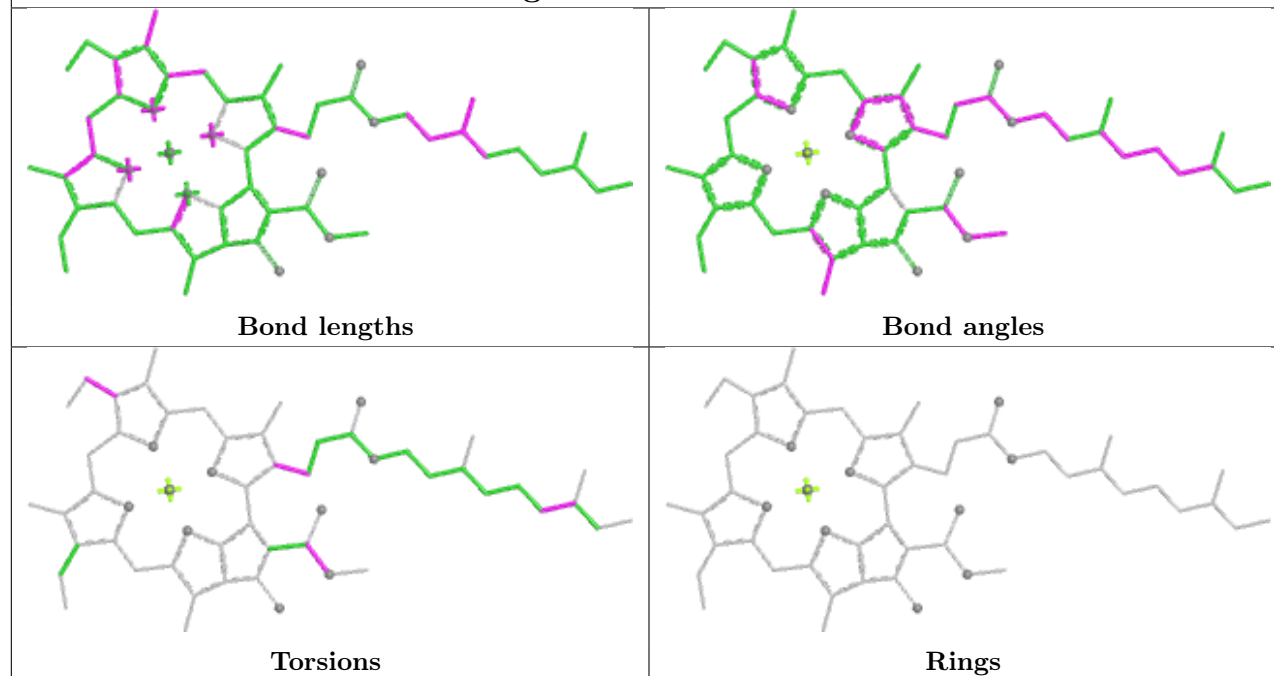
Torsions



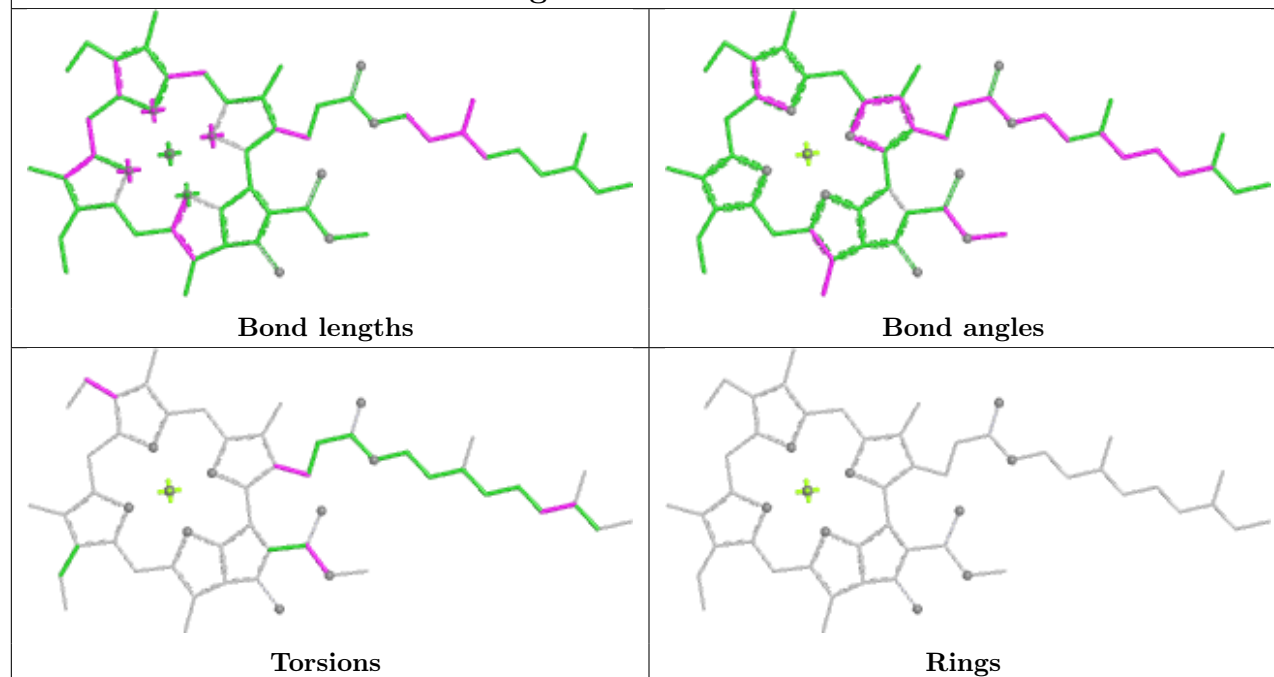
Rings



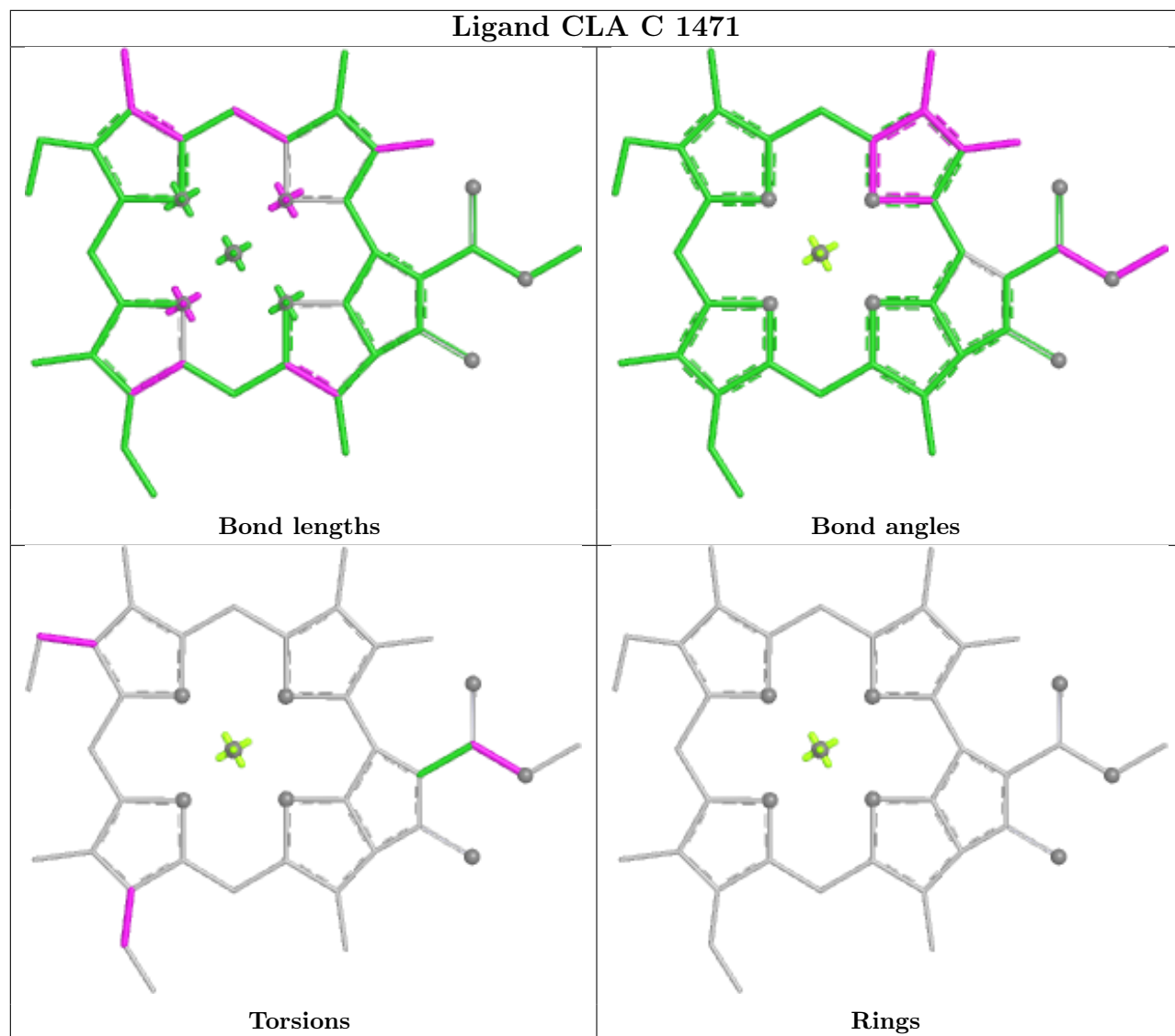
## Ligand CLA C 1462



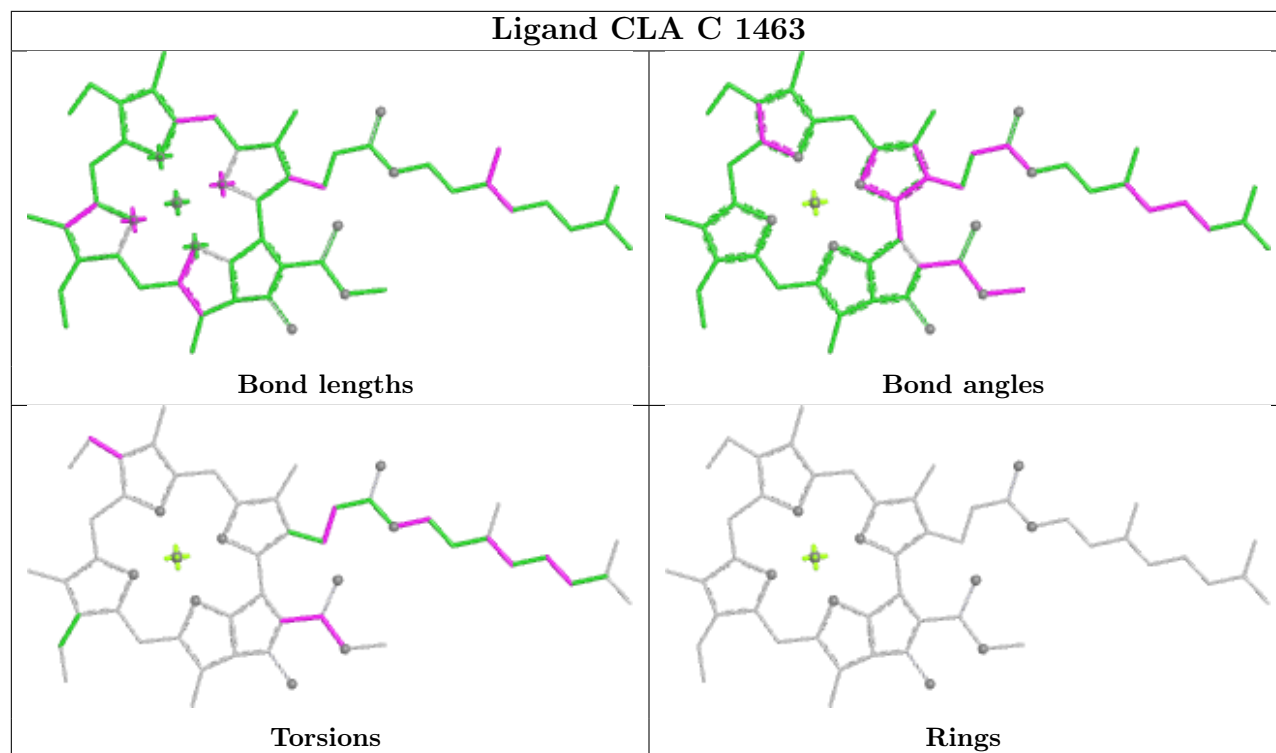
## Ligand CLA I 1462



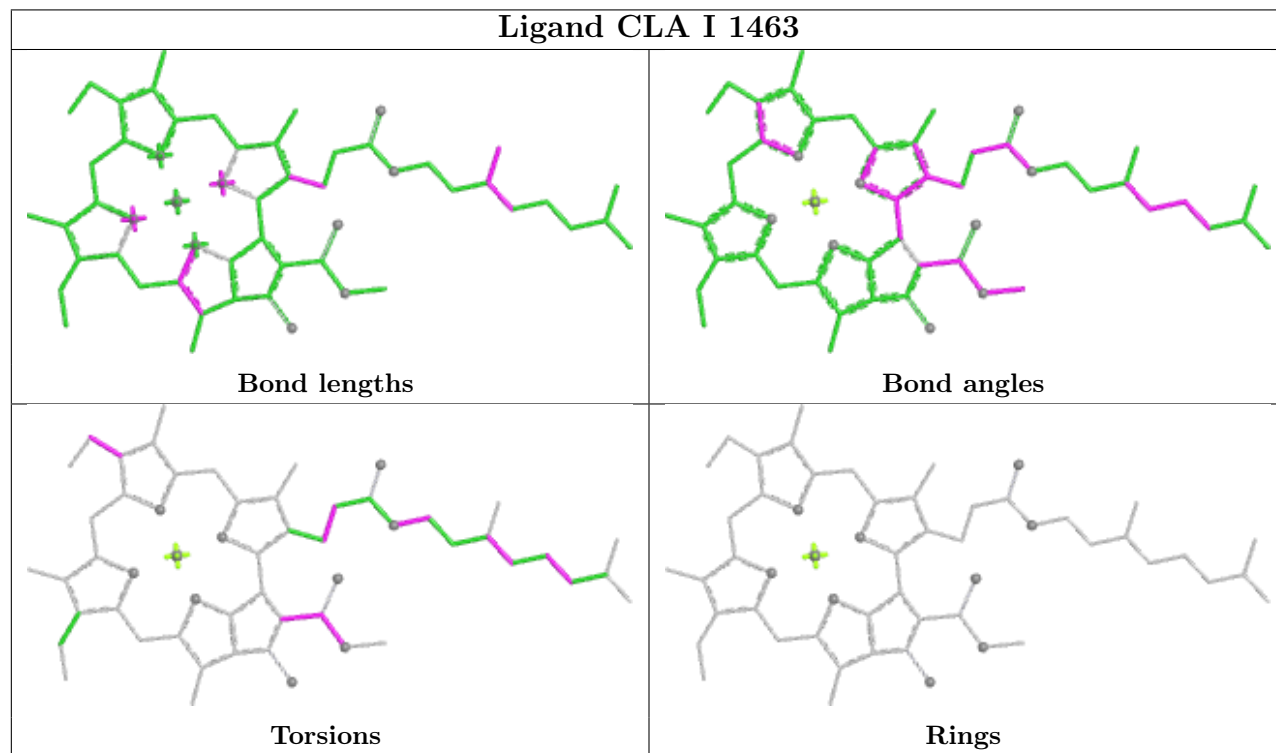
## Ligand CLA C 1471

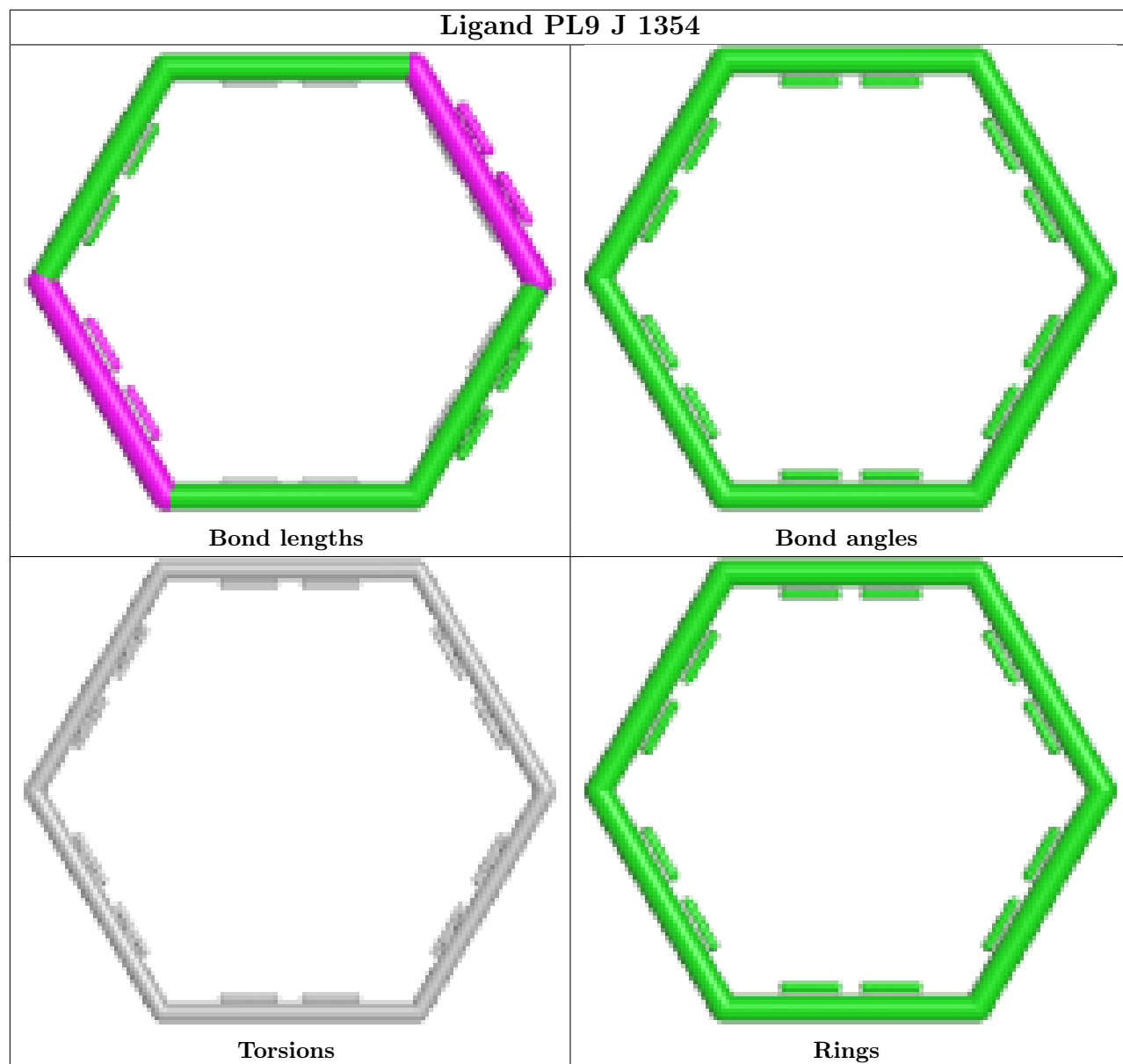


