



## Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 03:52 AM JST

PDB ID : 7CZL / pdb\_00007czl  
EMDB ID : EMD-30511  
Title : Structural insights into a dimeric Psb27-photosystem II complex from a cyanobacterium *Thermosynechococcus vulcanus*  
Authors : Pi, X.; Huang, G.; Xiao, Y.  
Deposited on : 2020-09-09  
Resolution : 3.78 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>  
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>.

---

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

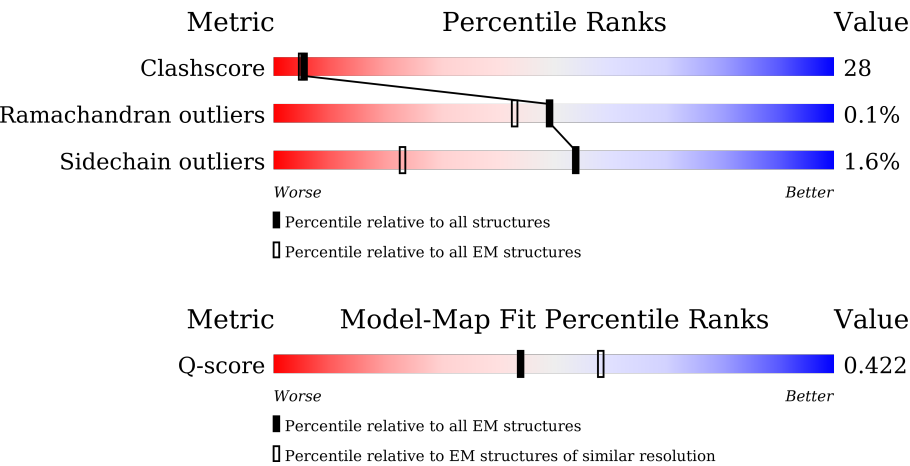
EMDB validation analysis : 0.0.1.dev133  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.50

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.78 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) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 10074 ( 3.28 - 4.27 )                                    |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                                |
|-----|-------|--------|-----------------------------------------------------------------|
| 1   | A     | 324    | <div><div></div><div>53%</div><div>46%</div><div>.</div></div>  |
| 1   | a     | 324    | <div><div></div><div>52%</div><div>47%</div><div>..</div></div> |
| 2   | B     | 505    | <div><div></div><div>54%</div><div>42%</div><div>.</div></div>  |
| 2   | b     | 505    | <div><div></div><div>53%</div><div>43%</div><div>.</div></div>  |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | C     | 446    |                  |
| 3   | c     | 446    |                  |
| 4   | D     | 339    |                  |
| 4   | d     | 339    |                  |
| 5   | E     | 65     |                  |
| 5   | e     | 65     |                  |
| 6   | F     | 31     |                  |
| 6   | f     | 31     |                  |
| 7   | H     | 62     |                  |
| 7   | h     | 62     |                  |
| 8   | I     | 34     |                  |
| 8   | i     | 34     |                  |
| 9   | K     | 37     |                  |
| 9   | k     | 37     |                  |
| 10  | L     | 37     |                  |
| 10  | l     | 37     |                  |
| 11  | M     | 33     |                  |
| 11  | m     | 33     |                  |
| 12  | T     | 30     |                  |
| 12  | t     | 30     |                  |
| 13  | Z     | 62     |                  |
| 13  | z     | 62     |                  |
| 14  | Y     | 30     |                  |
| 14  | y     | 30     |                  |
| 15  | N     | 108    |                  |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain                                                         |
|-----|-------|--------|--------------------------------------------------------------------------|
| 15  | n     | 108    | <div> <div>81%</div> <div>44%</div> <div>54%</div> </div>                |
| 16  | X     | 40     | <div> <div>20%</div> <div>48%</div> <div>20%</div> <div>12%</div> </div> |
| 16  | x     | 40     | <div> <div>30%</div> <div>40%</div> <div>18%</div> <div>12%</div> </div> |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 24  | BCT  | A     | 411  | -         | -        | X       | -                |
| 24  | BCT  | a     | 5412 | -         | -        | X       | -                |

## 2 Entry composition [i](#)

There are 30 unique types of molecules in this entry. The entry contains 40859 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem II protein D1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 324      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2533  | 1662 | 414 | 442 | 15 |         |       |
| 1   | a     | 322      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2523  | 1656 | 412 | 440 | 15 |         |       |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | 279     | PRO      | ARG    | conflict | UNP P51765 |
| A     | 286     | THR      | ALA    | conflict | UNP P51765 |
| a     | 5279    | PRO      | ARG    | conflict | UNP P51765 |
| a     | 5286    | THR      | ALA    | conflict | UNP P51765 |

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

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | B     | 484      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3784  | 2488 | 628 | 655 | 13 |         |       |
| 2   | b     | 484      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3780  | 2486 | 628 | 653 | 13 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| B     | 506     | ARG      | LYS    | conflict | UNP D0VWR1 |
| b     | 5506    | ARG      | LYS    | conflict | UNP D0VWR1 |

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

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | C     | 446      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3412  | 2240 | 570 | 589 | 13 |         |       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | c     | 446      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3412  | 2240 | 570 | 589 | 13 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | D     | 339      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2693  | 1786 | 438 | 457 | 12 |         |       |
| 4   | d     | 339      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2687  | 1783 | 435 | 457 | 12 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 5   | E     | 65       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 522   | 345 | 81 | 96 |         |       |
| 5   | e     | 65       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 522   | 345 | 81 | 96 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 6   | F     | 31       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 242   | 166 | 39 | 36 | 1 |         |       |
| 6   | f     | 28       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 219   | 149 | 36 | 33 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 7   | H     | 62       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 482   | 324 | 75 | 81 | 2 |         |       |
| 7   | h     | 62       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 482   | 324 | 75 | 81 | 2 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 8   | I     | 34       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 277   | 189 | 43 | 44 | 1 |         |       |
| 8   | i     | 34       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 277   | 189 | 43 | 44 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 9   | K     | 37       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 289   | 201 | 42 | 46 |         |       |
| 9   | k     | 34       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 264   | 186 | 36 | 42 |         |       |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| K     | 33      | LEU      | PHE    | conflict | UNP P19054 |
| K     | 39      | TRP      | VAL    | conflict | UNP P19054 |
| k     | 5033    | LEU      | PHE    | conflict | UNP P19054 |
| k     | 5039    | TRP      | VAL    | conflict | UNP P19054 |

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

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 10  | L     | 37       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 301   | 200 | 48 | 53 |         |       |
| 10  | l     | 37       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 301   | 200 | 48 | 53 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 11  | M     | 33       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 258   | 172 | 38 | 47 | 1 |         |       |
| 11  | m     | 33       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 258   | 172 | 38 | 47 | 1 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| M     | 8       | LEU      | PHE    | conflict | UNP P12312 |
| m     | 5008    | LEU      | PHE    | conflict | UNP P12312 |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 12  | T     | 30       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 254   | 179 | 36 | 37 | 2 |         |       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 12  | t     | 30       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 254   | 179 | 36 | 37 | 2 |         |       |

- Molecule 13 is a protein called Photosystem II reaction center protein Z.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 13  | Z     | 62       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 442   | 306 | 65 | 69 | 2 |         |       |
| 13  | z     | 62       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 442   | 306 | 65 | 69 | 2 |         |       |

- Molecule 14 is a protein called Photosystem II reaction center protein Ycf12.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 14  | Y     | 29       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 215   | 142 | 37 | 33 | 3 |         |       |
| 14  | y     | 29       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 215   | 142 | 37 | 33 | 3 |         |       |

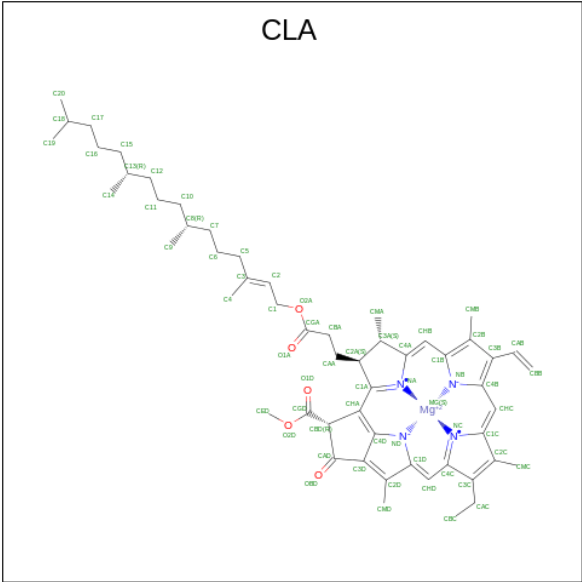
- Molecule 15 is a protein called Psb27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | n     | 108      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 860   | 536 | 155 | 167 | 2 |         |       |
| 15  | N     | 108      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 860   | 536 | 155 | 167 | 2 |         |       |

- Molecule 16 is a protein called Photosystem II reaction center protein X.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 16  | X     | 35       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 254   | 173 | 38 | 43 |         |       |
| 16  | x     | 35       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 254   | 173 | 38 | 43 |         |       |

- Molecule 17 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 |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 17  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 17  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 17  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 17  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 17  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 41    | 33 | 1  | 4 | 3 |         |
| 17  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 17  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 17  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 17  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 17  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 17  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 17  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 17  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 17  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 17  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 17  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 46 | 1  | 4 | 5 |         |
| 17  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 17  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 17  | C     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 17  | C     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 17  | C     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 17  | C     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 17  | C     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 17  | C     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 17  | C     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 17  | C     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 17  | C     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 37 | 1  | 4 | 5 |         |
| 17  | C     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 17  | C     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 17  | C     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |
| 17  | C     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 17  | D     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 17  | D     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |

*Continued on next page...*

*Continued from previous page...*

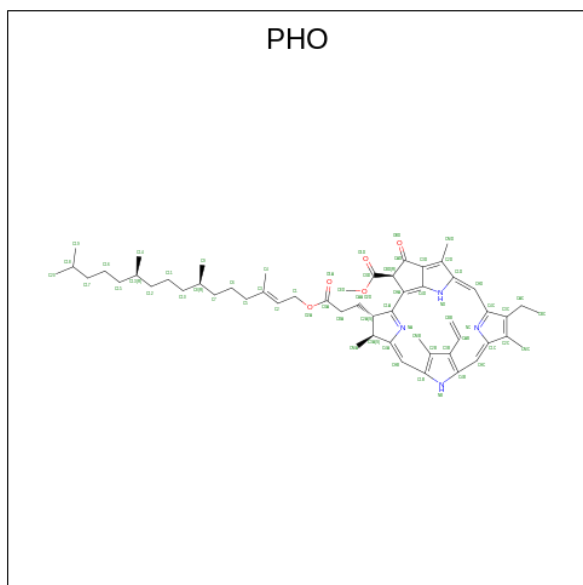
| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 17  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 17  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 17  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 17  | a     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 17  | b     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 17  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 17  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 17  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 17  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 17  | b     | 1        | Total<br>43 | C<br>35 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 17  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 17  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 17  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 17  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 17  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 17  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 17  | b     | 1        | Total<br>56 | C<br>46 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 17  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 17  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 17  | c     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

*Continued on next page...*

*Continued from previous page...*

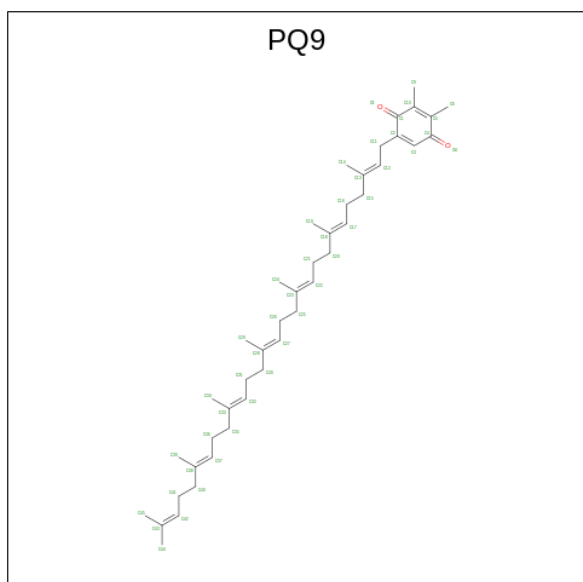
| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 17  | c     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 17  | c     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 17  | c     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 17  | c     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 17  | c     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 17  | c     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 17  | c     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 17  | c     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 37 | 1  | 4 | 5 |         |
| 17  | c     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 17  | c     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |
| 17  | c     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 17  | d     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 17  | d     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 17  | k     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |

- Molecule 18 is PHEOPHYTIN A (CCD ID: PHO) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>5</sub>).



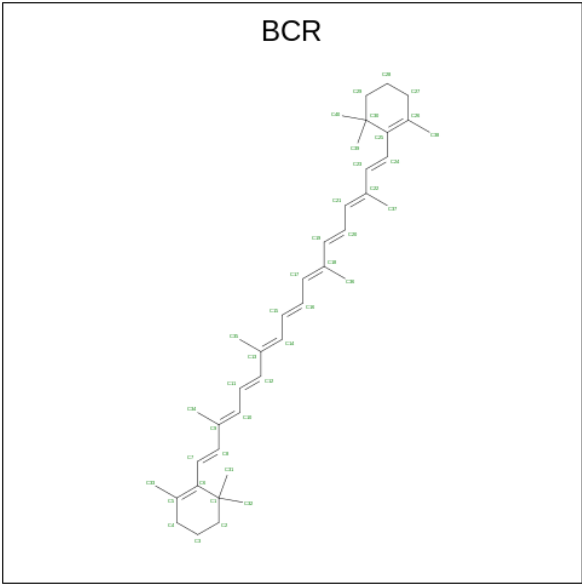
| Mol | Chain | Residues | Atoms |    |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 18  | A     | 1        | Total | C  | N | O | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |
| 18  | D     | 1        | Total | C  | N | O | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |
| 18  | a     | 1        | Total | C  | N | O | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |
| 18  | d     | 1        | Total | C  | N | O | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |

- Molecule 19 is 5-[(2E,6E,10E,14E,18E,22E)-3,7,11,15,19,23,27-HEPTAMETHYLOCTACOSA-2,6,10,14,18,22,26-HEPTAENYL]-2,3-DIMETHYLBENZO-1,4-QUINONE (CCD ID: PQ9) (formula:  $C_{43}H_{64}O_2$ ).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 19  | A     | 1        | Total | C  | O | 0       |
|     |       |          | 45    | 43 | 2 |         |
| 19  | D     | 1        | Total | C  | O | 0       |
|     |       |          | 45    | 43 | 2 |         |
| 19  | a     | 1        | Total | C  | O | 0       |
|     |       |          | 30    | 28 | 2 |         |
| 19  | d     | 1        | Total | C  | O | 0       |
|     |       |          | 45    | 43 | 2 |         |

- Molecule 20 is BETA-CAROTENE (CCD ID: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



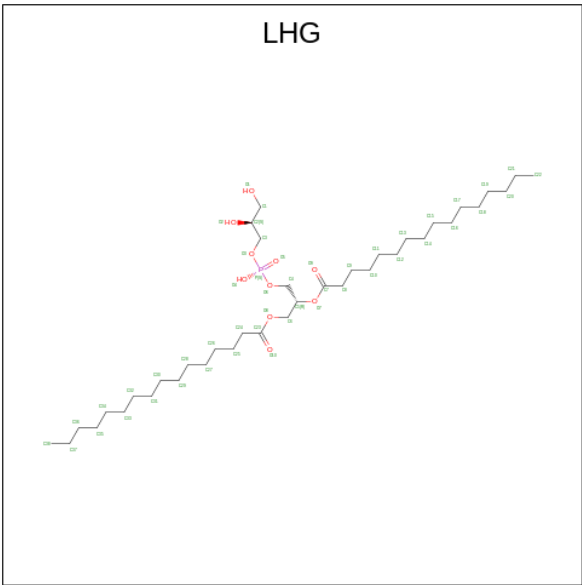
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 20  | A     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 20  | B     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 20  | B     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 20  | C     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 20  | C     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 20  | C     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 20  | D     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 20  | H     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |

Continued on next page...

*Continued from previous page...*

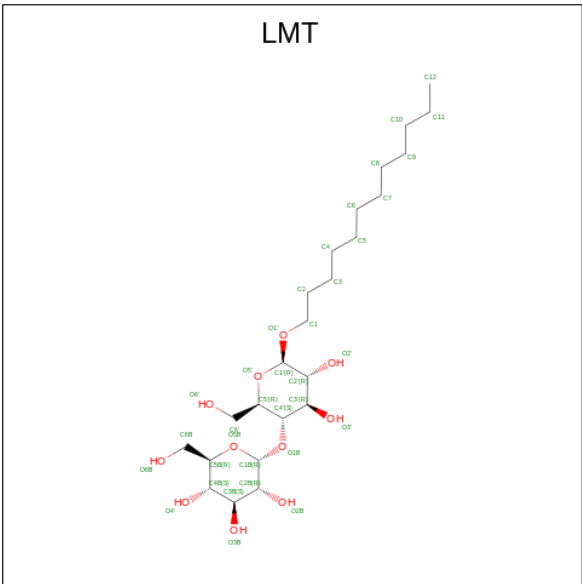
| Mol | Chain | Residues | Atoms            | AltConf |
|-----|-------|----------|------------------|---------|
| 20  | T     | 1        | Total C<br>40 40 | 0       |
| 20  | a     | 1        | Total C<br>40 40 | 0       |
| 20  | b     | 1        | Total C<br>40 40 | 0       |
| 20  | b     | 1        | Total C<br>40 40 | 0       |
| 20  | b     | 1        | Total C<br>40 40 | 0       |
| 20  | c     | 1        | Total C<br>40 40 | 0       |
| 20  | c     | 1        | Total C<br>40 40 | 0       |
| 20  | d     | 1        | Total C<br>40 40 | 0       |
| 20  | h     | 1        | Total C<br>40 40 | 0       |
| 20  | k     | 1        | Total C<br>40 40 | 0       |
| 20  | t     | 1        | Total C<br>40 40 | 0       |
| 20  | t     | 1        | Total C<br>40 40 | 0       |
| 20  | z     | 1        | Total C<br>40 40 | 0       |
| 20  | Y     | 1        | Total C<br>40 40 | 0       |

- Molecule 21 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 21  | A     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 39    | 28 | 10 | 1 |         |
| 21  | a     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 39    | 28 | 10 | 1 |         |

- Molecule 22 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>) (labeled as "Ligand of Interest" by depositor).



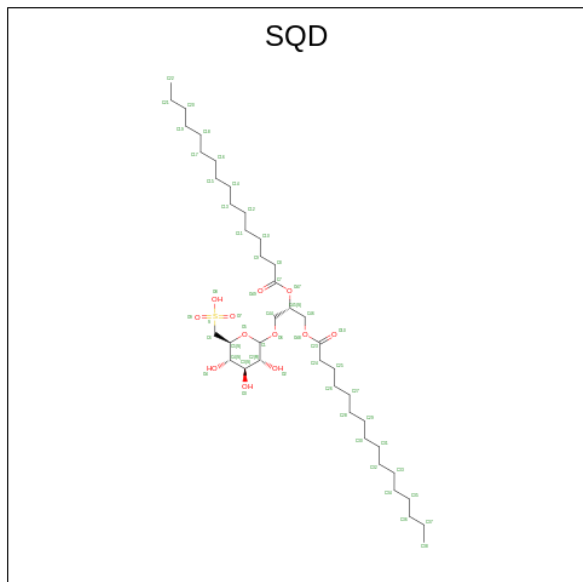
| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 22  | A     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |

Continued on next page...

Continued from previous page...

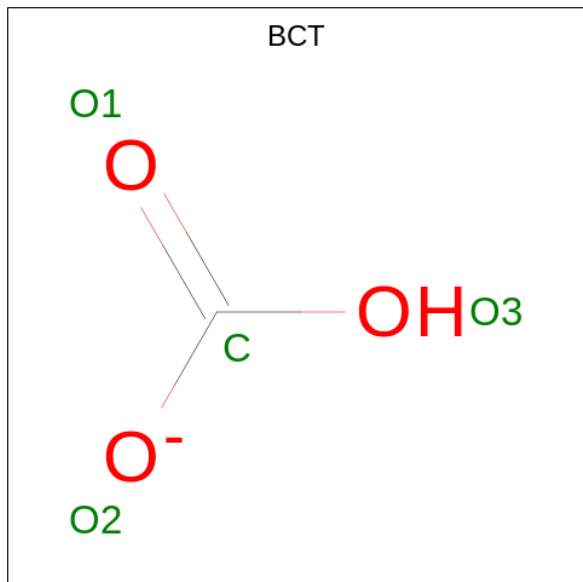
| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 22  | B     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 22  | M     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 22  | T     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 22  | a     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 22  | m     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |

- Molecule 23 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ).



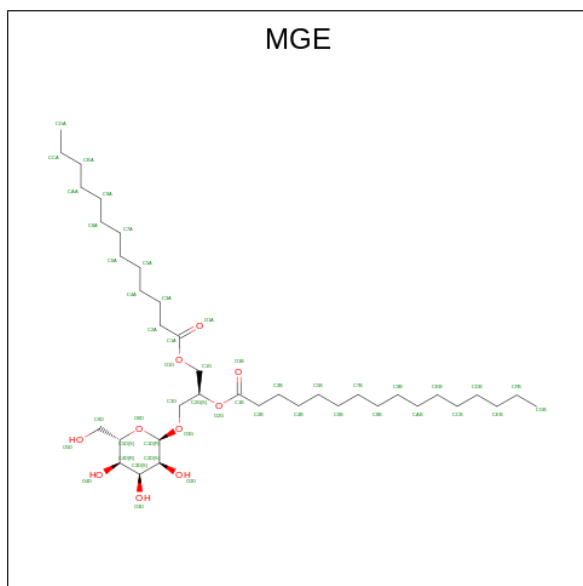
| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 23  | A     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 26    | 13 | 12 | 1 |         |
| 23  | D     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 54    | 41 | 12 | 1 |         |
| 23  | L     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 47    | 34 | 12 | 1 |         |
| 23  | a     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 26    | 13 | 12 | 1 |         |
| 23  | d     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 54    | 41 | 12 | 1 |         |
| 23  | l     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 47    | 34 | 12 | 1 |         |

- Molecule 24 is BICARBONATE ION (CCD ID: BCT) (formula:  $\text{CHO}_3$ ) (labeled as "Ligand of Interest" by depositor).



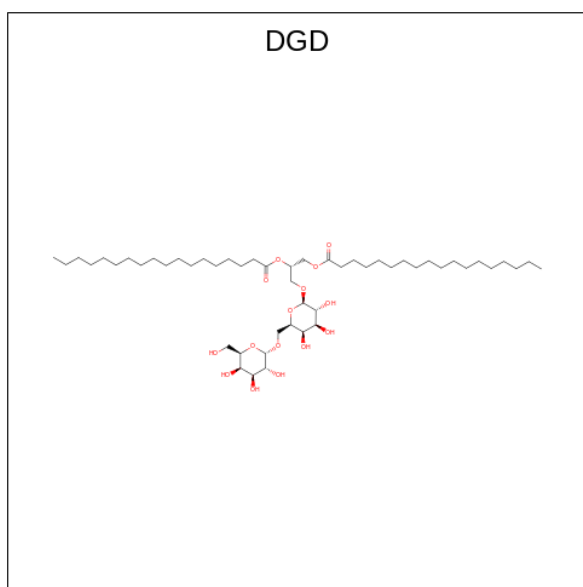
| Mol | Chain | Residues | Atoms |   |   | AltConf |
|-----|-------|----------|-------|---|---|---------|
| 24  | A     | 1        | Total | C | O | 0       |
|     |       |          | 4     | 1 | 3 |         |
| 24  | a     | 1        | Total | C | O | 0       |
|     |       |          | 4     | 1 | 3 |         |

- Molecule 25 is (1S)-2-(ALPHA-L-ALLOPYRANOSYLOXY)-1-[(TRIDECANOYLOXY)METHYL]ETHYL PALMITATE (CCD ID: MGE) (formula:  $\text{C}_{38}\text{H}_{72}\text{O}_{10}$ ).



| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 25  | A     | 1        | Total | C  | O  | 0       |
|     |       |          | 48    | 38 | 10 |         |
| 25  | B     | 1        | Total | C  | O  | 0       |
|     |       |          | 48    | 38 | 10 |         |
| 25  | C     | 1        | Total | C  | O  | 0       |
|     |       |          | 48    | 38 | 10 |         |
| 25  | D     | 1        | Total | C  | O  | 0       |
|     |       |          | 47    | 37 | 10 |         |
| 25  | D     | 1        | Total | C  | O  | 0       |
|     |       |          | 41    | 31 | 10 |         |
| 25  | D     | 1        | Total | C  | O  | 0       |
|     |       |          | 48    | 38 | 10 |         |
| 25  | b     | 1        | Total | C  | O  | 0       |
|     |       |          | 48    | 38 | 10 |         |
| 25  | c     | 1        | Total | C  | O  | 0       |
|     |       |          | 48    | 38 | 10 |         |
| 25  | d     | 1        | Total | C  | O  | 0       |
|     |       |          | 47    | 37 | 10 |         |
| 25  | d     | 1        | Total | C  | O  | 0       |
|     |       |          | 41    | 31 | 10 |         |
| 25  | d     | 1        | Total | C  | O  | 0       |
|     |       |          | 48    | 38 | 10 |         |
| 25  | l     | 1        | Total | C  | O  | 0       |
|     |       |          | 48    | 38 | 10 |         |
| 25  | m     | 1        | Total | C  | O  | 0       |
|     |       |          | 48    | 38 | 10 |         |
| 25  | m     | 1        | Total | C  | O  | 0       |
|     |       |          | 48    | 38 | 10 |         |

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



| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 26  | A     | 1        | Total | C  | O  | 0       |
|     |       |          | 53    | 38 | 15 |         |
| 26  | C     | 1        | Total | C  | O  | 0       |
|     |       |          | 47    | 32 | 15 |         |
| 26  | C     | 1        | Total | C  | O  | 0       |
|     |       |          | 57    | 42 | 15 |         |
| 26  | D     | 1        | Total | C  | O  | 0       |
|     |       |          | 54    | 39 | 15 |         |
| 26  | a     | 1        | Total | C  | O  | 0       |
|     |       |          | 57    | 42 | 15 |         |
| 26  | b     | 1        | Total | C  | O  | 0       |
|     |       |          | 54    | 39 | 15 |         |
| 26  | c     | 1        | Total | C  | O  | 0       |
|     |       |          | 53    | 38 | 15 |         |
| 26  | c     | 1        | Total | C  | O  | 0       |
|     |       |          | 47    | 32 | 15 |         |

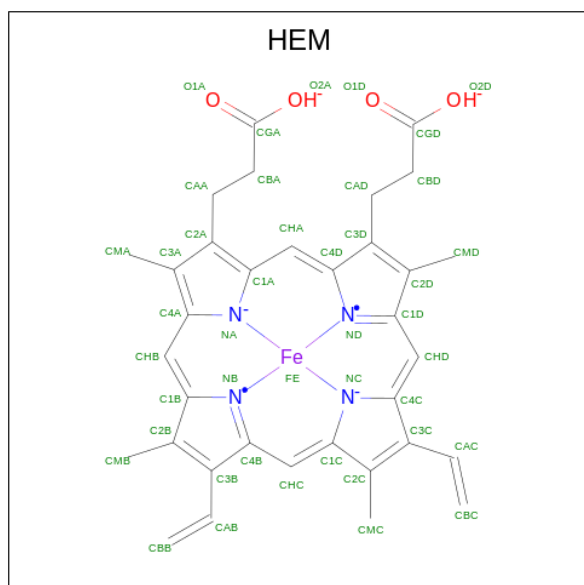
- Molecule 27 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 27  | C     | 1        | Total | Ca | 0       |
|     |       |          | 1     | 1  |         |
| 27  | c     | 1        | Total | Ca | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 28 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 28  | D     | 1        | Total | Fe | 0       |
|     |       |          | 1     | 1  |         |
| 28  | d     | 1        | Total | Fe | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 29 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 29  | F     | 1        | Total | C  | Fe | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |
| 29  | f     | 1        | Total | C  | Fe | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |

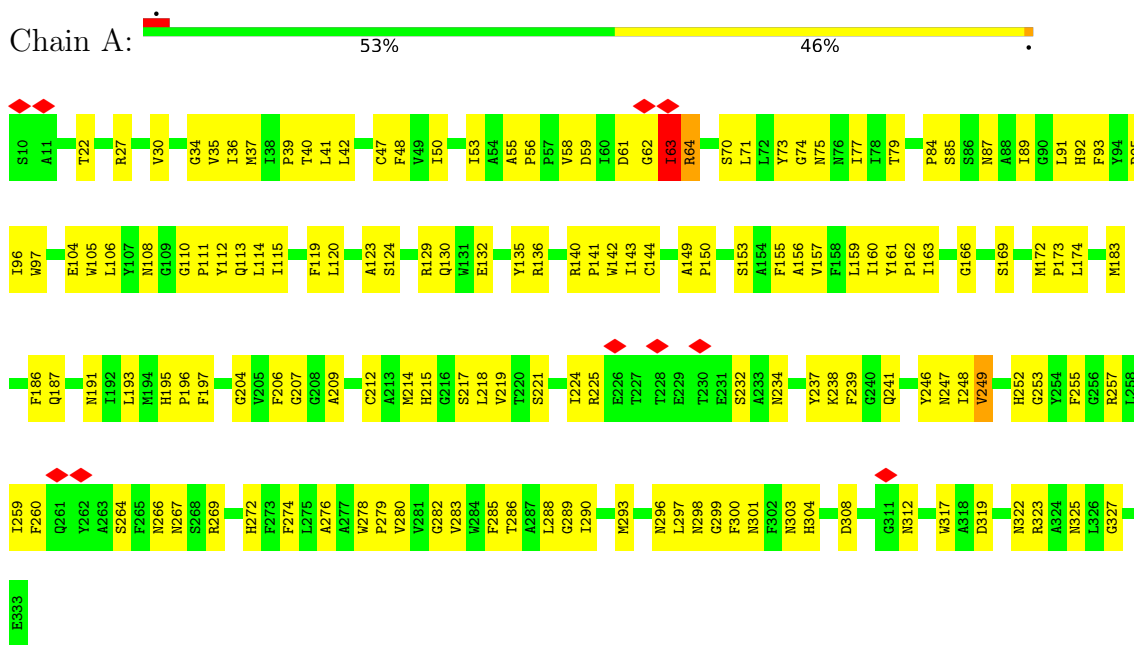
- Molecule 30 is CHLORIDE ION (CCD ID: CL) (formula:  $Cl$ ) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 30  | n     | 1        | Total | Cl | 0       |
|     |       |          | 1     | 1  |         |
| 30  | N     | 1        | Total | Cl | 0       |
|     |       |          | 1     | 1  |         |

### 3 Residue-property plots

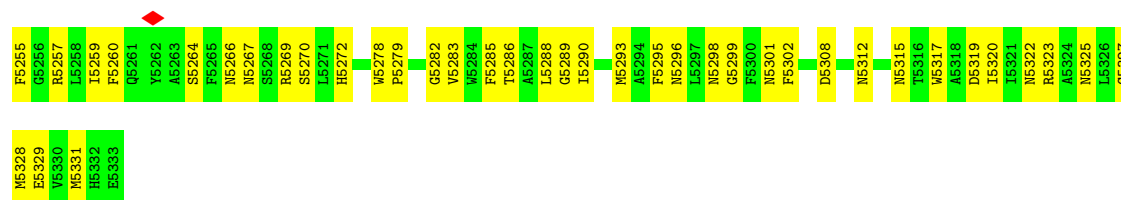
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Photosystem II protein D1