## Ligand CLA C 1463

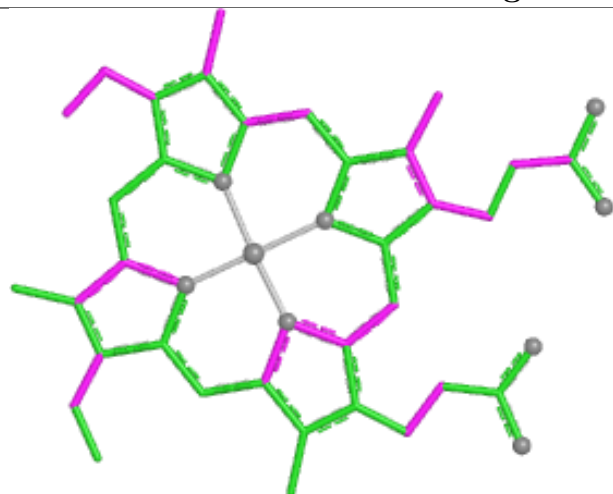


## Ligand CLA I 1463

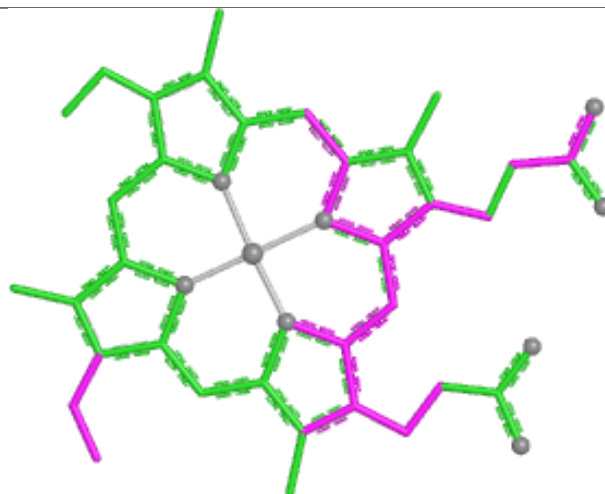




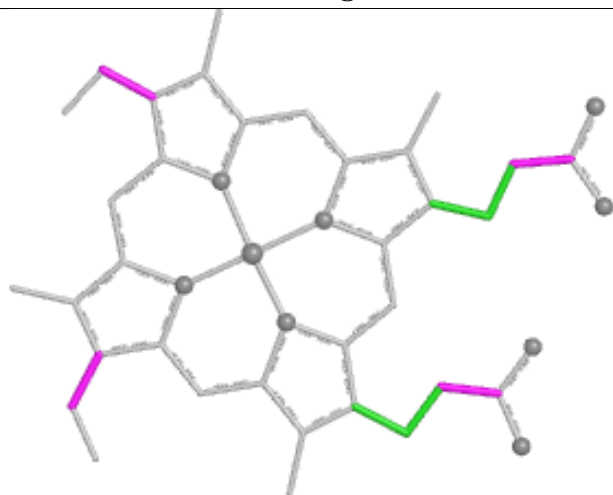
## Ligand HEC V 1138



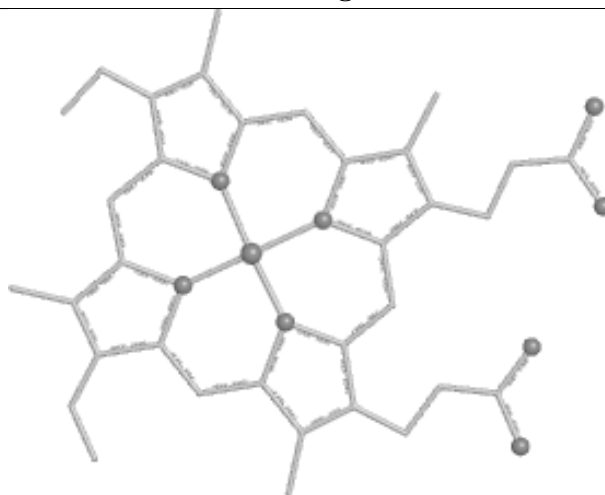
Bond lengths



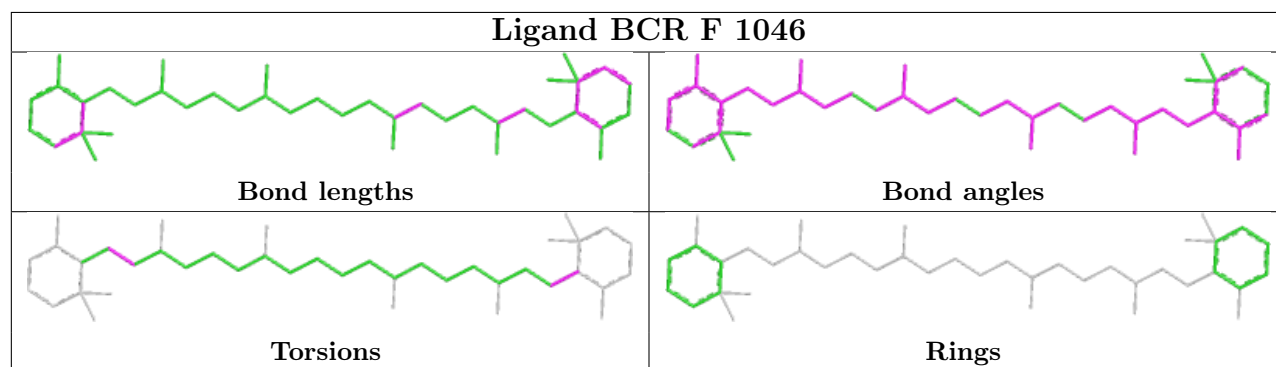
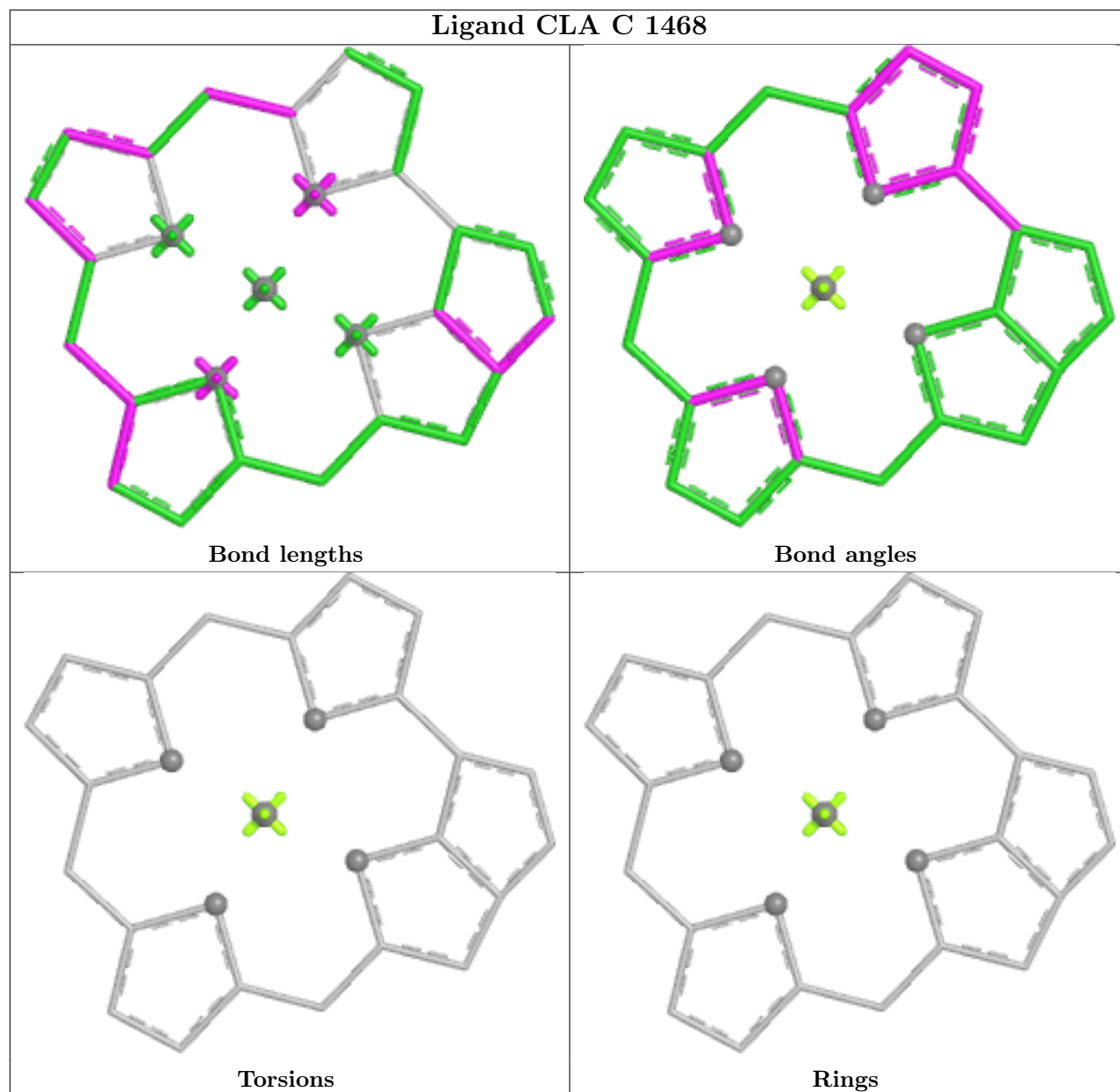
Bond angles



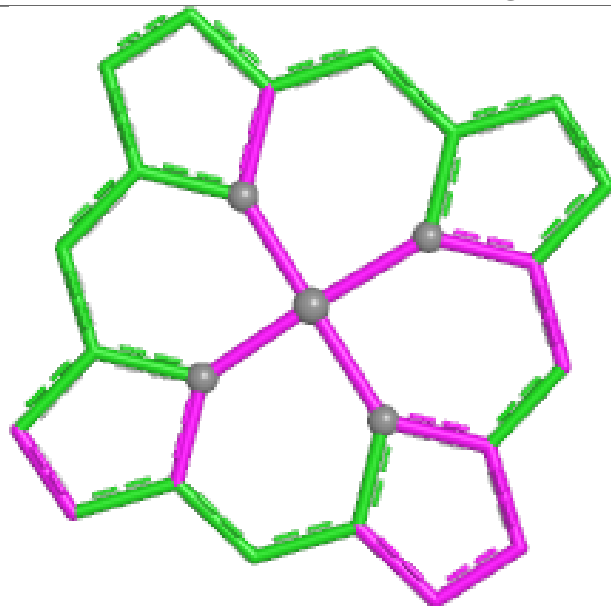
Torsions



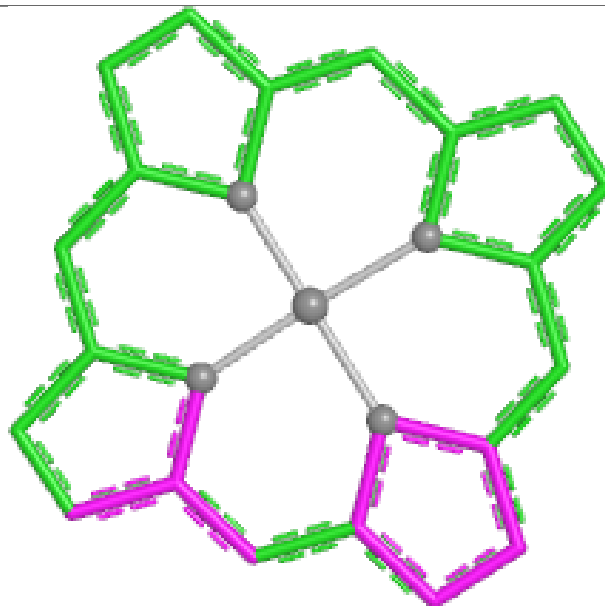
Rings



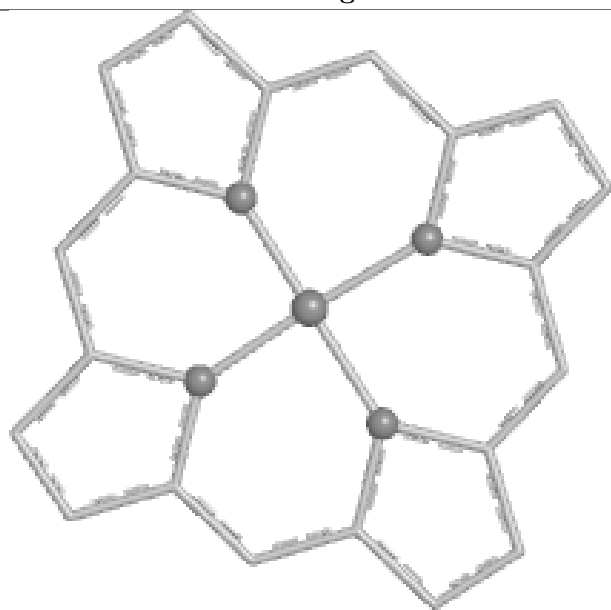
## Ligand HEM L 1046



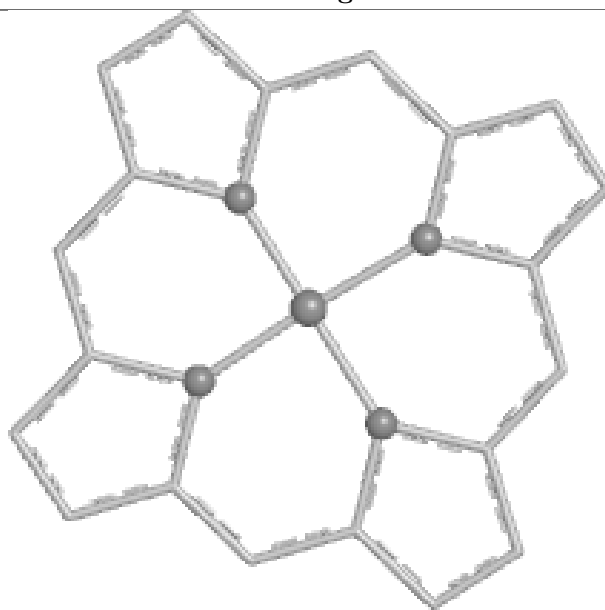
Bond lengths



Bond angles

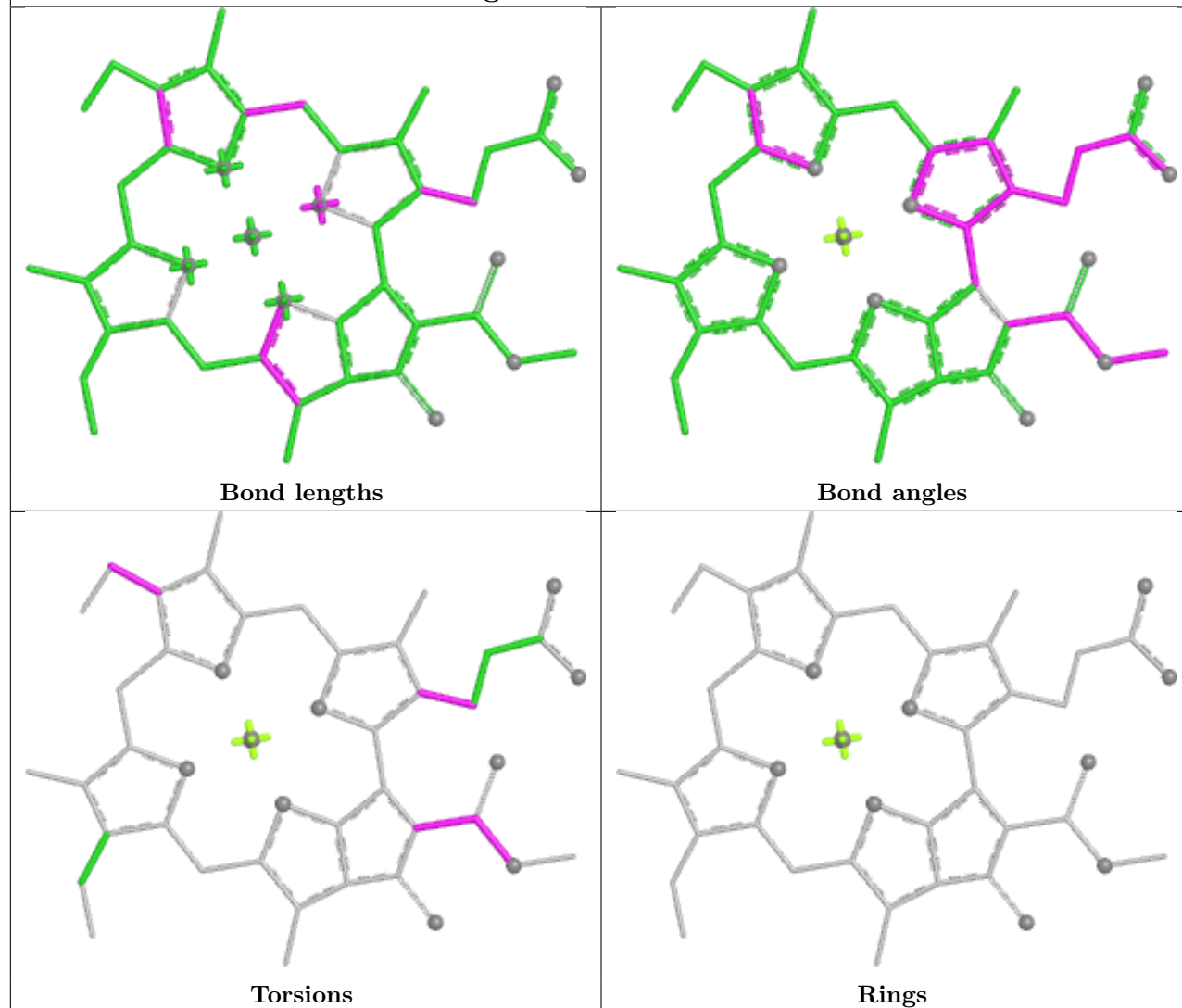


Torsions

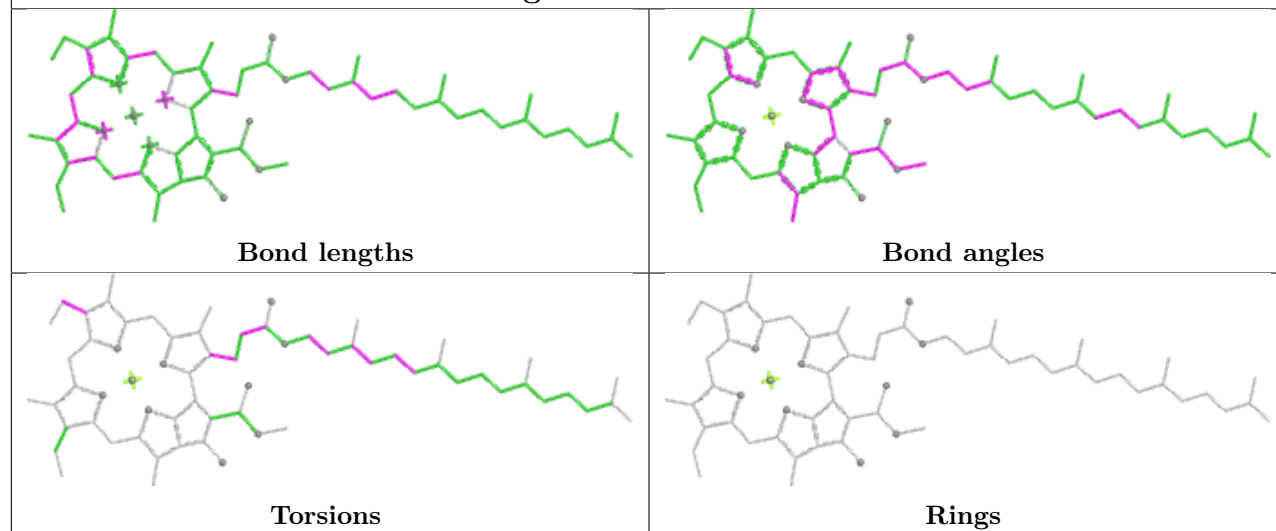


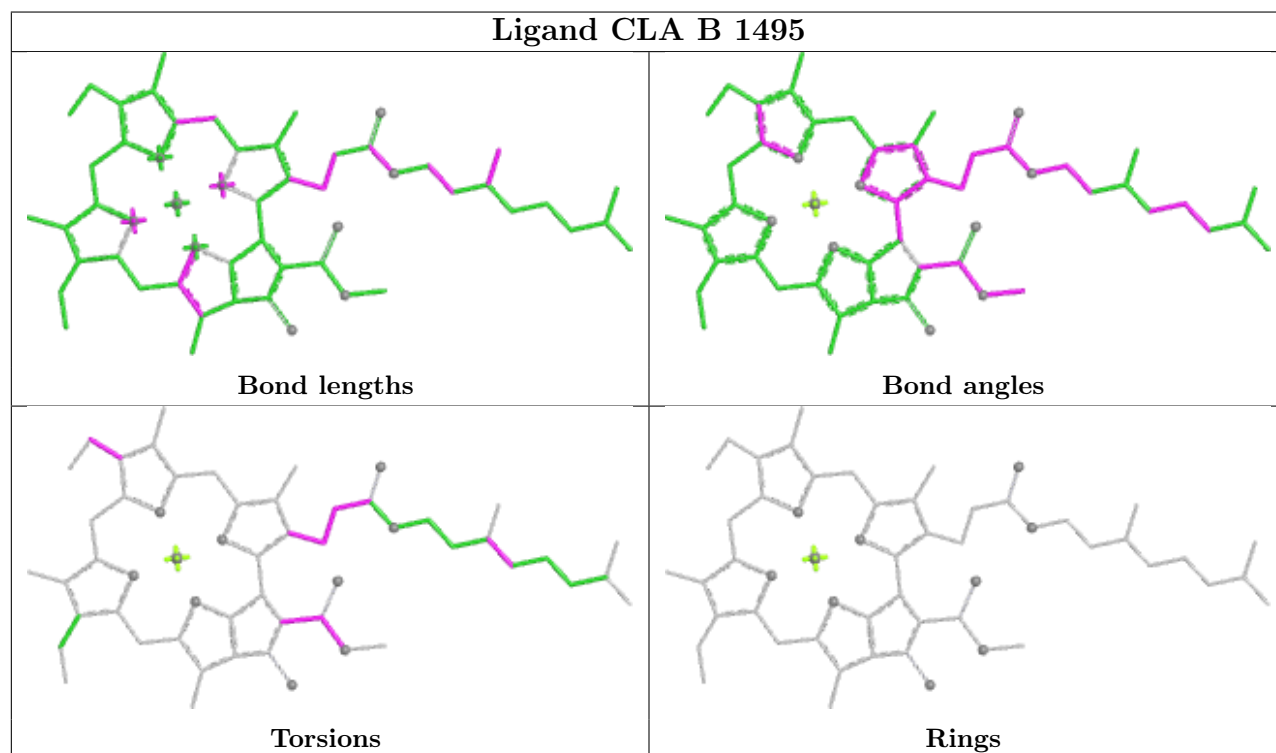
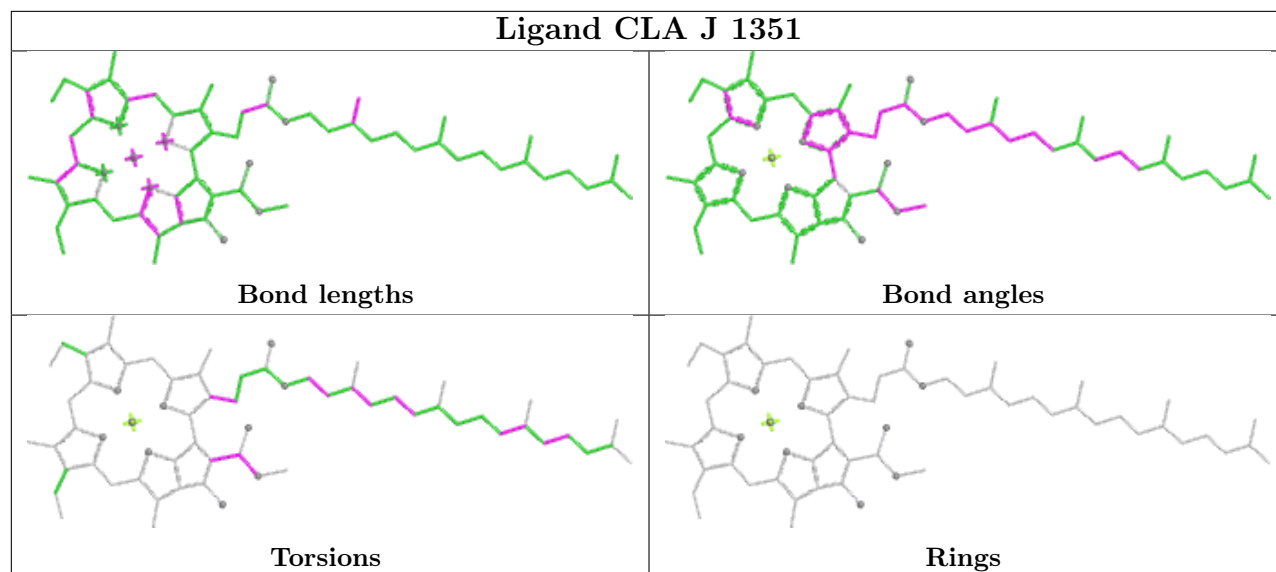
Rings