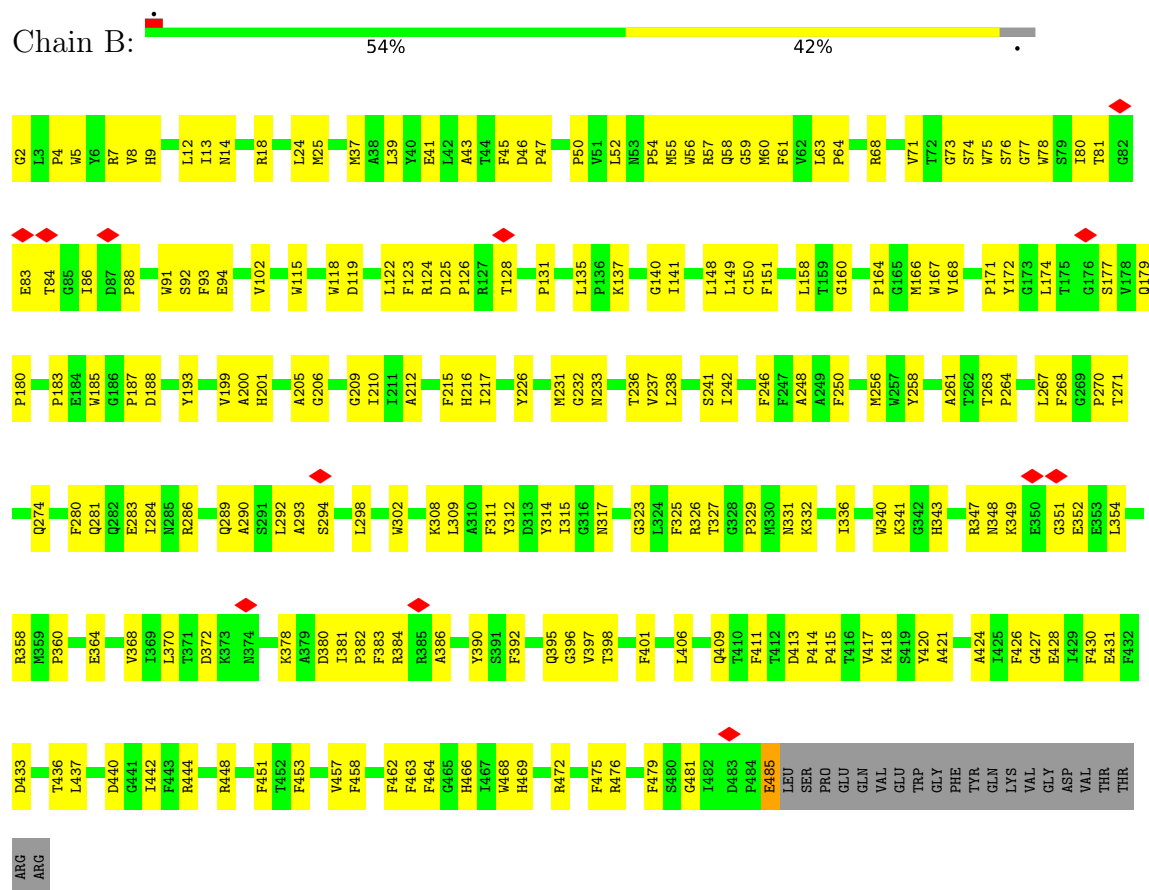


#### • Molecule 1: Photosystem II protein D1

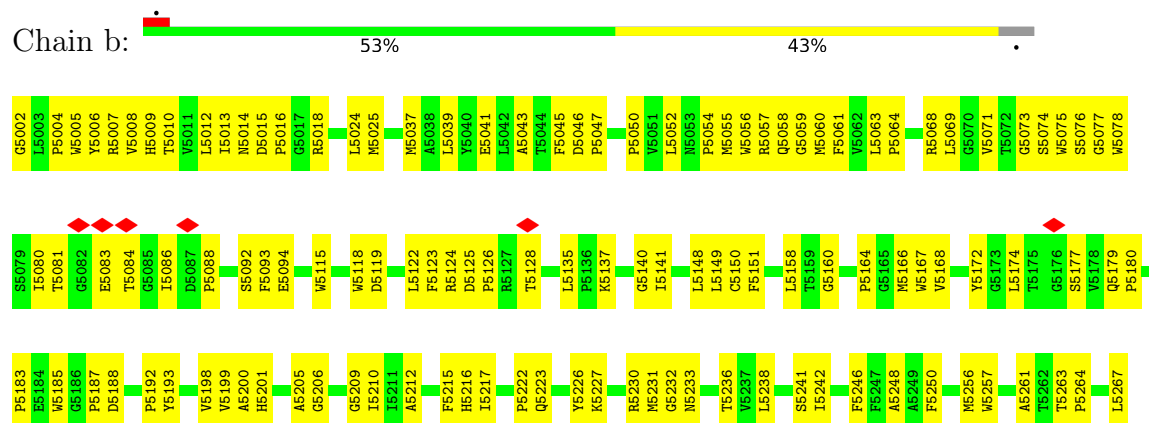


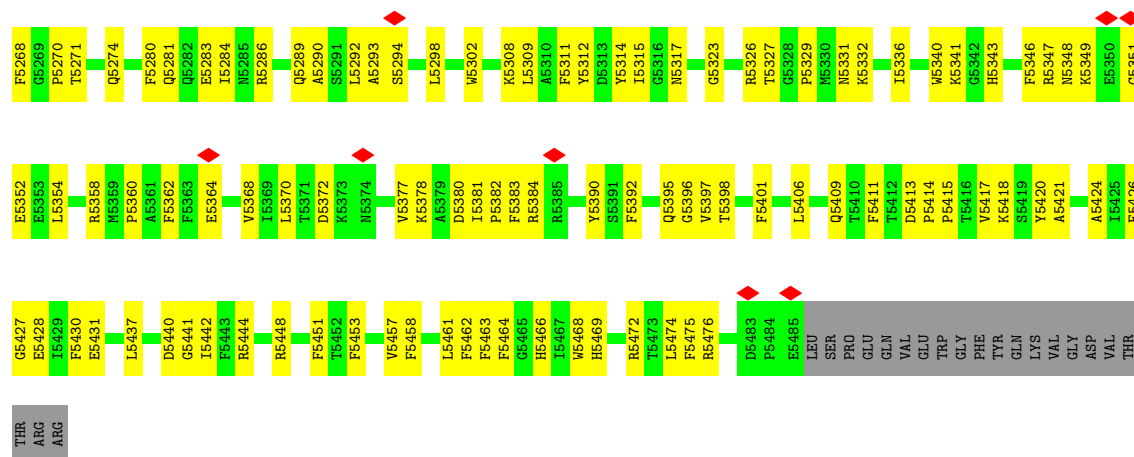


• Molecule 2: Photosystem II CP47 reaction center protein

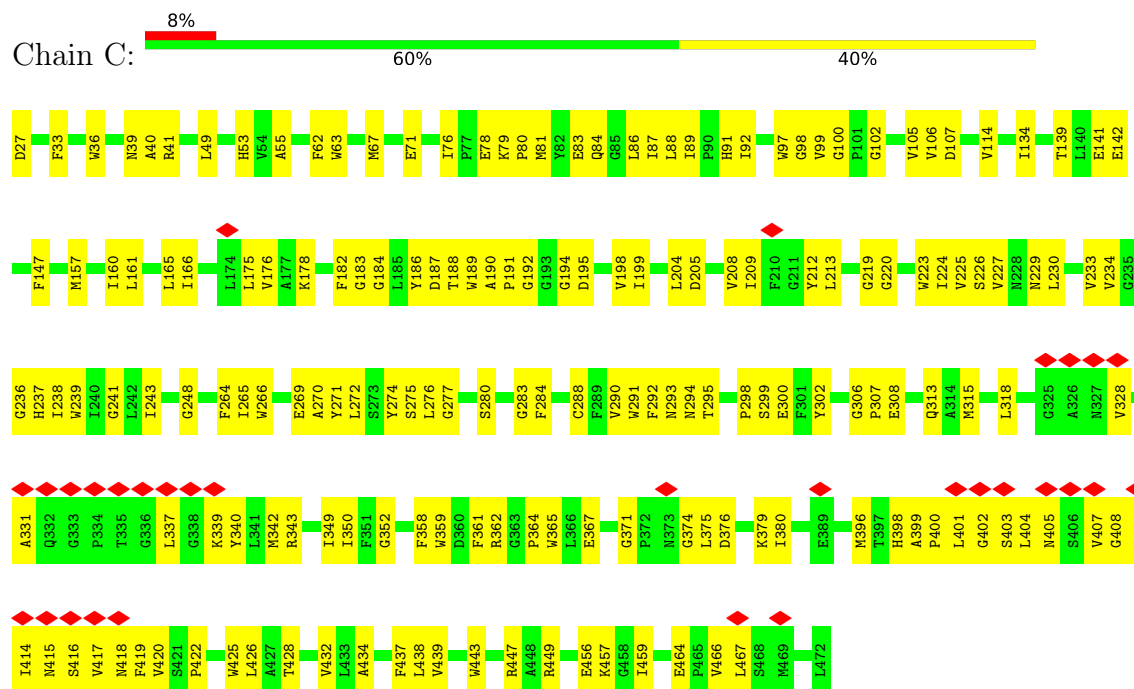


• Molecule 2: Photosystem II CP47 reaction center protein

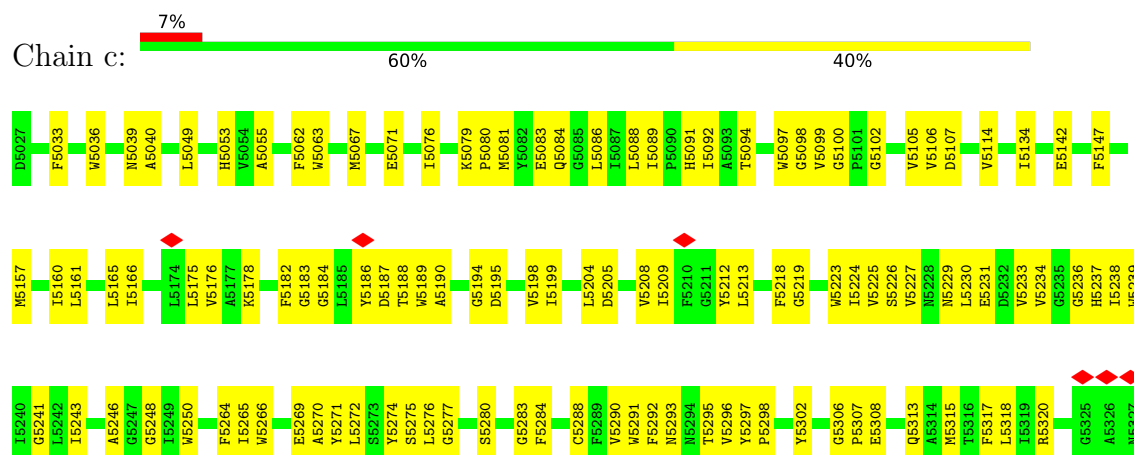




• Molecule 3: Photosystem II CP43 reaction center protein

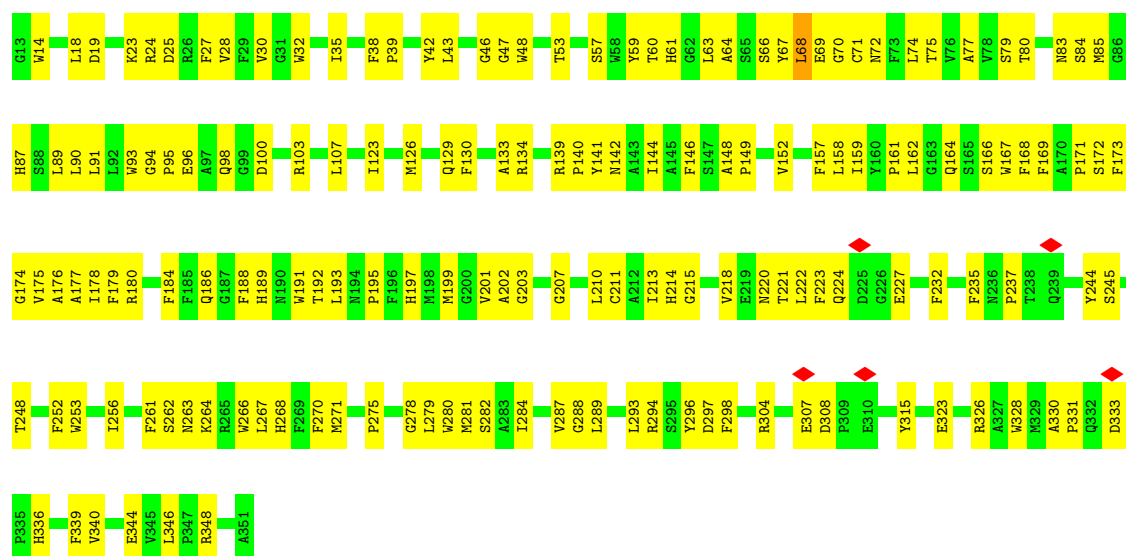


• Molecule 3: Photosystem II CP43 reaction center protein

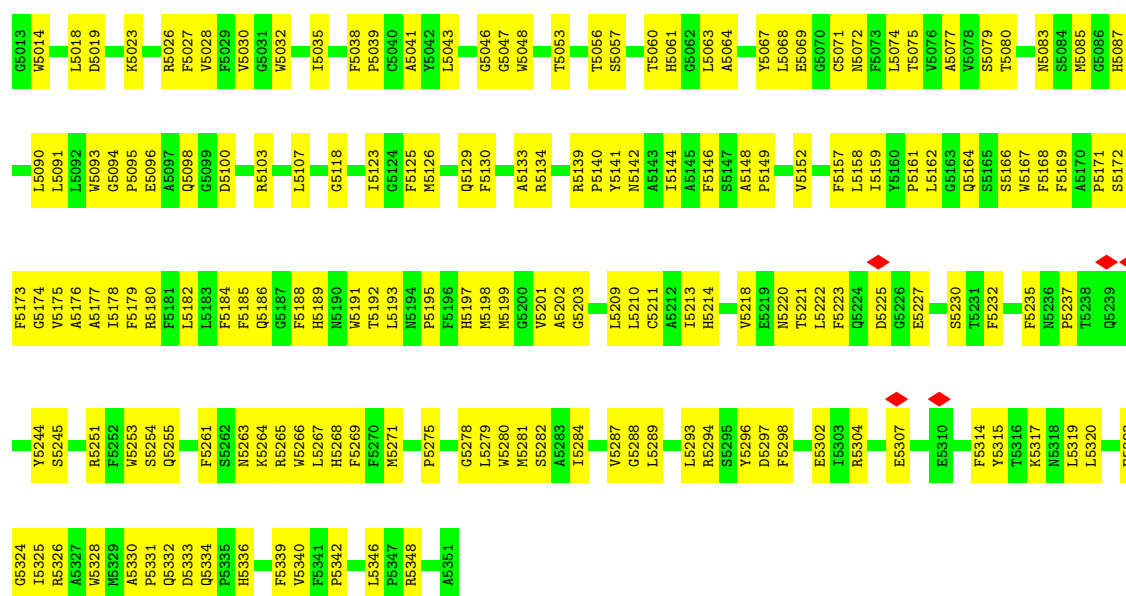




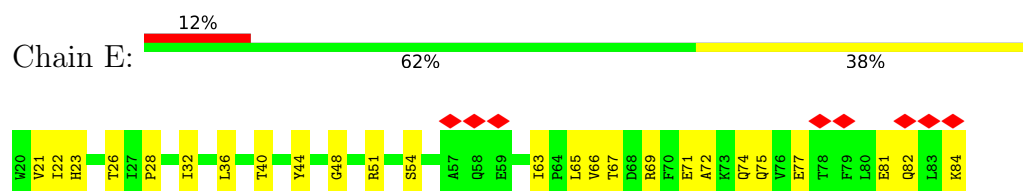
• Molecule 4: Photosystem II D2 protein



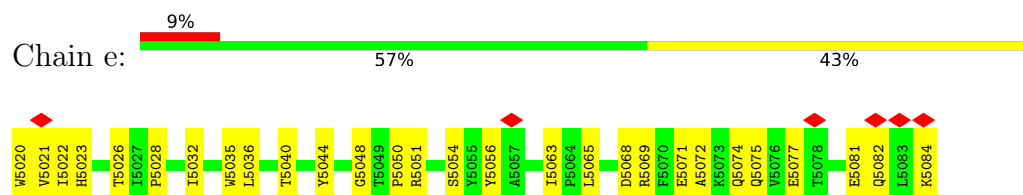
• Molecule 4: Photosystem II D2 protein



- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 5: Cytochrome b559 subunit alpha



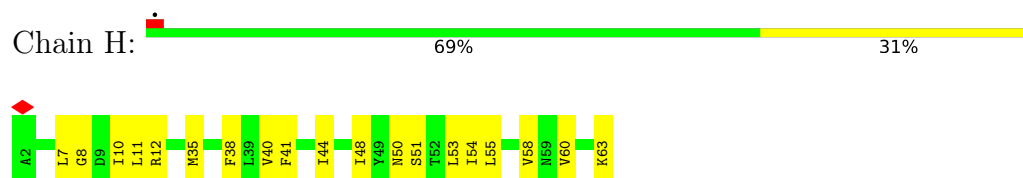
- Molecule 6: Cytochrome b559 subunit beta



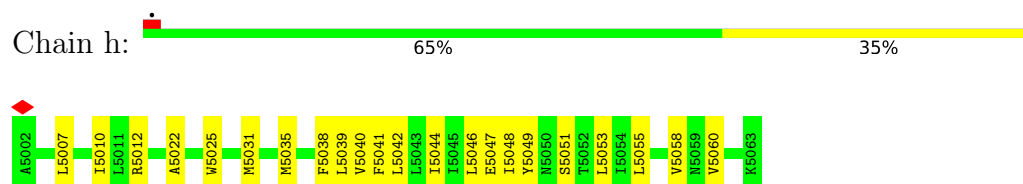
- Molecule 6: Cytochrome b559 subunit beta



- Molecule 7: Photosystem II reaction center protein H



- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I





- Molecule 8: Photosystem II reaction center protein I

Chain i: 76% 24%



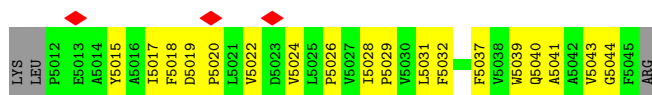
- Molecule 9: Photosystem II reaction center protein K

Chain K: 11% 51% 46%



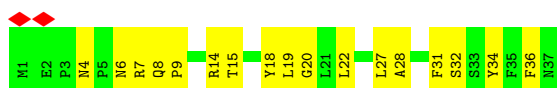
- Molecule 9: Photosystem II reaction center protein K

Chain k: 8% 43% 49% 8%



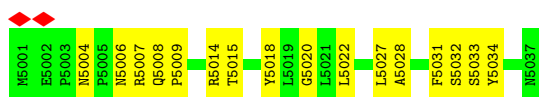
- Molecule 10: Photosystem II reaction center protein L

Chain L: 5% 54% 46%



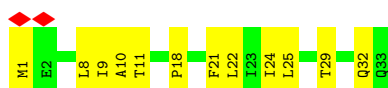
- Molecule 10: Photosystem II reaction center protein L

Chain l: 5% 57% 43%

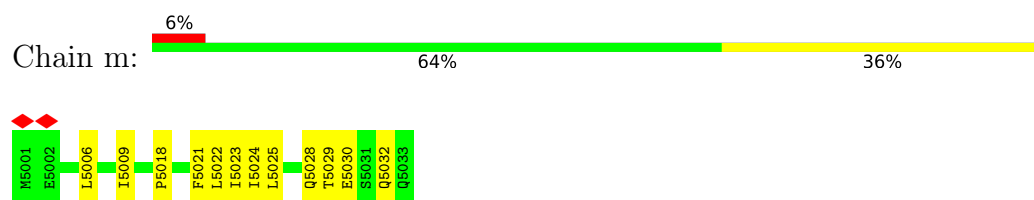


- Molecule 11: Photosystem II reaction center protein M

Chain M: 6% 64% 36%



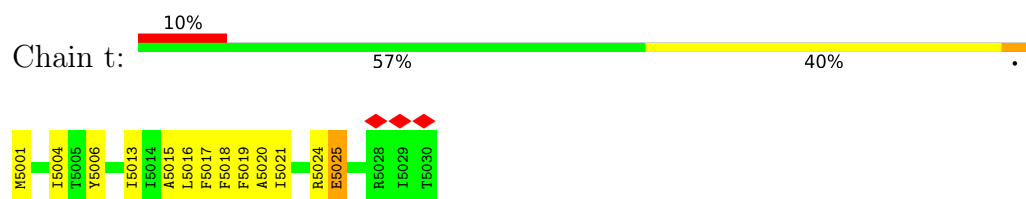
- Molecule 11: Photosystem II reaction center protein M



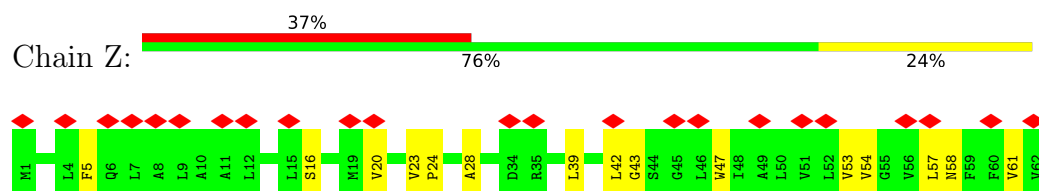
- Molecule 12: Photosystem II reaction center protein T



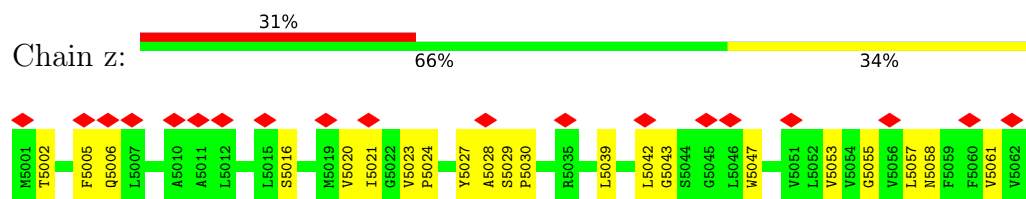
- Molecule 12: Photosystem II reaction center protein T



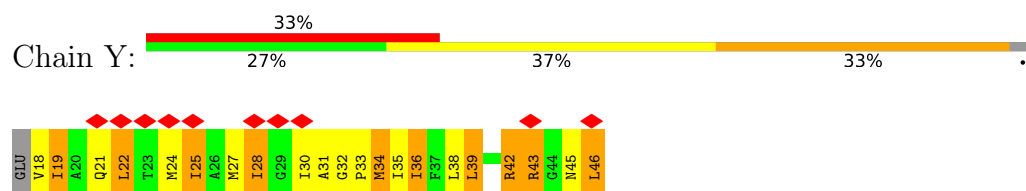
- Molecule 13: Photosystem II reaction center protein Z



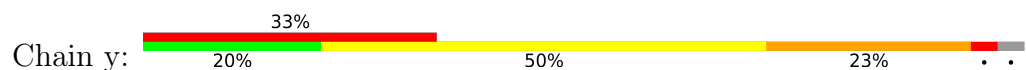
- Molecule 13: Photosystem II reaction center protein Z

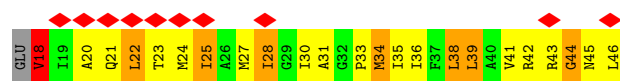


- Molecule 14: Photosystem II reaction center protein Ycf12

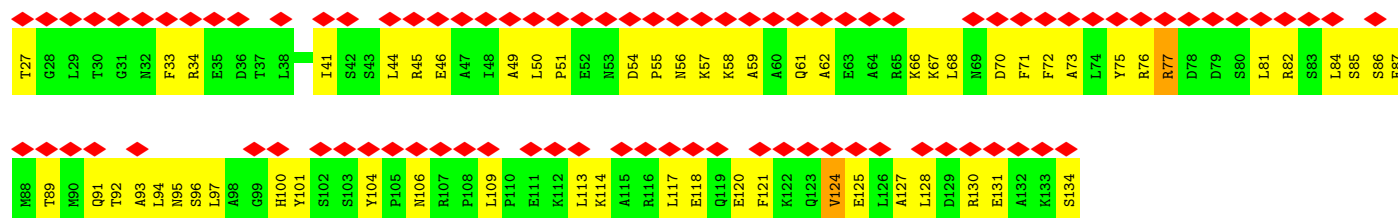
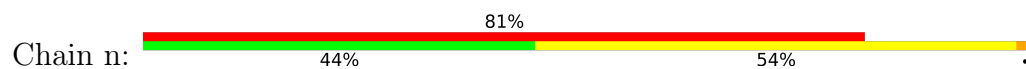


- Molecule 14: Photosystem II reaction center protein Ycf12

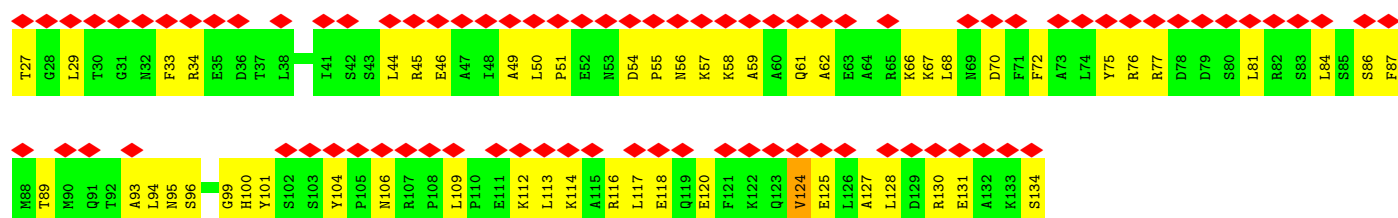
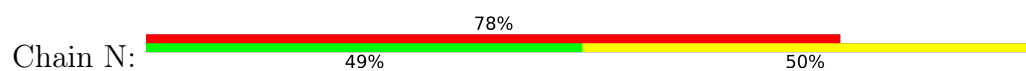




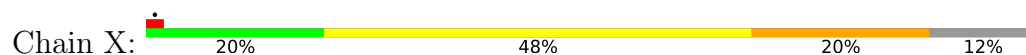
• Molecule 15: Psb27



• Molecule 15: Psb27



• Molecule 16: Photosystem II reaction center protein X



• Molecule 16: Photosystem II reaction center protein X



## 4 Experimental information

| Property                             | Value                        | Source    |
|--------------------------------------|------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE              | Depositor |
| Imposed symmetry                     | POINT, Not provided          |           |
| Number of particles used             | 87473                        | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF            | Depositor |
| CTF correction method                | NONE                         | Depositor |
| Microscope                           | FEI TITAN KRIOS              | Depositor |
| Voltage (kV)                         | 300                          | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                           | Depositor |
| Minimum defocus (nm)                 | Not provided                 |           |
| Maximum defocus (nm)                 | Not provided                 |           |
| Magnification                        | Not provided                 |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)    | Depositor |
| Maximum map value                    | 0.227                        | Depositor |
| Minimum map value                    | -0.125                       | Depositor |
| Average map value                    | 0.001                        | Depositor |
| Map value standard deviation         | 0.009                        | Depositor |
| Recommended contour level            | 0.038                        | Depositor |
| Map size ( $\text{\AA}$ )            | 313.5696, 313.5696, 313.5696 | wwPDB     |
| Map dimensions                       | 240, 240, 240                | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0             | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.30654, 1.30654, 1.30654    | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FE2, LHG, CL, CLA, PQ9, HEM, LMT, MGE, PHO, BCR, SQD, CA, DGD, BCT

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     | 0.44         | 0/2615        | 0.53        | 4/3568 (0.1%) |
| 1   | a     | 0.44         | 0/2605        | 0.50        | 1/3554 (0.0%) |
| 2   | B     | 0.45         | 0/3919        | 0.51        | 0/5343        |
| 2   | b     | 0.45         | 0/3915        | 0.51        | 0/5338        |
| 3   | C     | 0.38         | 0/3524        | 0.48        | 0/4804        |
| 3   | c     | 0.38         | 0/3524        | 0.49        | 1/4804 (0.0%) |
| 4   | D     | 0.48         | 1/2788 (0.0%) | 0.52        | 2/3802 (0.1%) |
| 4   | d     | 0.49         | 1/2782 (0.0%) | 0.50        | 0/3795        |
| 5   | E     | 0.29         | 0/538         | 0.50        | 0/737         |
| 5   | e     | 0.29         | 0/538         | 0.50        | 0/737         |
| 6   | F     | 0.30         | 0/250         | 0.50        | 0/342         |
| 6   | f     | 0.29         | 0/225         | 0.41        | 0/308         |
| 7   | H     | 0.37         | 0/495         | 0.49        | 0/678         |
| 7   | h     | 0.37         | 0/495         | 0.49        | 0/678         |
| 8   | I     | 0.36         | 0/284         | 0.40        | 0/384         |
| 8   | i     | 0.36         | 0/284         | 0.40        | 0/384         |
| 9   | K     | 0.37         | 0/299         | 0.65        | 0/412         |
| 9   | k     | 0.38         | 0/274         | 0.65        | 0/379         |
| 10  | L     | 0.41         | 0/308         | 0.47        | 0/419         |
| 10  | l     | 0.41         | 0/308         | 0.48        | 0/419         |
| 11  | M     | 0.39         | 0/261         | 0.51        | 0/356         |
| 11  | m     | 0.38         | 0/261         | 0.45        | 0/356         |
| 12  | T     | 0.51         | 0/263         | 0.48        | 0/356         |
| 12  | t     | 0.51         | 0/263         | 0.48        | 0/356         |
| 13  | Z     | 0.19         | 0/451         | 0.31        | 0/620         |
| 13  | z     | 0.19         | 0/451         | 0.32        | 0/620         |
| 14  | Y     | 0.30         | 0/216         | 0.70        | 0/289         |
| 14  | y     | 0.53         | 0/216         | 1.43        | 6/289 (2.1%)  |
| 15  | N     | 0.28         | 0/873         | 0.46        | 0/1172        |
| 15  | n     | 0.21         | 0/873         | 0.43        | 0/1172        |
| 16  | X     | 0.41         | 0/257         | 0.83        | 1/348 (0.3%)  |
| 16  | x     | 0.34         | 0/257         | 0.77        | 0/348         |

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5         |
| All | All   | 0.42         | 2/34612 (0.0%) | 0.51        | 15/47167 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 2                   |
| 1   | a     | 0                   | 2                   |
| 9   | K     | 0                   | 2                   |
| 9   | k     | 0                   | 2                   |
| 14  | y     | 0                   | 1                   |
| All | All   | 0                   | 9                   |

All (2) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 4   | D     | 340  | VAL  | C-N   | -5.98 | 1.21        | 1.33     |
| 4   | d     | 5340 | VAL  | C-N   | -5.96 | 1.21        | 1.33     |

All (15) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 14  | y     | 28   | ILE  | CA-C-N     | -8.76 | 104.23      | 121.41   |
| 14  | y     | 28   | ILE  | C-N-CA     | -8.76 | 104.23      | 121.41   |
| 1   | A     | 249  | VAL  | CG1-CB-CG2 | -7.19 | 94.98       | 110.80   |
| 14  | y     | 20   | ALA  | N-CA-C     | -7.07 | 103.51      | 111.14   |
| 1   | A     | 64   | ARG  | N-CA-C     | 6.17  | 123.94      | 110.80   |
| 14  | y     | 28   | ILE  | N-CA-C     | 6.17  | 116.91      | 110.62   |
| 3   | c     | 5410 | VAL  | CG1-CB-CG2 | -6.12 | 97.33       | 110.80   |
| 4   | D     | 68   | LEU  | CA-C-N     | -5.94 | 110.19      | 121.54   |
| 4   | D     | 68   | LEU  | C-N-CA     | -5.94 | 110.19      | 121.54   |
| 1   | A     | 63   | ILE  | CA-C-N     | 5.87  | 132.75      | 121.54   |
| 1   | A     | 63   | ILE  | C-N-CA     | 5.87  | 132.75      | 121.54   |
| 1   | a     | 5249 | VAL  | CG1-CB-CG2 | 5.61  | 123.14      | 110.80   |
| 16  | X     | 5    | PRO  | N-CA-C     | -5.48 | 105.91      | 113.53   |
| 14  | y     | 18   | VAL  | CA-C-N     | 5.38  | 128.05      | 120.42   |
| 14  | y     | 18   | VAL  | C-N-CA     | 5.38  | 128.05      | 120.42   |

There are no chirality outliers.

All (9) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | A     | 63   | ILE  | Mainchain |
| 1   | A     | 64   | ARG  | Peptide   |
| 9   | K     | 17   | ILE  | Peptide   |
| 9   | K     | 24   | VAL  | Peptide   |
| 1   | a     | 5063 | ILE  | Mainchain |
| 1   | a     | 5064 | ARG  | Peptide   |
| 9   | k     | 5017 | ILE  | Peptide   |
| 9   | k     | 5024 | VAL  | Peptide   |
| 14  | y     | 18   | VAL  | Mainchain |

## 5.2 Too-close contacts [i](#)

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     | 2533  | 0        | 2433     | 168     | 0            |
| 1   | a     | 2523  | 0        | 2426     | 161     | 0            |
| 2   | B     | 3784  | 0        | 3634     | 194     | 0            |
| 2   | b     | 3780  | 0        | 3630     | 197     | 0            |
| 3   | C     | 3412  | 0        | 3321     | 180     | 0            |
| 3   | c     | 3412  | 0        | 3321     | 175     | 0            |
| 4   | D     | 2693  | 0        | 2591     | 193     | 0            |
| 4   | d     | 2687  | 0        | 2580     | 215     | 0            |
| 5   | E     | 522   | 0        | 500      | 19      | 0            |
| 5   | e     | 522   | 0        | 500      | 20      | 0            |
| 6   | F     | 242   | 0        | 247      | 14      | 0            |
| 6   | f     | 219   | 0        | 228      | 11      | 0            |
| 7   | H     | 482   | 0        | 488      | 32      | 0            |
| 7   | h     | 482   | 0        | 488      | 38      | 0            |
| 8   | I     | 277   | 0        | 295      | 14      | 0            |
| 8   | i     | 277   | 0        | 292      | 7       | 0            |
| 9   | K     | 289   | 0        | 294      | 37      | 0            |
| 9   | k     | 264   | 0        | 269      | 44      | 0            |
| 10  | L     | 301   | 0        | 309      | 19      | 0            |
| 10  | l     | 301   | 0        | 306      | 19      | 0            |
| 11  | M     | 258   | 0        | 276      | 16      | 0            |
| 11  | m     | 258   | 0        | 273      | 11      | 0            |
| 12  | T     | 254   | 0        | 254      | 18      | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 12  | t     | 254   | 0        | 254      | 18      | 0            |
| 13  | Z     | 442   | 0        | 460      | 18      | 0            |
| 13  | z     | 442   | 0        | 457      | 38      | 0            |
| 14  | Y     | 215   | 0        | 246      | 60      | 0            |
| 14  | y     | 215   | 0        | 246      | 95      | 0            |
| 15  | N     | 860   | 0        | 864      | 54      | 0            |
| 15  | n     | 860   | 0        | 864      | 58      | 0            |
| 16  | X     | 254   | 0        | 284      | 60      | 0            |
| 16  | x     | 254   | 0        | 284      | 74      | 0            |
| 17  | A     | 250   | 0        | 265      | 28      | 0            |
| 17  | B     | 1007  | 0        | 1086     | 101     | 0            |
| 17  | C     | 774   | 0        | 781      | 65      | 0            |
| 17  | D     | 115   | 0        | 111      | 12      | 0            |
| 17  | a     | 250   | 0        | 265      | 28      | 0            |
| 17  | b     | 985   | 0        | 1045     | 96      | 0            |
| 17  | c     | 709   | 0        | 709      | 54      | 0            |
| 17  | d     | 115   | 0        | 111      | 9       | 0            |
| 17  | k     | 65    | 0        | 72       | 7       | 0            |
| 18  | A     | 64    | 0        | 74       | 7       | 0            |
| 18  | D     | 64    | 0        | 74       | 7       | 0            |
| 18  | a     | 64    | 0        | 74       | 9       | 0            |
| 18  | d     | 64    | 0        | 74       | 14      | 0            |
| 19  | A     | 45    | 0        | 64       | 7       | 0            |
| 19  | D     | 45    | 0        | 64       | 7       | 0            |
| 19  | a     | 30    | 0        | 37       | 2       | 0            |
| 19  | d     | 45    | 0        | 64       | 8       | 0            |
| 20  | A     | 40    | 0        | 56       | 3       | 0            |
| 20  | B     | 80    | 0        | 112      | 7       | 0            |
| 20  | C     | 120   | 0        | 168      | 12      | 0            |
| 20  | D     | 40    | 0        | 56       | 5       | 0            |
| 20  | H     | 40    | 0        | 54       | 6       | 0            |
| 20  | T     | 40    | 0        | 56       | 6       | 0            |
| 20  | Y     | 40    | 0        | 54       | 9       | 0            |
| 20  | a     | 40    | 0        | 56       | 5       | 0            |
| 20  | b     | 120   | 0        | 168      | 12      | 0            |
| 20  | c     | 80    | 0        | 112      | 9       | 0            |
| 20  | d     | 40    | 0        | 56       | 4       | 0            |
| 20  | h     | 40    | 0        | 54       | 7       | 0            |
| 20  | k     | 40    | 0        | 56       | 9       | 0            |
| 20  | t     | 80    | 0        | 112      | 9       | 0            |
| 20  | z     | 40    | 0        | 56       | 4       | 0            |
| 21  | A     | 39    | 0        | 51       | 2       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 21  | a     | 39    | 0        | 51       | 3       | 0            |
| 22  | A     | 35    | 0        | 45       | 3       | 0            |
| 22  | B     | 35    | 0        | 43       | 1       | 0            |
| 22  | M     | 35    | 0        | 44       | 2       | 0            |
| 22  | T     | 35    | 0        | 43       | 0       | 0            |
| 22  | a     | 35    | 0        | 45       | 0       | 0            |
| 22  | m     | 35    | 0        | 44       | 1       | 0            |
| 23  | A     | 26    | 0        | 15       | 0       | 0            |
| 23  | D     | 54    | 0        | 77       | 6       | 0            |
| 23  | L     | 47    | 0        | 61       | 16      | 0            |
| 23  | a     | 26    | 0        | 16       | 0       | 0            |
| 23  | d     | 54    | 0        | 77       | 2       | 0            |
| 23  | l     | 47    | 0        | 61       | 13      | 0            |
| 24  | A     | 4     | 0        | 1        | 8       | 0            |
| 24  | a     | 4     | 0        | 1        | 6       | 0            |
| 25  | A     | 48    | 0        | 69       | 12      | 0            |
| 25  | B     | 48    | 0        | 72       | 6       | 0            |
| 25  | C     | 48    | 0        | 72       | 5       | 0            |
| 25  | D     | 136   | 0        | 192      | 24      | 0            |
| 25  | b     | 48    | 0        | 72       | 6       | 0            |
| 25  | c     | 48    | 0        | 72       | 5       | 0            |
| 25  | d     | 136   | 0        | 194      | 25      | 0            |
| 25  | l     | 48    | 0        | 72       | 9       | 0            |
| 25  | m     | 96    | 0        | 143      | 19      | 0            |
| 26  | A     | 53    | 0        | 60       | 7       | 0            |
| 26  | C     | 104   | 0        | 124      | 3       | 0            |
| 26  | D     | 54    | 0        | 64       | 7       | 0            |
| 26  | a     | 57    | 0        | 72       | 2       | 0            |
| 26  | b     | 54    | 0        | 64       | 7       | 0            |
| 26  | c     | 100   | 0        | 112      | 7       | 0            |
| 27  | C     | 1     | 0        | 0        | 0       | 0            |
| 27  | c     | 1     | 0        | 0        | 0       | 0            |
| 28  | D     | 1     | 0        | 0        | 0       | 0            |
| 28  | d     | 1     | 0        | 0        | 0       | 0            |
| 29  | F     | 43    | 0        | 30       | 8       | 0            |
| 29  | f     | 43    | 0        | 30       | 4       | 0            |
| 30  | N     | 1     | 0        | 0        | 0       | 0            |
| 30  | n     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 40859 | 0        | 41299    | 2300    | 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 28.