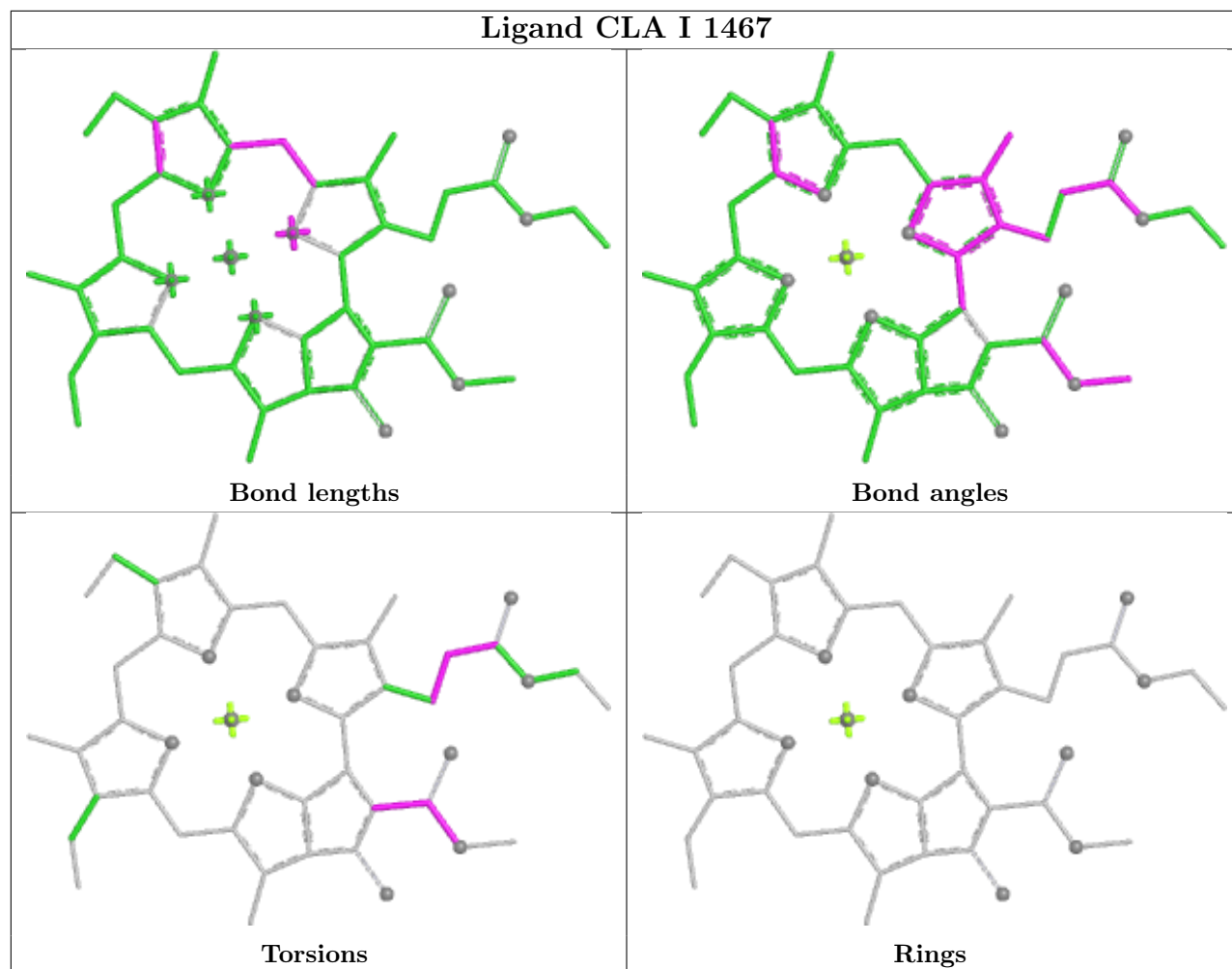
## Ligand CLA G 1344



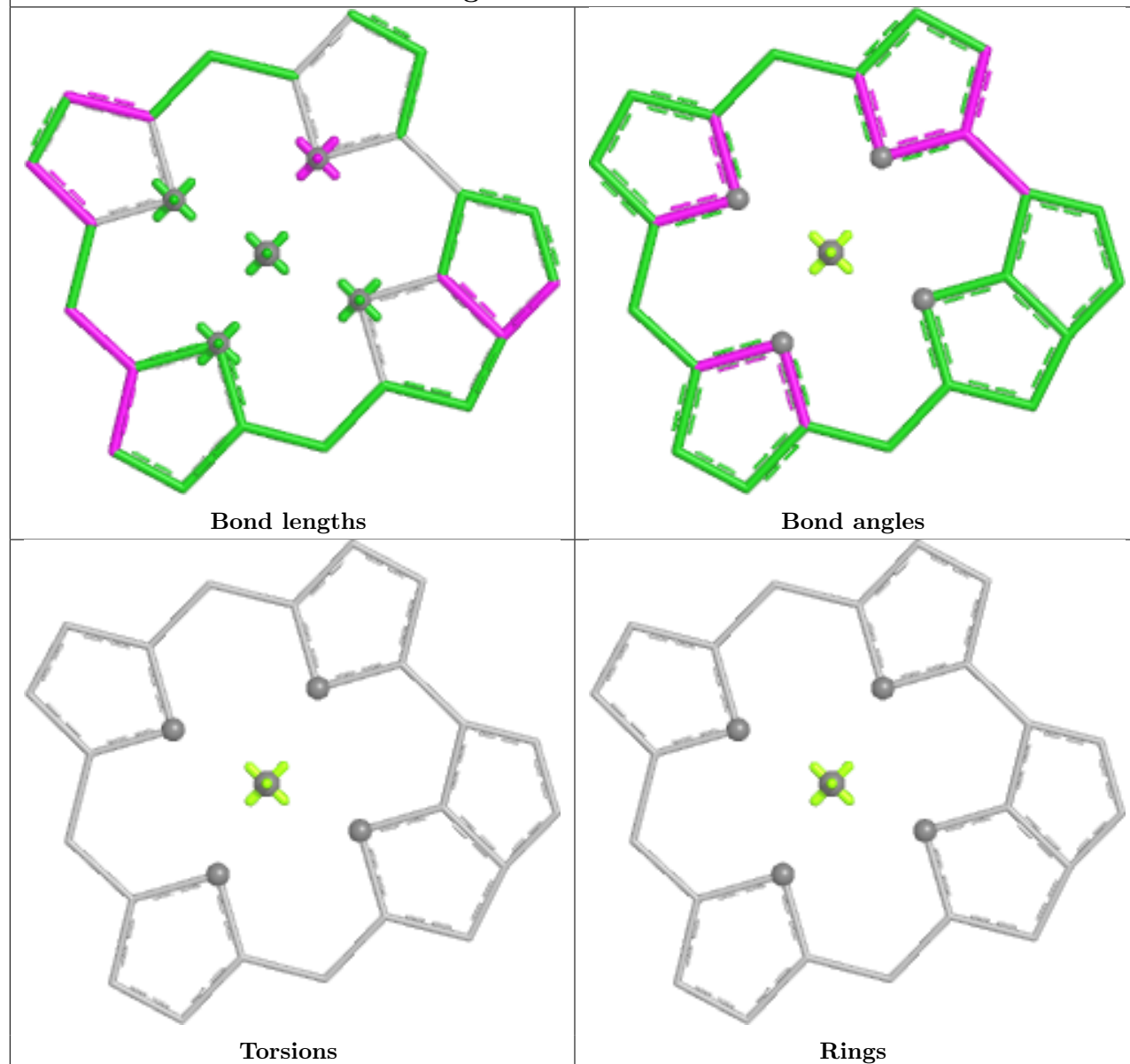
## Ligand CLA B 1487



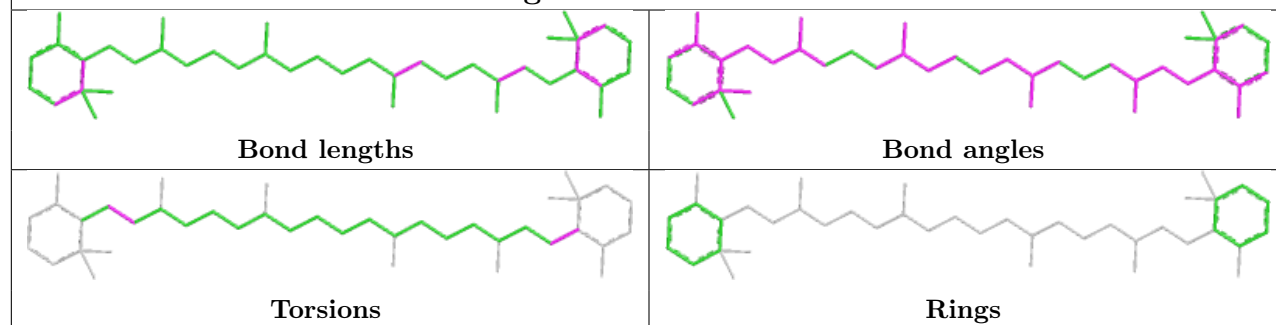




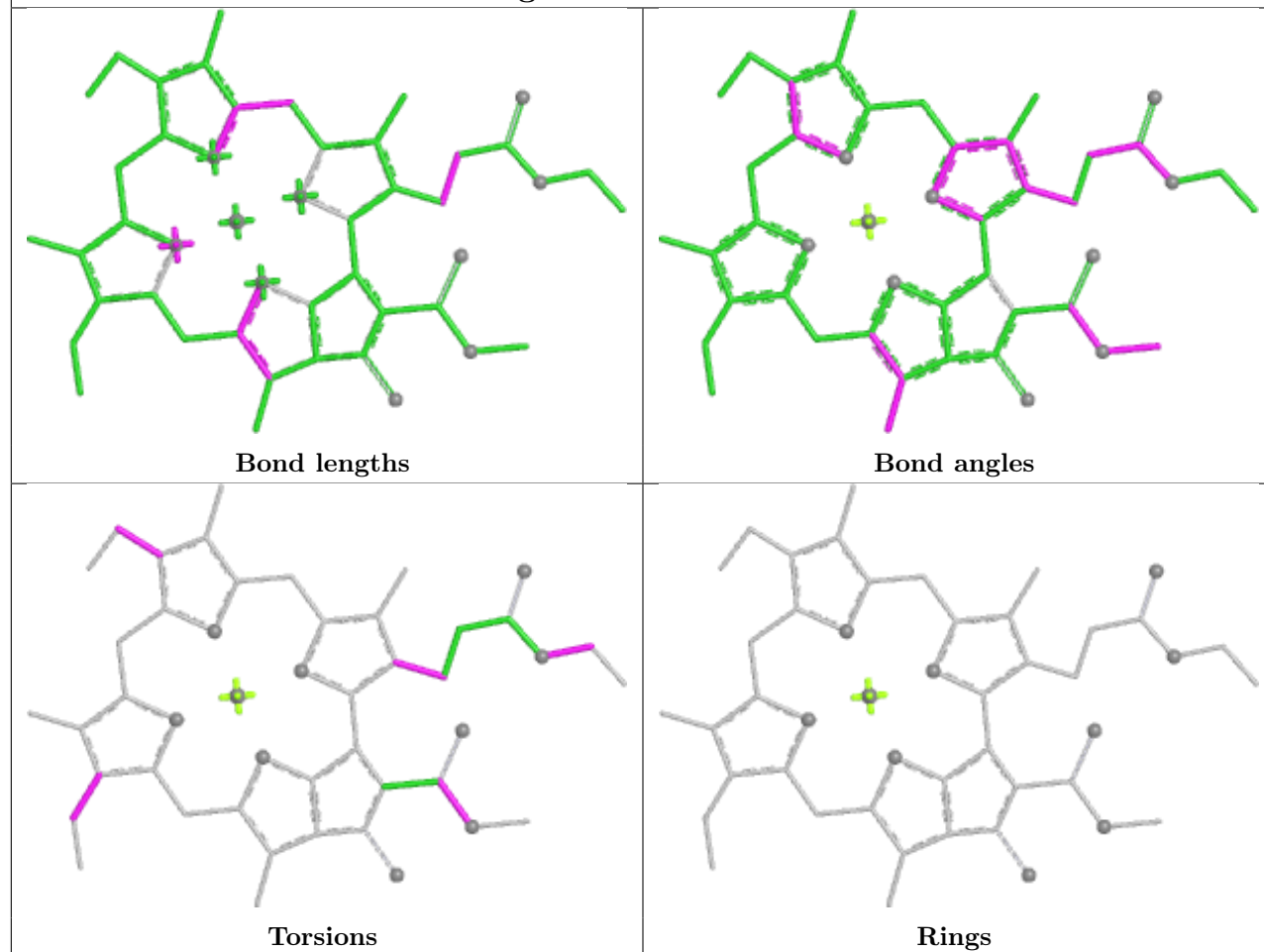
## Ligand CLA B 1491



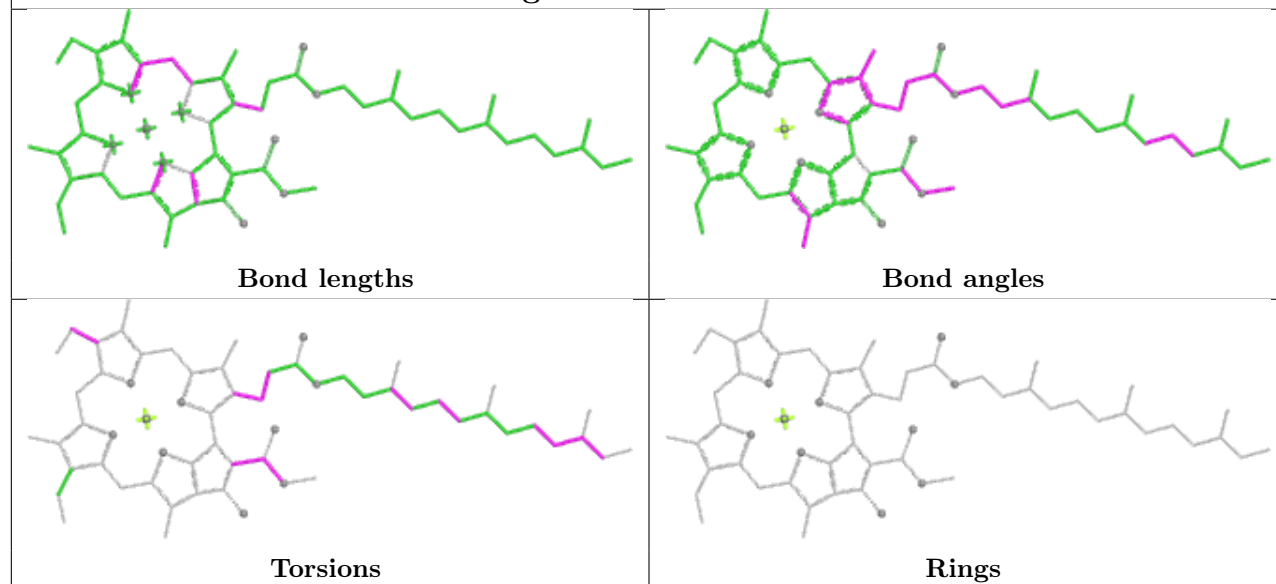
## Ligand BCR L 1047

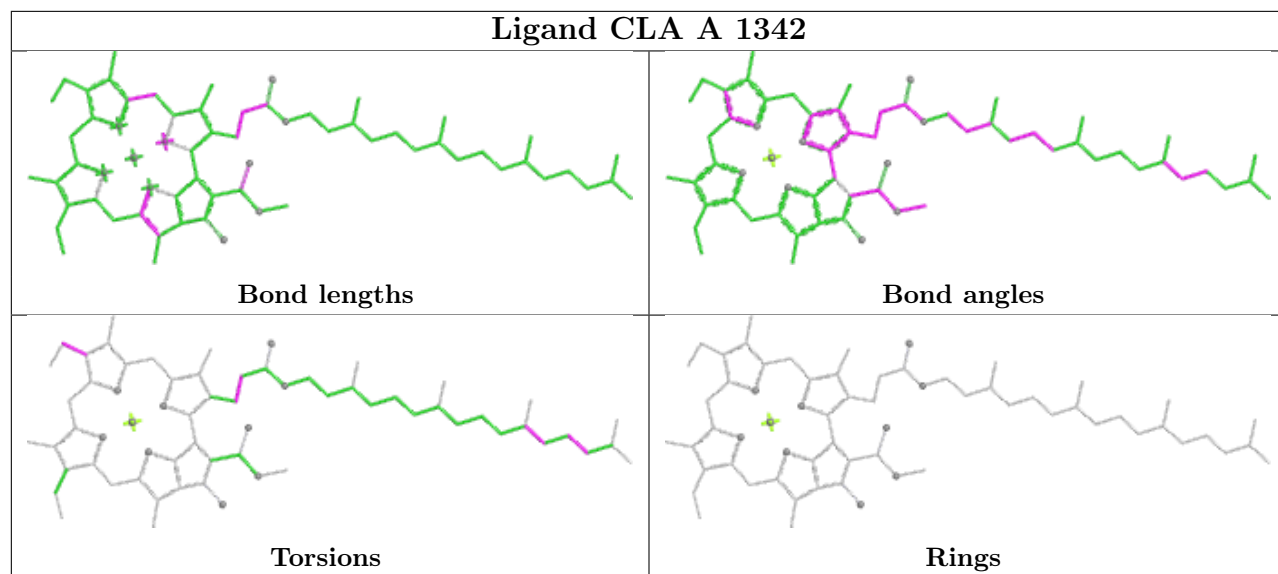


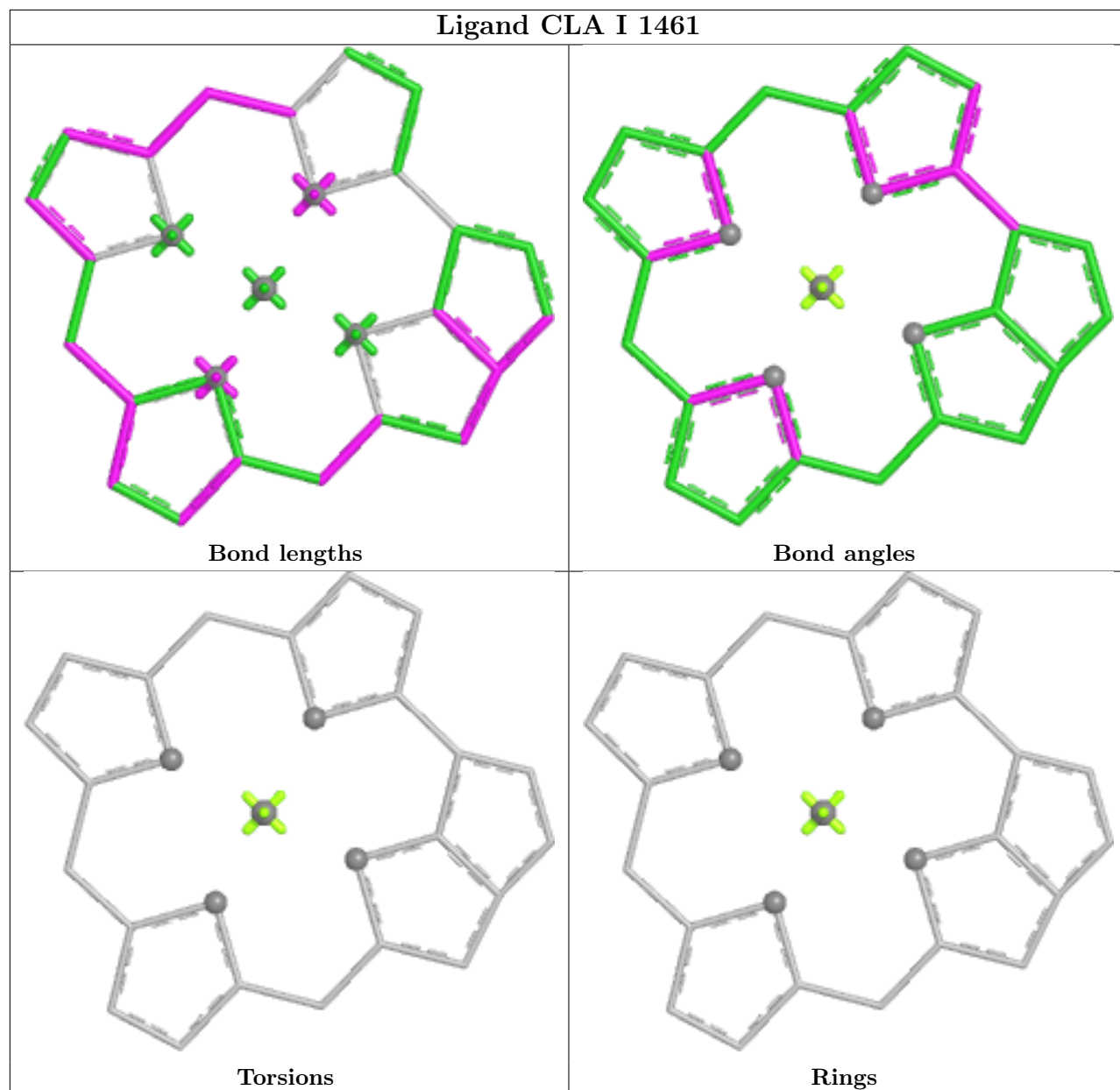
## Ligand CLA B 1485



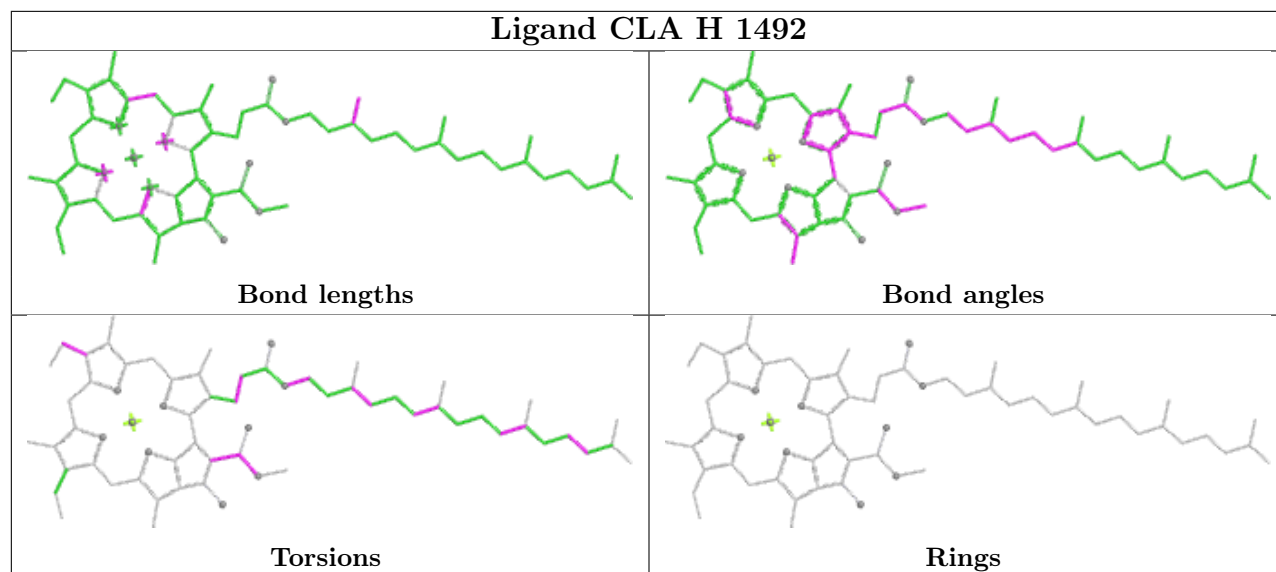
## Ligand CLA A 1343



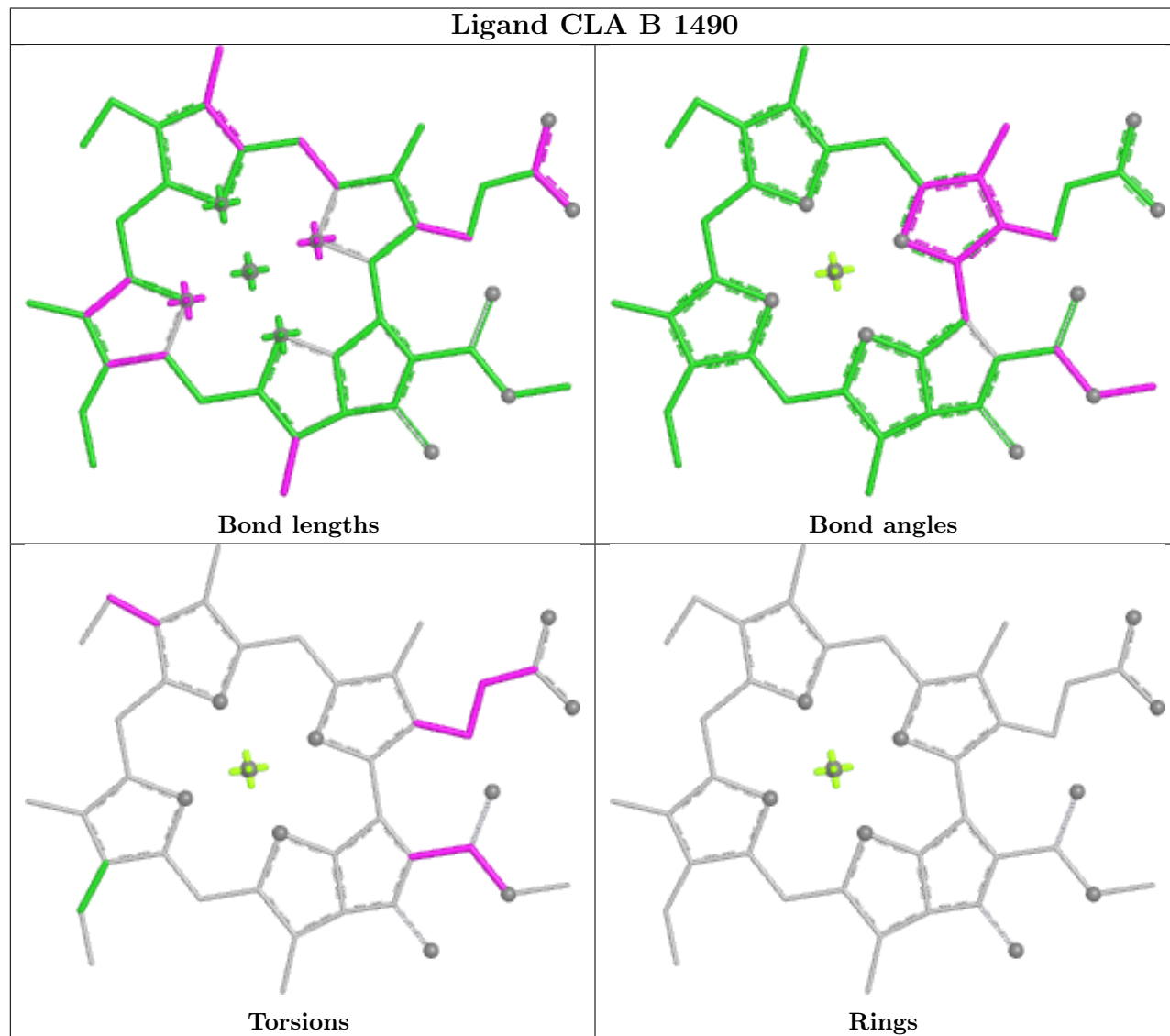


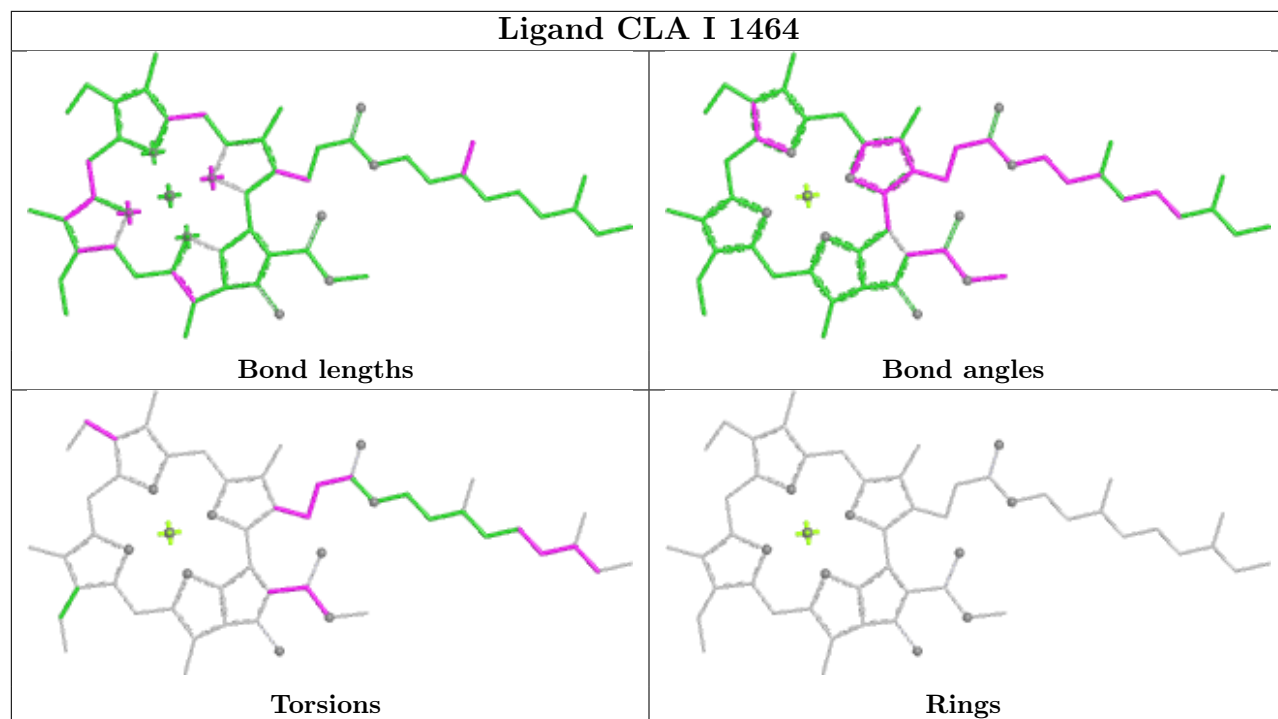


## Ligand CLA H 1492

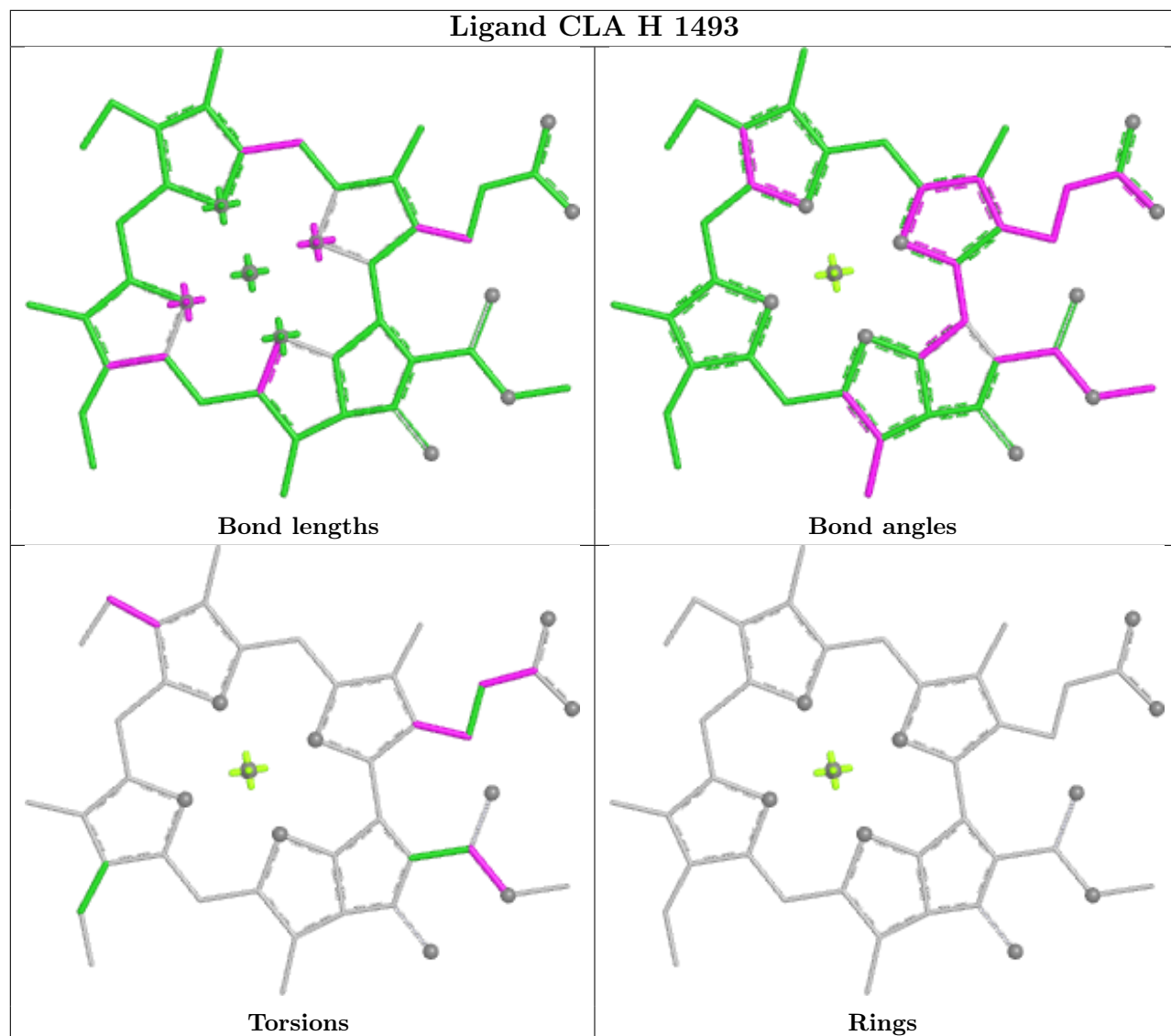


## Ligand CLA B 1490

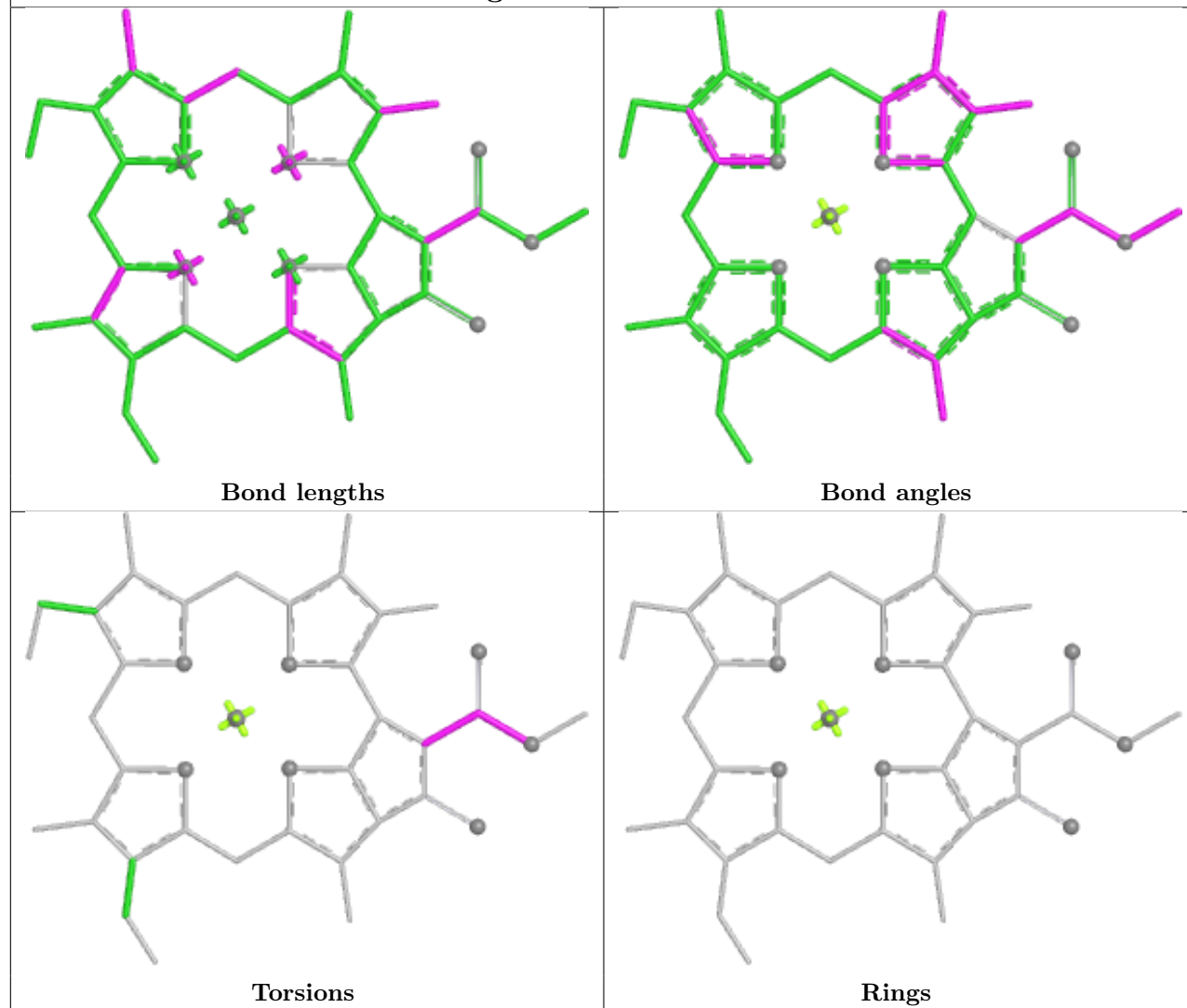




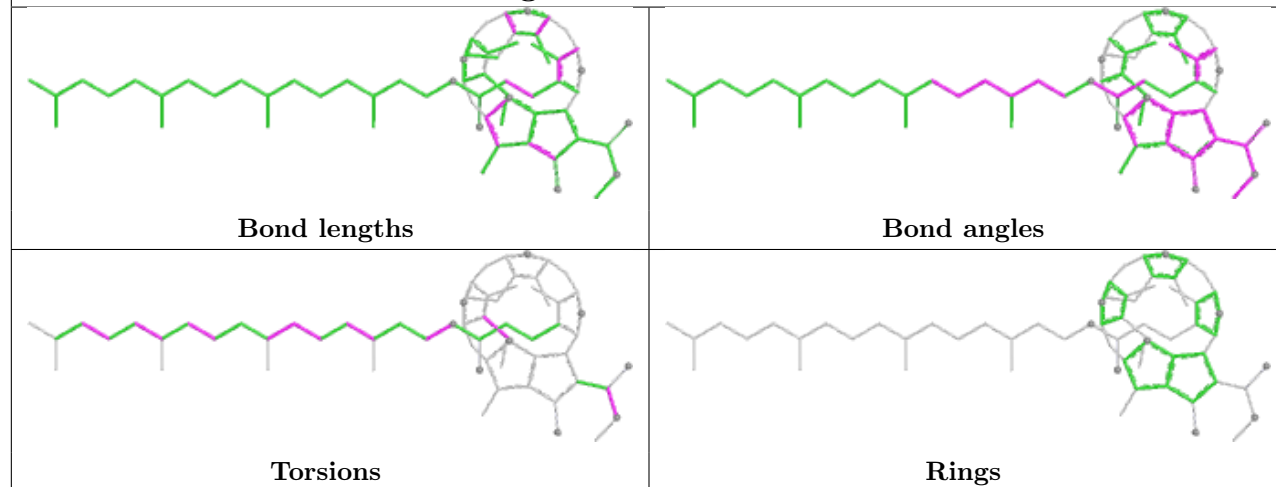
## Ligand CLA H 1493



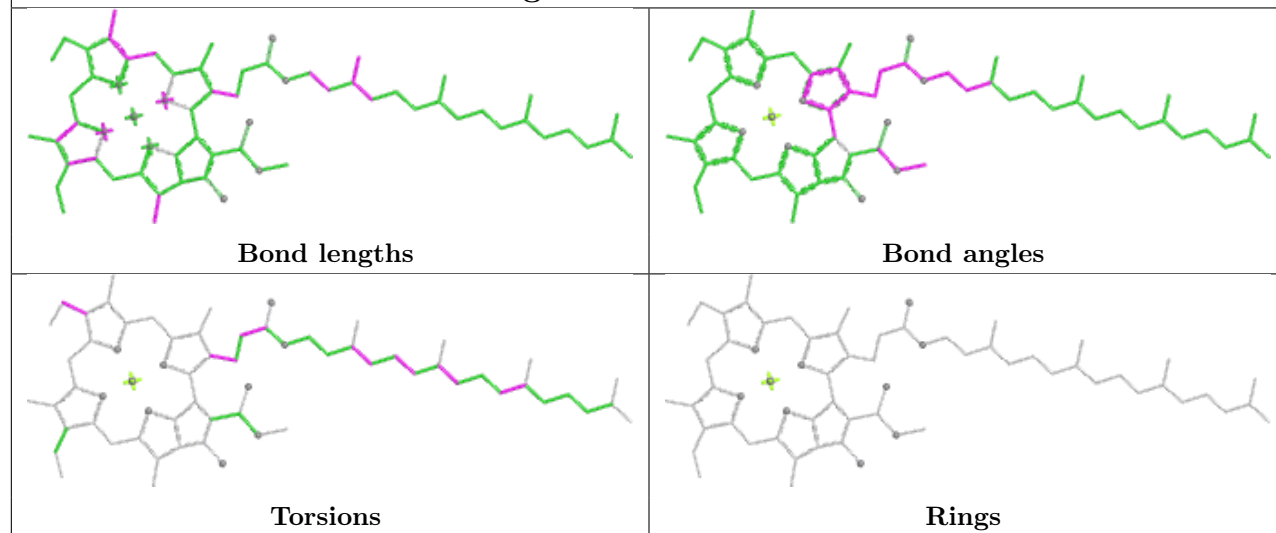
## Ligand CLA B 1497



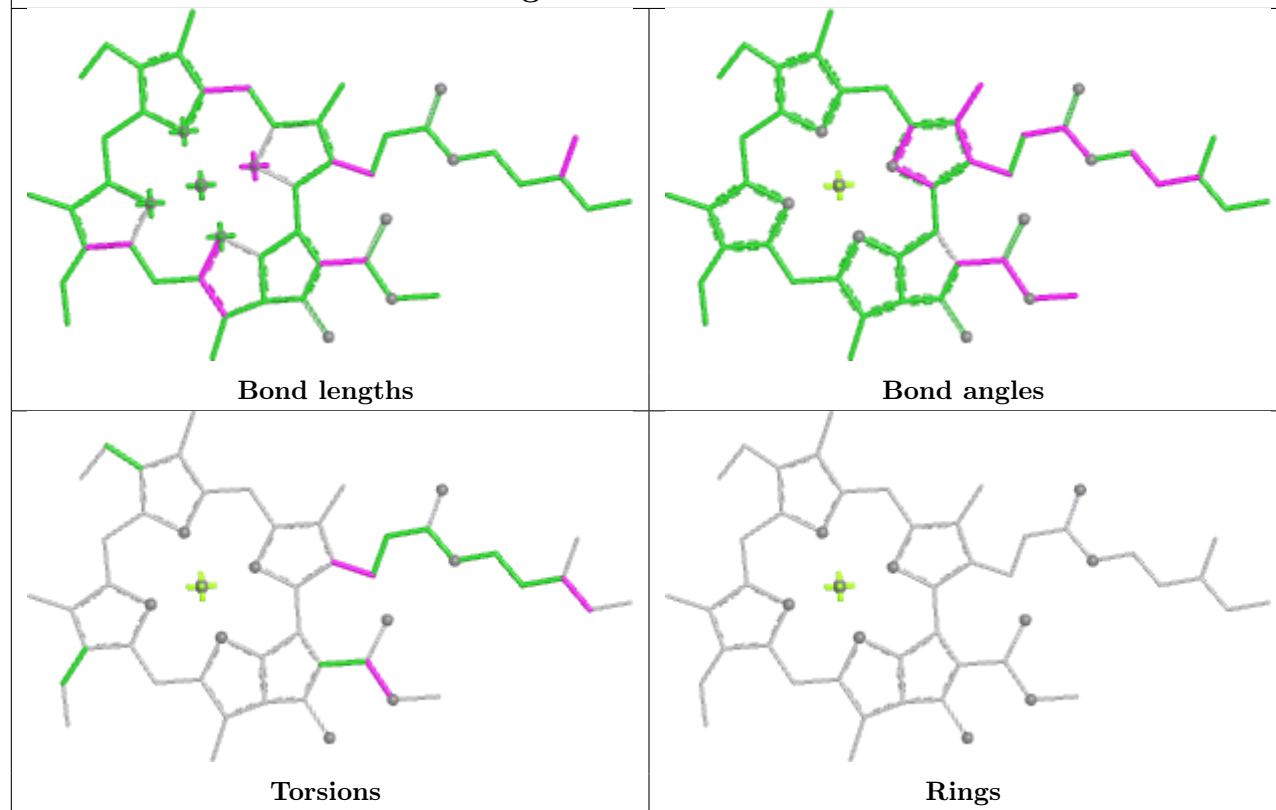
## Ligand PHO G 1345

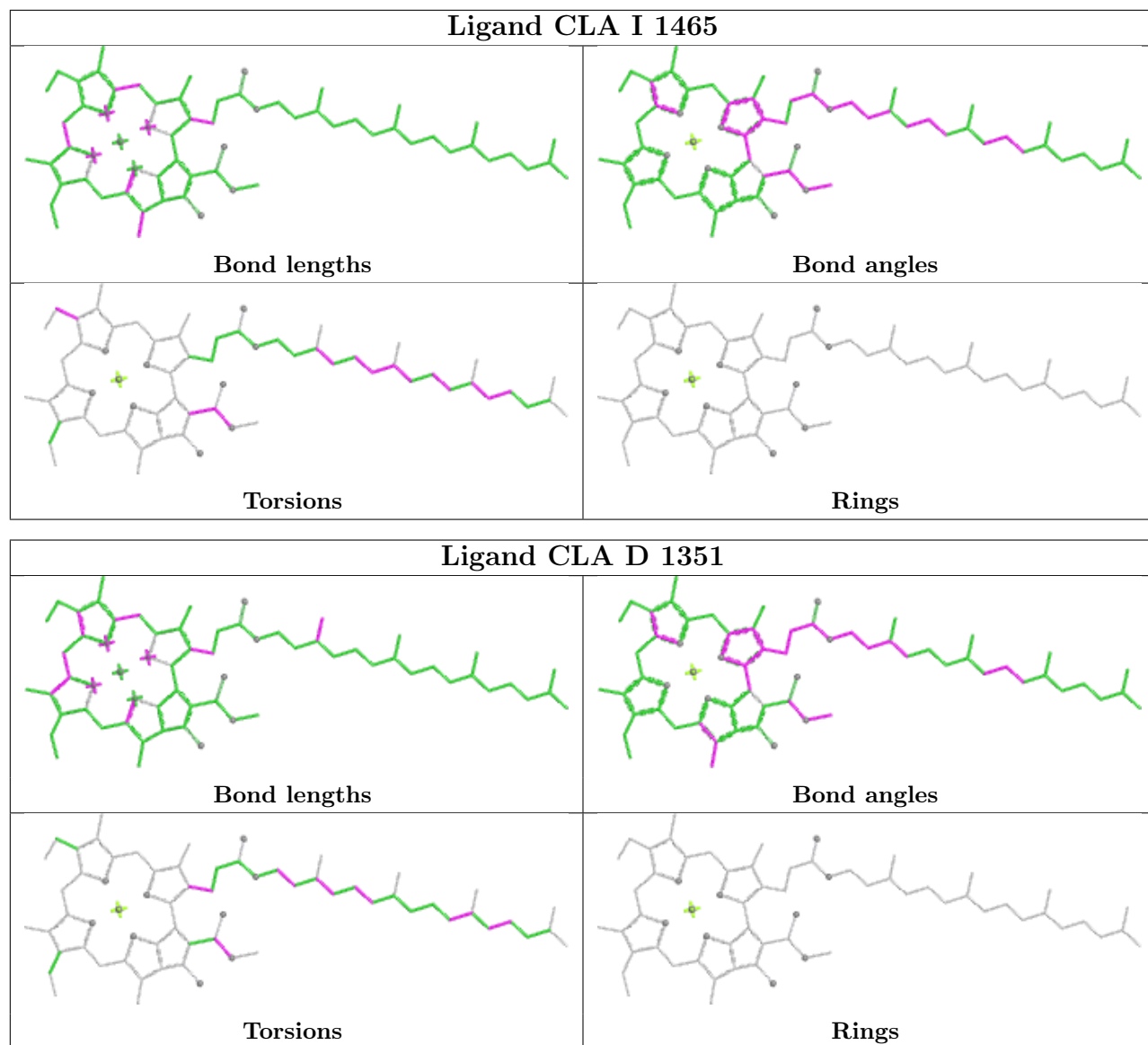


## Ligand CLA B 1482

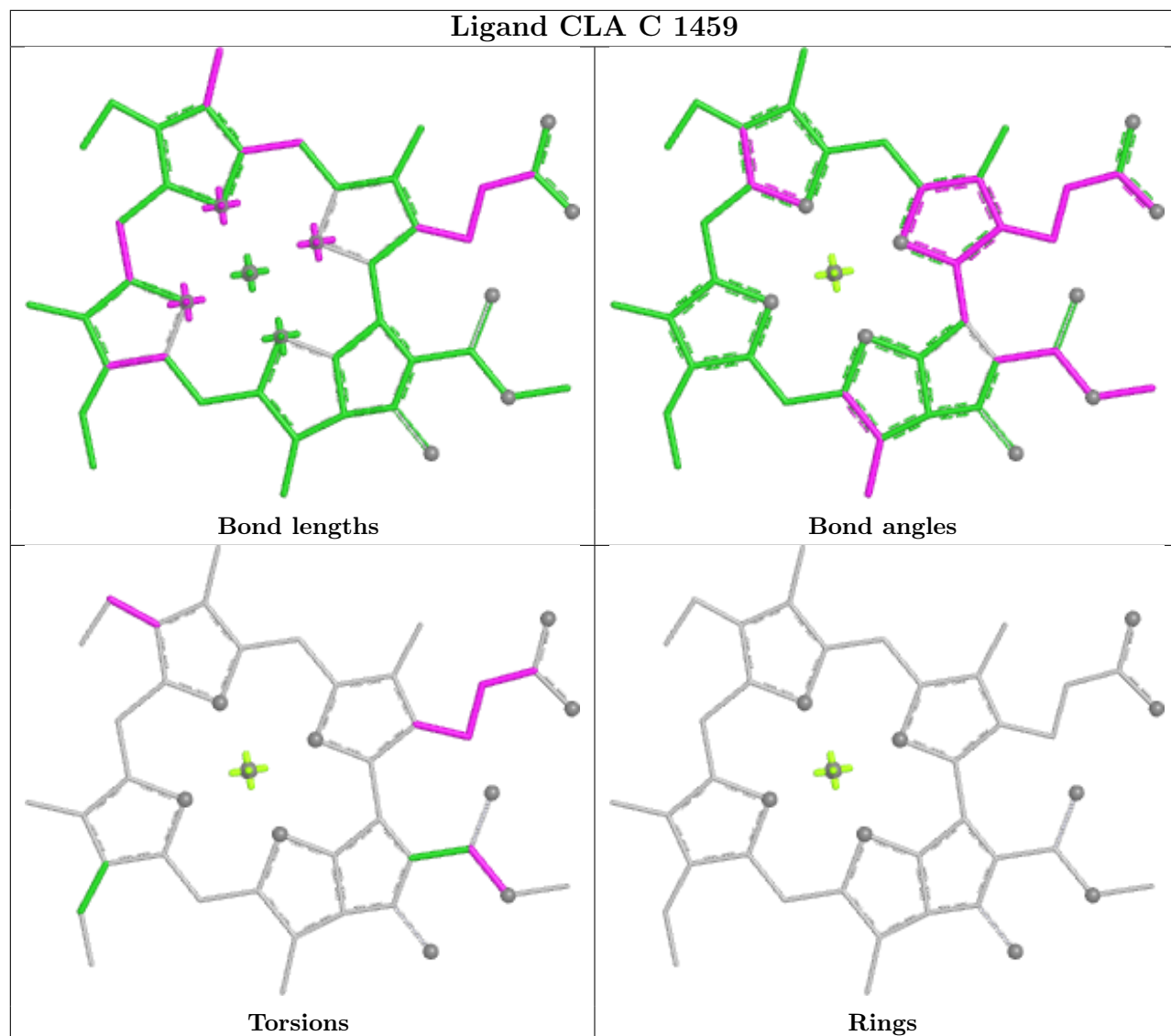


## Ligand CLA G 1346

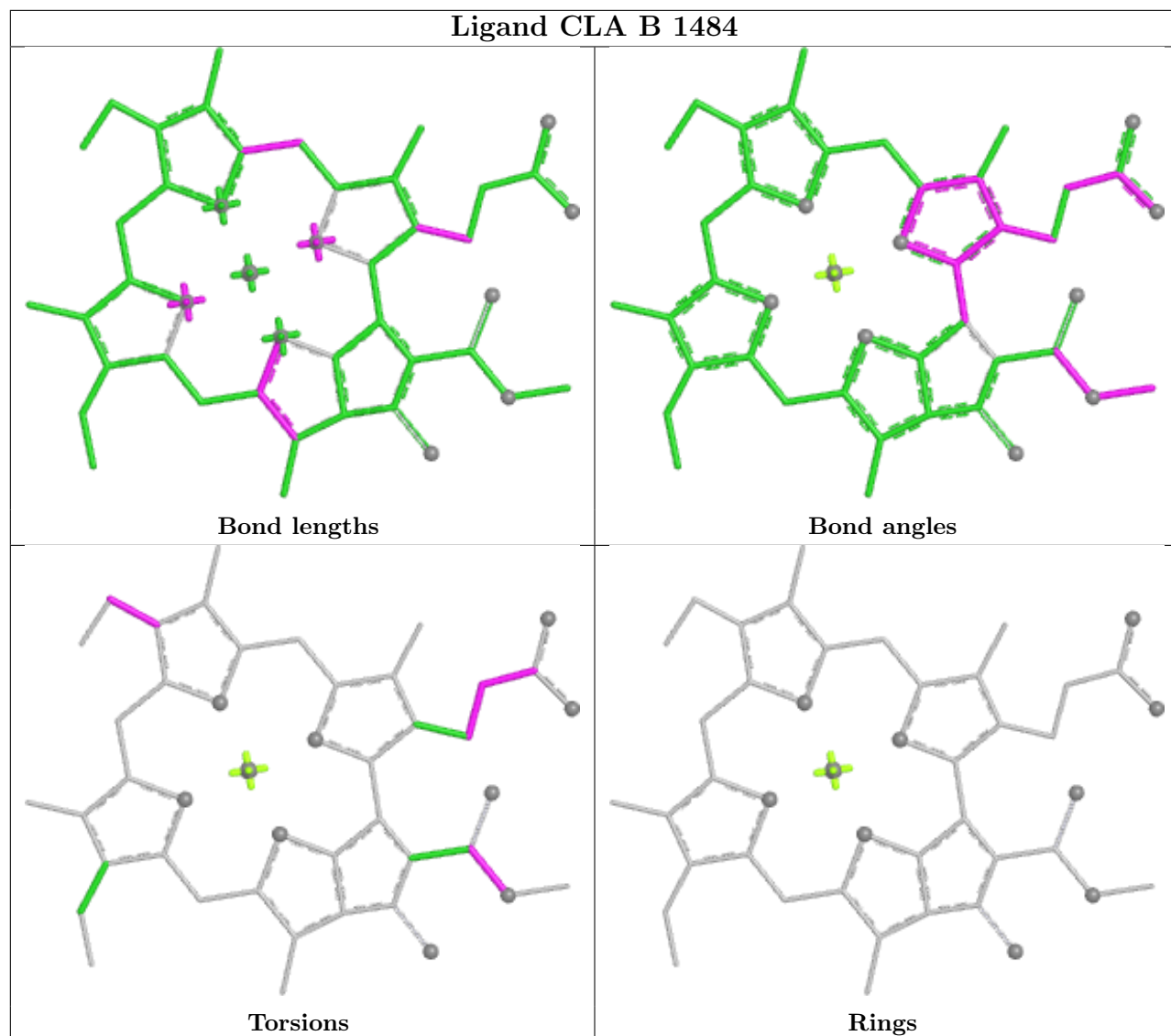




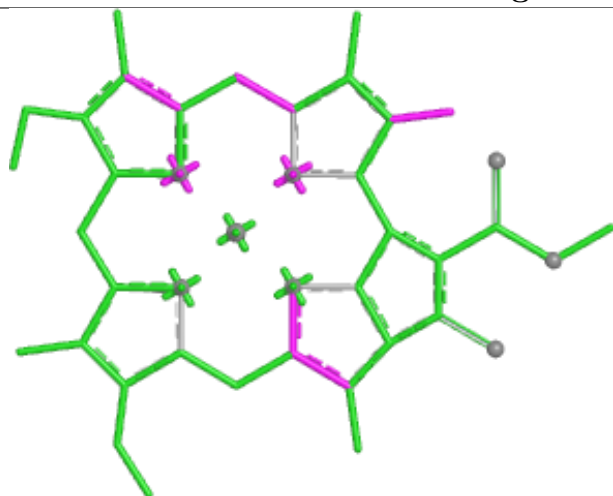
## Ligand CLA C 1459



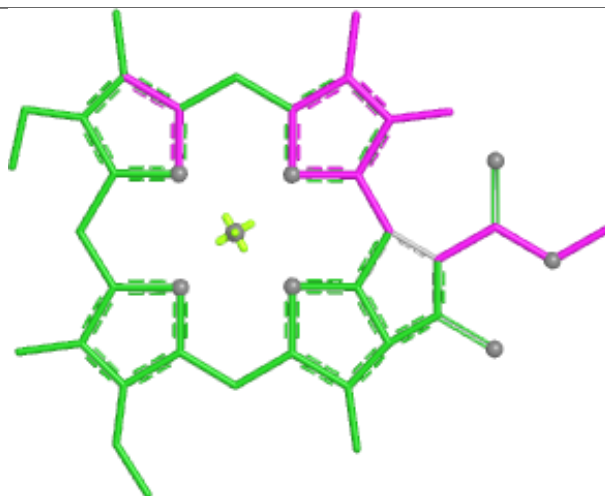
## Ligand CLA B 1484



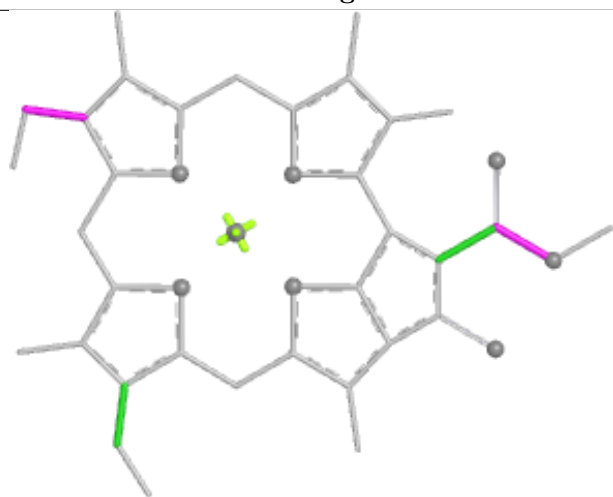
## Ligand CLA I 1469



Bond lengths



Bond angles

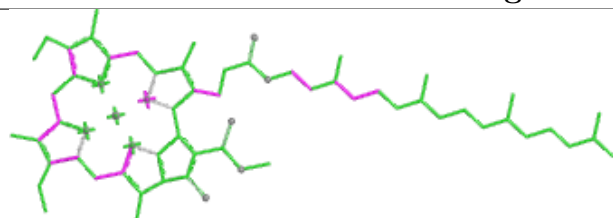


Torsions

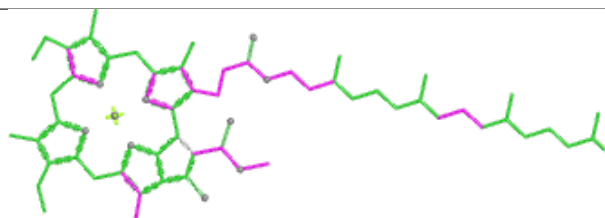


Rings

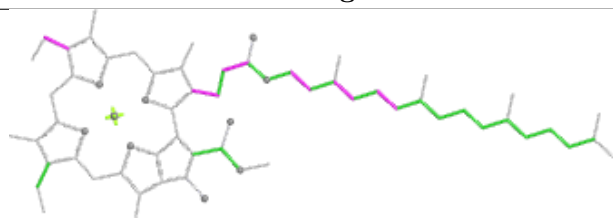
## Ligand CLA H 1487



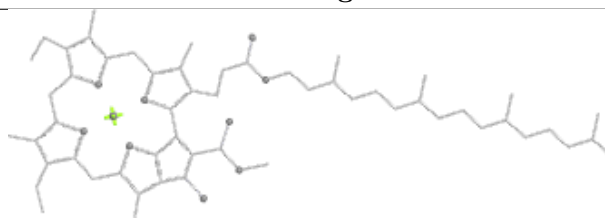
Bond lengths



Bond angles

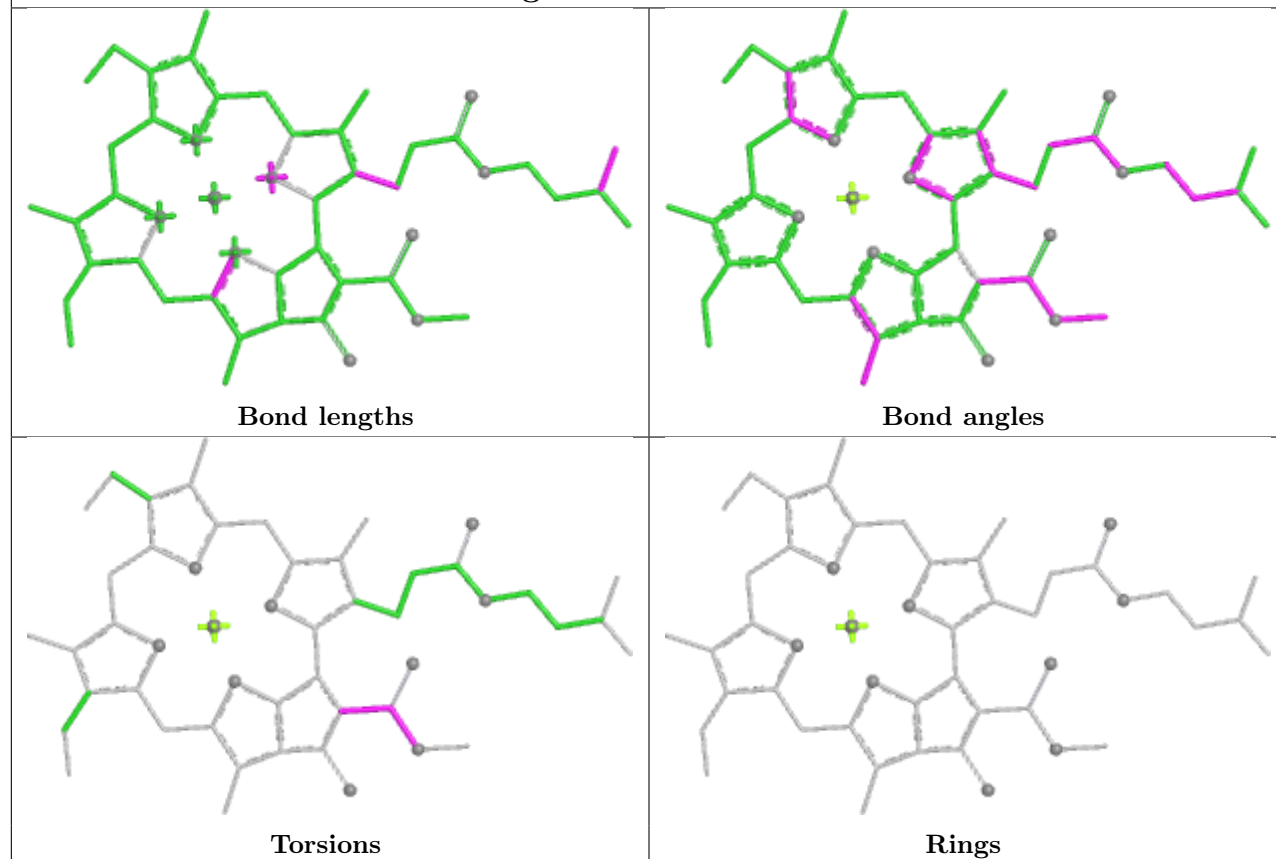


Torsions

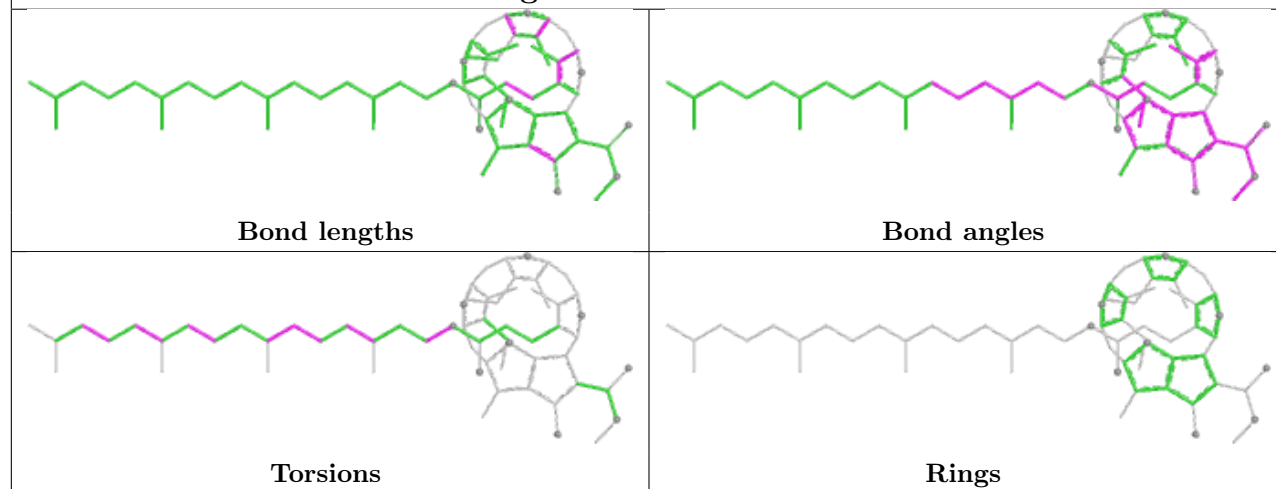


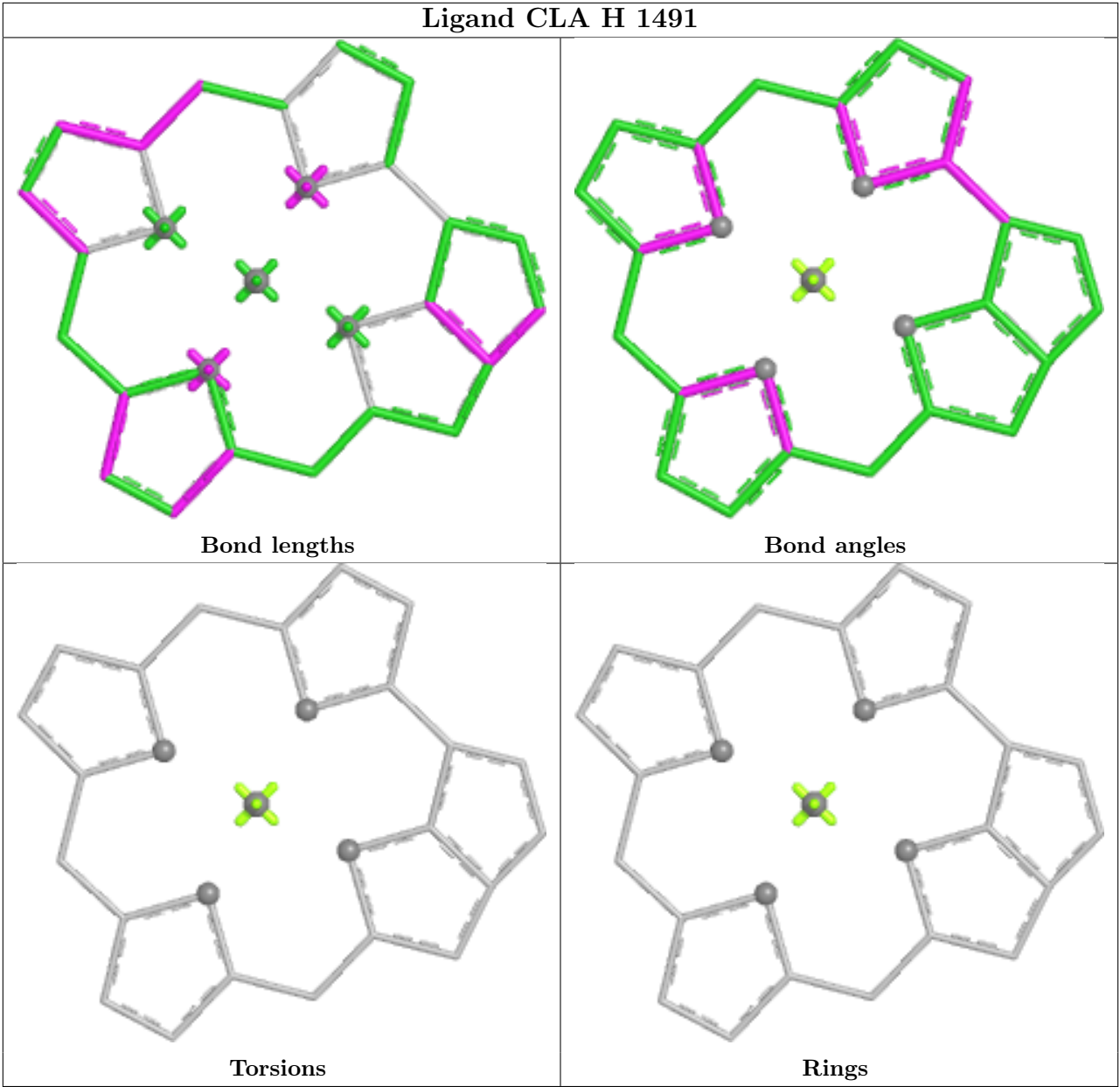
Rings

## Ligand CLA H 1489



## Ligand PHO A 1345





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 10  | Y     | 11               |