All (2300) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:k:5020:PRO:HG3  | 14:y:24:MET:CG    | 1.20                     | 1.58              |
| 9:k:5020:PRO:CG   | 14:y:24:MET:CG    | 1.81                     | 1.56              |
| 9:k:5039:TRP:NE1  | 14:y:46:LEU:CD2   | 1.68                     | 1.56              |
| 7:H:44:ILE:CD1    | 16:X:10:PHE:CZ    | 1.86                     | 1.53              |
| 9:k:5020:PRO:HG3  | 14:y:24:MET:CB    | 1.37                     | 1.51              |
| 13:z:5028:ALA:CB  | 14:y:39:LEU:HD21  | 1.41                     | 1.48              |
| 7:H:44:ILE:HD11   | 16:X:10:PHE:CZ    | 1.48                     | 1.45              |
| 14:y:35:ILE:CA    | 14:y:38:LEU:HD11  | 1.55                     | 1.34              |
| 16:X:27:VAL:O     | 16:X:31:ILE:HG12  | 1.26                     | 1.34              |
| 7:H:44:ILE:HD11   | 16:X:10:PHE:CE1   | 1.62                     | 1.34              |
| 16:x:8:LYS:O      | 16:x:12:ILE:CD1   | 1.79                     | 1.30              |
| 7:H:44:ILE:HD13   | 16:X:10:PHE:CZ    | 1.61                     | 1.22              |
| 16:x:9:GLY:CA     | 16:x:12:ILE:CD1   | 2.17                     | 1.22              |
| 2:B:258:TYR:CE2   | 26:D:411:DGD:HG32 | 1.75                     | 1.21              |
| 9:K:20:PRO:CG     | 14:Y:24:MET:HG3   | 1.72                     | 1.20              |
| 14:y:35:ILE:C     | 14:y:38:LEU:CD1   | 2.16                     | 1.19              |
| 13:z:5028:ALA:CB  | 14:y:39:LEU:CD2   | 2.20                     | 1.19              |
| 9:k:5020:PRO:CG   | 14:y:24:MET:HG3   | 1.57                     | 1.18              |
| 14:y:35:ILE:O     | 14:y:38:LEU:CD1   | 1.91                     | 1.18              |
| 9:k:5039:TRP:HE1  | 14:y:46:LEU:CD2   | 1.35                     | 1.17              |
| 16:x:9:GLY:HA2    | 16:x:12:ILE:CD1   | 1.73                     | 1.16              |
| 9:k:5020:PRO:HG2  | 14:y:24:MET:HG3   | 1.20                     | 1.16              |
| 16:X:3:ILE:HA     | 16:X:7:LEU:HD12   | 1.23                     | 1.15              |
| 9:k:5020:PRO:HG3  | 14:y:24:MET:HB3   | 1.25                     | 1.15              |
| 13:z:5028:ALA:HB2 | 14:y:39:LEU:CD2   | 1.75                     | 1.14              |
| 16:x:8:LYS:O      | 16:x:12:ILE:HD11  | 1.44                     | 1.14              |
| 7:H:44:ILE:CD1    | 16:X:10:PHE:CE1   | 2.21                     | 1.14              |
| 4:d:5035:ILE:CD1  | 16:x:28:LEU:HD11  | 1.78                     | 1.14              |
| 9:k:5039:TRP:NE1  | 14:y:46:LEU:HD21  | 1.38                     | 1.14              |
| 14:y:34:MET:O     | 14:y:38:LEU:CD1   | 1.96                     | 1.13              |
| 2:B:86:ILE:CG2    | 2:B:88:PRO:HD3    | 1.78                     | 1.13              |
| 16:x:9:GLY:CA     | 16:x:12:ILE:HD13  | 1.74                     | 1.13              |
| 7:h:5044:ILE:HD11 | 16:x:10:PHE:CZ    | 1.84                     | 1.12              |
| 14:y:35:ILE:HA    | 14:y:38:LEU:HD11  | 1.28                     | 1.12              |
| 9:k:5039:TRP:CD1  | 14:y:46:LEU:HD21  | 1.85                     | 1.10              |
| 9:k:5039:TRP:HE1  | 14:y:46:LEU:HD23  | 1.14                     | 1.10              |
| 7:h:5047:GLU:OE2  | 16:x:10:PHE:CE2   | 2.05                     | 1.10              |
| 16:x:8:LYS:C      | 16:x:12:ILE:HD11  | 1.76                     | 1.09              |
| 4:D:35:ILE:HD12   | 16:X:28:LEU:HD11  | 1.17                     | 1.09              |
| 14:y:18:VAL:O     | 14:y:22:LEU:HB2   | 1.52                     | 1.09              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:x:9:GLY:HA2    | 16:x:12:ILE:HD13  | 1.24                     | 1.09              |
| 16:x:9:GLY:C      | 16:x:12:ILE:CD1   | 2.26                     | 1.08              |
| 16:x:8:LYS:O      | 16:x:12:ILE:HD12  | 1.52                     | 1.08              |
| 9:k:5020:PRO:CG   | 14:y:24:MET:HG2   | 1.60                     | 1.07              |
| 9:K:20:PRO:HG2    | 14:Y:24:MET:HG3   | 1.35                     | 1.06              |
| 4:d:5035:ILE:HD12 | 16:x:28:LEU:HD11  | 1.11                     | 1.06              |
| 16:x:9:GLY:C      | 16:x:12:ILE:HD13  | 1.81                     | 1.06              |
| 16:x:12:ILE:HD12  | 16:x:12:ILE:H     | 1.21                     | 1.05              |
| 14:y:35:ILE:CA    | 14:y:38:LEU:CD1   | 2.33                     | 1.05              |
| 26:b:5621:DGD:O2D | 4:d:5087:HIS:HB2  | 1.55                     | 1.05              |
| 16:x:36:LYS:HD3   | 16:x:36:LYS:H     | 1.22                     | 1.03              |
| 2:b:5086:ILE:HG22 | 2:b:5088:PRO:HD3  | 1.36                     | 1.02              |
| 4:D:35:ILE:CD1    | 16:X:28:LEU:HD11  | 1.87                     | 1.02              |
| 7:h:5047:GLU:CD   | 16:x:10:PHE:CE2   | 2.37                     | 1.02              |
| 7:h:5047:GLU:OE1  | 16:x:10:PHE:CD2   | 2.12                     | 1.02              |
| 9:K:20:PRO:HG3    | 14:Y:24:MET:HG3   | 1.43                     | 1.01              |
| 9:k:5020:PRO:HG2  | 14:y:24:MET:CG    | 1.73                     | 1.00              |
| 16:x:9:GLY:O      | 16:x:12:ILE:HD13  | 1.62                     | 1.00              |
| 4:d:5035:ILE:CD1  | 16:x:28:LEU:CD1   | 2.39                     | 0.99              |
| 7:h:5044:ILE:CD1  | 16:x:10:PHE:CZ    | 2.45                     | 0.98              |
| 2:B:86:ILE:HG22   | 2:B:88:PRO:HD3    | 1.00                     | 0.98              |
| 14:y:35:ILE:O     | 14:y:38:LEU:HD13  | 1.59                     | 0.98              |
| 14:y:35:ILE:HA    | 14:y:38:LEU:CD1   | 1.93                     | 0.97              |
| 2:B:86:ILE:HG22   | 2:B:88:PRO:CD     | 1.94                     | 0.97              |
| 9:k:5039:TRP:NE1  | 14:y:46:LEU:HD22  | 1.79                     | 0.97              |
| 9:k:5039:TRP:CE2  | 14:y:46:LEU:CD2   | 2.47                     | 0.96              |
| 7:h:5047:GLU:OE2  | 16:x:10:PHE:HE2   | 1.49                     | 0.95              |
| 7:h:5047:GLU:OE1  | 16:x:10:PHE:CE2   | 2.18                     | 0.95              |
| 17:b:5612:CLA:H93 | 17:b:5612:CLA:H2  | 1.48                     | 0.95              |
| 7:H:44:ILE:CD1    | 16:X:10:PHE:HZ    | 1.69                     | 0.95              |
| 1:A:300:PHE:HA    | 3:C:403:SER:HB2   | 1.49                     | 0.94              |
| 7:h:5047:GLU:CD   | 16:x:10:PHE:CD2   | 2.45                     | 0.94              |
| 16:x:9:GLY:CA     | 16:x:12:ILE:HD11  | 1.97                     | 0.94              |
| 4:d:5141:TYR:HH   | 25:d:5409:MGE:H2  | 1.12                     | 0.94              |
| 4:d:5035:ILE:HD12 | 16:x:28:LEU:CD1   | 1.94                     | 0.93              |
| 16:X:27:VAL:O     | 16:X:31:ILE:CG1   | 2.16                     | 0.93              |
| 17:B:612:CLA:H93  | 17:B:612:CLA:H2   | 1.48                     | 0.93              |
| 4:D:35:ILE:CD1    | 16:X:28:LEU:CD1   | 2.46                     | 0.93              |
| 4:D:275:PRO:HB3   | 18:D:402:PHO:HBC1 | 1.51                     | 0.92              |
| 16:X:3:ILE:HG23   | 16:X:7:LEU:CD1    | 2.00                     | 0.92              |
| 16:x:9:GLY:O      | 16:x:12:ILE:CD1   | 2.17                     | 0.92              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:y:31:ALA:O      | 14:y:35:ILE:HG13   | 1.69                     | 0.92              |
| 7:h:5047:GLU:OE2   | 16:x:10:PHE:CD2    | 2.23                     | 0.91              |
| 4:D:35:ILE:HD12    | 16:X:28:LEU:CD1    | 1.99                     | 0.91              |
| 9:K:43:VAL:CG2     | 14:Y:46:LEU:HD13   | 2.00                     | 0.91              |
| 9:K:39:TRP:NE1     | 14:Y:46:LEU:HD21   | 1.84                     | 0.91              |
| 9:k:5020:PRO:CG    | 14:y:24:MET:HB3    | 1.98                     | 0.90              |
| 1:a:5143:ILE:HG23  | 4:d:5220:ASN:HD22  | 1.34                     | 0.90              |
| 14:y:34:MET:O      | 14:y:38:LEU:HD11   | 1.65                     | 0.90              |
| 14:y:35:ILE:C      | 14:y:38:LEU:HD11   | 1.90                     | 0.90              |
| 9:k:5020:PRO:CG    | 14:y:24:MET:CB     | 2.32                     | 0.90              |
| 9:k:5039:TRP:CE2   | 14:y:46:LEU:HD22   | 2.05                     | 0.90              |
| 14:Y:38:LEU:O      | 14:Y:42:ARG:HG3    | 1.72                     | 0.90              |
| 2:B:258:TYR:CZ     | 26:D:411:DGD:HG32  | 2.07                     | 0.89              |
| 14:y:34:MET:C      | 14:y:38:LEU:HD11   | 1.96                     | 0.89              |
| 3:c:5229:ASN:HD22  | 15:n:77:ARG:HG3    | 1.38                     | 0.88              |
| 9:K:43:VAL:HG23    | 14:Y:46:LEU:HD13   | 1.54                     | 0.88              |
| 16:X:3:ILE:HG23    | 16:X:7:LEU:HD13    | 1.53                     | 0.87              |
| 15:N:109:LEU:HB2   | 15:N:114:LYS:HE3   | 1.54                     | 0.87              |
| 9:K:39:TRP:NE1     | 14:Y:46:LEU:CD2    | 2.38                     | 0.87              |
| 1:A:212:CYS:HB2    | 4:D:211:CYS:HB2    | 1.57                     | 0.86              |
| 9:K:20:PRO:HG3     | 14:Y:24:MET:CG     | 2.03                     | 0.86              |
| 17:B:608:CLA:H201  | 26:D:411:DGD:HA81  | 1.57                     | 0.86              |
| 22:B:620:LMT:H6'   | 12:t:5001:MET:N    | 1.73                     | 0.86              |
| 4:d:5014:TRP:CZ2   | 16:x:29:ILE:HD12   | 2.10                     | 0.86              |
| 13:z:5028:ALA:HB1  | 14:y:39:LEU:CD2    | 2.04                     | 0.86              |
| 13:z:5028:ALA:HB1  | 14:y:39:LEU:HD21   | 1.58                     | 0.86              |
| 4:D:53:THR:HA      | 4:D:67:TYR:HB3     | 1.56                     | 0.86              |
| 9:k:5019:ASP:OD1   | 14:y:21:GLN:NE2    | 1.84                     | 0.86              |
| 14:y:35:ILE:O      | 14:y:38:LEU:HD12   | 1.73                     | 0.85              |
| 4:D:180:ARG:NH2    | 4:D:333:ASP:OD1    | 2.10                     | 0.85              |
| 15:N:109:LEU:HB2   | 15:N:114:LYS:CE    | 2.06                     | 0.85              |
| 9:K:20:PRO:CG      | 14:Y:24:MET:CG     | 2.54                     | 0.84              |
| 4:D:123:ILE:HD11   | 26:D:411:DGD:HAH2  | 1.57                     | 0.84              |
| 4:d:5053:THR:HA    | 4:d:5067:TYR:HB3   | 1.55                     | 0.84              |
| 4:d:5014:TRP:CZ2   | 16:x:29:ILE:CD1    | 2.61                     | 0.84              |
| 20:c:5513:BCR:H11C | 20:k:5502:BCR:H322 | 1.57                     | 0.84              |
| 4:d:5180:ARG:NH2   | 4:d:5333:ASP:OD1   | 2.10                     | 0.84              |
| 13:z:5021:ILE:HD11 | 14:y:31:ALA:HB1    | 1.59                     | 0.84              |
| 3:C:410:VAL:HG12   | 3:C:413:GLU:HB2    | 1.58                     | 0.83              |
| 14:y:35:ILE:N      | 14:y:38:LEU:HD11   | 1.92                     | 0.83              |
| 3:c:5102:GLY:N     | 3:c:5195:ASP:OD2   | 2.11                     | 0.83              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:Y:34:MET:N      | 14:Y:34:MET:HE3    | 1.92                     | 0.83              |
| 26:b:5621:DGD:O2D  | 4:d:5087:HIS:CB    | 2.26                     | 0.83              |
| 4:D:89:LEU:HD11    | 26:D:411:DGD:HA32  | 1.60                     | 0.83              |
| 3:C:102:GLY:N      | 3:C:195:ASP:OD2    | 2.11                     | 0.83              |
| 14:y:38:LEU:HD12   | 14:y:38:LEU:H      | 1.41                     | 0.82              |
| 2:B:77:GLY:HA2     | 2:B:86:ILE:CD1     | 2.10                     | 0.82              |
| 7:H:44:ILE:HD11    | 16:X:10:PHE:HZ     | 1.27                     | 0.82              |
| 7:H:44:ILE:HD13    | 16:X:10:PHE:CE2    | 2.14                     | 0.82              |
| 4:d:5035:ILE:HD11  | 16:x:28:LEU:HD13   | 1.62                     | 0.81              |
| 15:N:112:LYS:O     | 15:N:116:ARG:HG3   | 1.80                     | 0.81              |
| 20:b:5617:BCR:H10C | 25:b:5620:MGE:H241 | 1.62                     | 0.81              |
| 17:A:405:CLA:HHC   | 17:A:405:CLA:HBB1  | 1.63                     | 0.81              |
| 9:K:15:TYR:OH      | 13:Z:58:ASN:ND2    | 2.14                     | 0.81              |
| 4:d:5035:ILE:HD11  | 16:x:28:LEU:CD1    | 2.08                     | 0.81              |
| 1:a:5143:ILE:HG23  | 4:d:5220:ASN:ND2   | 1.95                     | 0.81              |
| 1:a:5315:ASN:O     | 4:d:5063:LEU:HB2   | 1.81                     | 0.81              |
| 15:N:34:ARG:HG3    | 15:N:128:LEU:HD21  | 1.63                     | 0.81              |
| 4:d:5071:CYS:SG    | 4:d:5075:THR:OG1   | 2.39                     | 0.81              |
| 14:Y:42:ARG:HG2    | 14:Y:42:ARG:HH11   | 1.45                     | 0.81              |
| 16:X:7:LEU:O       | 16:X:7:LEU:HD22    | 1.82                     | 0.81              |
| 9:k:5039:TRP:NE1   | 14:y:46:LEU:HD23   | 1.75                     | 0.80              |
| 20:B:618:BCR:H382  | 20:t:5102:BCR:H11C | 1.62                     | 0.80              |
| 4:D:71:CYS:SG      | 4:D:75:THR:OG1     | 2.39                     | 0.80              |
| 20:B:617:BCR:H10C  | 25:B:619:MGE:H241  | 1.62                     | 0.80              |
| 2:b:5188:ASP:HA    | 7:h:5058:VAL:HG12  | 1.64                     | 0.80              |
| 15:n:34:ARG:HG3    | 15:n:128:LEU:HD21  | 1.63                     | 0.80              |
| 3:C:308:GLU:OE2    | 3:C:365:TRP:NE1    | 2.11                     | 0.79              |
| 15:N:117:LEU:O     | 15:N:120:GLU:N     | 2.13                     | 0.79              |
| 14:y:18:VAL:O      | 14:y:22:LEU:N      | 2.15                     | 0.79              |
| 17:a:5406:CLA:HHC  | 17:a:5406:CLA:HBB1 | 1.63                     | 0.79              |
| 15:N:77:ARG:HD2    | 15:N:77:ARG:O      | 1.84                     | 0.79              |
| 1:A:143:ILE:HD13   | 4:D:252:PHE:HZ     | 1.47                     | 0.78              |
| 3:c:5308:GLU:OE2   | 3:c:5365:TRP:NE1   | 2.11                     | 0.78              |
| 9:k:5015:TYR:OH    | 13:z:5058:ASN:ND2  | 2.16                     | 0.78              |
| 1:A:272:HIS:NE2    | 24:A:411:BCT:O3    | 2.14                     | 0.78              |
| 16:x:36:LYS:H      | 16:x:36:LYS:CD     | 1.97                     | 0.78              |
| 4:D:189:HIS:HB3    | 4:D:289:LEU:HD11   | 1.65                     | 0.78              |
| 14:Y:19:ILE:HD12   | 14:Y:19:ILE:H      | 1.49                     | 0.78              |
| 16:X:3:ILE:CG2     | 16:X:8:LYS:HB2     | 2.14                     | 0.77              |
| 16:x:9:GLY:N       | 16:x:12:ILE:HD11   | 1.98                     | 0.77              |
| 1:A:288:LEU:HD13   | 3:C:432:VAL:HG13   | 1.66                     | 0.77              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 19:A:406:PQ9:H37   | 4:D:42:TYR:HB2     | 1.65                     | 0.77              |
| 3:C:189:TRP:HB2    | 15:N:76:ARG:CZ     | 2.15                     | 0.77              |
| 2:B:168:VAL:O      | 2:B:177:SER:OG     | 2.03                     | 0.77              |
| 1:a:5027:ARG:NH1   | 4:d:5254:SER:O     | 2.18                     | 0.77              |
| 17:B:606:CLA:H51   | 20:t:5101:BCR:H322 | 1.65                     | 0.77              |
| 4:d:5189:HIS:HB3   | 4:d:5289:LEU:HD11  | 1.65                     | 0.77              |
| 9:k:5020:PRO:HG3   | 14:y:24:MET:HG2    | 1.26                     | 0.77              |
| 13:z:5028:ALA:HB2  | 14:y:39:LEU:HD21   | 0.78                     | 0.77              |
| 9:K:39:TRP:HE1     | 14:Y:46:LEU:CD2    | 1.97                     | 0.77              |
| 4:d:5210:LEU:HD12  | 19:d:5405:PQ9:H17  | 1.67                     | 0.77              |
| 2:B:86:ILE:CG2     | 2:B:88:PRO:CD      | 2.60                     | 0.76              |
| 14:y:18:VAL:O      | 14:y:22:LEU:CB     | 2.33                     | 0.76              |
| 9:K:39:TRP:CD1     | 14:Y:46:LEU:HD21   | 2.20                     | 0.76              |
| 2:b:5168:VAL:O     | 2:b:5177:SER:OG    | 2.03                     | 0.76              |
| 4:D:172:SER:HB2    | 4:D:177:ALA:HB1    | 1.66                     | 0.76              |
| 4:D:93:TRP:CD1     | 4:D:94:GLY:H       | 2.04                     | 0.76              |
| 17:b:5611:CLA:H41  | 17:b:5614:CLA:HBC3 | 1.67                     | 0.76              |
| 21:a:5409:LHG:HC32 | 4:d:5230:SER:HA    | 1.68                     | 0.76              |
| 4:D:35:ILE:HD11    | 16:X:28:LEU:CD1    | 2.16                     | 0.76              |
| 4:D:210:LEU:HD12   | 19:D:406:PQ9:H17   | 1.67                     | 0.76              |
| 4:d:5172:SER:HB2   | 4:d:5177:ALA:HB1   | 1.67                     | 0.75              |
| 1:a:5269:ARG:HD2   | 4:d:5235:PHE:HB2   | 1.66                     | 0.75              |
| 14:y:34:MET:O      | 14:y:38:LEU:CG     | 2.33                     | 0.75              |
| 16:x:36:LYS:HD3    | 16:x:36:LYS:N      | 2.00                     | 0.75              |
| 12:T:25:GLU:OE1    | 12:T:25:GLU:N      | 2.19                     | 0.75              |
| 4:D:35:ILE:HD11    | 16:X:28:LEU:HD13   | 1.67                     | 0.75              |
| 16:X:3:ILE:CA      | 16:X:7:LEU:HD12    | 2.11                     | 0.75              |
| 3:C:342:MET:HE2    | 3:C:352:GLY:HA2    | 1.69                     | 0.75              |
| 7:h:5044:ILE:HD11  | 16:x:10:PHE:CE1    | 2.21                     | 0.75              |
| 1:a:5331:MET:HG3   | 4:d:5324:GLY:HA3   | 1.69                     | 0.74              |
| 3:c:5342:MET:HE2   | 3:c:5352:GLY:HA2   | 1.69                     | 0.74              |
| 14:Y:43:ARG:HB3    | 14:Y:43:ARG:NH1    | 2.02                     | 0.74              |
| 4:d:5093:TRP:CD1   | 4:d:5094:GLY:H     | 2.04                     | 0.74              |
| 17:B:611:CLA:H41   | 17:B:614:CLA:HBC3  | 1.67                     | 0.74              |
| 14:y:25:ILE:O      | 14:y:25:ILE:HD13   | 1.87                     | 0.74              |
| 4:D:69:GLU:HG2     | 4:D:70:GLY:H       | 1.50                     | 0.74              |
| 23:L:101:SQD:O7    | 10:l:5007:ARG:NH1  | 2.19                     | 0.74              |
| 16:x:8:LYS:C       | 16:x:12:ILE:CD1    | 2.48                     | 0.74              |
| 17:A:402:CLA:H13   | 19:D:406:PQ9:H452  | 1.70                     | 0.73              |
| 4:d:5297:ASP:HB3   | 4:d:5302:GLU:HG3   | 1.69                     | 0.73              |
| 4:D:77:ALA:HB2     | 4:D:174:GLY:HA3    | 1.70                     | 0.73              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:x:9:GLY:HA2     | 16:x:12:ILE:HD11   | 1.58                     | 0.73              |
| 20:k:5502:BCR:C33  | 14:y:28:ILE:O      | 2.36                     | 0.73              |
| 2:b:5086:ILE:HG22  | 2:b:5088:PRO:CD    | 2.15                     | 0.73              |
| 16:x:9:GLY:C       | 16:x:12:ILE:HD12   | 2.11                     | 0.73              |
| 1:a:5073:TYR:O     | 1:a:5075:ASN:ND2   | 2.21                     | 0.73              |
| 12:t:5025:GLU:OE1  | 12:t:5025:GLU:N    | 2.19                     | 0.73              |
| 25:D:410:MGE:H8A1  | 12:T:21:ILE:HD11   | 1.70                     | 0.73              |
| 14:y:35:ILE:C      | 14:y:38:LEU:HD12   | 2.05                     | 0.73              |
| 14:Y:43:ARG:HB3    | 14:Y:43:ARG:HH11   | 1.52                     | 0.73              |
| 16:x:15:LEU:C      | 16:x:15:LEU:HD22   | 2.14                     | 0.73              |
| 1:A:73:TYR:O       | 1:A:75:ASN:ND2     | 2.21                     | 0.72              |
| 16:X:27:VAL:HG13   | 16:X:31:ILE:HD11   | 1.70                     | 0.72              |
| 20:k:5502:BCR:H332 | 14:y:28:ILE:O      | 1.90                     | 0.72              |
| 2:B:472:ARG:NH2    | 17:B:611:CLA:O2D   | 2.21                     | 0.72              |
| 9:k:5020:PRO:CD    | 14:y:24:MET:HG2    | 2.19                     | 0.72              |
| 2:b:5472:ARG:NH2   | 17:b:5611:CLA:O2D  | 2.21                     | 0.72              |
| 17:b:5603:CLA:HAB  | 17:b:5605:CLA:H192 | 1.71                     | 0.72              |
| 14:y:38:LEU:HD12   | 14:y:38:LEU:N      | 2.05                     | 0.72              |
| 16:X:7:LEU:HD22    | 16:X:7:LEU:C       | 2.13                     | 0.72              |
| 16:x:21:LEU:HD23   | 16:x:21:LEU:C      | 2.14                     | 0.72              |
| 2:b:5064:PRO:HB2   | 2:b:5268:PHE:HE1   | 1.55                     | 0.72              |
| 7:H:40:VAL:HG13    | 16:X:14:LEU:CD1    | 2.20                     | 0.71              |
| 4:d:5077:ALA:HB2   | 4:d:5174:GLY:HA3   | 1.70                     | 0.71              |
| 17:B:603:CLA:HAB   | 17:B:605:CLA:H192  | 1.71                     | 0.71              |
| 2:B:64:PRO:HB2     | 2:B:268:PHE:HE1    | 1.55                     | 0.71              |
| 9:k:5039:TRP:CD1   | 14:y:46:LEU:CD2    | 2.57                     | 0.71              |
| 26:a:5411:DGD:HBE2 | 25:d:5408:MGE:H9B1 | 1.71                     | 0.71              |
| 3:C:191:PRO:O      | 15:N:95:ASN:HA     | 1.91                     | 0.71              |
| 7:H:53:LEU:CD1     | 16:X:7:LEU:HA      | 2.21                     | 0.71              |
| 14:Y:32:GLY:O      | 14:Y:35:ILE:HD12   | 1.89                     | 0.71              |
| 14:Y:34:MET:HE3    | 14:Y:34:MET:CA     | 2.21                     | 0.71              |
| 17:C:511:CLA:H72   | 14:Y:35:ILE:HG21   | 1.71                     | 0.70              |
| 17:C:503:CLA:H171  | 17:C:510:CLA:HBB2  | 1.73                     | 0.70              |
| 16:X:15:LEU:HD12   | 16:X:15:LEU:O      | 1.91                     | 0.70              |
| 5:e:5071:GLU:O     | 5:e:5074:GLN:N     | 2.25                     | 0.70              |
| 16:x:15:LEU:HD22   | 16:x:15:LEU:O      | 1.90                     | 0.70              |
| 14:y:34:MET:O      | 14:y:38:LEU:HG     | 1.90                     | 0.70              |
| 1:A:267:ASN:ND2    | 4:D:232:PHE:O      | 2.24                     | 0.70              |
| 5:E:71:GLU:O       | 5:E:74:GLN:N       | 2.25                     | 0.70              |
| 1:A:143:ILE:HG23   | 4:D:220:ASN:HD22   | 1.57                     | 0.70              |
| 1:A:215:HIS:NE2    | 24:A:411:BCT:O2    | 2.25                     | 0.70              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:b:5007:ARG:NH2   | 25:d:5409:MGE:O3D  | 2.23                     | 0.70              |
| 4:d:5046:GLY:HA2   | 20:d:5406:BCR:H12C | 1.73                     | 0.70              |
| 16:X:15:LEU:HD12   | 16:X:15:LEU:C      | 2.16                     | 0.69              |
| 4:D:141:TYR:HH     | 25:D:409:MGE:H2    | 1.39                     | 0.69              |
| 9:K:43:VAL:HG22    | 14:Y:46:LEU:HD13   | 1.75                     | 0.69              |
| 9:K:39:TRP:HD1     | 14:Y:36:ILE:HD11   | 1.57                     | 0.69              |
| 3:C:39:ASN:HB2     | 17:C:508:CLA:HBA1  | 1.74                     | 0.69              |
| 1:a:5076:ASN:HB3   | 10:l:5033:SER:HB2  | 1.75                     | 0.69              |
| 17:b:5603:CLA:HBB2 | 17:b:5605:CLA:H203 | 1.75                     | 0.69              |
| 3:c:5039:ASN:HB2   | 17:c:5508:CLA:HBA1 | 1.75                     | 0.69              |
| 13:z:5039:LEU:O    | 13:z:5043:GLY:N    | 2.21                     | 0.69              |
| 14:Y:46:LEU:O      | 14:Y:46:LEU:HD22   | 1.92                     | 0.69              |
| 2:B:280:PHE:CE2    | 2:B:312:TYR:HB3    | 2.27                     | 0.69              |
| 4:D:46:GLY:HA2     | 20:D:407:BCR:H12C  | 1.73                     | 0.69              |
| 4:d:5188:PHE:CD1   | 4:d:5326:ARG:HG2   | 2.28                     | 0.69              |
| 1:A:143:ILE:HD13   | 4:D:252:PHE:CZ     | 2.27                     | 0.69              |
| 2:b:5280:PHE:CE2   | 2:b:5312:TYR:HB3   | 2.27                     | 0.69              |
| 17:b:5602:CLA:H203 | 26:b:5621:DGD:HA62 | 1.75                     | 0.69              |
| 17:b:5616:CLA:H141 | 20:b:5619:BCR:HC8  | 1.75                     | 0.69              |
| 3:c:5187:ASP:N     | 3:c:5195:ASP:O     | 2.20                     | 0.69              |
| 3:c:5464:GLU:HB2   | 3:c:5467:LEU:HB2   | 1.74                     | 0.69              |
| 14:y:31:ALA:O      | 14:y:35:ILE:CG1    | 2.41                     | 0.69              |
| 16:X:21:LEU:HD23   | 16:X:21:LEU:H      | 1.58                     | 0.69              |
| 4:D:103:ARG:NH2    | 5:E:77:GLU:OE2     | 2.23                     | 0.69              |
| 17:k:5501:CLA:H42  | 14:y:46:LEU:HD23   | 1.75                     | 0.69              |
| 1:a:5130:GLN:HB3   | 1:a:5143:ILE:HD12  | 1.75                     | 0.68              |
| 17:c:5503:CLA:H171 | 17:c:5510:CLA:HBB2 | 1.73                     | 0.68              |
| 9:k:5039:TRP:HE1   | 14:y:46:LEU:HD21   | 1.16                     | 0.68              |
| 17:B:613:CLA:H51   | 25:D:409:MGE:H241  | 1.74                     | 0.68              |
| 3:C:464:GLU:HB2    | 3:C:467:LEU:HB2    | 1.74                     | 0.68              |
| 17:c:5505:CLA:HBD  | 17:c:5505:CLA:HBA1 | 1.75                     | 0.68              |
| 7:h:5044:ILE:HD11  | 16:x:10:PHE:HZ     | 1.54                     | 0.68              |
| 4:D:43:LEU:O       | 4:D:47:GLY:N       | 2.26                     | 0.68              |
| 4:D:188:PHE:CD1    | 4:D:326:ARG:HG2    | 2.28                     | 0.68              |
| 2:b:5323:GLY:HA3   | 2:b:5326:ARG:HH11  | 1.59                     | 0.68              |
| 17:B:603:CLA:HBB2  | 17:B:605:CLA:H203  | 1.75                     | 0.68              |
| 17:B:616:CLA:H141  | 20:t:5101:BCR:HC8  | 1.75                     | 0.68              |
| 7:H:54:ILE:O       | 16:X:4:THR:HG21    | 1.93                     | 0.68              |
| 13:Z:39:LEU:O      | 13:Z:43:GLY:N      | 2.21                     | 0.68              |
| 3:c:5265:ILE:HG13  | 3:c:5449:ARG:HG2   | 1.76                     | 0.68              |
| 14:Y:43:ARG:HH11   | 14:Y:43:ARG:CB     | 2.05                     | 0.68              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:N:58:LYS:O      | 15:N:62:ALA:N      | 2.24                     | 0.68              |
| 4:d:5176:ALA:HA    | 4:d:5179:PHE:HD2   | 1.59                     | 0.68              |
| 14:y:18:VAL:C      | 14:y:22:LEU:H      | 2.01                     | 0.68              |
| 1:A:166:GLY:HA3    | 3:C:358:PHE:HE1    | 1.58                     | 0.68              |
| 3:C:147:PHE:CD2    | 17:C:513:CLA:H3A   | 2.29                     | 0.68              |
| 3:C:265:ILE:HG13   | 3:C:449:ARG:HG2    | 1.76                     | 0.68              |
| 3:c:5362:ARG:HG3   | 15:n:82:ARG:HH11   | 1.59                     | 0.68              |
| 17:B:607:CLA:H203  | 4:D:281:MET:HE3    | 1.76                     | 0.67              |
| 12:t:5015:ALA:HB2  | 20:t:5102:BCR:H14C | 1.75                     | 0.67              |
| 17:C:505:CLA:HBD   | 17:C:505:CLA:HBA1  | 1.75                     | 0.67              |
| 3:c:5147:PHE:CD2   | 17:c:5512:CLA:H3A  | 2.29                     | 0.67              |
| 15:N:109:LEU:HD22  | 15:N:113:LEU:HD23  | 1.76                     | 0.67              |
| 4:D:24:ARG:NH2     | 16:X:37:VAL:HG21   | 2.10                     | 0.67              |
| 3:C:212:TYR:OH     | 3:C:227:VAL:N      | 2.18                     | 0.67              |
| 4:d:5043:LEU:O     | 4:d:5047:GLY:N     | 2.26                     | 0.67              |
| 15:N:44:LEU:HD21   | 15:N:68:LEU:HD21   | 1.76                     | 0.67              |
| 1:A:130:GLN:HB3    | 1:A:143:ILE:HD12   | 1.75                     | 0.67              |
| 2:B:149:LEU:HG     | 17:B:603:CLA:HBC1  | 1.77                     | 0.67              |
| 3:C:457:LYS:HE3    | 4:D:227:GLU:O      | 1.94                     | 0.67              |
| 23:D:403:SQD:H172  | 25:D:408:MGE:H242  | 1.77                     | 0.67              |
| 7:H:51:SER:HB2     | 7:H:60:VAL:HG21    | 1.77                     | 0.67              |
| 15:n:58:LYS:O      | 15:n:62:ALA:N      | 2.24                     | 0.67              |
| 4:D:14:TRP:CZ2     | 16:X:29:ILE:CD1    | 2.77                     | 0.67              |
| 13:z:5021:ILE:HD11 | 14:y:31:ALA:CB     | 2.24                     | 0.67              |
| 7:h:5051:SER:HB2   | 7:h:5060:VAL:HG21  | 1.77                     | 0.67              |
| 4:D:84:SER:OG      | 5:E:67:THR:O       | 2.10                     | 0.67              |
| 7:H:44:ILE:HD12    | 16:X:10:PHE:CE1    | 2.28                     | 0.67              |
| 4:d:5100:ASP:OD2   | 4:d:5103:ARG:NH1   | 2.26                     | 0.67              |
| 4:D:261:PHE:HA     | 25:D:410:MGE:H2D   | 1.76                     | 0.67              |
| 2:b:5149:LEU:HG    | 17:b:5603:CLA:HBC1 | 1.76                     | 0.67              |
| 20:C:515:BCR:H403  | 20:C:515:BCR:H371  | 1.77                     | 0.67              |
| 2:b:5004:PRO:HD2   | 2:b:5007:ARG:HD2   | 1.76                     | 0.67              |
| 16:X:3:ILE:HG22    | 16:X:8:LYS:HB2     | 1.77                     | 0.67              |
| 11:M:24:ILE:HD12   | 25:m:5103:MGE:H212 | 1.75                     | 0.66              |
| 13:z:5029:SER:HA   | 14:y:44:GLY:HA2    | 1.77                     | 0.66              |
| 15:N:130:ARG:O     | 15:N:134:SER:OG    | 2.10                     | 0.66              |
| 2:B:323:GLY:HA3    | 2:B:326:ARG:HH11   | 1.59                     | 0.66              |
| 1:a:5317:TRP:CZ3   | 4:d:5077:ALA:HB3   | 2.31                     | 0.66              |
| 24:a:5412:BCT:O2   | 4:d:5268:HIS:NE2   | 2.29                     | 0.66              |
| 13:z:5028:ALA:C    | 14:y:44:GLY:HA3    | 2.21                     | 0.66              |
| 15:n:109:LEU:HD22  | 15:n:113:LEU:HD23  | 1.76                     | 0.66              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:232:SER:HB2    | 2:B:4:PRO:HG3      | 1.77                     | 0.66              |
| 4:D:176:ALA:HA     | 4:D:179:PHE:HD2    | 1.59                     | 0.66              |
| 10:l:5004:ASN:HD22 | 10:l:5007:ARG:HE   | 1.42                     | 0.66              |
| 23:l:5102:SQD:H191 | 11:m:5023:ILE:HD11 | 1.78                     | 0.66              |
| 17:b:5604:CLA:HBB1 | 17:b:5607:CLA:HAB  | 1.78                     | 0.66              |
| 14:y:34:MET:O      | 14:y:38:LEU:HD12   | 1.90                     | 0.66              |
| 25:A:412:MGE:H122  | 11:M:18:PRO:HG3    | 1.77                     | 0.66              |
| 4:d:5139:ARG:NH2   | 4:d:5141:TYR:OH    | 2.29                     | 0.66              |
| 15:n:44:LEU:HD21   | 15:n:68:LEU:HD21   | 1.77                     | 0.66              |
| 13:z:5016:SER:OG   | 13:z:5047:TRP:NE1  | 2.22                     | 0.66              |
| 24:A:411:BCT:O2    | 4:D:268:HIS:NE2    | 2.29                     | 0.66              |
| 3:c:5208:VAL:O     | 3:c:5212:TYR:HB2   | 1.96                     | 0.66              |
| 20:z:5101:BCR:H403 | 20:z:5101:BCR:H371 | 1.77                     | 0.66              |
| 14:y:18:VAL:N      | 14:y:21:GLN:HB2    | 2.11                     | 0.66              |
| 2:B:4:PRO:HD2      | 2:B:7:ARG:HD2      | 1.76                     | 0.66              |
| 2:b:5192:PRO:HG3   | 7:h:5049:TYR:CD1   | 2.31                     | 0.66              |
| 3:c:5349:ILE:H     | 3:c:5374:GLY:HA3   | 1.61                     | 0.66              |
| 4:d:5275:PRO:HB3   | 18:d:5402:PHO:HBC1 | 1.76                     | 0.66              |
| 13:z:5005:PHE:CD1  | 13:z:5057:LEU:HD23 | 2.31                     | 0.66              |
| 4:D:139:ARG:NH2    | 4:D:141:TYR:OH     | 2.29                     | 0.65              |
| 4:D:24:ARG:CZ      | 16:X:37:VAL:HG21   | 2.26                     | 0.65              |
| 3:c:5388:GLN:NE2   | 15:n:95:ASN:HD21   | 1.95                     | 0.65              |
| 1:A:30:VAL:HG23    | 1:A:34:GLY:HA3     | 1.78                     | 0.65              |
| 3:C:187:ASP:N      | 3:C:195:ASP:O      | 2.20                     | 0.65              |
| 17:a:5403:CLA:H13  | 19:d:5405:PQ9:H452 | 1.77                     | 0.65              |
| 2:b:5187:PRO:HA    | 17:b:5601:CLA:HMA1 | 1.77                     | 0.65              |
| 3:C:208:VAL:O      | 3:C:212:TYR:HB2    | 1.96                     | 0.65              |
| 3:C:236:GLY:HA3    | 20:C:516:BCR:H393  | 1.79                     | 0.65              |
| 13:Z:58:ASN:HA     | 13:Z:61:VAL:HB     | 1.78                     | 0.65              |
| 2:b:5354:LEU:HD23  | 2:b:5370:LEU:HB3   | 1.78                     | 0.65              |
| 1:A:187:GLN:HG3    | 1:A:325:ASN:HD21   | 1.61                     | 0.65              |
| 2:B:354:LEU:HD23   | 2:B:370:LEU:HB3    | 1.78                     | 0.65              |
| 17:C:505:CLA:HBC3  | 17:C:505:CLA:HHD   | 1.79                     | 0.65              |
| 23:D:403:SQD:H381  | 20:Y:101:BCR:H21C  | 1.79                     | 0.65              |
| 5:E:36:LEU:O       | 5:E:40:THR:N       | 2.24                     | 0.65              |
| 9:K:20:PRO:HB2     | 14:Y:24:MET:HB2    | 1.77                     | 0.65              |
| 17:b:5613:CLA:H51  | 25:d:5409:MGE:H241 | 1.77                     | 0.65              |
| 17:B:604:CLA:HBB1  | 17:B:607:CLA:HAB   | 1.78                     | 0.65              |
| 17:c:5505:CLA:HBC3 | 17:c:5505:CLA:HHD  | 1.79                     | 0.65              |
| 5:e:5036:LEU:O     | 5:e:5040:THR:N     | 2.24                     | 0.65              |
| 2:b:5025:MET:HE2   | 20:b:5617:BCR:H23C | 1.79                     | 0.65              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 17:b:5607:CLA:H203 | 4:d:5281:MET:HE3   | 1.79                     | 0.65              |
| 17:b:5610:CLA:H141 | 17:b:5612:CLA:HBD  | 1.79                     | 0.65              |
| 2:B:187:PRO:HA     | 17:B:601:CLA:HMA1  | 1.77                     | 0.65              |
| 17:B:610:CLA:H141  | 17:B:612:CLA:HBD   | 1.79                     | 0.65              |
| 4:D:263:ASN:HB2    | 4:D:266:TRP:HB3    | 1.79                     | 0.65              |
| 1:a:5030:VAL:HG23  | 1:a:5034:GLY:HA3   | 1.78                     | 0.65              |
| 15:n:68:LEU:HD22   | 15:n:94:LEU:HD22   | 1.79                     | 0.65              |
| 1:A:156:ALA:HA     | 1:A:160:ILE:HD12   | 1.79                     | 0.65              |
| 2:B:124:ARG:O      | 7:H:12:ARG:NH2     | 2.30                     | 0.65              |
| 2:B:258:TYR:CE2    | 26:D:411:DGD:C3G   | 2.67                     | 0.65              |
| 2:B:68:ARG:NH2     | 17:B:603:CLA:O2D   | 2.30                     | 0.65              |
| 2:B:77:GLY:C       | 2:B:86:ILE:HD11    | 2.20                     | 0.65              |
| 3:c:5212:TYR:OH    | 3:c:5227:VAL:N     | 2.18                     | 0.65              |
| 4:d:5263:ASN:HB2   | 4:d:5266:TRP:HB3   | 1.79                     | 0.65              |
| 3:C:405:ASN:HD22   | 26:C:518:DGD:HD61  | 1.63                     | 0.64              |
| 16:x:7:LEU:O       | 16:x:7:LEU:HD13    | 1.96                     | 0.64              |
| 13:Z:16:SER:OG     | 13:Z:47:TRP:NE1    | 2.21                     | 0.64              |
| 4:d:5188:PHE:HD1   | 4:d:5326:ARG:HG2   | 1.62                     | 0.64              |
| 13:z:5058:ASN:HA   | 13:z:5061:VAL:HB   | 1.78                     | 0.64              |
| 5:e:5077:GLU:O     | 5:e:5081:GLU:N     | 2.31                     | 0.64              |
| 13:z:5021:ILE:CD1  | 14:y:31:ALA:HB1    | 2.26                     | 0.64              |
| 3:c:5033:PHE:CZ    | 3:c:5040:ALA:HB3   | 2.33                     | 0.64              |
| 2:B:25:MET:HE2     | 20:B:617:BCR:H23C  | 1.79                     | 0.64              |
| 4:D:100:ASP:OD2    | 4:D:103:ARG:NH1    | 2.26                     | 0.64              |
| 7:H:38:PHE:CD1     | 20:H:101:BCR:H10C  | 2.33                     | 0.64              |
| 10:L:14:ARG:NH2    | 23:L:101:SQD:O49   | 2.30                     | 0.64              |
| 1:a:5083:VAL:HG22  | 4:d:5314:PHE:CE2   | 2.33                     | 0.64              |
| 1:a:5143:ILE:N     | 4:d:5220:ASN:HD21  | 1.96                     | 0.64              |
| 1:a:5187:GLN:HG3   | 1:a:5325:ASN:HD21  | 1.61                     | 0.64              |
| 2:b:5068:ARG:NH2   | 17:b:5603:CLA:O2D  | 2.30                     | 0.64              |
| 1:A:297:LEU:HD23   | 3:C:428:THR:HG21   | 1.79                     | 0.64              |
| 1:a:5156:ALA:HA    | 1:a:5160:ILE:HD12  | 1.79                     | 0.64              |
| 15:N:68:LEU:HD22   | 15:N:94:LEU:HD22   | 1.79                     | 0.64              |
| 2:B:440:ASP:OD1    | 2:B:442:ILE:N      | 2.30                     | 0.64              |
| 2:B:462:PHE:O      | 2:B:466:HIS:N      | 2.30                     | 0.64              |
| 3:C:349:ILE:H      | 3:C:374:GLY:HA3    | 1.61                     | 0.64              |
| 4:D:202:ALA:HB2    | 19:D:406:PQ9:H342  | 1.80                     | 0.64              |
| 26:a:5411:DGD:HD61 | 3:c:5405:ASN:HD22  | 1.62                     | 0.64              |
| 3:c:5372:PRO:HB3   | 15:n:85:SER:HA     | 1.80                     | 0.64              |
| 4:d:5041:ALA:HB1   | 18:d:5402:PHO:H42  | 1.80                     | 0.64              |
| 4:d:5202:ALA:HB2   | 19:d:5405:PQ9:H342 | 1.80                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:z:5028:ALA:O    | 14:y:45:ASN:N      | 2.31                     | 0.64              |
| 25:D:410:MGE:H2B1  | 10:L:19:LEU:HD21   | 1.78                     | 0.63              |
| 16:x:7:LEU:HD13    | 16:x:7:LEU:C       | 2.22                     | 0.63              |
| 3:C:33:PHE:CZ      | 3:C:40:ALA:HB3     | 2.33                     | 0.63              |
| 1:a:5296:ASN:HB3   | 3:c:5401:LEU:HA    | 1.79                     | 0.63              |
| 2:B:160:GLY:HA3    | 2:B:180:PRO:HB3    | 1.80                     | 0.63              |
| 17:b:5603:CLA:H201 | 7:h:5035:MET:HG3   | 1.79                     | 0.63              |
| 3:c:5236:GLY:HA3   | 20:c:5514:BCR:H393 | 1.79                     | 0.63              |
| 26:b:5621:DGD:O2D  | 4:d:5087:HIS:CG    | 2.52                     | 0.63              |
| 4:D:188:PHE:HD1    | 4:D:326:ARG:HG2    | 1.62                     | 0.63              |
| 4:d:5060:THR:HG23  | 4:d:5061:HIS:H     | 1.64                     | 0.63              |
| 15:n:130:ARG:O     | 15:n:134:SER:OG    | 2.10                     | 0.63              |
| 17:B:605:CLA:HBB1  | 17:B:606:CLA:H43   | 1.80                     | 0.63              |
| 3:C:187:ASP:HA     | 3:C:230:LEU:HD11   | 1.81                     | 0.63              |
| 4:D:130:PHE:O      | 4:D:133:ALA:N      | 2.32                     | 0.63              |
| 17:b:5601:CLA:H2A  | 17:b:5601:CLA:CED  | 2.29                     | 0.63              |
| 3:c:5187:ASP:HA    | 3:c:5230:LEU:HD11  | 1.81                     | 0.63              |
| 17:B:601:CLA:CED   | 17:B:601:CLA:H2A   | 2.29                     | 0.63              |
| 2:b:5002:GLY:N     | 10:l:5009:PRO:O    | 2.32                     | 0.63              |
| 20:b:5617:BCR:HC22 | 25:b:5620:MGE:H5B1 | 1.81                     | 0.63              |
| 16:x:12:ILE:HD12   | 16:x:12:ILE:N      | 2.04                     | 0.63              |
| 2:B:468:TRP:CE3    | 4:D:144:ILE:HD13   | 2.34                     | 0.63              |
| 16:x:12:ILE:CD1    | 16:x:12:ILE:H      | 1.95                     | 0.63              |
| 2:B:2:GLY:N        | 10:L:9:PRO:O       | 2.31                     | 0.62              |
| 2:B:75:TRP:CZ3     | 2:B:94:GLU:HB2     | 2.34                     | 0.62              |
| 4:D:91:LEU:HD23    | 4:D:93:TRP:CZ2     | 2.34                     | 0.62              |
| 3:C:293:ASN:OD1    | 3:C:295:THR:N      | 2.32                     | 0.62              |
| 4:D:72:ASN:HD21    | 4:D:74:LEU:HB2     | 1.63                     | 0.62              |
| 10:L:8:GLN:NE2     | 10:L:9:PRO:HD2     | 2.15                     | 0.62              |
| 15:n:86:SER:O      | 15:n:89:THR:OG1    | 2.17                     | 0.62              |
| 1:A:105:TRP:HE3    | 1:A:106:LEU:HD12   | 1.64                     | 0.62              |
| 4:D:60:THR:HG23    | 4:D:61:HIS:H       | 1.64                     | 0.62              |
| 15:n:124:VAL:O     | 15:n:128:LEU:N     | 2.18                     | 0.62              |
| 3:C:33:PHE:HZ      | 3:C:40:ALA:HB3     | 1.64                     | 0.62              |
| 3:c:5293:ASN:OD1   | 3:c:5295:THR:N     | 2.32                     | 0.62              |
| 4:d:5091:LEU:HD23  | 4:d:5093:TRP:CZ2   | 2.34                     | 0.62              |
| 4:d:5192:THR:HG23  | 17:d:5403:CLA:HBC2 | 1.82                     | 0.62              |
| 4:D:192:THR:HG23   | 17:D:404:CLA:HBC2  | 1.81                     | 0.62              |
| 4:D:297:ASP:HA     | 4:D:315:TYR:OH     | 2.00                     | 0.62              |
| 2:b:5256:MET:HG3   | 2:b:5451:PHE:CE1   | 2.34                     | 0.62              |
| 7:H:38:PHE:HD1     | 20:H:101:BCR:H10C  | 1.65                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:a:5329:GLU:OE1   | 3:c:5412:THR:OG1   | 2.09                     | 0.62              |
| 4:d:5072:ASN:HD21  | 4:d:5074:LEU:HB2   | 1.63                     | 0.62              |
| 7:h:5038:PHE:CD1   | 20:h:5101:BCR:H10C | 2.33                     | 0.62              |
| 2:B:122:LEU:HD12   | 7:H:8:GLY:HA2      | 1.82                     | 0.62              |
| 17:B:608:CLA:H51   | 17:B:609:CLA:H112  | 1.82                     | 0.62              |
| 3:C:157:MET:HE1    | 3:C:271:TYR:CG     | 2.35                     | 0.62              |
| 4:d:5244:TYR:OH    | 4:d:5264:LYS:NZ    | 2.32                     | 0.62              |
| 5:e:5074:GLN:NE2   | 5:e:5077:GLU:OE1   | 2.33                     | 0.62              |
| 20:k:5502:BCR:H16C | 14:y:33:PRO:HD3    | 1.82                     | 0.62              |
| 10:l:5008:GLN:NE2  | 10:l:5009:PRO:HD2  | 2.14                     | 0.62              |
| 15:N:109:LEU:CB    | 15:N:114:LYS:HE3   | 2.26                     | 0.62              |
| 12:T:18:PHE:HB2    | 20:T:102:BCR:HC7   | 1.81                     | 0.62              |
| 2:b:5160:GLY:HA3   | 2:b:5180:PRO:HB3   | 1.80                     | 0.62              |
| 3:c:5402:GLY:HA3   | 3:c:5420:VAL:HG22  | 1.81                     | 0.62              |
| 4:D:66:SER:OG      | 4:D:69:GLU:OE1     | 2.18                     | 0.62              |
| 1:a:5105:TRP:HE3   | 1:a:5106:LEU:HD12  | 1.64                     | 0.62              |
| 2:b:5292:LEU:HD21  | 2:b:5298:LEU:HA    | 1.81                     | 0.62              |
| 1:A:253:GLY:O      | 1:A:257:ARG:N      | 2.31                     | 0.61              |
| 2:B:256:MET:HG3    | 2:B:451:PHE:CE1    | 2.34                     | 0.61              |
| 2:b:5440:ASP:OD1   | 2:b:5442:ILE:N     | 2.31                     | 0.61              |
| 3:c:5461:ARG:NH1   | 4:d:5225:ASP:OD1   | 2.32                     | 0.61              |
| 1:a:5024:THR:O     | 4:d:5255:GLN:NE2   | 2.32                     | 0.61              |
| 1:a:5083:VAL:HG22  | 4:d:5314:PHE:HE2   | 1.64                     | 0.61              |
| 1:a:5253:GLY:O     | 1:a:5257:ARG:N     | 2.31                     | 0.61              |
| 2:b:5080:ILE:HD11  | 2:b:5093:PHE:CZ    | 2.35                     | 0.61              |
| 2:B:80:ILE:HD11    | 2:B:93:PHE:CZ      | 2.35                     | 0.61              |
| 17:b:5608:CLA:H51  | 17:b:5609:CLA:H112 | 1.82                     | 0.61              |
| 5:e:5021:VAL:HG23  | 5:e:5022:ILE:H     | 1.65                     | 0.61              |
| 20:B:617:BCR:HC22  | 25:B:619:MGE:H5B1  | 1.81                     | 0.61              |
| 4:D:244:TYR:OH     | 4:D:264:LYS:NZ     | 2.32                     | 0.61              |
| 17:a:5403:CLA:H161 | 25:d:5410:MGE:H252 | 1.83                     | 0.61              |
| 4:D:189:HIS:CG     | 4:D:289:LEU:HD21   | 2.36                     | 0.61              |
| 3:c:5033:PHE:HZ    | 3:c:5040:ALA:HB3   | 1.64                     | 0.61              |
| 3:c:5157:MET:HE1   | 3:c:5271:TYR:CG    | 2.35                     | 0.61              |
| 2:B:46:ASP:OD1     | 2:B:58:GLN:NE2     | 2.33                     | 0.61              |
| 4:D:223:PHE:HE1    | 4:D:245:SER:HB3    | 1.65                     | 0.61              |
| 2:b:5046:ASP:OD1   | 2:b:5058:GLN:NE2   | 2.33                     | 0.61              |
| 4:d:5068:LEU:HA    | 6:f:5040:MET:SD    | 2.41                     | 0.61              |
| 5:e:5020:TRP:N     | 5:e:5023:HIS:HD2   | 1.97                     | 0.61              |
| 7:h:5038:PHE:HD1   | 20:h:5101:BCR:H10C | 1.65                     | 0.61              |
| 10:L:14:ARG:NH1    | 23:L:101:SQD:O10   | 2.32                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:b:5075:TRP:CZ3  | 2:b:5094:GLU:HB2   | 2.34                     | 0.61              |
| 4:d:5297:ASP:HA   | 4:d:5315:TYR:OH    | 2.00                     | 0.61              |
| 13:z:5028:ALA:HB1 | 14:y:39:LEU:CD1    | 2.31                     | 0.61              |
| 15:n:62:ALA:O     | 15:n:66:LYS:HG2    | 2.01                     | 0.61              |
| 16:x:3:ILE:O      | 16:x:3:ILE:HG22    | 2.00                     | 0.61              |
| 1:A:285:PHE:O     | 1:A:289:GLY:N      | 2.33                     | 0.61              |
| 2:B:80:ILE:HD11   | 2:B:93:PHE:HZ      | 1.66                     | 0.61              |
| 2:B:292:LEU:HD21  | 2:B:298:LEU:HA     | 1.81                     | 0.61              |
| 4:D:210:LEU:HD22  | 4:D:271:MET:HG2    | 1.83                     | 0.61              |
| 3:c:5189:TRP:HB3  | 15:n:76:ARG:NE     | 2.16                     | 0.61              |
| 13:z:5039:LEU:HA  | 13:z:5042:LEU:HB2  | 1.83                     | 0.61              |
| 23:L:101:SQD:H81  | 25:m:5101:MGE:H6B2 | 1.82                     | 0.60              |
| 14:Y:18:VAL:O     | 14:Y:18:VAL:HG12   | 2.01                     | 0.60              |
| 15:N:124:VAL:O    | 15:N:128:LEU:N     | 2.18                     | 0.60              |
| 4:d:5189:HIS:CG   | 4:d:5289:LEU:HD21  | 2.36                     | 0.60              |
| 4:d:5223:PHE:HE1  | 4:d:5245:SER:HB3   | 1.65                     | 0.60              |
| 1:A:272:HIS:CD2   | 4:D:218:VAL:HG11   | 2.35                     | 0.60              |
| 2:B:61:PHE:O      | 2:B:64:PRO:HD2     | 2.02                     | 0.60              |
| 4:d:5130:PHE:O    | 4:d:5133:ALA:N     | 2.32                     | 0.60              |
| 15:N:86:SER:O     | 15:N:89:THR:OG1    | 2.17                     | 0.60              |
| 16:X:37:VAL:O     | 16:X:37:VAL:HG12   | 2.01                     | 0.60              |
| 17:B:608:CLA:H72  | 17:B:609:CLA:H121  | 1.83                     | 0.60              |
| 2:b:5185:TRP:HE1  | 17:b:5601:CLA:HBC3 | 1.66                     | 0.60              |
| 9:k:5020:PRO:CB   | 14:y:24:MET:HB3    | 2.30                     | 0.60              |
| 3:C:402:GLY:HA3   | 3:C:420:VAL:HG22   | 1.81                     | 0.60              |
| 12:T:4:ILE:HD11   | 20:T:102:BCR:H272  | 1.81                     | 0.60              |
| 2:b:5462:PHE:O    | 2:b:5466:HIS:N     | 2.30                     | 0.60              |
| 13:Z:28:ALA:HB1   | 14:Y:39:LEU:CD1    | 2.31                     | 0.60              |
| 2:b:5080:ILE:HD11 | 2:b:5093:PHE:HZ    | 1.66                     | 0.60              |
| 15:N:62:ALA:O     | 15:N:66:LYS:HG2    | 2.01                     | 0.60              |
| 2:B:75:TRP:HZ3    | 2:B:94:GLU:HB2     | 1.67                     | 0.60              |
| 5:E:21:VAL:HG23   | 5:E:22:ILE:H       | 1.65                     | 0.60              |
| 13:Z:39:LEU:HA    | 13:Z:42:LEU:HB2    | 1.83                     | 0.60              |
| 1:a:5328:MET:HE2  | 4:d:5325:ILE:HD11  | 1.83                     | 0.60              |
| 2:b:5420:TYR:O    | 2:b:5424:ALA:N     | 2.33                     | 0.60              |
| 4:d:5261:PHE:HE1  | 25:d:5410:MGE:C1B  | 2.15                     | 0.60              |
| 5:e:5063:ILE:HG22 | 5:e:5065:LEU:HB2   | 1.83                     | 0.60              |
| 2:B:380:ASP:N     | 2:B:390:TYR:O      | 2.34                     | 0.60              |
| 3:C:178:LYS:HD2   | 3:C:182:PHE:O      | 2.02                     | 0.60              |
| 15:N:112:LYS:O    | 15:N:116:ARG:CG    | 2.48                     | 0.60              |
| 1:a:5104:GLU:OE2  | 1:a:5108:ASN:ND2   | 2.34                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:b:5256:MET:SD    | 2:b:5263:THR:HG21  | 2.42                     | 0.60              |
| 4:d:5074:LEU:HD22  | 4:d:5175:VAL:HG11  | 1.84                     | 0.60              |
| 16:X:9:GLY:HA2     | 16:X:12:ILE:HD12   | 1.82                     | 0.60              |
| 2:b:5061:PHE:O     | 2:b:5064:PRO:HD2   | 2.02                     | 0.60              |
| 2:b:5075:TRP:HZ3   | 2:b:5094:GLU:HB2   | 1.67                     | 0.60              |
| 2:b:5167:TRP:CD1   | 2:b:5264:PRO:HG3   | 2.37                     | 0.60              |
| 2:b:5340:TRP:HE1   | 2:b:5428:GLU:HB3   | 1.67                     | 0.60              |
| 2:B:167:TRP:CD1    | 2:B:264:PRO:HG3    | 2.37                     | 0.59              |
| 2:B:185:TRP:HE1    | 17:B:601:CLA:HBC3  | 1.66                     | 0.59              |
| 4:D:261:PHE:HE1    | 25:D:410:MGE:C1B   | 2.15                     | 0.59              |
| 1:a:5288:LEU:HD22  | 3:c:5432:VAL:HG22  | 1.84                     | 0.59              |
| 1:A:104:GLU:OE2    | 1:A:108:ASN:ND2    | 2.34                     | 0.59              |
| 2:B:420:TYR:O      | 2:B:424:ALA:N      | 2.33                     | 0.59              |
| 24:A:411:BCT:O2    | 4:D:214:HIS:NE2    | 2.35                     | 0.59              |
| 18:D:402:PHO:H152  | 17:D:404:CLA:H172  | 1.83                     | 0.59              |
| 2:B:256:MET:SD     | 2:B:263:THR:HG21   | 2.42                     | 0.59              |
| 1:a:5084:PRO:HA    | 1:a:5112:TYR:CG    | 2.38                     | 0.59              |
| 3:c:5466:VAL:HG13  | 4:d:5251:ARG:HD3   | 1.84                     | 0.59              |
| 4:D:103:ARG:HH21   | 5:E:77:GLU:CD      | 2.09                     | 0.59              |
| 1:a:5283:VAL:O     | 1:a:5286:THR:OG1   | 2.19                     | 0.59              |
| 2:b:5271:THR:HG22  | 2:b:5274:GLN:HG2   | 1.84                     | 0.59              |
| 23:l:5102:SQD:H101 | 25:m:5103:MGE:H6A2 | 1.84                     | 0.59              |
| 5:E:63:ILE:HG22    | 5:E:65:LEU:HB2     | 1.83                     | 0.59              |
| 3:c:5367:GLU:HG3   | 15:n:91:GLN:HE22   | 1.66                     | 0.59              |
| 17:c:5512:CLA:C4B  | 20:z:5101:BCR:H383 | 2.33                     | 0.59              |
| 17:b:5608:CLA:H72  | 17:b:5609:CLA:H121 | 1.83                     | 0.59              |
| 16:X:36:LYS:N      | 16:X:36:LYS:HD2    | 2.18                     | 0.59              |
| 1:A:35:VAL:HG11    | 8:I:18:LEU:HD22    | 1.85                     | 0.59              |
| 1:A:259:ILE:HG22   | 1:A:260:PHE:H      | 1.68                     | 0.59              |
| 20:C:514:BCR:H11C  | 20:Y:101:BCR:H322  | 1.84                     | 0.59              |
| 1:a:5195:HIS:ND1   | 1:a:5196:PRO:HD2   | 2.18                     | 0.59              |
| 2:b:5341:LYS:HD3   | 2:b:5431:GLU:HG3   | 1.84                     | 0.59              |
| 2:B:39:LEU:O       | 2:B:43:ALA:N       | 2.35                     | 0.59              |
| 2:B:135:LEU:HD22   | 2:B:232:GLY:H      | 1.68                     | 0.59              |
| 2:B:340:TRP:HE1    | 2:B:428:GLU:HB3    | 1.67                     | 0.59              |
| 2:B:341:LYS:HD3    | 2:B:431:GLU:HG3    | 1.84                     | 0.59              |
| 4:D:74:LEU:HD22    | 4:D:175:VAL:HG11   | 1.84                     | 0.59              |
| 29:F:101:HEM:HBC2  | 29:F:101:HEM:HHD   | 1.84                     | 0.59              |
| 1:a:5218:LEU:O     | 1:a:5221:SER:OG    | 2.18                     | 0.59              |
| 2:b:5055:MET:HE1   | 2:b:5080:ILE:HA    | 1.85                     | 0.59              |
| 29:f:5101:HEM:HBC2 | 29:f:5101:HEM:HHD  | 1.84                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:x:4:THR:HB      | 16:x:5:PRO:HD2     | 1.83                     | 0.59              |
| 1:A:53:ILE:HA      | 1:A:71:LEU:HB3     | 1.85                     | 0.58              |
| 2:B:150:CYS:HA     | 17:B:603:CLA:HBC2  | 1.85                     | 0.58              |
| 2:B:271:THR:HG22   | 2:B:274:GLN:HG2    | 1.84                     | 0.58              |
| 2:B:464:PHE:HB2    | 4:D:280:TRP:CH2    | 2.38                     | 0.58              |
| 3:C:225:VAL:HG21   | 3:C:288:CYS:SG     | 2.43                     | 0.58              |
| 3:C:239:TRP:O      | 3:C:243:ILE:N      | 2.32                     | 0.58              |
| 29:F:101:HEM:HBB2  | 29:F:101:HEM:HMB2  | 1.85                     | 0.58              |
| 2:b:5135:LEU:HD22  | 2:b:5232:GLY:H     | 1.68                     | 0.58              |
| 2:b:5283:GLU:HA    | 2:b:5286:ARG:HG2   | 1.85                     | 0.58              |
| 4:d:5210:LEU:HD22  | 4:d:5271:MET:HG2   | 1.83                     | 0.58              |
| 7:h:5044:ILE:HD13  | 16:x:10:PHE:CZ     | 2.36                     | 0.58              |
| 14:y:25:ILE:HA     | 14:y:28:ILE:HG12   | 1.85                     | 0.58              |
| 2:b:5349:LYS:HD3   | 2:b:5396:GLY:HA3   | 1.85                     | 0.58              |
| 29:f:5101:HEM:HMB2 | 29:f:5101:HEM:HBB2 | 1.85                     | 0.58              |
| 9:K:39:TRP:CD1     | 14:Y:36:ILE:HD11   | 2.38                     | 0.58              |
| 1:a:5136:ARG:NH2   | 8:i:5027:ASP:OD1   | 2.37                     | 0.58              |
| 2:b:5418:LYS:HA    | 2:b:5421:ALA:HB3   | 1.85                     | 0.58              |
| 4:d:5018:LEU:CD1   | 16:x:29:ILE:HG12   | 2.33                     | 0.58              |
| 17:B:602:CLA:H112  | 17:B:602:CLA:H171  | 1.85                     | 0.58              |
| 4:D:218:VAL:HG23   | 4:D:244:TYR:CG     | 2.38                     | 0.58              |
| 6:F:24:HIS:NE2     | 29:F:101:HEM:ND    | 2.51                     | 0.58              |
| 2:b:5012:LEU:HB2   | 17:b:5612:CLA:HMC2 | 1.84                     | 0.58              |
| 3:c:5106:VAL:HG23  | 3:c:5107:ASP:H     | 1.69                     | 0.58              |
| 26:A:413:DGD:HB71  | 25:C:519:MGE:H7A1  | 1.84                     | 0.58              |
| 17:C:513:CLA:C4B   | 20:C:515:BCR:H383  | 2.33                     | 0.58              |
| 5:E:22:ILE:HG22    | 5:E:26:THR:HG23    | 1.85                     | 0.58              |
| 2:b:5222:PRO:HB3   | 7:h:5025:TRP:C     | 2.29                     | 0.58              |
| 2:b:5290:ALA:O     | 2:b:5294:SER:N     | 2.33                     | 0.58              |
| 17:b:5611:CLA:H172 | 17:b:5613:CLA:H8   | 1.85                     | 0.58              |
| 2:B:205:ALA:O      | 2:B:209:GLY:N      | 2.34                     | 0.58              |
| 2:B:280:PHE:O      | 2:B:284:ILE:N      | 2.37                     | 0.58              |
| 2:B:349:LYS:HD3    | 2:B:396:GLY:HA3    | 1.85                     | 0.58              |
| 3:C:331:ALA:HB1    | 3:C:339:LYS:HE3    | 1.86                     | 0.58              |
| 1:a:5159:LEU:HD23  | 26:c:5515:DGD:HAT1 | 1.85                     | 0.58              |
| 2:b:5360:PRO:HG2   | 4:d:5339:PHE:HZ    | 1.69                     | 0.58              |
| 3:c:5225:VAL:HG21  | 3:c:5288:CYS:SG    | 2.43                     | 0.58              |
| 16:X:21:LEU:HD23   | 16:X:21:LEU:N      | 2.19                     | 0.58              |
| 3:c:5331:ALA:HB1   | 3:c:5339:LYS:HE3   | 1.86                     | 0.58              |
| 4:d:5018:LEU:HD12  | 16:x:29:ILE:HG12   | 1.85                     | 0.58              |
| 4:d:5146:PHE:HD1   | 18:d:5402:PHO:C3D  | 2.17                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:55:MET:HE1     | 2:B:80:ILE:HA      | 1.85                     | 0.58              |
| 3:C:290:VAL:HG11   | 3:C:426:LEU:HB2    | 1.86                     | 0.58              |
| 11:M:9:ILE:HG13    | 11:m:5009:ILE:HG13 | 1.86                     | 0.58              |
| 24:a:5412:BCT:O2   | 4:d:5214:HIS:NE2   | 2.36                     | 0.58              |
| 3:c:5178:LYS:HD2   | 3:c:5182:PHE:O     | 2.02                     | 0.58              |
| 4:d:5129:GLN:HE21  | 4:d:5142:ASN:CG    | 2.12                     | 0.58              |
| 6:f:5017:THR:OG1   | 6:f:5018:VAL:N     | 2.37                     | 0.58              |
| 16:X:29:ILE:O      | 16:X:32:SER:OG     | 2.18                     | 0.58              |
| 1:A:84:PRO:HA      | 1:A:112:TYR:CG     | 2.38                     | 0.58              |
| 1:A:218:LEU:O      | 1:A:221:SER:OG     | 2.18                     | 0.58              |
| 25:A:412:MGE:H3A2  | 11:M:22:LEU:HD11   | 1.86                     | 0.58              |
| 2:B:418:LYS:HA     | 2:B:421:ALA:HB3    | 1.85                     | 0.58              |
| 3:C:212:TYR:HH     | 3:C:227:VAL:H      | 1.50                     | 0.58              |
| 4:D:195:PRO:HB2    | 10:L:31:PHE:HE1    | 1.69                     | 0.58              |
| 1:a:5259:ILE:HG22  | 1:a:5260:PHE:H     | 1.68                     | 0.58              |
| 2:b:5150:CYS:HA    | 17:b:5603:CLA:HBC2 | 1.86                     | 0.58              |
| 17:b:5602:CLA:H171 | 17:b:5602:CLA:H112 | 1.85                     | 0.58              |
| 19:d:5405:PQ9:H301 | 25:l:5101:MGE:H241 | 1.86                     | 0.58              |
| 14:Y:42:ARG:HH11   | 14:Y:42:ARG:CG     | 2.14                     | 0.58              |
| 1:A:195:HIS:ND1    | 1:A:196:PRO:HD2    | 2.18                     | 0.58              |
| 2:B:12:LEU:HB2     | 17:B:612:CLA:HMC2  | 1.85                     | 0.58              |
| 2:B:413:ASP:HB2    | 2:B:415:PRO:HD2    | 1.86                     | 0.58              |
| 3:C:229:ASN:HD22   | 15:N:77:ARG:HB2    | 1.68                     | 0.58              |
| 1:a:5053:ILE:HA    | 1:a:5071:LEU:HB3   | 1.85                     | 0.58              |
| 25:d:5410:MGE:H6A2 | 12:t:5017:PHE:CD1  | 2.39                     | 0.58              |
| 1:A:272:HIS:CD2    | 24:A:411:BCT:HO3   | 2.18                     | 0.57              |
| 3:C:106:VAL:HG23   | 3:C:107:ASP:H      | 1.69                     | 0.57              |
| 3:C:459:ILE:HG22   | 4:D:222:LEU:O      | 2.04                     | 0.57              |
| 3:c:5376:ASP:O     | 3:c:5380:ILE:HG12  | 2.04                     | 0.57              |
| 2:B:283:GLU:HA     | 2:B:286:ARG:HG2    | 1.85                     | 0.57              |