| 10  | X     | 11               |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 7   | O     | 5                |
| 7   | P     | 5                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | Y     | 185:UNK   | C      | 200:UNK   | N      | 108.56       |
| 1     | X     | 185:UNK   | C      | 200:UNK   | N      | 108.51       |
| 1     | X     | 374:UNK   | C      | 400:UNK   | N      | 87.82        |
| 1     | Y     | 374:UNK   | C      | 400:UNK   | N      | 87.78        |
| 1     | X     | 475:UNK   | C      | 501:UNK   | N      | 66.94        |
| 1     | Y     | 475:UNK   | C      | 501:UNK   | N      | 66.93        |
| 1     | Y     | 37:UNK    | C      | 52:UNK    | N      | 65.23        |
| 1     | X     | 37:UNK    | C      | 52:UNK    | N      | 65.16        |
| 1     | X     | 281:UNK   | C      | 310:UNK   | N      | 51.09        |
| 1     | Y     | 281:UNK   | C      | 310:UNK   | N      | 51.09        |
| 1     | X     | 537:UNK   | C      | 552:UNK   | N      | 45.76        |
| 1     | Y     | 537:UNK   | C      | 552:UNK   | N      | 45.74        |
| 1     | X     | 440:UNK   | C      | 451:UNK   | N      | 26.17        |
| 1     | Y     | 440:UNK   | C      | 451:UNK   | N      | 26.11        |
| 1     | Y     | 337:UNK   | C      | 355:UNK   | N      | 23.96        |
| 1     | X     | 337:UNK   | C      | 355:UNK   | N      | 23.90        |
| 1     | X     | 79:UNK    | C      | 106:UNK   | N      | 19.50        |
| 1     | Y     | 79:UNK    | C      | 106:UNK   | N      | 19.46        |
| 1     | O     | 95:UNK    | C      | 96:UNK    | N      | 11.66        |
| 1     | P     | 95:UNK    | C      | 96:UNK    | N      | 11.66        |
| 1     | P     | 85:UNK    | C      | 86:UNK    | N      | 9.75         |
| 1     | O     | 85:UNK    | C      | 86:UNK    | N      | 9.73         |
| 1     | P     | 36:UNK    | C      | 37:UNK    | N      | 9.25         |
| 1     | O     | 36:UNK    | C      | 37:UNK    | N      | 9.24         |
| 1     | Y     | 129:UNK   | C      | 157:UNK   | N      | 9.15         |
| 1     | X     | 129:UNK   | C      | 157:UNK   | N      | 9.11         |
| 1     | Y     | 227:UNK   | C      | 252:UNK   | N      | 8.97         |
| 1     | X     | 227:UNK   | C      | 252:UNK   | N      | 8.93         |
| 1     | P     | 146:UNK   | C      | 147:UNK   | N      | 5.82         |
| 1     | O     | 146:UNK   | C      | 147:UNK   | N      | 5.80         |
| 1     | O     | 47:UNK    | C      | 48:UNK    | N      | 4.68         |
| 1     | P     | 47:UNK    | C      | 48:UNK    | N      | 4.68         |

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.