| 23:L:101:SQD:H101  | 25:m:5101:MGE:H4B2 | 1.86                     | 0.57              |
| 15:N:54:ASP:HB2    | 15:N:55:PRO:HD2    | 1.87                     | 0.57              |
| 26:A:413:DGD:HA51  | 3:C:284:PHE:HB3    | 1.86                     | 0.57              |
| 26:C:518:DGD:HBE2  | 25:D:408:MGE:H9B1  | 1.86                     | 0.57              |
| 3:C:99:VAL:O       | 3:C:105:VAL:N      | 2.36                     | 0.57              |
| 2:b:5380:ASP:N     | 2:b:5390:TYR:O     | 2.34                     | 0.57              |
| 4:d:5218:VAL:HG23  | 4:d:5244:TYR:CG    | 2.38                     | 0.57              |
| 24:A:411:BCT:C     | 4:D:214:HIS:HE2    | 2.17                     | 0.57              |
| 2:B:13:ILE:HG23    | 2:B:14:ASN:H       | 1.70                     | 0.57              |
| 2:B:78:TRP:HA      | 2:B:84:THR:HG22    | 1.86                     | 0.57              |
| 3:C:376:ASP:O      | 3:C:380:ILE:HG12   | 2.04                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:D:42:TYR:OH      | 6:F:25:THR:O       | 2.14                     | 0.57              |
| 3:c:5284:PHE:HB3   | 26:c:5515:DGD:HA51 | 1.86                     | 0.57              |
| 19:d:5405:PQ9:H241 | 25:l:5101:MGE:H242 | 1.87                     | 0.57              |
| 9:k:5043:VAL:HG23  | 14:y:46:LEU:HD13   | 1.86                     | 0.57              |
| 4:D:87:HIS:CE1     | 4:D:162:LEU:HA     | 2.40                     | 0.57              |
| 7:H:53:LEU:HD11    | 16:X:7:LEU:HA      | 1.85                     | 0.57              |
| 2:b:5238:LEU:O     | 2:b:5242:ILE:HG12  | 2.05                     | 0.57              |
| 5:e:5022:ILE:HG22  | 5:e:5026:THR:HG23  | 1.85                     | 0.57              |
| 1:A:303:ASN:ND2    | 3:C:414:ILE:HG13   | 2.20                     | 0.57              |
| 4:D:129:GLN:HE21   | 4:D:142:ASN:CG     | 2.12                     | 0.57              |
| 1:a:5238:LYS:O     | 1:a:5241:GLN:HG3   | 2.05                     | 0.57              |
| 3:c:5178:LYS:HZ2   | 3:c:5183:GLY:HA3   | 1.70                     | 0.57              |
| 4:d:5087:HIS:CE1   | 4:d:5162:LEU:HA    | 2.40                     | 0.57              |
| 17:B:611:CLA:H172  | 17:B:613:CLA:H8    | 1.85                     | 0.57              |
| 3:c:5097:TRP:HE1   | 3:c:5178:LYS:NZ    | 2.03                     | 0.57              |
| 4:d:5093:TRP:CG    | 4:d:5094:GLY:H     | 2.23                     | 0.57              |
| 9:k:5026:PRO:O     | 9:k:5029:PRO:HD2   | 2.05                     | 0.57              |
| 15:n:51:PRO:HG2    | 15:n:54:ASP:HB3    | 1.87                     | 0.57              |
| 1:A:238:LYS:O      | 1:A:241:GLN:HG3    | 2.05                     | 0.57              |
| 9:K:43:VAL:HG23    | 14:Y:46:LEU:CD1    | 2.30                     | 0.57              |
| 1:a:5144:CYS:HB2   | 3:c:5442:LEU:HD21  | 1.87                     | 0.57              |
| 17:a:5404:CLA:HMB2 | 18:d:5402:PHO:H161 | 1.87                     | 0.57              |
| 2:b:5005:TRP:HE1   | 25:l:5101:MGE:H3G2 | 1.68                     | 0.57              |
| 7:h:5047:GLU:OE2   | 16:x:10:PHE:HD2    | 1.86                     | 0.57              |
| 2:B:122:LEU:HD11   | 7:H:11:LEU:HB2     | 1.87                     | 0.57              |
| 2:B:401:PHE:CD2    | 2:B:406:LEU:HD11   | 2.39                     | 0.57              |
| 20:H:101:BCR:H331  | 20:H:101:BCR:H343  | 1.87                     | 0.57              |
| 1:a:5087:ASN:ND2   | 1:a:5169:SER:OG    | 2.38                     | 0.57              |
| 13:z:5028:ALA:O    | 14:y:44:GLY:CA     | 2.53                     | 0.57              |
| 14:y:30:ILE:HG12   | 14:y:30:ILE:O      | 2.04                     | 0.57              |
| 2:B:7:ARG:NH1      | 17:B:611:CLA:HED1  | 2.20                     | 0.56              |
| 2:B:81:THR:OG1     | 2:B:83:GLU:OE1     | 2.18                     | 0.56              |
| 3:C:97:TRP:HE1     | 3:C:178:LYS:NZ     | 2.03                     | 0.56              |
| 9:K:26:PRO:O       | 9:K:29:PRO:HD2     | 2.05                     | 0.56              |
| 1:a:5320:ILE:HD11  | 4:d:5063:LEU:HD21  | 1.87                     | 0.56              |
| 24:a:5412:BCT:C    | 4:d:5214:HIS:HE2   | 2.17                     | 0.56              |
| 14:Y:33:PRO:HD3    | 20:Y:101:BCR:H16C  | 1.87                     | 0.56              |
| 1:A:87:ASN:ND2     | 1:A:169:SER:OG     | 2.38                     | 0.56              |
| 20:D:407:BCR:H11C  | 6:F:29:PRO:CB      | 2.36                     | 0.56              |
| 10:L:7:ARG:NH1     | 23:l:5102:SQD:O7   | 2.38                     | 0.56              |
| 14:Y:34:MET:HA     | 14:Y:34:MET:CE     | 2.35                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:C:398:HIS:HA     | 3:C:419:PHE:CZ     | 2.40                     | 0.56              |
| 4:D:93:TRP:CG      | 4:D:94:GLY:H       | 2.23                     | 0.56              |
| 2:b:5280:PHE:O     | 2:b:5284:ILE:N     | 2.37                     | 0.56              |
| 17:b:5609:CLA:CGA  | 7:h:5031:MET:HE1   | 2.35                     | 0.56              |
| 3:c:5099:VAL:O     | 3:c:5105:VAL:N     | 2.36                     | 0.56              |
| 3:c:5368:PRO:HG3   | 15:n:91:GLN:HE21   | 1.70                     | 0.56              |
| 4:d:5195:PRO:HB2   | 10:l:5031:PHE:HE1  | 1.70                     | 0.56              |
| 16:X:3:ILE:HG22    | 16:X:8:LYS:CB      | 2.35                     | 0.56              |
| 17:A:401:CLA:C2    | 18:A:404:PHO:HBB1  | 2.36                     | 0.56              |
| 2:B:314:TYR:HB3    | 2:B:317:ASN:HB2    | 1.88                     | 0.56              |
| 2:b:5078:TRP:HA    | 2:b:5084:THR:HG22  | 1.86                     | 0.56              |
| 2:b:5241:SER:OG    | 17:b:5612:CLA:O1D  | 2.19                     | 0.56              |
| 2:b:5401:PHE:CD2   | 2:b:5406:LEU:HD11  | 2.39                     | 0.56              |
| 3:c:5398:HIS:HA    | 3:c:5419:PHE:CZ    | 2.40                     | 0.56              |
| 4:d:5093:TRP:CZ2   | 16:x:13:GLY:HA3    | 2.40                     | 0.56              |
| 3:C:165:LEU:HD13   | 17:C:506:CLA:HAB   | 1.87                     | 0.56              |
| 5:E:77:GLU:O       | 5:E:81:GLU:HB2     | 2.06                     | 0.56              |
| 3:c:5230:LEU:O     | 3:c:5233:VAL:HG22  | 2.06                     | 0.56              |
| 4:d:5189:HIS:HA    | 4:d:5294:ARG:HD2   | 1.87                     | 0.56              |
| 1:A:187:GLN:HE21   | 1:A:325:ASN:HD21   | 1.54                     | 0.56              |
| 1:A:283:VAL:O      | 1:A:286:THR:OG1    | 2.19                     | 0.56              |
| 1:a:5285:PHE:O     | 1:a:5289:GLY:N     | 2.33                     | 0.56              |
| 2:b:5071:VAL:HG22  | 17:b:5606:CLA:HED1 | 1.88                     | 0.56              |
| 3:c:5165:LEU:HD13  | 17:c:5506:CLA:HAB  | 1.87                     | 0.56              |
| 3:c:5290:VAL:HG11  | 3:c:5426:LEU:HB2   | 1.86                     | 0.56              |
| 4:d:5261:PHE:HA    | 25:d:5410:MGE:H2D  | 1.88                     | 0.56              |
| 15:n:72:PHE:O      | 15:n:76:ARG:HG3    | 2.06                     | 0.56              |
| 2:B:71:VAL:HG22    | 17:B:606:CLA:HED1  | 1.88                     | 0.56              |
| 2:B:241:SER:OG     | 17:B:612:CLA:O1D   | 2.19                     | 0.56              |
| 4:D:189:HIS:HA     | 4:D:294:ARG:HD2    | 1.87                     | 0.56              |
| 1:A:162:PRO:O      | 1:A:166:GLY:N      | 2.39                     | 0.56              |
| 2:B:290:ALA:HA     | 2:B:293:ALA:HB3    | 1.87                     | 0.56              |
| 2:B:302:TRP:CE3    | 2:B:343:HIS:CD2    | 2.94                     | 0.56              |
| 3:C:63:TRP:CZ2     | 3:C:67:MET:HG3     | 2.41                     | 0.56              |
| 3:C:178:LYS:HZ2    | 3:C:183:GLY:HA3    | 1.70                     | 0.56              |
| 4:D:223:PHE:CE1    | 4:D:245:SER:HB3    | 2.41                     | 0.56              |
| 1:a:5162:PRO:O     | 1:a:5166:GLY:N     | 2.39                     | 0.56              |
| 1:a:5187:GLN:HE21  | 1:a:5325:ASN:HD21  | 1.54                     | 0.56              |
| 2:b:5413:ASP:HB2   | 2:b:5415:PRO:HD2   | 1.86                     | 0.56              |
| 17:b:5612:CLA:HBB1 | 17:b:5612:CLA:HMB1 | 1.88                     | 0.56              |
| 17:c:5501:CLA:H93  | 20:c:5514:BCR:H19C | 1.88                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:D:403:SQD:H371  | 20:Y:101:BCR:H23C  | 1.88                     | 0.56              |
| 9:K:35:LEU:HB2     | 20:Y:101:BCR:H351  | 1.88                     | 0.56              |
| 2:B:238:LEU:O      | 2:B:242:ILE:HG12   | 2.05                     | 0.56              |
| 2:b:5013:ILE:HG23  | 2:b:5014:ASN:H     | 1.70                     | 0.56              |
| 2:b:5364:GLU:HG3   | 4:d:5296:TYR:CE2   | 2.41                     | 0.56              |
| 3:c:5147:PHE:CE2   | 17:c:5512:CLA:H3A  | 2.41                     | 0.56              |
| 1:A:293:MET:SD     | 1:A:298:ASN:HA     | 2.47                     | 0.55              |
| 2:b:5302:TRP:CE3   | 2:b:5343:HIS:CD2   | 2.94                     | 0.55              |
| 20:h:5101:BCR:H331 | 20:h:5101:BCR:H343 | 1.87                     | 0.55              |
| 3:C:230:LEU:O      | 3:C:233:VAL:HG22   | 2.06                     | 0.55              |
| 17:C:511:CLA:H42   | 14:Y:46:LEU:HD23   | 1.87                     | 0.55              |
| 4:D:304:ARG:HG2    | 11:M:1:MET:CE      | 2.36                     | 0.55              |
| 17:a:5402:CLA:C2   | 18:a:5405:PHO:HBB1 | 2.36                     | 0.55              |
| 2:b:5007:ARG:NH1   | 17:b:5611:CLA:HED1 | 2.20                     | 0.55              |
| 2:b:5372:ASP:OD2   | 2:b:5378:LYS:HD3   | 2.07                     | 0.55              |
| 17:b:5608:CLA:H13  | 7:h:5039:LEU:HD21  | 1.88                     | 0.55              |
| 1:A:132:GLU:HB2    | 1:A:136:ARG:HH12   | 1.72                     | 0.55              |
| 2:b:5290:ALA:HA    | 2:b:5293:ALA:HB3   | 1.87                     | 0.55              |
| 3:c:5063:TRP:CZ2   | 3:c:5067:MET:HG3   | 2.41                     | 0.55              |
| 5:e:5020:TRP:CD1   | 5:e:5021:VAL:HG13  | 2.41                     | 0.55              |
| 13:z:5016:SER:HG   | 13:z:5047:TRP:HE1  | 1.51                     | 0.55              |
| 15:n:54:ASP:HB2    | 15:n:55:PRO:HD2    | 1.87                     | 0.55              |
| 16:x:9:GLY:O       | 16:x:12:ILE:HD12   | 1.98                     | 0.55              |
| 2:B:263:THR:HB     | 2:B:268:PHE:CD2    | 2.41                     | 0.55              |
| 2:b:5039:LEU:O     | 2:b:5043:ALA:N     | 2.35                     | 0.55              |
| 2:b:5064:PRO:HB2   | 2:b:5268:PHE:CE1   | 2.41                     | 0.55              |
| 2:b:5081:THR:OG1   | 2:b:5083:GLU:OE1   | 2.18                     | 0.55              |
| 4:d:5223:PHE:CE1   | 4:d:5245:SER:HB3   | 2.41                     | 0.55              |
| 15:N:45:ARG:HG3    | 15:N:118:GLU:HG2   | 1.89                     | 0.55              |
| 2:B:289:GLN:O      | 2:B:293:ALA:N      | 2.27                     | 0.55              |
| 2:B:372:ASP:OD2    | 2:B:378:LYS:HD3    | 2.06                     | 0.55              |
| 3:C:147:PHE:CE2    | 17:C:513:CLA:H3A   | 2.41                     | 0.55              |
| 3:C:223:TRP:NE1    | 25:C:519:MGE:H8B1  | 2.22                     | 0.55              |
| 17:C:506:CLA:HBA1  | 17:C:506:CLA:CHA   | 2.37                     | 0.55              |
| 1:a:5293:MET:SD    | 1:a:5298:ASN:HA    | 2.47                     | 0.55              |
| 4:d:5271:MET:O     | 4:d:5275:PRO:HD2   | 2.06                     | 0.55              |
| 16:X:3:ILE:HG21    | 16:X:8:LYS:HB2     | 1.88                     | 0.55              |
| 1:A:135:TYR:CE2    | 8:I:31:ASN:HB3     | 2.41                     | 0.55              |
| 1:A:246:TYR:HE2    | 1:A:248:ILE:HD11   | 1.71                     | 0.55              |
| 25:A:412:MGE:H3G2  | 2:B:5:TRP:HE1      | 1.70                     | 0.55              |
| 4:D:191:TRP:CZ2    | 4:D:197:HIS:HB2    | 2.42                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:a:5022:THR:HG21  | 8:i:5030:ARG:HD3   | 1.89                     | 0.55              |
| 2:b:5314:TYR:HB3   | 2:b:5317:ASN:HB2   | 1.88                     | 0.55              |
| 15:N:51:PRO:HG2    | 15:N:54:ASP:HB3    | 1.87                     | 0.55              |
| 17:A:405:CLA:H52   | 8:I:9:TYR:CD1      | 2.42                     | 0.55              |
| 17:B:612:CLA:HMB1  | 17:B:612:CLA:HBB1  | 1.88                     | 0.55              |
| 17:C:501:CLA:HBB1  | 20:C:516:BCR:H23C  | 1.89                     | 0.55              |
| 4:D:67:TYR:OH      | 25:D:408:MGE:H3G1  | 2.06                     | 0.55              |
| 2:b:5205:ALA:O     | 2:b:5209:GLY:N     | 2.34                     | 0.55              |
| 17:b:5614:CLA:H2   | 25:m:5101:MGE:H211 | 1.89                     | 0.55              |
| 2:B:77:GLY:CA      | 2:B:86:ILE:CD1     | 2.85                     | 0.55              |
| 1:a:5063:ILE:HG13  | 1:a:5064:ARG:N     | 2.22                     | 0.55              |
| 1:a:5246:TYR:HE2   | 1:a:5248:ILE:HD11  | 1.71                     | 0.55              |
| 2:b:5263:THR:HB    | 2:b:5268:PHE:CD2   | 2.41                     | 0.55              |
| 3:c:5376:ASP:HB2   | 3:c:5379:LYS:HE2   | 1.89                     | 0.55              |
| 2:B:290:ALA:O      | 2:B:294:SER:N      | 2.33                     | 0.55              |
| 3:C:376:ASP:HB2    | 3:C:379:LYS:HE2    | 1.89                     | 0.55              |
| 4:d:5191:TRP:CZ2   | 4:d:5197:HIS:HB2   | 2.42                     | 0.55              |
| 17:C:501:CLA:H93   | 20:C:516:BCR:H19C  | 1.88                     | 0.55              |
| 7:H:44:ILE:HD11    | 16:X:10:PHE:HE1    | 1.53                     | 0.55              |
| 1:a:5056:PRO:O     | 1:a:5058:VAL:N     | 2.40                     | 0.55              |
| 2:b:5464:PHE:HB2   | 4:d:5280:TRP:CH2   | 2.42                     | 0.55              |
| 17:c:5501:CLA:HBB1 | 20:c:5514:BCR:H23C | 1.89                     | 0.55              |
| 17:c:5506:CLA:HBA1 | 17:c:5506:CLA:CHA  | 2.37                     | 0.55              |
| 3:C:223:TRP:CE2    | 25:C:519:MGE:H8B1  | 2.42                     | 0.54              |
| 4:D:19:ASP:OD1     | 4:D:23:LYS:NZ      | 2.39                     | 0.54              |
| 4:D:271:MET:O      | 4:D:275:PRO:HD2    | 2.06                     | 0.54              |
| 3:C:186:TYR:OH     | 3:C:300:GLU:OE1    | 2.26                     | 0.54              |
| 1:a:5132:GLU:HB2   | 1:a:5136:ARG:HH12  | 1.72                     | 0.54              |
| 17:c:5501:CLA:H161 | 17:c:5507:CLA:H102 | 1.89                     | 0.54              |
| 23:l:5102:SQD:H91  | 25:m:5103:MGE:H4A1 | 1.89                     | 0.54              |
| 1:a:5317:TRP:HZ3   | 4:d:5077:ALA:HB3   | 1.69                     | 0.54              |
| 4:d:5056:THR:HG21  | 5:e:5050:PRO:HD3   | 1.89                     | 0.54              |
| 15:n:45:ARG:HG3    | 15:n:118:GLU:HG2   | 1.89                     | 0.54              |
| 17:A:401:CLA:C3    | 18:A:404:PHO:HBB1  | 2.37                     | 0.54              |
| 2:B:212:ALA:HB2    | 17:B:609:CLA:HMC2  | 1.90                     | 0.54              |
| 4:D:83:ASN:HA      | 4:D:166:SER:OG     | 2.08                     | 0.54              |
| 2:b:5074:SER:HA    | 2:b:5092:SER:HB2   | 1.90                     | 0.54              |
| 17:b:5613:CLA:O1D  | 17:b:5613:CLA:H2A  | 2.08                     | 0.54              |
| 1:A:96:ILE:HD13    | 1:A:105:TRP:CE2    | 2.43                     | 0.54              |
| 2:B:401:PHE:HD2    | 2:B:406:LEU:HD11   | 1.72                     | 0.54              |
| 17:a:5402:CLA:C3   | 18:a:5405:PHO:HBB1 | 2.37                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:c:5239:TRP:O    | 3:c:5243:ILE:N     | 2.33                     | 0.54              |
| 6:f:5040:MET:O    | 6:f:5043:ILE:HG12  | 2.07                     | 0.54              |
| 1:A:56:PRO:O      | 1:A:58:VAL:N       | 2.40                     | 0.54              |
| 2:b:5212:ALA:HB2  | 17:b:5609:CLA:HMC2 | 1.90                     | 0.54              |
| 3:c:5277:GLY:C    | 17:c:5505:CLA:HBC2 | 2.32                     | 0.54              |
| 3:c:5340:TYR:O    | 3:c:5352:GLY:N     | 2.41                     | 0.54              |
| 17:A:402:CLA:H71  | 25:D:410:MGE:H221  | 1.88                     | 0.54              |
| 2:B:74:SER:HA     | 2:B:92:SER:HB2     | 1.90                     | 0.54              |
| 3:C:277:GLY:C     | 17:C:505:CLA:HBC2  | 2.32                     | 0.54              |
| 17:C:501:CLA:H161 | 17:C:507:CLA:H102  | 1.89                     | 0.54              |
| 1:a:5053:ILE:O    | 1:a:5070:SER:OG    | 2.25                     | 0.54              |
| 1:A:53:ILE:O      | 1:A:70:SER:OG      | 2.25                     | 0.54              |
| 1:A:119:PHE:HD2   | 1:A:120:LEU:HD12   | 1.73                     | 0.54              |
| 1:A:142:TRP:HH2   | 3:C:447:ARG:HB2    | 1.73                     | 0.54              |
| 2:B:77:GLY:HA2    | 2:B:86:ILE:HD12    | 1.89                     | 0.54              |
| 6:F:43:ILE:HG13   | 6:F:44:GLN:HG3     | 1.90                     | 0.54              |
| 7:h:5035:MET:HB2  | 20:h:5101:BCR:HC42 | 1.89                     | 0.54              |
| 13:z:5005:PHE:CE1 | 13:z:5057:LEU:HD23 | 2.43                     | 0.54              |
| 13:z:5028:ALA:CB  | 14:y:39:LEU:HD22   | 2.31                     | 0.54              |
| 15:n:97:LEU:HD12  | 15:n:117:LEU:HD13  | 1.90                     | 0.54              |
| 4:D:304:ARG:HG2   | 11:M:1:MET:HE2     | 1.90                     | 0.54              |
| 6:F:40:MET:O      | 6:F:43:ILE:HG12    | 2.07                     | 0.54              |
| 7:H:35:MET:HB2    | 20:H:101:BCR:HC42  | 1.89                     | 0.54              |
| 1:a:5290:ILE:HD11 | 17:a:5402:CLA:OBD  | 2.08                     | 0.54              |
| 1:A:143:ILE:HG13  | 1:A:144:CYS:H      | 1.73                     | 0.53              |
| 1:a:5096:ILE:HD13 | 1:a:5105:TRP:CE2   | 2.43                     | 0.53              |
| 4:d:5232:PHE:CE2  | 23:d:5407:SQD:H461 | 2.43                     | 0.53              |
| 13:z:5028:ALA:O   | 14:y:44:GLY:C      | 2.50                     | 0.53              |
| 15:N:109:LEU:CA   | 15:N:114:LYS:HE3   | 2.37                     | 0.53              |
| 16:X:14:LEU:C     | 16:X:14:LEU:HD23   | 2.32                     | 0.53              |
| 1:A:91:LEU:HB2    | 1:A:166:GLY:O      | 2.09                     | 0.53              |
| 1:A:143:ILE:CD1   | 4:D:252:PHE:HZ     | 2.21                     | 0.53              |
| 2:B:47:PRO:HB3    | 2:B:78:TRP:CE3     | 2.43                     | 0.53              |
| 4:D:263:ASN:N     | 25:D:410:MGE:O3D   | 2.41                     | 0.53              |
| 2:b:5406:LEU:HD13 | 2:b:5409:GLN:HB3   | 1.90                     | 0.53              |
| 4:d:5093:TRP:O    | 4:d:5098:GLN:N     | 2.41                     | 0.53              |
| 15:n:50:LEU:HB2   | 15:n:57:LYS:HE3    | 1.90                     | 0.53              |
| 1:A:22:THR:HG21   | 8:I:30:ARG:HD3     | 1.90                     | 0.53              |
| 2:B:18:ARG:HD2    | 2:B:115:TRP:CZ3    | 2.44                     | 0.53              |
| 2:B:406:LEU:HD13  | 2:B:409:GLN:HB3    | 1.90                     | 0.53              |
| 4:D:14:TRP:CZ2    | 16:X:29:ILE:HD12   | 2.43                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:M:101:LMT:H4O1  | 22:M:101:LMT:H6B   | 1.55                     | 0.53              |
| 4:d:5199:MET:HE2   | 10:l:5027:LEU:HD22 | 1.90                     | 0.53              |
| 14:Y:34:MET:CA     | 14:Y:34:MET:CE     | 2.85                     | 0.53              |
| 1:A:142:TRP:CH2    | 3:C:447:ARG:HB2    | 2.43                     | 0.53              |
| 11:M:21:PHE:HD1    | 25:m:5103:MGE:H202 | 1.73                     | 0.53              |
| 23:d:5407:SQD:H371 | 20:k:5502:BCR:H23C | 1.89                     | 0.53              |
| 3:C:192:GLY:HA3    | 15:N:99:GLY:HA2    | 1.89                     | 0.53              |
| 3:C:340:TYR:O      | 3:C:352:GLY:N      | 2.41                     | 0.53              |
| 1:a:5119:PHE:HD2   | 1:a:5120:LEU:HD12  | 1.73                     | 0.53              |
| 2:b:5047:PRO:HB3   | 2:b:5078:TRP:CE3   | 2.43                     | 0.53              |
| 17:b:5614:CLA:C4A  | 17:b:5614:CLA:HBA2 | 2.39                     | 0.53              |
| 3:c:5134:ILE:HD11  | 17:k:5501:CLA:H12  | 1.91                     | 0.53              |
| 3:c:5189:TRP:CD1   | 3:c:5364:PRO:HA    | 2.44                     | 0.53              |
| 6:f:5043:ILE:HG13  | 6:f:5044:GLN:HG3   | 1.90                     | 0.53              |
| 15:n:73:ALA:HA     | 15:n:76:ARG:HH21   | 1.72                     | 0.53              |
| 1:A:55:ALA:HB3     | 1:A:70:SER:HB2     | 1.90                     | 0.53              |
| 2:B:347:ARG:HB2    | 2:B:398:THR:OG1    | 2.09                     | 0.53              |
| 3:C:79:LYS:HB3     | 3:C:80:PRO:HD2     | 1.91                     | 0.53              |
| 4:D:24:ARG:NH1     | 16:X:37:VAL:HG21   | 2.24                     | 0.53              |
| 4:D:328:TRP:CE2    | 4:D:346:LEU:HD23   | 2.44                     | 0.53              |
| 17:b:5602:CLA:H172 | 26:b:5621:DGD:HAT1 | 1.90                     | 0.53              |
| 4:d:5080:THR:HG21  | 4:d:5167:TRP:O     | 2.08                     | 0.53              |
| 4:d:5083:ASN:HA    | 4:d:5166:SER:OG    | 2.08                     | 0.53              |
| 6:f:5019:ARG:NH1   | 29:f:5101:HEM:O1D  | 2.41                     | 0.53              |
| 2:B:18:ARG:HE      | 2:B:118:TRP:HB3    | 1.73                     | 0.53              |
| 17:B:613:CLA:H2A   | 17:B:613:CLA:O1D   | 2.08                     | 0.53              |
| 9:K:28:ILE:HA      | 9:K:31:LEU:HD13    | 1.91                     | 0.53              |
| 17:c:5511:CLA:H2A  | 17:c:5511:CLA:O2D  | 2.09                     | 0.53              |
| 4:d:5035:ILE:CD1   | 16:x:28:LEU:HD13   | 2.25                     | 0.53              |
| 17:B:607:CLA:H171  | 4:D:199:MET:HE1    | 1.91                     | 0.53              |
| 17:C:512:CLA:O2D   | 17:C:512:CLA:H2A   | 2.09                     | 0.53              |
| 1:a:5055:ALA:HB3   | 1:a:5070:SER:HB2   | 1.90                     | 0.53              |
| 2:b:5018:ARG:HH22  | 10:l:5007:ARG:HH21 | 1.56                     | 0.53              |
| 2:b:5281:GLN:HE22  | 2:b:5358:ARG:HD3   | 1.74                     | 0.53              |
| 3:c:5343:ARG:HA    | 3:c:5349:ILE:HG22  | 1.91                     | 0.53              |
| 15:N:120:GLU:O     | 15:N:124:VAL:HG23  | 2.09                     | 0.53              |
| 17:B:603:CLA:H172  | 17:B:609:CLA:H8    | 1.91                     | 0.53              |
| 4:D:93:TRP:O       | 4:D:98:GLN:N       | 2.41                     | 0.53              |
| 9:K:20:PRO:HB3     | 14:Y:21:GLN:HA     | 1.90                     | 0.53              |
| 1:a:5091:LEU:HB2   | 1:a:5166:GLY:O     | 2.09                     | 0.53              |
| 2:b:5401:PHE:HD2   | 2:b:5406:LEU:HD11  | 1.73                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 4:d:5210:LEU:HA    | 4:d:5213:ILE:HG22 | 1.91                     | 0.53              |
| 4:d:5328:TRP:CE2   | 4:d:5346:LEU:HD23 | 2.44                     | 0.53              |
| 13:z:5028:ALA:HB1  | 14:y:39:LEU:HD11  | 1.91                     | 0.53              |
| 4:D:323:GLU:HA     | 4:D:326:ARG:HE    | 1.74                     | 0.53              |
| 1:a:5301:ASN:HB2   | 1:a:5322:ASN:HD21 | 1.74                     | 0.53              |
| 2:b:5174:LEU:HA    | 2:b:5308:LYS:HE3  | 1.91                     | 0.53              |
| 14:Y:31:ALA:O      | 14:Y:34:MET:HB2   | 2.09                     | 0.53              |
| 25:A:412:MGE:H242  | 19:D:406:PQ9:H241 | 1.91                     | 0.52              |
| 2:B:358:ARG:NH1    | 2:B:427:GLY:HA2   | 2.24                     | 0.52              |
| 17:B:614:CLA:C4A   | 17:B:614:CLA:HBA2 | 2.39                     | 0.52              |
| 4:D:80:THR:HG21    | 4:D:167:TRP:O     | 2.08                     | 0.52              |
| 1:a:5093:PHE:HB2   | 3:c:5218:PHE:CB   | 2.39                     | 0.52              |
| 3:c:5457:LYS:NZ    | 4:d:5227:GLU:O    | 2.41                     | 0.52              |
| 15:n:50:LEU:H      | 15:n:57:LYS:NZ    | 2.07                     | 0.52              |
| 15:N:50:LEU:H      | 15:N:57:LYS:NZ    | 2.07                     | 0.52              |
| 2:B:392:PHE:HZ     | 2:B:418:LYS:HB3   | 1.75                     | 0.52              |
| 2:B:475:PHE:HD2    | 4:D:140:PRO:HG3   | 1.73                     | 0.52              |
| 4:D:85:MET:HE2     | 4:D:90:LEU:HD21   | 1.91                     | 0.52              |
| 1:a:5163:ILE:HD11  | 26:c:5515:DGD:O1B | 2.10                     | 0.52              |
| 1:a:5193:LEU:HD21  | 17:a:5402:CLA:C2C | 2.40                     | 0.52              |
| 4:d:5026:ARG:HD2   | 6:f:5018:VAL:HG21 | 1.91                     | 0.52              |
| 2:B:174:LEU:HA     | 2:B:308:LYS:HE3   | 1.91                     | 0.52              |
| 6:F:20:TRP:CD1     | 6:F:24:HIS:CE1    | 2.97                     | 0.52              |
| 6:F:26:LEU:O       | 6:F:29:PRO:HD2    | 2.10                     | 0.52              |
| 2:b:5018:ARG:HD2   | 2:b:5115:TRP:CZ3  | 2.44                     | 0.52              |
| 2:b:5018:ARG:HE    | 2:b:5118:TRP:HB3  | 1.73                     | 0.52              |
| 4:d:5221:THR:C     | 4:d:5222:LEU:HD12 | 2.35                     | 0.52              |
| 20:k:5502:BCR:H333 | 14:y:28:ILE:O     | 2.08                     | 0.52              |
| 15:n:120:GLU:O     | 15:n:124:VAL:HG23 | 2.09                     | 0.52              |
| 3:C:62:PHE:CZ      | 9:K:28:ILE:HD11   | 2.44                     | 0.52              |
| 2:b:5347:ARG:HB2   | 2:b:5398:THR:OG1  | 2.09                     | 0.52              |
| 2:b:5358:ARG:NH1   | 2:b:5427:GLY:HA2  | 2.24                     | 0.52              |
| 1:A:149:ALA:HB3    | 1:A:150:PRO:HD3   | 1.92                     | 0.52              |
| 3:C:408:GLY:HA3    | 3:C:418:ASN:HA    | 1.92                     | 0.52              |
| 4:D:199:MET:HE2    | 10:L:27:LEU:HD22  | 1.91                     | 0.52              |
| 3:c:5403:SER:OG    | 3:c:5407:VAL:N    | 2.25                     | 0.52              |
| 4:d:5085:MET:HE2   | 4:d:5090:LEU:HD21 | 1.91                     | 0.52              |
| 15:N:50:LEU:HB2    | 15:N:57:LYS:HE3   | 1.90                     | 0.52              |
| 1:A:193:LEU:HD21   | 17:A:401:CLA:C2C  | 2.40                     | 0.52              |
| 1:A:204:GLY:HA3    | 1:A:282:GLY:HA3   | 1.91                     | 0.52              |
| 2:B:364:GLU:HG3    | 4:D:296:TYR:CE2   | 2.45                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:C:157:MET:HE2    | 17:C:507:CLA:HAC1  | 1.92                     | 0.52              |
| 3:C:437:PHE:CE2    | 17:C:502:CLA:HAC2  | 2.45                     | 0.52              |
| 1:a:5039:PRO:HB3   | 20:a:5408:BCR:H10C | 1.90                     | 0.52              |
| 17:b:5612:CLA:H171 | 17:b:5613:CLA:HBB2 | 1.91                     | 0.52              |
| 3:c:5157:MET:HE2   | 17:c:5507:CLA:HAC1 | 1.92                     | 0.52              |
| 4:D:93:TRP:CZ2     | 16:X:13:GLY:HA3    | 2.45                     | 0.52              |
| 4:D:221:THR:C      | 4:D:222:LEU:HD12   | 2.34                     | 0.52              |
| 25:D:410:MGE:H6A1  | 12:T:17:PHE:CD1    | 2.45                     | 0.52              |
| 1:a:5143:ILE:HG13  | 1:a:5144:CYS:H     | 1.73                     | 0.52              |
| 1:a:5149:ALA:HB3   | 1:a:5150:PRO:HD3   | 1.92                     | 0.52              |
| 2:b:5045:PHE:HA    | 2:b:5060:MET:HE3   | 1.91                     | 0.52              |
| 2:b:5392:PHE:HZ    | 2:b:5418:LYS:HB3   | 1.75                     | 0.52              |
| 4:d:5323:GLU:HA    | 4:d:5326:ARG:HE    | 1.75                     | 0.52              |
| 7:h:5047:GLU:CD    | 16:x:10:PHE:HE2    | 2.01                     | 0.52              |
| 9:k:5028:ILE:HA    | 9:k:5031:LEU:HD13  | 1.91                     | 0.52              |
| 11:m:5028:GLN:NE2  | 25:m:5101:MGE:H1G2 | 2.25                     | 0.52              |
| 15:N:27:THR:HG23   | 15:N:70:ASP:HB3    | 1.92                     | 0.52              |
| 1:a:5217:SER:OG    | 4:d:5142:ASN:HA    | 2.10                     | 0.52              |
| 3:c:5408:GLY:HA3   | 3:c:5418:ASN:HA    | 1.92                     | 0.52              |
| 6:f:5026:LEU:O     | 6:f:5029:PRO:HD2   | 2.10                     | 0.52              |
| 10:l:5004:ASN:ND2  | 10:l:5006:ASN:O    | 2.43                     | 0.52              |
| 14:Y:28:ILE:N      | 14:Y:28:ILE:CD1    | 2.73                     | 0.52              |
| 1:A:290:ILE:HD11   | 17:A:401:CLA:OBD   | 2.08                     | 0.52              |
| 1:A:301:ASN:HB2    | 1:A:322:ASN:HD21   | 1.74                     | 0.52              |
| 2:B:397:VAL:HG11   | 2:B:417:VAL:HG11   | 1.92                     | 0.52              |
| 3:C:55:ALA:HB1     | 20:C:514:BCR:H373  | 1.91                     | 0.52              |
| 3:C:134:ILE:HD11   | 17:C:511:CLA:H12   | 1.91                     | 0.52              |
| 5:E:23:HIS:HE1     | 29:F:101:HEM:ND    | 2.07                     | 0.52              |
| 3:c:5055:ALA:HB1   | 20:c:5513:BCR:H373 | 1.91                     | 0.52              |
| 3:c:5264:PHE:HE1   | 20:c:5514:BCR:H313 | 1.75                     | 0.52              |
| 10:l:5014:ARG:NH1  | 23:l:5102:SQD:O48  | 2.43                     | 0.52              |
| 15:n:27:THR:HG23   | 15:n:70:ASP:HB3    | 1.92                     | 0.52              |
| 16:X:21:LEU:N      | 16:X:21:LEU:CD2    | 2.73                     | 0.52              |
| 1:A:39:PRO:HB3     | 20:A:407:BCR:H10C  | 1.90                     | 0.52              |
| 2:B:64:PRO:HB2     | 2:B:268:PHE:CE1    | 2.41                     | 0.52              |
| 17:B:614:CLA:H2    | 25:m:5103:MGE:H8A1 | 1.91                     | 0.52              |
| 10:L:4:ASN:ND2     | 10:L:6:ASN:O       | 2.43                     | 0.52              |
| 2:b:5289:GLN:O     | 2:b:5293:ALA:N     | 2.27                     | 0.52              |
| 17:b:5603:CLA:H172 | 17:b:5609:CLA:H8   | 1.91                     | 0.52              |
| 3:c:5079:LYS:HB3   | 3:c:5080:PRO:HD2   | 1.91                     | 0.52              |
| 4:d:5186:GLN:HB2   | 17:d:5403:CLA:HBC1 | 1.92                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:n:75:TYR:HB3    | 15:n:87:PHE:CE1    | 2.45                     | 0.52              |
| 1:A:27:ARG:NH2     | 12:T:21:ILE:O      | 2.42                     | 0.51              |
| 1:A:269:ARG:HD3    | 4:D:222:LEU:HD23   | 1.92                     | 0.51              |
| 2:B:45:PHE:HA      | 2:B:60:MET:HE3     | 1.91                     | 0.51              |
| 1:a:5204:GLY:HA3   | 1:a:5282:GLY:HA3   | 1.91                     | 0.51              |
| 3:c:5188:THR:OG1   | 3:c:5295:THR:O     | 2.28                     | 0.51              |
| 1:A:274:PHE:HD1    | 23:D:403:SQD:H82   | 1.75                     | 0.51              |
| 1:A:304:HIS:CD2    | 3:C:415:ASN:OD1    | 2.64                     | 0.51              |
| 3:C:204:LEU:HA     | 3:C:209:ILE:HD11   | 1.93                     | 0.51              |
| 10:L:14:ARG:HH22   | 23:L:101:SQD:C7    | 2.23                     | 0.51              |
| 13:Z:5:PHE:CZ      | 13:Z:54:VAL:HA     | 2.46                     | 0.51              |
| 17:b:5607:CLA:H171 | 4:d:5199:MET:HE1   | 1.90                     | 0.51              |
| 4:D:48:TRP:CG      | 18:D:402:PHO:H13   | 2.46                     | 0.51              |
| 1:a:5093:PHE:HB2   | 3:c:5218:PHE:CG    | 2.45                     | 0.51              |
| 2:b:5222:PRO:HA    | 7:h:5022:ALA:HB3   | 1.93                     | 0.51              |
| 17:B:612:CLA:H171  | 17:B:613:CLA:HBB2  | 1.91                     | 0.51              |
| 4:D:69:GLU:HG2     | 4:D:70:GLY:N       | 2.22                     | 0.51              |
| 4:d:5019:ASP:OD1   | 4:d:5023:LYS:NZ    | 2.39                     | 0.51              |
| 1:A:195:HIS:CD2    | 1:A:197:PHE:HB2    | 2.46                     | 0.51              |
| 12:T:18:PHE:HB2    | 20:T:102:BCR:C7    | 2.40                     | 0.51              |
| 1:a:5195:HIS:CD2   | 1:a:5197:PHE:HB2   | 2.46                     | 0.51              |
| 17:a:5402:CLA:H201 | 25:d:5410:MGE:H232 | 1.92                     | 0.51              |
| 4:d:5014:TRP:CZ2   | 16:x:29:ILE:HD11   | 2.44                     | 0.51              |
| 1:A:219:VAL:HG11   | 4:D:268:HIS:CE1    | 2.45                     | 0.51              |
| 3:C:188:THR:OG1    | 3:C:295:THR:O      | 2.28                     | 0.51              |
| 4:D:186:GLN:HB2    | 17:D:404:CLA:HBC1  | 1.91                     | 0.51              |
| 1:a:5293:MET:HE1   | 1:a:5299:GLY:N     | 2.26                     | 0.51              |
| 17:a:5403:CLA:H91  | 17:a:5403:CLA:H3A  | 1.93                     | 0.51              |
| 1:A:97:TRP:NE1     | 25:C:519:MGE:O5D   | 2.39                     | 0.51              |
| 2:B:368:VAL:HG11   | 2:B:381:ILE:HD12   | 1.92                     | 0.51              |
| 3:C:343:ARG:HA     | 3:C:349:ILE:HG22   | 1.91                     | 0.51              |
| 25:D:410:MGE:H222  | 12:T:17:PHE:HZ     | 1.74                     | 0.51              |
| 3:c:5437:PHE:CE2   | 17:c:5502:CLA:HAC2 | 2.45                     | 0.51              |
| 1:A:42:LEU:HD22    | 20:A:407:BCR:H11C  | 1.93                     | 0.51              |
| 7:H:40:VAL:CG1     | 16:X:14:LEU:CD1    | 2.87                     | 0.51              |
| 1:a:5143:ILE:HG13  | 1:a:5144:CYS:N     | 2.26                     | 0.51              |
| 3:c:5401:LEU:HD22  | 3:c:5409:GLY:O     | 2.11                     | 0.51              |
| 14:Y:42:ARG:CG     | 14:Y:42:ARG:NH1    | 2.73                     | 0.51              |
| 3:c:5204:LEU:HB2   | 3:c:5239:TRP:HE1   | 1.76                     | 0.51              |
| 25:d:5410:MGE:H8A1 | 12:t:5021:ILE:HD11 | 1.93                     | 0.51              |
| 5:e:5035:TRP:CE3   | 6:f:5039:ALA:HB2   | 2.45                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:143:ILE:HG13   | 1:A:144:CYS:N      | 2.26                     | 0.51              |
| 2:B:475:PHE:HE1    | 4:D:134:ARG:HB2    | 1.76                     | 0.51              |
| 4:D:175:VAL:O      | 4:D:178:ILE:HG22   | 2.11                     | 0.51              |
| 4:D:210:LEU:HA     | 4:D:213:ILE:HG22   | 1.91                     | 0.51              |
| 1:a:5042:LEU:HD22  | 20:a:5408:BCR:H11C | 1.93                     | 0.51              |
| 2:b:5368:VAL:HG11  | 2:b:5381:ILE:HD12  | 1.92                     | 0.51              |
| 4:D:164:GLN:HB3    | 4:D:169:PHE:HD2    | 1.76                     | 0.50              |
| 7:H:55:LEU:O       | 7:H:58:VAL:HG22    | 2.10                     | 0.50              |
| 8:I:21:PHE:HA      | 8:I:24:LEU:HB2     | 1.93                     | 0.50              |
| 4:d:5175:VAL:O     | 4:d:5178:ILE:HG22  | 2.11                     | 0.50              |
| 22:m:5102:LMT:H1'  | 12:t:5001:MET:HB2  | 1.92                     | 0.50              |
| 7:h:5055:LEU:O     | 7:h:5058:VAL:HG22  | 2.10                     | 0.50              |
| 23:l:5102:SQD:H141 | 25:m:5103:MGE:H7B1 | 1.93                     | 0.50              |
| 15:N:75:TYR:HB3    | 15:N:87:PHE:CE1    | 2.45                     | 0.50              |
| 2:B:281:GLN:HE22   | 2:B:358:ARG:HD3    | 1.74                     | 0.50              |
| 3:C:243:ILE:HG22   | 17:C:506:CLA:HMC3  | 1.93                     | 0.50              |
| 2:b:5377:VAL:HG11  | 4:d:5342:PRO:HG3   | 1.92                     | 0.50              |
| 1:A:163:ILE:HD11   | 26:A:413:DGD:HB31  | 1.93                     | 0.50              |
| 1:A:207:GLY:HA3    | 1:A:278:TRP:NE1    | 2.27                     | 0.50              |
| 1:A:219:VAL:HG13   | 1:A:246:TYR:CG     | 2.46                     | 0.50              |
| 2:B:172:TYR:HB3    | 2:B:174:LEU:HD13   | 1.93                     | 0.50              |
| 4:D:61:HIS:CE1     | 4:D:79:SER:HB3     | 2.47                     | 0.50              |
| 4:D:85:MET:HE1     | 4:D:96:GLU:HG2     | 1.93                     | 0.50              |
| 6:F:18:VAL:HG13    | 6:F:19:ARG:H       | 1.76                     | 0.50              |
| 2:b:5397:VAL:HG11  | 2:b:5417:VAL:HG11  | 1.92                     | 0.50              |
| 20:c:5514:BCR:H341 | 20:c:5514:BCR:H352 | 1.93                     | 0.50              |
| 1:A:293:MET:HE1    | 1:A:299:GLY:N      | 2.26                     | 0.50              |
| 1:a:5219:VAL:HG13  | 1:a:5246:TYR:CG    | 2.46                     | 0.50              |
| 14:Y:34:MET:HE3    | 14:Y:34:MET:HA     | 1.93                     | 0.50              |
| 2:B:215:PHE:HD2    | 2:B:216:HIS:CD2    | 2.29                     | 0.50              |
| 3:C:264:PHE:HE1    | 20:C:516:BCR:H313  | 1.75                     | 0.50              |
| 1:A:73:TYR:HE1     | 22:A:409:LMT:H5'   | 1.77                     | 0.50              |
| 1:A:74:GLY:HA3     | 11:M:1:MET:SD      | 2.51                     | 0.50              |
| 6:F:19:ARG:NH1     | 29:F:101:HEM:O1D   | 2.40                     | 0.50              |
| 9:K:18:PHE:O       | 9:K:22:VAL:HG12    | 2.12                     | 0.50              |
| 1:a:5233:ALA:O     | 4:d:5265:ARG:NH1   | 2.44                     | 0.50              |
| 2:b:5246:PHE:CE1   | 2:b:5463:PHE:HB2   | 2.47                     | 0.50              |
| 2:b:5475:PHE:HD2   | 4:d:5140:PRO:HG3   | 1.76                     | 0.50              |
| 4:d:5061:HIS:CE1   | 4:d:5079:SER:HB3   | 2.47                     | 0.50              |
| 12:t:5004:ILE:HD11 | 20:t:5102:BCR:H272 | 1.93                     | 0.50              |
| 15:N:113:LEU:O     | 15:N:117:LEU:HG    | 2.12                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:272:HIS:NE2    | 24:A:411:BCT:C     | 2.74                     | 0.50              |
| 4:d:5085:MET:HE1   | 4:d:5096:GLU:HG2   | 1.93                     | 0.50              |
| 4:d:5095:PRO:HG2   | 4:d:5096:GLU:CD    | 2.37                     | 0.50              |
| 8:i:5021:PHE:HA    | 8:i:5024:LEU:HB2   | 1.93                     | 0.50              |
| 23:l:5102:SQD:H121 | 23:l:5102:SQD:H242 | 1.94                     | 0.50              |
| 1:A:283:VAL:HG21   | 18:A:404:PHO:HAC2  | 1.94                     | 0.50              |
| 17:A:402:CLA:H91   | 17:A:402:CLA:H3A   | 1.93                     | 0.50              |
| 3:C:438:LEU:HD11   | 17:C:505:CLA:HBB1  | 1.94                     | 0.50              |
| 4:D:95:PRO:HG2     | 4:D:96:GLU:CD      | 2.37                     | 0.50              |
| 2:b:5233:ASN:HD21  | 2:b:5476:ARG:HG2   | 1.77                     | 0.50              |
| 3:c:5176:VAL:HG11  | 3:c:5238:ILE:HD11  | 1.93                     | 0.50              |
| 3:c:5243:ILE:HG22  | 17:c:5506:CLA:HMC3 | 1.93                     | 0.50              |
| 3:c:5372:PRO:HB3   | 15:n:85:SER:CA     | 2.42                     | 0.50              |
| 1:A:63:ILE:CG2     | 3:C:337:LEU:HB3    | 2.42                     | 0.49              |
| 1:A:130:GLN:NE2    | 18:A:404:PHO:O1D   | 2.45                     | 0.49              |
| 17:A:401:CLA:H8    | 17:A:402:CLA:HBB1  | 1.94                     | 0.49              |
| 2:B:52:LEU:O       | 2:B:54:PRO:HD3     | 2.12                     | 0.49              |
| 2:B:348:ASN:O      | 2:B:349:LYS:HG2    | 2.12                     | 0.49              |
| 17:B:608:CLA:CBB   | 4:D:123:ILE:HG12   | 2.42                     | 0.49              |
| 1:a:5331:MET:CG    | 4:d:5324:GLY:HA3   | 2.40                     | 0.49              |
| 2:b:5223:GLN:N     | 7:h:5022:ALA:O     | 2.45                     | 0.49              |
| 3:c:5204:LEU:HA    | 3:c:5209:ILE:HD11  | 1.93                     | 0.49              |
| 4:d:5203:GLY:HA3   | 4:d:5278:GLY:HA3   | 1.94                     | 0.49              |
| 23:L:101:SQD:H162  | 23:L:101:SQD:H261  | 1.93                     | 0.49              |
| 12:T:25:GLU:H      | 12:T:25:GLU:CD     | 2.17                     | 0.49              |
| 1:a:5283:VAL:HG21  | 18:a:5405:PHO:HAC2 | 1.94                     | 0.49              |
| 3:c:5175:LEU:HD12  | 17:c:5501:CLA:C2D  | 2.42                     | 0.49              |
| 3:c:5190:ALA:H     | 3:c:5194:GLY:HA2   | 1.76                     | 0.49              |
| 4:d:5164:GLN:HB3   | 4:d:5169:PHE:HD2   | 1.76                     | 0.49              |
| 5:e:5069:ARG:O     | 5:e:5071:GLU:HG2   | 2.12                     | 0.49              |
| 16:x:7:LEU:C       | 16:x:7:LEU:CD1     | 2.86                     | 0.49              |
| 17:A:401:CLA:NB    | 17:D:404:CLA:HBB1  | 2.27                     | 0.49              |
| 2:B:233:ASN:HD21   | 2:B:476:ARG:HG2    | 1.77                     | 0.49              |
| 2:b:5174:LEU:HD11  | 2:b:5309:LEU:HB2   | 1.94                     | 0.49              |
| 3:c:5189:TRP:NE1   | 3:c:5364:PRO:HA    | 2.26                     | 0.49              |
| 3:c:5438:LEU:HD11  | 17:c:5505:CLA:HBB1 | 1.94                     | 0.49              |
| 17:B:602:CLA:H101  | 17:B:609:CLA:H203  | 1.95                     | 0.49              |
| 3:C:237:HIS:O      | 3:C:241:GLY:N      | 2.39                     | 0.49              |
| 17:a:5402:CLA:H8   | 17:a:5403:CLA:HBB1 | 1.94                     | 0.49              |
| 2:b:5172:TYR:HB3   | 2:b:5174:LEU:HD13  | 1.93                     | 0.49              |
| 4:d:5048:TRP:CG    | 18:d:5402:PHO:H13  | 2.48                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:485:GLU:O      | 2:B:485:GLU:HG3    | 2.11                     | 0.49              |
| 20:C:516:BCR:H341  | 20:C:516:BCR:H352  | 1.93                     | 0.49              |
| 4:D:157:PHE:HE1    | 4:D:171:PRO:HB2    | 1.76                     | 0.49              |
| 5:E:69:ARG:O       | 5:E:71:GLU:HG2     | 2.12                     | 0.49              |
| 2:b:5215:PHE:HD2   | 2:b:5216:HIS:CD2   | 2.29                     | 0.49              |
| 25:d:5410:MGE:O2D  | 25:d:5410:MGE:O4D  | 2.28                     | 0.49              |
| 1:A:187:GLN:HG3    | 1:A:325:ASN:ND2    | 2.28                     | 0.49              |
| 2:B:158:LEU:HB3    | 2:B:199:VAL:HG22   | 1.94                     | 0.49              |
| 3:C:176:VAL:HG11   | 3:C:238:ILE:HD11   | 1.93                     | 0.49              |
| 3:C:189:TRP:HD1    | 15:N:76:ARG:NH2    | 2.10                     | 0.49              |
| 4:D:14:TRP:CZ2     | 16:X:29:ILE:HD11   | 2.47                     | 0.49              |
| 1:a:5130:GLN:NE2   | 18:a:5405:PHO:O1D  | 2.45                     | 0.49              |
| 2:b:5158:LEU:HB3   | 2:b:5199:VAL:HG22  | 1.94                     | 0.49              |
| 17:b:5602:CLA:H101 | 17:b:5609:CLA:H203 | 1.95                     | 0.49              |
| 14:y:35:ILE:HA     | 14:y:38:LEU:HD13   | 1.91                     | 0.49              |
| 2:B:76:SER:HB2     | 2:B:78:TRP:CD1     | 2.48                     | 0.49              |
| 2:B:125:ASP:HB2    | 2:B:126:PRO:HD2    | 1.95                     | 0.49              |
| 17:B:615:CLA:O1A   | 17:B:615:CLA:H2A   | 2.13                     | 0.49              |
| 3:C:175:LEU:HD12   | 17:C:501:CLA:C2D   | 2.42                     | 0.49              |
| 3:C:459:ILE:N      | 4:D:222:LEU:O      | 2.46                     | 0.49              |
| 2:b:5052:LEU:O     | 2:b:5054:PRO:HD3   | 2.12                     | 0.49              |
| 2:b:5270:PRO:HG3   | 2:b:5317:ASN:HD21  | 1.78                     | 0.49              |
| 4:d:5157:PHE:HE1   | 4:d:5171:PRO:HB2   | 1.76                     | 0.49              |
| 9:k:5018:PHE:O     | 9:k:5022:VAL:HG12  | 2.12                     | 0.49              |
| 15:n:100:HIS:HE1   | 15:n:104:TYR:CE2   | 2.31                     | 0.49              |
| 15:N:117:LEU:O     | 15:N:118:GLU:C     | 2.55                     | 0.49              |
| 17:C:511:CLA:H41   | 14:Y:39:LEU:HD12   | 1.94                     | 0.49              |
| 4:D:71:CYS:O       | 25:D:408:MGE:H3D   | 2.13                     | 0.49              |
| 1:a:5077:ILE:HD11  | 12:t:5006:TYR:CD1  | 2.48                     | 0.49              |
| 2:b:5076:SER:HB2   | 2:b:5078:TRP:CD1   | 2.48                     | 0.49              |
| 4:d:5069:GLU:O     | 6:f:5040:MET:HE1   | 2.12                     | 0.49              |
| 16:X:3:ILE:HD12    | 16:X:7:LEU:HD11    | 1.94                     | 0.49              |
| 3:C:204:LEU:HB2    | 3:C:239:TRP:HE1    | 1.76                     | 0.49              |
| 1:a:5088:ALA:HA    | 3:c:5356:MET:HE2   | 1.94                     | 0.49              |
| 1:a:5174:LEU:O     | 1:a:5174:LEU:HD12  | 2.13                     | 0.49              |
| 1:a:5207:GLY:HA3   | 1:a:5278:TRP:NE1   | 2.27                     | 0.49              |
| 2:b:5468:TRP:CE3   | 4:d:5144:ILE:HD13  | 2.47                     | 0.49              |
| 4:d:5027:PHE:CD2   | 4:d:5028:VAL:HG13  | 2.48                     | 0.49              |
| 17:k:5501:CLA:H42  | 14:y:46:LEU:CD2    | 2.41                     | 0.49              |
| 1:A:174:LEU:HD12   | 1:A:174:LEU:O      | 2.13                     | 0.49              |
| 2:B:172:TYR:HE1    | 2:B:283:GLU:CD     | 2.21                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:L:101:SQD:H162  | 23:L:101:SQD:H242  | 1.94                     | 0.49              |
| 1:a:5252:HIS:CE1   | 1:a:5264:SER:HB3   | 2.48                     | 0.49              |
| 15:N:100:HIS:HE1   | 15:N:104:TYR:CE2   | 2.31                     | 0.49              |
| 2:B:246:PHE:CE1    | 2:B:463:PHE:HB2    | 2.47                     | 0.48              |
| 2:B:281:GLN:HE22   | 2:B:358:ARG:CD     | 2.26                     | 0.48              |
| 3:C:223:TRP:CE3    | 3:C:224:ILE:HG12   | 2.48                     | 0.48              |
| 21:a:5409:LHG:O3   | 21:a:5409:LHG:O1   | 2.19                     | 0.48              |
| 2:b:5125:ASP:HB2   | 2:b:5126:PRO:HD2   | 1.95                     | 0.48              |
| 4:d:5075:THR:HA    | 4:d:5176:ALA:HB3   | 1.95                     | 0.48              |
| 4:d:5107:LEU:HD21  | 5:e:5072:ALA:CB    | 2.42                     | 0.48              |
| 4:d:5269:PHE:HZ    | 25:d:5409:MGE:H3G2 | 1.78                     | 0.48              |
| 7:h:5044:ILE:CD1   | 16:x:10:PHE:CE1    | 2.89                     | 0.48              |
| 1:A:252:HIS:CE1    | 1:A:264:SER:HB3    | 2.48                     | 0.48              |
| 1:A:267:ASN:ND2    | 4:D:235:PHE:HB3    | 2.27                     | 0.48              |
| 2:B:457:VAL:HG13   | 4:D:284:ILE:HD12   | 1.94                     | 0.48              |
| 3:C:459:ILE:HG22   | 4:D:222:LEU:C      | 2.38                     | 0.48              |
| 2:b:5074:SER:OG    | 2:b:5094:GLU:OE1   | 2.26                     | 0.48              |
| 26:b:5621:DGD:O2D  | 4:d:5087:HIS:CD2   | 2.65                     | 0.48              |
| 3:c:5223:TRP:CE3   | 3:c:5224:ILE:HG12  | 2.48                     | 0.48              |
| 3:c:5337:LEU:HB2   | 3:c:5342:MET:SD    | 2.54                     | 0.48              |
| 20:c:5513:BCR:H272 | 17:k:5501:CLA:H61  | 1.95                     | 0.48              |
| 1:A:187:GLN:NE2    | 1:A:191:ASN:HA     | 2.28                     | 0.48              |
| 2:B:174:LEU:HD11   | 2:B:309:LEU:HB2    | 1.94                     | 0.48              |
| 3:C:190:ALA:H      | 3:C:194:GLY:HA2    | 1.78                     | 0.48              |
| 4:D:75:THR:HA      | 4:D:176:ALA:HB3    | 1.95                     | 0.48              |
| 5:E:28:PRO:O       | 5:E:32:ILE:HG12    | 2.14                     | 0.48              |
| 3:c:5212:TYR:HH    | 3:c:5227:VAL:H     | 1.50                     | 0.48              |
| 2:B:47:PRO:O       | 2:B:50:PRO:HD3     | 2.13                     | 0.48              |
| 2:B:74:SER:OG      | 2:B:94:GLU:OE1     | 2.26                     | 0.48              |
| 17:C:502:CLA:H12   | 17:C:503:CLA:C3    | 2.44                     | 0.48              |
| 4:D:27:PHE:CD2     | 4:D:28:VAL:HG13    | 2.48                     | 0.48              |
| 1:a:5187:GLN:HG3   | 1:a:5325:ASN:ND2   | 2.28                     | 0.48              |
| 1:a:5315:ASN:ND2   | 4:d:5332:GLN:OE1   | 2.47                     | 0.48              |
| 3:c:5237:HIS:O     | 3:c:5241:GLY:N     | 2.39                     | 0.48              |
| 5:e:5072:ALA:HA    | 5:e:5075:GLN:HB3   | 1.95                     | 0.48              |
| 15:n:58:LYS:NZ     | 15:n:106:ASN:OD1   | 2.29                     | 0.48              |
| 1:A:97:TRP:CD1     | 8:I:5:LYS:HD2      | 2.48                     | 0.48              |
| 17:B:608:CLA:H102  | 17:B:609:CLA:H142  | 1.95                     | 0.48              |
| 3:C:275:SER:OG     | 17:C:509:CLA:O2D   | 2.26                     | 0.48              |
| 20:D:407:BCR:H11C  | 6:F:29:PRO:HB3     | 1.95                     | 0.48              |
| 1:a:5278:TRP:HB3   | 1:a:5279:PRO:HD3   | 1.96                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 17:b:5612:CLA:H71  | 17:b:5612:CLA:H162 | 1.95                     | 0.48              |
| 3:c:5062:PHE:CZ    | 9:k:5028:ILE:HD11  | 2.48                     | 0.48              |
| 3:c:5371:GLY:HA3   | 3:c:5376:ASP:CG    | 2.38                     | 0.48              |
| 26:c:5515:DGD:HB71 | 25:c:5517:MGE:H7A1 | 1.95                     | 0.48              |
| 4:d:5061:HIS:CD2   | 4:d:5168:PHE:HE1   | 2.31                     | 0.48              |
| 10:l:5028:ALA:O    | 10:l:5032:SER:N    | 2.40                     | 0.48              |
| 17:A:401:CLA:HBD   | 17:A:402:CLA:HAC2  | 1.96                     | 0.48              |
| 2:B:77:GLY:C       | 2:B:86:ILE:CD1     | 2.87                     | 0.48              |
| 17:B:601:CLA:H2A   | 17:B:601:CLA:O2D   | 2.13                     | 0.48              |
| 17:B:602:CLA:H2A   | 17:B:602:CLA:O2D   | 2.14                     | 0.48              |
| 3:C:40:ALA:HB2     | 17:C:508:CLA:H2A   | 1.96                     | 0.48              |
| 3:C:337:LEU:HB2    | 3:C:342:MET:SD     | 2.54                     | 0.48              |
| 3:C:371:GLY:HA3    | 3:C:376:ASP:CG     | 2.38                     | 0.48              |
| 3:C:403:SER:OG     | 3:C:407:VAL:N      | 2.25                     | 0.48              |
| 4:D:203:GLY:HA3    | 4:D:278:GLY:HA3    | 1.94                     | 0.48              |
| 17:D:405:CLA:O2D   | 17:D:405:CLA:H2A   | 2.14                     | 0.48              |
| 2:b:5008:VAL:HG23  | 2:b:5009:HIS:CD2   | 2.49                     | 0.48              |
| 2:b:5281:GLN:HE22  | 2:b:5358:ARG:CD    | 2.26                     | 0.48              |
| 2:b:5475:PHE:CD2   | 4:d:5140:PRO:HG3   | 2.49                     | 0.48              |
| 17:b:5601:CLA:H2A  | 17:b:5601:CLA:O2D  | 2.13                     | 0.48              |
| 1:A:37:MET:SD      | 1:A:129:ARG:NE     | 2.82                     | 0.48              |
| 1:A:296:ASN:HB3    | 3:C:401:LEU:HD23   | 1.95                     | 0.48              |
| 17:B:612:CLA:H71   | 17:B:612:CLA:H162  | 1.95                     | 0.48              |
| 2:b:5047:PRO:O     | 2:b:5050:PRO:HD3   | 2.13                     | 0.48              |
| 3:c:5040:ALA:HB2   | 17:c:5508:CLA:H2A  | 1.96                     | 0.48              |
| 20:d:5406:BCR:H372 | 25:d:5408:MGE:H2A2 | 1.95                     | 0.48              |
| 2:B:270:PRO:HG3    | 2:B:317:ASN:HD21   | 1.78                     | 0.48              |
| 6:F:34:LEU:HD23    | 6:F:37:ILE:HD12    | 1.96                     | 0.48              |
| 1:a:5050:ILE:HG21  | 20:a:5408:BCR:H393 | 1.96                     | 0.48              |
| 1:a:5160:ILE:O     | 1:a:5163:ILE:N     | 2.46                     | 0.48              |
| 1:a:5212:CYS:HB2   | 4:d:5211:CYS:HB2   | 1.96                     | 0.48              |
| 1:a:5289:GLY:O     | 1:a:5293:MET:HG2   | 2.13                     | 0.48              |
| 2:b:5172:TYR:HE1   | 2:b:5283:GLU:CD    | 2.21                     | 0.48              |
| 2:b:5348:ASN:O     | 2:b:5349:LYS:HG2   | 2.12                     | 0.48              |
| 17:b:5608:CLA:H102 | 17:b:5609:CLA:H142 | 1.95                     | 0.48              |
| 17:b:5615:CLA:H2A  | 17:b:5615:CLA:O1A  | 2.13                     | 0.48              |
| 3:c:5413:GLU:OE2   | 3:c:5416:SER:OG    | 2.31                     | 0.48              |
| 13:z:5043:GLY:O    | 13:z:5047:TRP:N    | 2.47                     | 0.48              |
| 14:Y:38:LEU:O      | 14:Y:42:ARG:CG     | 2.55                     | 0.48              |
| 4:D:60:THR:HG23    | 4:D:61:HIS:N       | 2.28                     | 0.48              |
| 17:a:5403:CLA:H152 | 17:a:5403:CLA:H111 | 1.42                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 17:c:5503:CLA:H13  | 17:c:5503:CLA:H101 | 1.47                     | 0.48              |
| 6:f:5034:LEU:HD23  | 6:f:5037:ILE:HD12  | 1.96                     | 0.48              |
| 13:z:5028:ALA:O    | 14:y:44:GLY:HA3    | 2.14                     | 0.48              |
| 15:N:93:ALA:O      | 15:N:96:SER:OG     | 2.25                     | 0.48              |
| 1:A:140:ARG:HD3    | 1:A:142:TRP:HE1    | 1.79                     | 0.48              |
| 5:E:72:ALA:HA      | 5:E:75:GLN:HB3     | 1.95                     | 0.48              |
| 9:K:20:PRO:HG3     | 14:Y:24:MET:HG2    | 1.93                     | 0.48              |
| 23:L:101:SQD:O8    | 23:L:101:SQD:O3    | 2.19                     | 0.48              |
| 11:M:24:ILE:HG12   | 11:m:5024:ILE:HG12 | 1.96                     | 0.48              |
| 13:Z:43:GLY:O      | 13:Z:47:TRP:N      | 2.47                     | 0.48              |
| 1:a:5037:MET:HE1   | 1:a:5129:ARG:HH21  | 1.79                     | 0.48              |
| 1:a:5140:ARG:HD3   | 1:a:5142:TRP:HE1   | 1.79                     | 0.48              |
| 1:a:5187:GLN:NE2   | 1:a:5191:ASN:HA    | 2.28                     | 0.48              |
| 5:e:5028:PRO:O     | 5:e:5032:ILE:HG12  | 2.14                     | 0.48              |
| 1:a:5063:ILE:HD12  | 3:c:5335:THR:HB    | 1.96                     | 0.47              |
| 1:a:5138:GLY:HA2   | 3:c:5455:PHE:CE1   | 2.49                     | 0.47              |
| 17:a:5402:CLA:HBD  | 17:a:5403:CLA:HAC2 | 1.96                     | 0.47              |
| 17:b:5611:CLA:CBB  | 17:b:5613:CLA:HHB  | 2.44                     | 0.47              |
| 3:c:5134:ILE:HG21  | 13:z:5027:TYR:HB3  | 1.96                     | 0.47              |
| 17:c:5510:CLA:H122 | 17:c:5510:CLA:H162 | 1.72                     | 0.47              |
| 4:d:5085:MET:HE2   | 4:d:5107:LEU:HD23  | 1.97                     | 0.47              |
| 4:d:5157:PHE:CE1   | 4:d:5171:PRO:HB2   | 2.49                     | 0.47              |
| 4:d:5263:ASN:N     | 25:d:5410:MGE:O3D  | 2.47                     | 0.47              |
| 17:d:5404:CLA:H2A  | 17:d:5404:CLA:O2D  | 2.14                     | 0.47              |
| 1:A:278:TRP:HB3    | 1:A:279:PRO:HD3    | 1.96                     | 0.47              |
| 2:B:233:ASN:O      | 2:B:236:THR:HG22   | 2.14                     | 0.47              |
| 4:D:214:HIS:O      | 4:D:218:VAL:HG12   | 2.14                     | 0.47              |
| 13:Z:28:ALA:HB1    | 14:Y:39:LEU:HD13   | 1.95                     | 0.47              |
| 17:a:5403:CLA:H52  | 19:d:5405:PQ9:H242 | 1.95                     | 0.47              |
| 2:b:5326:ARG:HH22  | 4:d:5297:ASP:N     | 2.12                     | 0.47              |
| 17:c:5502:CLA:H12  | 17:c:5503:CLA:C3   | 2.43                     | 0.47              |
| 18:d:5402:PHO:H143 | 18:d:5402:PHO:H111 | 1.65                     | 0.47              |
| 17:B:611:CLA:CBB   | 17:B:613:CLA:HHB   | 2.44                     | 0.47              |
| 3:C:229:ASN:HD22   | 15:N:77:ARG:CB     | 2.28                     | 0.47              |
| 3:C:274:TYR:HD1    | 17:C:505:CLA:HMD2  | 1.80                     | 0.47              |
| 3:C:413:GLU:OE2    | 3:C:416:SER:OG     | 2.31                     | 0.47              |
| 9:K:31:LEU:HB3     | 20:Y:101:BCR:C13   | 2.44                     | 0.47              |
| 1:a:5319:ASP:O     | 1:a:5323:ARG:N     | 2.46                     | 0.47              |
| 1:a:5323:ARG:O     | 1:a:5327:GLY:N     | 2.43                     | 0.47              |
| 16:x:21:LEU:C      | 16:x:21:LEU:CD2    | 2.86                     | 0.47              |
| 1:A:143:ILE:HG23   | 4:D:220:ASN:ND2    | 2.27                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 17:C:511:CLA:H61   | 20:C:514:BCR:H272  | 1.95                     | 0.47              |
| 4:D:85:MET:HE2     | 4:D:107:LEU:HD23   | 1.97                     | 0.47              |
| 1:a:5084:PRO:HD3   | 1:a:5173:PRO:HB3   | 1.97                     | 0.47              |
| 2:b:5409:GLN:HG3   | 2:b:5411:PHE:CE1   | 2.50                     | 0.47              |
| 17:b:5602:CLA:H172 | 26:b:5621:DGD:HA82 | 1.96                     | 0.47              |
| 17:b:5602:CLA:O2D  | 17:b:5602:CLA:H2A  | 2.14                     | 0.47              |
| 4:d:5159:ILE:HG21  | 4:d:5287:VAL:HG22  | 1.97                     | 0.47              |
| 4:d:5193:LEU:O     | 10:l:5034:TYR:OH   | 2.31                     | 0.47              |
| 9:k:5020:PRO:HB3   | 14:y:21:GLN:O      | 2.15                     | 0.47              |
| 11:m:5030:GLU:O    | 25:m:5103:MGE:O3D  | 2.32                     | 0.47              |
| 14:y:38:LEU:CD1    | 14:y:38:LEU:H      | 2.06                     | 0.47              |
| 4:D:157:PHE:CE1    | 4:D:171:PRO:HB2    | 2.49                     | 0.47              |
| 4:D:261:PHE:HD2    | 4:D:267:LEU:HG     | 1.79                     | 0.47              |
| 1:a:5165:GLN:O     | 3:c:5357:ARG:NH1   | 2.44                     | 0.47              |
| 4:d:5297:ASP:HB3   | 4:d:5302:GLU:CG    | 2.40                     | 0.47              |
| 16:x:36:LYS:HG2    | 16:x:36:LYS:O      | 2.14                     | 0.47              |
| 1:A:37:MET:HE1     | 1:A:129:ARG:HH21   | 1.79                     | 0.47              |
| 2:B:8:VAL:HG23     | 2:B:9:HIS:CD2      | 2.49                     | 0.47              |
| 2:b:5215:PHE:HD2   | 2:b:5216:HIS:HD2   | 1.62                     | 0.47              |
| 2:b:5233:ASN:O     | 2:b:5236:THR:HG22  | 2.15                     | 0.47              |
| 17:b:5607:CLA:H61  | 17:b:5607:CLA:H41  | 1.52                     | 0.47              |
| 4:d:5067:TYR:OH    | 25:d:5408:MGE:H3G1 | 2.15                     | 0.47              |
| 9:k:5040:GLN:O     | 9:k:5044:GLY:N     | 2.38                     | 0.47              |
| 15:N:58:LYS:NZ     | 15:N:106:ASN:OD1   | 2.29                     | 0.47              |
| 1:A:79:THR:HG22    | 4:D:315:TYR:HB2    | 1.96                     | 0.47              |
| 1:A:187:GLN:HE21   | 1:A:325:ASN:ND2    | 2.13                     | 0.47              |
| 1:A:289:GLY:O      | 1:A:293:MET:HG2    | 2.13                     | 0.47              |
| 26:A:413:DGD:HA72  | 3:C:284:PHE:HB3    | 1.97                     | 0.47              |
| 2:B:59:GLY:HA3     | 2:B:329:PRO:HB3    | 1.97                     | 0.47              |
| 2:B:91:TRP:CH2     | 17:B:606:CLA:H12   | 2.49                     | 0.47              |
| 2:B:414:PRO:O      | 2:B:418:LYS:HG2    | 2.14                     | 0.47              |
| 2:B:475:PHE:CD2    | 4:D:140:PRO:HG3    | 2.49                     | 0.47              |
| 17:B:608:CLA:HBB2  | 4:D:123:ILE:HG12   | 1.96                     | 0.47              |
| 17:C:505:CLA:HBA1  | 17:C:505:CLA:CBD   | 2.44                     | 0.47              |
| 5:E:23:HIS:CE1     | 29:F:101:HEM:ND    | 2.83                     | 0.47              |
| 2:b:5457:VAL:HG13  | 4:d:5284:ILE:HD12  | 1.97                     | 0.47              |
| 20:b:5617:BCR:H383 | 25:m:5101:MGE:H202 | 1.97                     | 0.47              |
| 20:b:5617:BCR:HC41 | 11:m:5006:LEU:HD21 | 1.96                     | 0.47              |
| 3:c:5080:PRO:HG2   | 3:c:5083:GLU:HB2   | 1.97                     | 0.47              |
| 3:c:5274:TYR:HD1   | 17:c:5505:CLA:HMD2 | 1.80                     | 0.47              |
| 17:c:5505:CLA:HBA1 | 17:c:5505:CLA:CBD  | 2.44                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 17:c:5505:CLA:H52  | 17:c:5505:CLA:H8   | 1.52                     | 0.47              |
| 4:d:5282:SER:OG    | 17:d:5403:CLA:O1D  | 2.27                     | 0.47              |
| 25:d:5410:MGE:H262 | 12:t:5013:ILE:HG21 | 1.96                     | 0.47              |
| 1:A:84:PRO:HD3     | 1:A:173:PRO:HB3    | 1.97                     | 0.47              |
| 1:A:140:ARG:NH2    | 3:C:456:GLU:O      | 2.48                     | 0.47              |
| 1:A:183:MET:HB3    | 17:A:401:CLA:HBC2  | 1.96                     | 0.47              |
| 17:B:604:CLA:H161  | 17:B:616:CLA:H192  | 1.97                     | 0.47              |
| 3:C:36:TRP:O       | 17:C:508:CLA:H12   | 2.15                     | 0.47              |
| 4:D:61:HIS:CD2     | 4:D:168:PHE:HE1    | 2.31                     | 0.47              |
| 12:T:25:GLU:N      | 12:T:25:GLU:CD     | 2.73                     | 0.47              |
| 17:k:5501:CLA:H112 | 17:k:5501:CLA:H91  | 1.68                     | 0.47              |
| 12:t:5025:GLU:H    | 12:t:5025:GLU:CD   | 2.17                     | 0.47              |
| 16:X:20:VAL:O      | 16:X:21:LEU:C      | 2.58                     | 0.47              |
| 2:B:392:PHE:CZ     | 2:B:418:LYS:HB3    | 2.50                     | 0.47              |
| 3:C:166:ILE:HG13   | 3:C:248:GLY:HA3    | 1.95                     | 0.47              |
| 3:C:205:ASP:OD1    | 3:C:208:VAL:HG22   | 2.15                     | 0.47              |
| 13:Z:28:ALA:CB     | 14:Y:39:LEU:HD11   | 2.45                     | 0.47              |
| 2:b:5125:ASP:OD1   | 2:b:5128:THR:OG1   | 2.31                     | 0.47              |
| 2:b:5347:ARG:HD3   | 2:b:5351:GLY:HA2   | 1.97                     | 0.47              |
| 3:c:5184:GLY:HA3   | 3:c:5198:VAL:HG22  | 1.97                     | 0.47              |
| 3:c:5318:LEU:HD11  | 3:c:5328:VAL:HG21  | 1.97                     | 0.47              |
| 4:d:5214:HIS:O     | 4:d:5218:VAL:HG12  | 2.14                     | 0.47              |
| 14:Y:28:ILE:N      | 14:Y:28:ILE:HD12   | 2.29                     | 0.47              |
| 15:N:61:GLN:NE2    | 15:N:101:TYR:OH    | 2.46                     | 0.47              |
| 17:B:607:CLA:H41   | 17:B:607:CLA:H61   | 1.52                     | 0.47              |
| 3:c:5166:ILE:HG13  | 3:c:5248:GLY:HA3   | 1.95                     | 0.47              |
| 9:k:5031:LEU:HD23  | 20:k:5502:BCR:C14  | 2.45                     | 0.47              |
| 1:A:300:PHE:CD2    | 3:C:404:LEU:HD12   | 2.50                     | 0.46              |
| 17:C:503:CLA:H13   | 17:C:503:CLA:H101  | 1.47                     | 0.46              |
| 14:y:25:ILE:HA     | 14:y:28:ILE:CD1    | 2.45                     | 0.46              |
| 1:A:34:GLY:HA2     | 1:A:37:MET:HB3     | 1.97                     | 0.46              |
| 1:A:50:ILE:HG21    | 20:A:407:BCR:H393  | 1.96                     | 0.46              |
| 1:A:317:TRP:CH2    | 4:D:77:ALA:HB3     | 2.49                     | 0.46              |
| 2:B:347:ARG:HD3    | 2:B:351:GLY:HA2    | 1.97                     | 0.46              |
| 17:B:604:CLA:HMD1  | 17:B:612:CLA:H193  | 1.97                     | 0.46              |
| 3:C:264:PHE:HE2    | 17:C:506:CLA:HAA2  | 1.80                     | 0.46              |
| 4:D:83:ASN:ND2     | 4:D:336:HIS:CE1    | 2.83                     | 0.46              |
| 4:D:159:ILE:HG21   | 4:D:287:VAL:HG22   | 1.97                     | 0.46              |
| 4:D:221:THR:O      | 4:D:222:LEU:HD12   | 2.15                     | 0.46              |
| 4:D:282:SER:OG     | 17:D:404:CLA:O1D   | 2.26                     | 0.46              |
| 1:a:5218:LEU:HD21  | 1:a:5255:PHE:HB2   | 1.97                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:b:5414:PRO:O     | 2:b:5418:LYS:HG2   | 2.14                     | 0.46              |
| 3:c:5275:SER:OG    | 17:c:5509:CLA:O2D  | 2.26                     | 0.46              |
| 3:c:5284:PHE:HB3   | 26:c:5515:DGD:HA72 | 1.97                     | 0.46              |
| 3:c:5461:ARG:HH11  | 4:d:5223:PHE:HB2   | 1.80                     | 0.46              |
| 4:d:5221:THR:O     | 4:d:5222:LEU:HD12  | 2.15                     | 0.46              |
| 15:N:109:LEU:HB2   | 15:N:114:LYS:CG    | 2.46                     | 0.46              |
| 1:A:142:TRP:HZ3    | 3:C:443:TRP:O      | 1.98                     | 0.46              |
| 2:B:381:ILE:HG12   | 2:B:392:PHE:HE1    | 1.80                     | 0.46              |
| 2:B:475:PHE:O      | 2:B:479:PHE:N      | 2.44                     | 0.46              |
| 3:C:349:ILE:HG13   | 3:C:374:GLY:HA3    | 1.97                     | 0.46              |
| 17:C:505:CLA:H152  | 17:C:505:CLA:H18   | 1.68                     | 0.46              |
| 17:C:505:CLA:H52   | 17:C:505:CLA:H8    | 1.52                     | 0.46              |
| 9:K:29:PRO:HA      | 9:K:32:PHE:CD2     | 2.51                     | 0.46              |
| 1:a:5063:ILE:HG21  | 3:c:5337:LEU:HD23  | 1.97                     | 0.46              |
| 17:b:5604:CLA:H161 | 17:b:5616:CLA:H192 | 1.97                     | 0.46              |
| 17:b:5609:CLA:C3B  | 20:h:5101:BCR:H323 | 2.45                     | 0.46              |
| 3:c:5264:PHE:HE2   | 17:c:5506:CLA:HAA2 | 1.80                     | 0.46              |
| 4:d:5083:ASN:ND2   | 4:d:5336:HIS:CE1   | 2.83                     | 0.46              |
| 14:y:18:VAL:O      | 14:y:22:LEU:CA     | 2.63                     | 0.46              |
| 1:A:160:ILE:O      | 1:A:163:ILE:N      | 2.46                     | 0.46              |
| 22:A:409:LMT:H111  | 2:b:5094:GLU:HG2   | 1.97                     | 0.46              |
| 2:B:409:GLN:HG3    | 2:B:411:PHE:CE1    | 2.50                     | 0.46              |
| 17:B:606:CLA:H162  | 17:B:606:CLA:H122  | 1.64                     | 0.46              |
| 3:C:362:ARG:HD2    | 3:C:367:GLU:OE1    | 2.16                     | 0.46              |
| 1:a:5295:PHE:HD2   | 3:c:5428:THR:OG1   | 1.98                     | 0.46              |
| 17:b:5616:CLA:O2D  | 17:b:5616:CLA:H2A  | 2.15                     | 0.46              |
| 3:c:5036:TRP:O     | 17:c:5508:CLA:H12  | 2.15                     | 0.46              |
| 17:c:5510:CLA:H61  | 17:c:5510:CLA:H2   | 1.63                     | 0.46              |
| 4:d:5279:LEU:HD11  | 18:d:5402:PHO:HMC3 | 1.97                     | 0.46              |
| 12:t:5025:GLU:N    | 12:t:5025:GLU:CD   | 2.73                     | 0.46              |
| 14:Y:24:MET:HA     | 14:Y:27:MET:SD     | 2.56                     | 0.46              |
| 1:A:218:LEU:HD21   | 1:A:255:PHE:HB2    | 1.96                     | 0.46              |
| 25:A:412:MGE:H241  | 19:D:406:PQ9:H301  | 1.97                     | 0.46              |
| 2:B:77:GLY:HA2     | 2:B:86:ILE:HD13    | 1.91                     | 0.46              |
| 2:B:215:PHE:HD2    | 2:B:216:HIS:HD2    | 1.62                     | 0.46              |
| 17:B:605:CLA:H41   | 17:B:605:CLA:H61   | 1.54                     | 0.46              |
| 3:C:161:LEU:HD13   | 17:C:507:CLA:C1D   | 2.46                     | 0.46              |
| 3:C:439:VAL:O      | 3:C:443:TRP:N      | 2.47                     | 0.46              |
| 9:K:24:VAL:HG11    | 14:Y:25:ILE:HD11   | 1.97                     | 0.46              |
| 12:T:16:LEU:O      | 12:T:20:ALA:N      | 2.45                     | 0.46              |
| 1:a:5328:MET:HE2   | 4:d:5325:ILE:CD1   | 2.45                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:b:5392:PHE:CZ    | 2:b:5418:LYS:HB3   | 2.50                     | 0.46              |
| 17:b:5601:CLA:H2A  | 17:b:5601:CLA:HED3 | 1.98                     | 0.46              |
| 17:b:5602:CLA:H51  | 7:h:5042:LEU:HD11  | 1.98                     | 0.46              |
| 9:k:5029:PRO:HA    | 9:k:5032:PHE:CD2   | 2.51                     | 0.46              |
| 9:k:5043:VAL:HG22  | 14:y:46:LEU:HB3    | 1.98                     | 0.46              |
| 10:l:5020:GLY:HA3  | 11:m:5022:LEU:HD13 | 1.98                     | 0.46              |
| 3:C:318:LEU:HD11   | 3:C:328:VAL:HG21   | 1.97                     | 0.46              |
| 4:D:139:ARG:NH2    | 4:D:141:TYR:HH     | 2.14                     | 0.46              |
| 19:D:406:PQ9:H361  | 19:D:406:PQ9:H341  | 1.64                     | 0.46              |
| 13:Z:53:VAL:O      | 13:Z:57:LEU:HB2    | 2.16                     | 0.46              |
| 18:a:5405:PHO:H51  | 18:a:5405:PHO:H8   | 1.72                     | 0.46              |
| 2:b:5381:ILE:HG12  | 2:b:5392:PHE:HE1   | 1.80                     | 0.46              |
| 3:c:5276:LEU:O     | 3:c:5280:SER:N     | 2.39                     | 0.46              |
| 4:d:5146:PHE:O     | 4:d:5149:PRO:HD2   | 2.16                     | 0.46              |
| 9:k:5019:ASP:HB3   | 14:y:21:GLN:HG2    | 1.95                     | 0.46              |
| 15:n:93:ALA:O      | 15:n:96:SER:OG     | 2.25                     | 0.46              |
| 1:A:130:GLN:HG2    | 4:D:256:ILE:HG21   | 1.98                     | 0.46              |
| 19:A:406:PQ9:H161  | 19:A:406:PQ9:H141  | 1.62                     | 0.46              |
| 2:B:24:LEU:HD21    | 17:B:616:CLA:CAB   | 2.46                     | 0.46              |
| 2:B:458:PHE:HB3    | 17:B:604:CLA:HMC2  | 1.97                     | 0.46              |
| 4:D:193:LEU:HD21   | 4:D:298:PHE:CZ     | 2.51                     | 0.46              |
| 9:K:39:TRP:HE1     | 14:Y:46:LEU:HD23   | 1.78                     | 0.46              |
| 10:L:36:PHE:HE1    | 11:M:8:LEU:HA      | 1.80                     | 0.46              |
| 2:b:5063:LEU:HB3   | 2:b:5064:PRO:HD3   | 1.98                     | 0.46              |
| 4:d:5141:TYR:OH    | 25:d:5409:MGE:O2D  | 2.34                     | 0.46              |
| 1:A:237:TYR:CE2    | 4:D:263:ASN:HA     | 2.50                     | 0.46              |
| 1:A:276:ALA:HB2    | 4:D:215:GLY:C      | 2.40                     | 0.46              |
| 2:B:226:TYR:CD1    | 2:B:231:MET:HB2    | 2.51                     | 0.46              |
| 17:C:501:CLA:H2A   | 17:C:501:CLA:O1D   | 2.16                     | 0.46              |
| 17:C:508:CLA:H202  | 17:C:508:CLA:H161  | 1.84                     | 0.46              |
| 4:D:18:LEU:HD12    | 16:X:29:ILE:HG12   | 1.96                     | 0.46              |
| 23:D:403:SQD:H342  | 9:K:37:PHE:CE2     | 2.51                     | 0.46              |
| 17:D:404:CLA:H201  | 25:D:408:MGE:H8A1  | 1.98                     | 0.46              |
| 11:M:21:PHE:CZ     | 11:M:25:LEU:HD11   | 2.51                     | 0.46              |
| 1:a:5183:MET:HB3   | 17:a:5402:CLA:HBC2 | 1.96                     | 0.46              |
| 1:a:5207:GLY:HA3   | 1:a:5278:TRP:HE1   | 1.80                     | 0.46              |
| 2:b:5312:TYR:O     | 2:b:5317:ASN:ND2   | 2.49                     | 0.46              |
| 2:b:5458:PHE:HB3   | 17:b:5604:CLA:HMC2 | 1.97                     | 0.46              |
| 3:c:5205:ASP:OD1   | 3:c:5208:VAL:HG22  | 2.15                     | 0.46              |
| 4:d:5193:LEU:HD21  | 4:d:5298:PHE:CZ    | 2.51                     | 0.46              |
| 23:l:5102:SQD:H262 | 12:t:5019:PHE:HE2  | 1.80                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:392:PHE:O      | 2:B:396:GLY:N      | 2.49                     | 0.46              |
| 3:C:86:LEU:HD21    | 3:C:89:ILE:HB      | 1.98                     | 0.46              |
| 4:D:146:PHE:O      | 4:D:149:PRO:HD2    | 2.16                     | 0.46              |
| 23:L:101:SQD:H45   | 25:m:5101:MGE:H8B1 | 1.98                     | 0.46              |
| 1:a:5140:ARG:O     | 4:d:5220:ASN:HB3   | 2.16                     | 0.46              |
| 20:b:5617:BCR:H20C | 20:b:5617:BCR:H361 | 1.81                     | 0.46              |
| 3:c:5157:MET:HE1   | 3:c:5271:TYR:CD2   | 2.51                     | 0.46              |
| 3:c:5362:ARG:HD2   | 3:c:5367:GLU:OE1   | 2.16                     | 0.46              |
| 17:c:5501:CLA:H2A  | 17:c:5501:CLA:O1D  | 2.16                     | 0.46              |
| 4:d:5060:THR:HG23  | 4:d:5061:HIS:N     | 2.28                     | 0.46              |
| 5:e:5051:ARG:O     | 5:e:5054:SER:N     | 2.40                     | 0.46              |
| 9:k:5031:LEU:HD23  | 20:k:5502:BCR:H14C | 1.98                     | 0.46              |
| 1:A:91:LEU:HD22    | 26:A:413:DGD:O2D   | 2.15                     | 0.46              |
| 2:B:63:LEU:HB3     | 2:B:64:PRO:HD3     | 1.98                     | 0.46              |
| 17:B:610:CLA:H111  | 17:B:610:CLA:H143  | 1.70                     | 0.46              |
| 2:b:5315:ILE:HG21  | 2:b:5426:PHE:CD1   | 2.51                     | 0.46              |
| 17:b:5604:CLA:HMD1 | 17:b:5612:CLA:H193 | 1.97                     | 0.46              |
| 17:b:5611:CLA:H141 | 17:b:5611:CLA:H162 | 1.59                     | 0.46              |
| 3:c:5212:TYR:OH    | 3:c:5226:SER:HB2   | 2.16                     | 0.46              |
| 3:c:5306:GLY:N     | 3:c:5307:PRO:HD2   | 2.31                     | 0.46              |
| 17:B:616:CLA:O2D   | 17:B:616:CLA:H2A   | 2.15                     | 0.45              |
| 4:D:61:HIS:CD2     | 4:D:168:PHE:CE1    | 3.04                     | 0.45              |
| 23:L:101:SQD:H82   | 23:L:101:SQD:H62   | 1.98                     | 0.45              |
| 2:b:5024:LEU:HD21  | 17:b:5616:CLA:CAB  | 2.46                     | 0.45              |
| 2:b:5059:GLY:HA3   | 2:b:5329:PRO:HB3   | 1.97                     | 0.45              |
| 17:b:5604:CLA:H92  | 17:b:5604:CLA:H62  | 1.75                     | 0.45              |
| 3:c:5229:ASN:OD1   | 3:c:5230:LEU:N     | 2.49                     | 0.45              |
| 4:d:5118:GLY:HA3   | 18:d:5402:PHO:H93  | 1.97                     | 0.45              |
| 15:n:61:GLN:NE2    | 15:n:101:TYR:OH    | 2.46                     | 0.45              |
| 3:C:184:GLY:HA3    | 3:C:198:VAL:HG22   | 1.97                     | 0.45              |
| 3:C:283:GLY:HA3    | 3:C:434:ALA:HB2    | 1.99                     | 0.45              |
| 4:D:168:PHE:HD2    | 4:D:169:PHE:CE1    | 2.34                     | 0.45              |
| 9:K:29:PRO:HA      | 9:K:32:PHE:HD2     | 1.81                     | 0.45              |
| 1:a:5034:GLY:HA2   | 1:a:5037:MET:HB3   | 1.97                     | 0.45              |
| 1:a:5048:PHE:HA    | 1:a:5115:ILE:HD11  | 1.99                     | 0.45              |
| 1:a:5246:TYR:CE2   | 1:a:5248:ILE:HD11  | 2.51                     | 0.45              |
| 21:a:5409:LHG:HC11 | 17:c:5508:CLA:O1D  | 2.16                     | 0.45              |
| 3:c:5349:ILE:HG13  | 3:c:5374:GLY:HA3   | 1.97                     | 0.45              |
| 23:l:5102:SQD:H112 | 23:l:5102:SQD:H82  | 1.56                     | 0.45              |
| 14:y:25:ILE:HD13   | 14:y:25:ILE:C      | 2.41                     | 0.45              |
| 21:A:408:LHG:H02   | 21:A:408:LHG:P     | 2.39                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:C:80:PRO:HG2     | 3:C:83:GLU:HB2     | 1.97                     | 0.45              |
| 3:C:205:ASP:H      | 3:C:209:ILE:HD12   | 1.82                     | 0.45              |
| 3:C:274:TYR:HE1    | 17:C:505:CLA:OBD   | 1.99                     | 0.45              |
| 17:C:511:CLA:H91   | 17:C:511:CLA:H112  | 1.68                     | 0.45              |
| 1:a:5120:LEU:O     | 1:a:5123:ALA:N     | 2.49                     | 0.45              |
| 1:a:5187:GLN:HE21  | 1:a:5325:ASN:ND2   | 2.13                     | 0.45              |
| 2:b:5226:TYR:CD1   | 2:b:5231:MET:HB2   | 2.51                     | 0.45              |
| 3:c:5086:LEU:HD21  | 3:c:5089:ILE:HB    | 1.98                     | 0.45              |
| 3:c:5399:ALA:O     | 3:c:5401:LEU:HD23  | 2.16                     | 0.45              |
| 15:n:75:TYR:HB3    | 15:n:87:PHE:HE1    | 1.81                     | 0.45              |
| 15:N:75:TYR:HB3    | 15:N:87:PHE:HE1    | 1.81                     | 0.45              |
| 15:N:84:LEU:HD22   | 15:N:131:GLU:HG3   | 1.98                     | 0.45              |
| 2:B:312:TYR:O      | 2:B:317:ASN:ND2    | 2.49                     | 0.45              |
| 17:B:603:CLA:H142  | 17:B:603:CLA:H112  | 1.69                     | 0.45              |
| 3:C:49:LEU:HD11    | 3:C:53:HIS:HE1     | 1.82                     | 0.45              |
| 3:C:229:ASN:OD1    | 3:C:230:LEU:N      | 2.49                     | 0.45              |
| 3:C:306:GLY:N      | 3:C:307:PRO:HD2    | 2.30                     | 0.45              |
| 8:I:31:ASN:ND2     | 8:I:33:LYS:O       | 2.50                     | 0.45              |
| 9:K:37:PHE:O       | 9:K:41:ALA:N       | 2.50                     | 0.45              |
| 1:a:5091:LEU:O     | 1:a:5091:LEU:HD23  | 2.16                     | 0.45              |
| 3:c:5307:PRO:HA    | 3:c:5358:PHE:CD2   | 2.51                     | 0.45              |
| 4:d:5261:PHE:HD2   | 4:d:5267:LEU:HG    | 1.79                     | 0.45              |
| 25:d:5410:MGE:H2A2 | 25:d:5410:MGE:H5A2 | 1.68                     | 0.45              |
| 11:m:5029:THR:HA   | 11:m:5032:GLN:HG2  | 1.98                     | 0.45              |
| 13:z:5029:SER:CA   | 14:y:44:GLY:HA2    | 2.45                     | 0.45              |
| 1:A:234:ASN:HB2    | 25:A:412:MGE:O3D   | 2.17                     | 0.45              |
| 17:B:613:CLA:H41   | 17:B:613:CLA:H61   | 1.70                     | 0.45              |
| 3:C:276:LEU:O      | 3:C:280:SER:N      | 2.39                     | 0.45              |
| 10:L:28:ALA:O      | 10:L:32:SER:N      | 2.40                     | 0.45              |
| 1:a:5060:ILE:HD12  | 4:d:5317:LYS:NZ    | 2.31                     | 0.45              |
| 1:a:5085:SER:HB2   | 1:a:5089:ILE:HG21  | 1.99                     | 0.45              |
| 2:b:5124:ARG:O     | 7:h:5012:ARG:NH2   | 2.46                     | 0.45              |
| 2:b:5392:PHE:O     | 2:b:5396:GLY:N     | 2.49                     | 0.45              |
| 3:c:5161:LEU:HD13  | 17:c:5507:CLA:C1D  | 2.46                     | 0.45              |
| 4:d:5014:TRP:HZ2   | 16:x:29:ILE:HD12   | 1.73                     | 0.45              |
| 9:k:5029:PRO:HA    | 9:k:5032:PHE:HD2   | 1.81                     | 0.45              |
| 23:l:5102:SQD:H272 | 23:l:5102:SQD:H151 | 1.98                     | 0.45              |
| 1:A:207:GLY:HA3    | 1:A:278:TRP:HE1    | 1.80                     | 0.45              |
| 1:A:300:PHE:HD2    | 3:C:404:LEU:HD12   | 1.81                     | 0.45              |
| 26:C:518:DGD:HBN1  | 25:D:408:MGE:H211  | 1.97                     | 0.45              |
| 25:D:410:MGE:H5B2  | 25:D:410:MGE:H8B1  | 1.70                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:a:5036:ILE:O     | 1:a:5040:THR:HG22  | 2.16                     | 0.45              |
| 2:b:5140:GLY:HA3   | 2:b:5217:ILE:HG13  | 1.99                     | 0.45              |
| 2:b:5437:LEU:HD23  | 2:b:5437:LEU:O     | 2.17                     | 0.45              |
| 2:b:5451:PHE:HE2   | 17:b:5604:CLA:HMA3 | 1.81                     | 0.45              |
| 3:c:5372:PRO:HG3   | 15:n:85:SER:OG     | 2.17                     | 0.45              |
| 4:d:5061:HIS:CD2   | 4:d:5168:PHE:CE1   | 3.04                     | 0.45              |
| 1:A:48:PHE:HA      | 1:A:115:ILE:HD11   | 1.99                     | 0.45              |
| 1:A:120:LEU:O      | 1:A:123:ALA:N      | 2.49                     | 0.45              |
| 1:A:219:VAL:HG11   | 4:D:268:HIS:ND1    | 2.32                     | 0.45              |
| 19:A:406:PQ9:H191  | 19:A:406:PQ9:H211  | 1.69                     | 0.45              |
| 21:A:408:LHG:O3    | 21:A:408:LHG:O1    | 2.19                     | 0.45              |
| 17:B:611:CLA:H162  | 17:B:611:CLA:H141  | 1.59                     | 0.45              |
| 3:C:212:TYR:OH     | 3:C:226:SER:HB2    | 2.16                     | 0.45              |
| 4:D:141:TYR:OH     | 25:D:409:MGE:O4D   | 2.19                     | 0.45              |
| 18:D:402:PHO:H143  | 18:D:402:PHO:H111  | 1.65                     | 0.45              |
| 1:a:5290:ILE:O     | 1:a:5293:MET:N     | 2.50                     | 0.45              |
| 2:b:5326:ARG:NH2   | 4:d:5297:ASP:HB2   | 2.31                     | 0.45              |
| 4:d:5168:PHE:HD2   | 4:d:5169:PHE:CE1   | 2.34                     | 0.45              |
| 17:d:5403:CLA:H202 | 17:d:5403:CLA:H162 | 1.73                     | 0.45              |
| 11:m:5021:PHE:CZ   | 11:m:5025:LEU:HD11 | 2.51                     | 0.45              |
| 19:A:406:PQ9:H341  | 19:A:406:PQ9:H361  | 1.67                     | 0.45              |
| 5:E:44:TYR:O       | 5:E:48:GLY:N       | 2.50                     | 0.45              |
| 11:M:29:THR:HA     | 11:M:32:GLN:HG2    | 1.98                     | 0.45              |
| 13:Z:5:PHE:HZ      | 13:Z:54:VAL:HA     | 1.80                     | 0.45              |
| 2:b:5006:TYR:OH    | 25:d:5409:MGE:H6D1 | 2.16                     | 0.45              |
| 2:b:5326:ARG:HH21  | 4:d:5297:ASP:HB2   | 1.81                     | 0.45              |
| 2:b:5360:PRO:HG2   | 4:d:5339:PHE:CZ    | 2.51                     | 0.45              |
| 3:c:5049:LEU:HD11  | 3:c:5053:HIS:HE1   | 1.82                     | 0.45              |
| 3:c:5362:ARG:HG3   | 15:n:82:ARG:NH1    | 2.30                     | 0.45              |
| 3:c:5379:LYS:HD2   | 15:n:92:THR:HG21   | 1.99                     | 0.45              |
| 4:d:5148:ALA:HB3   | 4:d:5149:PRO:HD3   | 1.98                     | 0.45              |
| 1:A:36:ILE:O       | 1:A:40:THR:HG22    | 2.16                     | 0.45              |
| 4:D:24:ARG:HG2     | 4:D:25:ASP:H       | 1.81                     | 0.45              |
| 2:b:5326:ARG:HB3   | 2:b:5444:ARG:HG2   | 1.99                     | 0.45              |
| 17:b:5605:CLA:H61  | 17:b:5605:CLA:H41  | 1.54                     | 0.45              |
| 17:c:5502:CLA:H12  | 17:c:5503:CLA:C2   | 2.47                     | 0.45              |
| 4:d:5334:GLN:HB3   | 4:d:5336:HIS:CE1   | 2.52                     | 0.45              |
| 17:d:5403:CLA:H201 | 25:d:5408:MGE:H8A2 | 1.98                     | 0.45              |
| 5:e:5044:TYR:O     | 5:e:5048:GLY:N     | 2.50                     | 0.45              |
| 1:A:91:LEU:HD23    | 1:A:91:LEU:O       | 2.16                     | 0.45              |
| 2:B:469:HIS:O      | 2:B:472:ARG:N      | 2.50                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 17:B:609:CLA:H92   | 17:B:609:CLA:H62   | 1.77                     | 0.45              |
| 3:C:308:GLU:HB2    | 3:C:361:PHE:CZ     | 2.52                     | 0.45              |
| 4:D:141:TYR:OH     | 25:D:409:MGE:O2D   | 2.28                     | 0.45              |
| 4:D:148:ALA:HB3    | 4:D:149:PRO:HD3    | 1.98                     | 0.45              |
| 4:D:157:PHE:CE1    | 4:D:173:PHE:HE1    | 2.35                     | 0.45              |
| 4:D:334:GLN:HB3    | 4:D:336:HIS:CE1    | 2.52                     | 0.45              |
| 25:D:409:MGE:H2A1  | 25:D:409:MGE:H252  | 1.99                     | 0.45              |
| 9:K:40:GLN:O       | 9:K:44:GLY:N       | 2.38                     | 0.45              |
| 2:b:5122:LEU:HD22  | 2:b:5123:PHE:CE1   | 2.52                     | 0.45              |
| 2:b:5185:TRP:HB3   | 2:b:5200:ALA:HB1   | 1.98                     | 0.45              |
| 3:c:5283:GLY:HA3   | 3:c:5434:ALA:HB2   | 1.98                     | 0.45              |
| 9:k:5037:PHE:O     | 9:k:5041:ALA:N     | 2.50                     | 0.45              |
| 13:z:5028:ALA:C    | 14:y:44:GLY:CA     | 2.90                     | 0.45              |
| 15:n:84:LEU:HD22   | 15:n:131:GLU:HG3   | 1.98                     | 0.45              |
| 16:X:20:VAL:HG12   | 16:X:21:LEU:N      | 2.32                     | 0.45              |
| 1:A:92:HIS:ND1     | 3:C:219:GLY:O      | 2.51                     | 0.44              |
| 17:B:607:CLA:H122  | 25:B:619:MGE:H132  | 1.99                     | 0.44              |
| 17:B:612:CLA:HBA1  | 17:B:612:CLA:H3A   | 1.54                     | 0.44              |
| 17:B:615:CLA:H13   | 17:B:615:CLA:H172  | 1.73                     | 0.44              |
| 3:C:276:LEU:HA     | 3:C:276:LEU:HD23   | 1.75                     | 0.44              |
| 20:D:407:BCR:H371  | 20:D:407:BCR:H24C  | 1.75                     | 0.44              |
| 2:b:5056:TRP:HB3   | 2:b:5267:LEU:O     | 2.17                     | 0.44              |
| 3:c:5081:MET:HE3   | 3:c:5105:VAL:HG21  | 1.99                     | 0.44              |
| 3:c:5229:ASN:OD1   | 3:c:5231:GLU:N     | 2.43                     | 0.44              |
| 3:c:5308:GLU:HB2   | 3:c:5361:PHE:CZ    | 2.52                     | 0.44              |
| 4:d:5297:ASP:OD1   | 4:d:5315:TYR:OH    | 2.33                     | 0.44              |
| 9:k:5028:ILE:CG1   | 9:k:5029:PRO:HD3   | 2.48                     | 0.44              |
| 11:m:5028:GLN:NE2  | 25:m:5101:MGE:H3G2 | 2.33                     | 0.44              |
| 14:Y:18:VAL:HG13   | 14:Y:21:GLN:HE21   | 1.82                     | 0.44              |
| 14:Y:32:GLY:O      | 14:Y:35:ILE:CD1    | 2.64                     | 0.44              |
| 1:A:119:PHE:O      | 1:A:123:ALA:N      | 2.45                     | 0.44              |
| 2:B:451:PHE:HE2    | 17:B:604:CLA:HMA3  | 1.81                     | 0.44              |
| 4:D:93:TRP:CD1     | 4:D:94:GLY:N       | 2.81                     | 0.44              |
| 2:b:5263:THR:HB    | 2:b:5268:PHE:HD2   | 1.82                     | 0.44              |
| 17:b:5610:CLA:H8   | 17:b:5610:CLA:H51  | 1.66                     | 0.44              |
| 4:d:5176:ALA:HA    | 4:d:5179:PHE:CD2   | 2.45                     | 0.44              |
| 20:t:5101:BCR:H20C | 20:t:5101:BCR:H361 | 1.80                     | 0.44              |
| 13:z:5053:VAL:O    | 13:z:5057:LEU:HB2  | 2.16                     | 0.44              |
| 1:A:85:SER:HB2     | 1:A:89:ILE:HG21    | 1.99                     | 0.44              |
| 3:C:142:GLU:OE1    | 3:C:142:GLU:N      | 2.51                     | 0.44              |
| 17:C:508:CLA:C4A   | 17:C:508:CLA:HBA2  | 2.47                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:D:346:LEU:O      | 4:D:348:ARG:N      | 2.48                     | 0.44              |
| 1:a:5037:MET:SD    | 1:a:5129:ARG:NE    | 2.82                     | 0.44              |
| 17:b:5603:CLA:C3D  | 17:b:5605:CLA:H43  | 2.48                     | 0.44              |
| 17:b:5604:CLA:H62  | 17:b:5604:CLA:H41  | 1.59                     | 0.44              |
| 3:c:5098:GLY:O     | 3:c:5106:VAL:N     | 2.49                     | 0.44              |
| 3:c:5274:TYR:HE1   | 17:c:5505:CLA:OBD  | 1.99                     | 0.44              |
| 20:h:5101:BCR:H371 | 20:h:5101:BCR:H24C | 1.75                     | 0.44              |
| 8:i:5015:PHE:O     | 8:i:5019:PHE:N     | 2.50                     | 0.44              |
| 9:k:5020:PRO:HB3   | 14:y:24:MET:HB3    | 1.98                     | 0.44              |
| 9:k:5028:ILE:HG13  | 9:k:5029:PRO:HD3   | 2.00                     | 0.44              |
| 15:n:72:PHE:HB2    | 15:n:94:LEU:HD13   | 1.99                     | 0.44              |
| 2:B:56:TRP:HB3     | 2:B:267:LEU:O      | 2.17                     | 0.44              |
| 2:B:315:ILE:HG21   | 2:B:426:PHE:CD1    | 2.51                     | 0.44              |
| 2:B:433:ASP:OD2    | 2:B:436:THR:OG1    | 2.26                     | 0.44              |
| 2:B:437:LEU:HD23   | 2:B:437:LEU:O      | 2.17                     | 0.44              |
| 3:C:92:ILE:HD12    | 3:C:114:VAL:HG11   | 1.99                     | 0.44              |
| 3:C:189:TRP:HH2    | 3:C:367:GLU:HB3    | 1.81                     | 0.44              |
| 20:T:102:BCR:H24C  | 20:b:5617:BCR:H341 | 2.00                     | 0.44              |
| 20:a:5408:BCR:H312 | 8:i:5015:PHE:CE1   | 2.53                     | 0.44              |
| 3:c:5234:VAL:O     | 3:c:5238:ILE:HG12  | 2.17                     | 0.44              |
| 3:c:5317:PHE:HD1   | 3:c:5320:ARG:HE    | 1.65                     | 0.44              |
| 17:d:5403:CLA:H62  | 17:d:5403:CLA:H93  | 1.64                     | 0.44              |
| 16:X:3:ILE:CG2     | 16:X:7:LEU:CD1     | 2.86                     | 0.44              |
| 1:A:166:GLY:HA3    | 3:C:358:PHE:CE1    | 2.47                     | 0.44              |
| 1:A:323:ARG:O      | 1:A:327:GLY:N      | 2.43                     | 0.44              |
| 2:B:13:ILE:HG23    | 2:B:14:ASN:N       | 2.32                     | 0.44              |
| 2:B:118:TRP:CD1    | 2:B:118:TRP:H      | 2.35                     | 0.44              |
| 2:B:140:GLY:HA3    | 2:B:217:ILE:HG13   | 1.99                     | 0.44              |
| 2:B:164:PRO:HG3    | 17:B:606:CLA:O1D   | 2.18                     | 0.44              |
| 2:B:185:TRP:HB3    | 2:B:200:ALA:HB1    | 1.98                     | 0.44              |
| 2:B:326:ARG:HB3    | 2:B:444:ARG:HG2    | 1.99                     | 0.44              |
| 3:C:264:PHE:O      | 3:C:274:TYR:OH     | 2.33                     | 0.44              |
| 3:C:307:PRO:HA     | 3:C:358:PHE:CD2    | 2.51                     | 0.44              |
| 4:D:201:VAL:HG22   | 17:D:404:CLA:C2B   | 2.48                     | 0.44              |
| 4:D:262:SER:H      | 25:D:410:MGE:C2D   | 2.30                     | 0.44              |
| 9:K:28:ILE:HG13    | 9:K:29:PRO:HD3     | 2.00                     | 0.44              |
| 1:a:5317:TRP:CZ3   | 4:d:5177:ALA:HB2   | 2.52                     | 0.44              |
| 2:b:5164:PRO:HG3   | 17:b:5606:CLA:O1D  | 2.18                     | 0.44              |
| 2:b:5390:TYR:HA    | 2:b:5395:GLN:OE1   | 2.18                     | 0.44              |
| 17:b:5608:CLA:H202 | 17:b:5608:CLA:H162 | 1.78                     | 0.44              |
| 17:b:5611:CLA:HBB1 | 17:b:5613:CLA:H3A  | 2.00                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:c:5205:ASP:H     | 3:c:5209:ILE:HD12  | 1.82                     | 0.44              |
| 4:d:5087:HIS:CD2   | 4:d:5166:SER:HA    | 2.52                     | 0.44              |
| 4:d:5157:PHE:CE1   | 4:d:5173:PHE:HE1   | 2.35                     | 0.44              |
| 4:d:5279:LEU:CD1   | 18:d:5402:PHO:HAC2 | 2.48                     | 0.44              |
| 16:x:14:LEU:C      | 16:x:14:LEU:HD23   | 2.42                     | 0.44              |
| 17:A:401:CLA:H122  | 18:A:404:PHO:HBA2  | 2.00                     | 0.44              |
| 26:A:413:DGD:HA81  | 26:A:413:DGD:HAE1  | 1.83                     | 0.44              |
| 17:B:601:CLA:H2A   | 17:B:601:CLA:HED3  | 1.98                     | 0.44              |
| 17:B:613:CLA:H101  | 17:B:613:CLA:H62   | 1.68                     | 0.44              |
| 17:B:613:CLA:H111  | 17:B:613:CLA:H142  | 1.76                     | 0.44              |
| 3:C:234:VAL:O      | 3:C:238:ILE:HG12   | 2.17                     | 0.44              |
| 3:C:408:GLY:CA     | 3:C:418:ASN:HA     | 2.47                     | 0.44              |
| 18:D:402:PHO:HBA1  | 18:D:402:PHO:H3A   | 1.71                     | 0.44              |
| 9:K:28:ILE:CG1     | 9:K:29:PRO:HD3     | 2.47                     | 0.44              |
| 18:a:5405:PHO:H41  | 18:a:5405:PHO:H61  | 1.74                     | 0.44              |
| 17:b:5614:CLA:HBA1 | 25:m:5101:MGE:H7B2 | 2.00                     | 0.44              |
| 17:c:5508:CLA:C4A  | 17:c:5508:CLA:HBA2 | 2.47                     | 0.44              |
| 4:d:5168:PHE:HD2   | 4:d:5169:PHE:CD1   | 2.36                     | 0.44              |
| 4:d:5201:VAL:HG22  | 17:d:5403:CLA:C2B  | 2.48                     | 0.44              |
| 20:d:5406:BCR:H15C | 20:d:5406:BCR:H351 | 1.90                     | 0.44              |
| 1:A:246:TYR:CE2    | 1:A:248:ILE:HD11   | 2.51                     | 0.44              |
| 17:A:402:CLA:H18   | 12:T:10:PHE:HZ     | 1.82                     | 0.44              |
| 17:B:603:CLA:C3D   | 17:B:605:CLA:H43   | 2.48                     | 0.44              |
| 3:C:157:MET:HE1    | 3:C:271:TYR:CD2    | 2.51                     | 0.44              |
| 17:b:5607:CLA:H122 | 25:b:5620:MGE:H132 | 1.99                     | 0.44              |
| 17:b:5615:CLA:H13  | 17:b:5615:CLA:H172 | 1.73                     | 0.44              |
| 25:d:5410:MGE:H222 | 25:l:5101:MGE:H262 | 2.00                     | 0.44              |
| 14:Y:42:ARG:HG2    | 14:Y:42:ARG:NH1    | 2.20                     | 0.44              |
| 1:A:93:PHE:CD2     | 1:A:95:PRO:HD3     | 2.53                     | 0.44              |
| 2:B:18:ARG:HD2     | 2:B:115:TRP:CE3    | 2.53                     | 0.44              |
| 2:B:122:LEU:HD22   | 2:B:123:PHE:CE1    | 2.52                     | 0.44              |
| 2:B:141:ILE:HA     | 2:B:217:ILE:HD11   | 2.00                     | 0.44              |
| 3:C:160:ILE:HD13   | 17:C:512:CLA:HAC2  | 2.00                     | 0.44              |
| 17:C:508:CLA:H111  | 17:C:508:CLA:H91   | 1.73                     | 0.44              |
| 4:D:235:PHE:CE2    | 4:D:237:PRO:HB3    | 2.53                     | 0.44              |
| 4:D:297:ASP:OD1    | 4:D:315:TYR:OH     | 2.33                     | 0.44              |
| 23:L:101:SQD:H271  | 12:T:19:PHE:CZ     | 2.52                     | 0.44              |
| 13:Z:28:ALA:CB     | 14:Y:39:LEU:HD21   | 2.48                     | 0.44              |
| 1:a:5161:TYR:CE1   | 1:a:5186:PHE:HE1   | 2.36                     | 0.44              |
| 1:a:5193:LEU:HD22  | 4:d:5179:PHE:CE1   | 2.52                     | 0.44              |
| 1:a:5312:ASN:HB3   | 5:e:5056:TYR:HE2   | 1.83                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:b:5018:ARG:HD2   | 2:b:5115:TRP:CE3   | 2.53                     | 0.44              |
| 17:b:5608:CLA:CGA  | 17:b:5608:CLA:C1A  | 2.96                     | 0.44              |
| 17:b:5614:CLA:H71  | 20:b:5617:BCR:H362 | 1.99                     | 0.44              |
| 3:c:5408:GLY:CA    | 3:c:5418:ASN:HA    | 2.47                     | 0.44              |
| 26:c:5515:DGD:HAE1 | 26:c:5515:DGD:HA81 | 1.83                     | 0.44              |
| 15:n:27:THR:HG22   | 15:n:67:LYS:HB3    | 2.00                     | 0.44              |
| 15:N:27:THR:HG22   | 15:N:67:LYS:HB3    | 2.00                     | 0.44              |
| 1:A:290:ILE:O      | 1:A:293:MET:N      | 2.50                     | 0.44              |
| 1:A:303:ASN:HD21   | 3:C:414:ILE:HG13   | 1.79                     | 0.44              |
| 2:B:226:TYR:CE1    | 2:B:231:MET:HB2    | 2.53                     | 0.44              |
| 3:C:27:ASP:O       | 3:C:41:ARG:NH1     | 2.51                     | 0.44              |
| 3:C:79:LYS:HE2     | 3:C:83:GLU:HG2     | 1.99                     | 0.44              |
| 4:D:39:PRO:O       | 4:D:43:LEU:HD13    | 2.18                     | 0.44              |
| 4:D:87:HIS:CD2     | 4:D:166:SER:HA     | 2.52                     | 0.44              |
| 8:I:15:PHE:O       | 8:I:19:PHE:N       | 2.50                     | 0.44              |
| 2:b:5192:PRO:HG3   | 7:h:5049:TYR:CE1   | 2.52                     | 0.44              |
| 17:b:5603:CLA:O1D  | 17:b:5603:CLA:H2A  | 2.18                     | 0.44              |
| 17:b:5608:CLA:CBB  | 4:d:5123:ILE:HG12  | 2.48                     | 0.44              |
| 3:c:5175:LEU:HD11  | 17:c:5501:CLA:HED2 | 2.00                     | 0.44              |
| 17:c:5507:CLA:H91  | 17:c:5507:CLA:H112 | 1.68                     | 0.44              |
| 4:d:5174:GLY:N     | 18:d:5402:PHO:H203 | 2.33                     | 0.44              |
| 8:i:5031:ASN:ND2   | 8:i:5033:LYS:O     | 2.50                     | 0.44              |
| 13:z:5002:THR:O    | 13:z:5006:GLN:N    | 2.42                     | 0.44              |
| 25:A:412:MGE:H121  | 17:B:613:CLA:H18   | 1.99                     | 0.43              |
| 3:C:71:GLU:CD      | 3:C:86:LEU:HD12    | 2.43                     | 0.43              |
| 4:D:59:TYR:O       | 5:E:66:VAL:HG12    | 2.18                     | 0.43              |
| 6:F:18:VAL:HG13    | 6:F:19:ARG:N       | 2.33                     | 0.43              |
| 17:a:5404:CLA:H62  | 17:a:5404:CLA:H101 | 1.81                     | 0.43              |
| 2:b:5469:HIS:O     | 2:b:5472:ARG:N     | 2.50                     | 0.43              |
| 17:b:5613:CLA:H142 | 17:b:5613:CLA:H111 | 1.76                     | 0.43              |
| 25:b:5620:MGE:O2D  | 25:b:5620:MGE:O4D  | 2.36                     | 0.43              |
| 3:c:5106:VAL:HG23  | 3:c:5107:ASP:N     | 2.33                     | 0.43              |
| 3:c:5142:GLU:N     | 3:c:5142:GLU:OE1   | 2.50                     | 0.43              |
| 3:c:5409:GLY:N     | 3:c:5417:VAL:O     | 2.50                     | 0.43              |
| 18:A:404:PHO:HBA2  | 18:A:404:PHO:H3A   | 1.39                     | 0.43              |
| 2:B:390:TYR:HA     | 2:B:395:GLN:OE1    | 2.18                     | 0.43              |
| 17:B:611:CLA:HBB1  | 17:B:613:CLA:H3A   | 2.00                     | 0.43              |
| 17:C:502:CLA:H12   | 17:C:503:CLA:C2    | 2.48                     | 0.43              |
| 17:C:505:CLA:H102  | 17:C:505:CLA:H13   | 1.85                     | 0.43              |
| 4:D:168:PHE:HD2    | 4:D:169:PHE:CD1    | 2.36                     | 0.43              |
| 7:H:38:PHE:O       | 7:H:41:PHE:HB3     | 2.19                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:L:101:SQD:O9    | 10:l:5007:ARG:NH2  | 2.48                     | 0.43              |
| 17:a:5402:CLA:H122 | 18:a:5405:PHO:HBA2 | 2.00                     | 0.43              |
| 3:c:5071:GLU:CD    | 3:c:5086:LEU:HD12  | 2.43                     | 0.43              |
| 3:c:5094:THR:O     | 3:c:5186:TYR:HB3   | 2.18                     | 0.43              |
| 3:c:5401:LEU:HD22  | 3:c:5409:GLY:C     | 2.42                     | 0.43              |
| 17:c:5506:CLA:H202 | 17:c:5506:CLA:H161 | 1.73                     | 0.43              |
| 29:f:5101:HEM:HBC2 | 29:f:5101:HEM:CHD  | 2.48                     | 0.43              |
| 7:h:5040:VAL:O     | 7:h:5044:ILE:HG12  | 2.18                     | 0.43              |
| 13:z:5053:VAL:HA   | 13:z:5057:LEU:HD13 | 2.01                     | 0.43              |
| 15:n:100:HIS:HE1   | 15:n:104:TYR:CZ    | 2.36                     | 0.43              |
| 16:x:9:GLY:N       | 16:x:12:ILE:CD1    | 2.65                     | 0.43              |
| 17:B:603:CLA:H61   | 17:B:603:CLA:H41   | 1.83                     | 0.43              |
| 17:B:604:CLA:H41   | 17:B:604:CLA:H62   | 1.59                     | 0.43              |
| 17:B:609:CLA:HBA1  | 17:B:609:CLA:H3A   | 1.60                     | 0.43              |
| 17:B:612:CLA:H2A   | 17:B:612:CLA:O2D   | 2.18                     | 0.43              |
| 17:B:614:CLA:H71   | 20:B:617:BCR:H362  | 1.99                     | 0.43              |
| 3:C:81:MET:HE3     | 3:C:105:VAL:HG21   | 1.99                     | 0.43              |
| 3:C:189:TRP:CH2    | 3:C:367:GLU:HB3    | 2.52                     | 0.43              |
| 4:D:57:SER:O       | 4:D:64:ALA:HA      | 2.18                     | 0.43              |
| 18:D:402:PHO:H2A   | 18:D:402:PHO:CED   | 2.48                     | 0.43              |
| 17:a:5403:CLA:H61  | 17:a:5403:CLA:H93  | 1.74                     | 0.43              |
| 18:a:5405:PHO:HBA2 | 18:a:5405:PHO:H3A  | 1.39                     | 0.43              |
| 2:b:5248:ALA:HB2   | 17:b:5603:CLA:H52  | 2.01                     | 0.43              |
| 17:b:5612:CLA:H2   | 17:b:5612:CLA:H62  | 1.32                     | 0.43              |
| 3:c:5079:LYS:HE2   | 3:c:5083:GLU:HG2   | 1.99                     | 0.43              |
| 3:c:5160:ILE:HD13  | 17:c:5511:CLA:HAC2 | 2.00                     | 0.43              |
| 4:d:5235:PHE:CE2   | 4:d:5237:PRO:HB3   | 2.53                     | 0.43              |
| 15:n:127:ALA:HA    | 15:n:130:ARG:HD2   | 2.00                     | 0.43              |
| 2:B:201:HIS:O      | 2:B:205:ALA:N      | 2.43                     | 0.43              |
| 17:B:602:CLA:H62   | 17:B:602:CLA:H41   | 1.71                     | 0.43              |
| 3:C:189:TRP:CH2    | 3:C:364:PRO:HA     | 2.53                     | 0.43              |
| 17:C:510:CLA:H122  | 17:C:510:CLA:H162  | 1.72                     | 0.43              |
| 4:D:123:ILE:O      | 4:D:126:MET:N      | 2.52                     | 0.43              |
| 5:E:82:GLN:C       | 5:E:84:LYS:H       | 2.27                     | 0.43              |
| 7:H:40:VAL:O       | 7:H:44:ILE:HG12    | 2.18                     | 0.43              |
| 1:a:5266:ASN:OD1   | 1:a:5267:ASN:N     | 2.52                     | 0.43              |
| 2:b:5141:ILE:HA    | 2:b:5217:ILE:HD11  | 2.00                     | 0.43              |
| 3:c:5313:GLN:HG3   | 3:c:5396:MET:HG3   | 2.00                     | 0.43              |
| 10:l:5015:THR:O    | 10:l:5018:TYR:N    | 2.51                     | 0.43              |
| 13:z:5055:GLY:HA3  | 20:z:5101:BCR:C5   | 2.48                     | 0.43              |
| 15:N:72:PHE:HB2    | 15:N:94:LEU:HD13   | 1.99                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:N:100:HIS:HE1   | 15:N:104:TYR:CZ    | 2.36                     | 0.43              |
| 1:A:161:TYR:CE1    | 1:A:186:PHE:HE1    | 2.36                     | 0.43              |
| 2:B:256:MET:O      | 2:B:448:ARG:NH1    | 2.47                     | 0.43              |
| 3:C:350:ILE:HG21   | 3:C:359:TRP:HB2    | 2.00                     | 0.43              |
| 3:C:409:GLY:N      | 3:C:417:VAL:O      | 2.51                     | 0.43              |
| 1:a:5089:ILE:HD12  | 1:a:5089:ILE:HA    | 1.85                     | 0.43              |
| 2:b:5013:ILE:HG23  | 2:b:5014:ASN:N     | 2.32                     | 0.43              |
| 17:c:5503:CLA:HBD  | 17:c:5503:CLA:HBA1 | 2.01                     | 0.43              |
| 20:c:5513:BCR:H24C | 20:c:5513:BCR:H371 | 1.84                     | 0.43              |
| 12:t:5018:PHE:HB2  | 20:t:5102:BCR:C8   | 2.48                     | 0.43              |
| 1:A:239:PHE:HE2    | 12:T:29:ILE:HG13   | 1.83                     | 0.43              |
| 1:A:319:ASP:O      | 1:A:323:ARG:N      | 2.46                     | 0.43              |
| 17:A:403:CLA:H2A   | 17:A:403:CLA:CED   | 2.49                     | 0.43              |
| 17:B:604:CLA:H62   | 17:B:604:CLA:H92   | 1.75                     | 0.43              |
| 3:C:98:GLY:O       | 3:C:106:VAL:N      | 2.49                     | 0.43              |
| 3:C:313:GLN:HG3    | 3:C:396:MET:HG3    | 2.00                     | 0.43              |
| 3:C:318:LEU:CD1    | 3:C:328:VAL:HG21   | 2.48                     | 0.43              |
| 5:E:51:ARG:O       | 5:E:54:SER:N       | 2.40                     | 0.43              |
| 1:a:5018:CYS:SG    | 8:i:5030:ARG:NH2   | 2.92                     | 0.43              |
| 2:b:5226:TYR:CE1   | 2:b:5231:MET:HB2   | 2.53                     | 0.43              |
| 17:b:5602:CLA:H62  | 17:b:5602:CLA:H41  | 1.71                     | 0.43              |
| 17:b:5603:CLA:H112 | 17:b:5603:CLA:H142 | 1.69                     | 0.43              |
| 3:c:5092:ILE:HD12  | 3:c:5114:VAL:HG11  | 1.99                     | 0.43              |
| 3:c:5318:LEU:CD1   | 3:c:5328:VAL:HG21  | 2.48                     | 0.43              |
| 26:c:5515:DGD:HB71 | 25:c:5517:MGE:H5A2 | 2.00                     | 0.43              |
| 4:d:5039:PRO:O     | 4:d:5043:LEU:HD13  | 2.18                     | 0.43              |
| 4:d:5346:LEU:O     | 4:d:5348:ARG:N     | 2.48                     | 0.43              |
| 20:d:5406:BCR:H24C | 20:d:5406:BCR:H371 | 1.75                     | 0.43              |
| 15:N:127:ALA:HA    | 15:N:130:ARG:HD2   | 2.00                     | 0.43              |
| 3:C:400:PRO:O      | 3:C:401:LEU:HG     | 2.19                     | 0.43              |
| 1:a:5272:HIS:NE2   | 24:a:5412:BCT:O3   | 2.48                     | 0.43              |
| 2:b:5037:MET:HE1   | 17:b:5607:CLA:CHD  | 2.49                     | 0.43              |
| 3:c:5350:ILE:HG21  | 3:c:5359:TRP:HB2   | 2.00                     | 0.43              |
| 14:Y:18:VAL:HG13   | 14:Y:21:GLN:NE2    | 2.34                     | 0.43              |
| 16:x:7:LEU:HD22    | 16:x:7:LEU:HA      | 1.90                     | 0.43              |
| 1:A:266:ASN:OD1    | 1:A:267:ASN:N      | 2.52                     | 0.43              |
| 17:A:402:CLA:H111  | 17:A:402:CLA:H152  | 1.42                     | 0.43              |
| 2:B:188:ASP:HA     | 7:H:58:VAL:HG12    | 2.01                     | 0.43              |
| 3:C:147:PHE:HD2    | 17:C:513:CLA:H3A   | 1.82                     | 0.43              |
| 3:C:187:ASP:OD1    | 3:C:189:TRP:N      | 2.52                     | 0.43              |
| 3:C:226:SER:O      | 3:C:227:VAL:C      | 2.62                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 29:F:101:HEM:HBC2 | 29:F:101:HEM:CHD   | 2.48                     | 0.43              |
| 10:L:15:THR:O     | 10:L:18:TYR:N      | 2.51                     | 0.43              |
| 1:a:5093:PHE:CD2  | 1:a:5095:PRO:HD3   | 2.53                     | 0.43              |
| 1:a:5097:TRP:NE1  | 25:c:5517:MGE:O5D  | 2.43                     | 0.43              |
| 17:a:5403:CLA:O1A | 4:d:5202:ALA:HA    | 2.18                     | 0.43              |
| 17:a:5403:CLA:H12 | 4:d:5202:ALA:HA    | 2.00                     | 0.43              |
| 2:b:5005:TRP:CZ2  | 25:l:5101:MGE:H2A2 | 2.54                     | 0.43              |
| 2:b:5256:MET:O    | 2:b:5448:ARG:NH1   | 2.47                     | 0.43              |
| 4:d:5057:SER:O    | 4:d:5064:ALA:HA    | 2.18                     | 0.43              |
| 4:d:5235:PHE:HE2  | 4:d:5237:PRO:HB3   | 1.84                     | 0.43              |
| 5:e:5082:GLN:C    | 5:e:5084:LYS:H     | 2.27                     | 0.43              |
| 7:h:5038:PHE:O    | 7:h:5041:PHE:HB3   | 2.18                     | 0.43              |
| 23:l:5102:SQD:H62 | 25:m:5103:MGE:H2A1 | 2.01                     | 0.43              |
| 15:n:67:LYS:O     | 15:n:71:PHE:N      | 2.32                     | 0.43              |
| 14:y:34:MET:HE2   | 14:y:34:MET:HB2    | 1.79                     | 0.43              |
| 16:x:3:ILE:CD1    | 16:x:7:LEU:HD12    | 2.48                     | 0.43              |
| 1:A:124:SER:OG    | 1:A:155:PHE:HZ     | 2.02                     | 0.43              |
| 17:A:402:CLA:H61  | 17:A:402:CLA:H93   | 1.74                     | 0.43              |
| 17:B:606:CLA:O2D  | 17:B:606:CLA:H2A   | 2.18                     | 0.43              |
| 17:B:614:CLA:C2   | 25:m:5103:MGE:H8A1 | 2.49                     | 0.43              |
| 3:C:175:LEU:HD11  | 17:C:501:CLA:HED2  | 2.00                     | 0.43              |
| 4:D:30:VAL:HG22   | 4:D:38:PHE:HE2     | 1.84                     | 0.43              |
| 1:a:5214:MET:O    | 1:a:5217:SER:N     | 2.52                     | 0.43              |
| 2:b:5332:LYS:HA   | 2:b:5437:LEU:HD22  | 2.01                     | 0.43              |
| 2:b:5347:ARG:HA   | 2:b:5352:GLU:O     | 2.19                     | 0.43              |
| 17:b:5612:CLA:H2A | 17:b:5612:CLA:O2D  | 2.18                     | 0.43              |
| 3:c:5186:TYR:OH   | 3:c:5296:VAL:HA    | 2.19                     | 0.43              |
| 18:d:5402:PHO:CED | 18:d:5402:PHO:H2A  | 2.48                     | 0.43              |
| 1:A:264:SER:OG    | 19:A:406:PQ9:O4    | 2.29                     | 0.43              |
| 2:B:74:SER:OG     | 2:B:75:TRP:N       | 2.52                     | 0.43              |
| 20:C:514:BCR:H20C | 20:C:514:BCR:H361  | 1.84                     | 0.43              |
| 4:D:235:PHE:HE2   | 4:D:237:PRO:HB3    | 1.84                     | 0.43              |
| 7:H:48:ILE:HG13   | 7:H:53:LEU:HD23    | 2.01                     | 0.43              |
| 1:a:5143:ILE:H    | 4:d:5220:ASN:ND2   | 2.17                     | 0.43              |
| 2:b:5368:VAL:CG1  | 2:b:5381:ILE:HD12  | 2.49                     | 0.43              |
| 17:b:5606:CLA:O2D | 17:b:5606:CLA:H2A  | 2.18                     | 0.43              |
| 4:d:5018:LEU:HD12 | 16:x:29:ILE:HA     | 2.01                     | 0.43              |
| 1:A:89:ILE:HD12   | 1:A:89:ILE:HA      | 1.85                     | 0.42              |
| 18:A:404:PHO:H51  | 18:A:404:PHO:H8    | 1.72                     | 0.42              |
| 2:B:256:MET:HG3   | 2:B:451:PHE:CD1    | 2.54                     | 0.42              |
| 3:C:189:TRP:HB2   | 15:N:76:ARG:NH1    | 2.34                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:D:93:TRP:CG      | 4:D:94:GLY:N       | 2.87                     | 0.42              |
| 9:K:31:LEU:HD23    | 20:Y:101:BCR:H14C  | 2.01                     | 0.42              |
| 11:M:11:THR:HG21   | 12:T:9:ILE:HD11    | 2.00                     | 0.42              |
| 13:Z:23:VAL:HB     | 13:Z:24:PRO:HD3    | 2.01                     | 0.42              |
| 1:a:5077:ILE:HD12  | 1:a:5077:ILE:H     | 1.84                     | 0.42              |
| 1:a:5124:SER:OG    | 1:a:5155:PHE:HZ    | 2.02                     | 0.42              |
| 1:a:5193:LEU:HD21  | 17:a:5402:CLA:HMC2 | 2.01                     | 0.42              |
| 1:a:5317:TRP:CH2   | 4:d:5077:ALA:HB3   | 2.52                     | 0.42              |
| 1:a:5331:MET:HE2   | 4:d:5320:LEU:O     | 2.19                     | 0.42              |
| 2:b:5118:TRP:H     | 2:b:5118:TRP:CD1   | 2.35                     | 0.42              |
| 2:b:5475:PHE:HE1   | 4:d:5134:ARG:HB3   | 1.84                     | 0.42              |
| 17:b:5607:CLA:H92  | 17:b:5607:CLA:H62  | 1.61                     | 0.42              |
| 3:c:5097:TRP:HE1   | 3:c:5178:LYS:HZ1   | 1.65                     | 0.42              |
| 3:c:5439:VAL:O     | 3:c:5443:TRP:N     | 2.52                     | 0.42              |
| 19:d:5405:PQ9:H212 | 19:d:5405:PQ9:H191 | 1.86                     | 0.42              |
| 7:h:5047:GLU:CD    | 16:x:10:PHE:HD2    | 2.16                     | 0.42              |
| 23:l:5102:SQD:H241 | 23:l:5102:SQD:H271 | 1.73                     | 0.42              |
| 23:l:5102:SQD:C23  | 12:t:5019:PHE:HZ   | 2.31                     | 0.42              |
| 1:A:74:GLY:HA3     | 11:M:1:MET:CE      | 2.50                     | 0.42              |
| 25:A:412:MGE:H102  | 25:A:412:MGE:H7A1  | 1.71                     | 0.42              |
| 2:B:7:ARG:HH11     | 17:B:611:CLA:HED1  | 1.84                     | 0.42              |
| 2:B:37:MET:HE1     | 17:B:607:CLA:CHD   | 2.49                     | 0.42              |
| 2:B:58:GLN:HG3     | 2:B:60:MET:HE2     | 2.01                     | 0.42              |
| 3:C:315:MET:O      | 3:C:318:LEU:HB3    | 2.19                     | 0.42              |
| 3:C:349:ILE:HD11   | 3:C:375:LEU:O      | 2.19                     | 0.42              |
| 17:C:507:CLA:H91   | 17:C:507:CLA:H112  | 1.69                     | 0.42              |
| 10:L:20:GLY:HA3    | 11:M:22:LEU:HD13   | 2.00                     | 0.42              |
| 1:a:5047:CYS:SG    | 1:a:5114:LEU:HD22  | 2.59                     | 0.42              |
| 1:a:5319:ASP:HA    | 1:a:5322:ASN:HB2   | 2.01                     | 0.42              |
| 17:a:5402:CLA:H191 | 25:d:5410:MGE:H212 | 2.02                     | 0.42              |
| 18:a:5405:PHO:NB   | 4:d:5209:LEU:HD12  | 2.34                     | 0.42              |
| 4:d:5030:VAL:HG22  | 4:d:5038:PHE:HE2   | 1.84                     | 0.42              |
| 4:d:5269:PHE:CZ    | 25:d:5409:MGE:H3G2 | 2.54                     | 0.42              |
| 5:e:5068:ASP:OD1   | 5:e:5068:ASP:N     | 2.51                     | 0.42              |
| 12:t:5016:LEU:O    | 12:t:5020:ALA:N    | 2.45                     | 0.42              |
| 2:B:248:ALA:HB2    | 17:B:603:CLA:H52   | 2.01                     | 0.42              |
| 2:B:332:LYS:HA     | 2:B:437:LEU:HD22   | 2.01                     | 0.42              |
| 2:B:347:ARG:HA     | 2:B:352:GLU:O      | 2.19                     | 0.42              |
| 17:B:610:CLA:H62   | 17:B:610:CLA:H41   | 1.81                     | 0.42              |
| 3:C:189:TRP:CZ3    | 3:C:364:PRO:HA     | 2.54                     | 0.42              |
| 13:Z:28:ALA:HB1    | 14:Y:39:LEU:HD11   | 2.01                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:b:5047:PRO:HB3   | 2:b:5078:TRP:CD2   | 2.54                     | 0.42              |
| 3:c:5223:TRP:CE2   | 25:c:5517:MGE:H8B1 | 2.55                     | 0.42              |
| 17:c:5512:CLA:CAB  | 20:z:5101:BCR:H24C | 2.50                     | 0.42              |
| 4:d:5023:LYS:NZ    | 4:d:5032:TRP:HE1   | 2.17                     | 0.42              |
| 4:d:5123:ILE:O     | 4:d:5126:MET:N     | 2.52                     | 0.42              |
| 4:d:5304:ARG:HH11  | 4:d:5307:GLU:HB2   | 1.84                     | 0.42              |
| 7:h:5048:ILE:HG13  | 7:h:5053:LEU:HD23  | 2.01                     | 0.42              |
| 15:n:46:GLU:OE2    | 15:n:50:LEU:HD11   | 2.20                     | 0.42              |
| 15:N:46:GLU:OE2    | 15:N:50:LEU:HD11   | 2.19                     | 0.42              |
| 16:X:3:ILE:HG23    | 16:X:7:LEU:HD12    | 1.94                     | 0.42              |
| 1:A:47:CYS:SG      | 1:A:114:LEU:HD22   | 2.59                     | 0.42              |
| 17:A:401:CLA:H202  | 17:A:401:CLA:H161  | 1.76                     | 0.42              |
| 2:B:381:ILE:HG22   | 2:B:382:PRO:O      | 2.20                     | 0.42              |
| 17:C:503:CLA:H202  | 17:C:503:CLA:H162  | 1.82                     | 0.42              |
| 17:D:404:CLA:H61   | 17:D:404:CLA:H41   | 1.62                     | 0.42              |
| 6:F:24:HIS:NE2     | 29:F:101:HEM:C1D   | 2.87                     | 0.42              |
| 23:L:101:SQD:O9    | 10:l:5007:ARG:NH1  | 2.52                     | 0.42              |
| 13:Z:53:VAL:HA     | 13:Z:57:LEU:HD13   | 2.00                     | 0.42              |
| 17:a:5404:CLA:H112 | 17:a:5404:CLA:H91  | 1.84                     | 0.42              |
| 2:b:5256:MET:HG3   | 2:b:5451:PHE:CD1   | 2.54                     | 0.42              |
| 3:c:5315:MET:O     | 3:c:5318:LEU:HB3   | 2.19                     | 0.42              |
| 17:c:5503:CLA:H161 | 17:c:5503:CLA:H122 | 1.67                     | 0.42              |
| 4:d:5026:ARG:CD    | 6:f:5018:VAL:HG21  | 2.50                     | 0.42              |
| 25:l:5101:MGE:H263 | 25:l:5101:MGE:H231 | 1.82                     | 0.42              |
| 13:z:5016:SER:O    | 13:z:5020:VAL:HG23 | 2.20                     | 0.42              |
| 15:n:27:THR:N      | 15:n:67:LYS:HG2    | 2.35                     | 0.42              |
| 15:N:56:ASN:HB3    | 15:N:59:ALA:HB3    | 2.01                     | 0.42              |
| 1:A:153:SER:O      | 1:A:157:VAL:HG12   | 2.19                     | 0.42              |
| 1:A:224:ILE:HD11   | 1:A:247:ASN:OD1    | 2.20                     | 0.42              |
| 2:B:137:LYS:HE3    | 2:B:217:ILE:HG23   | 2.02                     | 0.42              |
| 2:B:360:PRO:HG2    | 4:D:339:PHE:HZ     | 1.84                     | 0.42              |
| 17:B:603:CLA:O1D   | 17:B:603:CLA:H2A   | 2.18                     | 0.42              |
| 4:D:23:LYS:NZ      | 4:D:32:TRP:HE1     | 2.17                     | 0.42              |
| 13:Z:16:SER:O      | 13:Z:20:VAL:HG23   | 2.20                     | 0.42              |
| 3:c:5408:GLY:N     | 3:c:5418:ASN:HA    | 2.35                     | 0.42              |
| 17:d:5403:CLA:H61  | 17:d:5403:CLA:H41  | 1.62                     | 0.42              |
| 12:t:5018:PHE:HB2  | 20:t:5102:BCR:HC8  | 2.00                     | 0.42              |
| 15:n:56:ASN:HB3    | 15:n:59:ALA:HB3    | 2.01                     | 0.42              |
| 1:A:97:TRP:CG      | 8:I:5:LYS:HB2      | 2.55                     | 0.42              |
| 1:A:159:LEU:HD23   | 26:A:413:DGD:HAT1  | 2.00                     | 0.42              |
| 2:B:102:VAL:HG12   | 17:B:606:CLA:H91   | 2.01                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:119:ASP:OD1   | 2:B:119:ASP:N     | 2.51                     | 0.42              |
| 3:C:291:TRP:HD1   | 3:C:292:PHE:CE2   | 2.37                     | 0.42              |
| 3:C:422:PRO:HA    | 3:C:425:TRP:HD1   | 1.85                     | 0.42              |
| 17:C:513:CLA:H2A  | 17:C:513:CLA:HED3 | 2.02                     | 0.42              |
| 17:D:404:CLA:H162 | 17:D:404:CLA:H202 | 1.73                     | 0.42              |
| 1:a:5027:ARG:NH2  | 12:t:5024:ARG:HE  | 2.17                     | 0.42              |
| 17:a:5404:CLA:H2A | 17:a:5404:CLA:CED | 2.49                     | 0.42              |
| 2:b:5058:GLN:HG3  | 2:b:5060:MET:HE2  | 2.01                     | 0.42              |
| 2:b:5119:ASP:N    | 2:b:5119:ASP:OD1  | 2.50                     | 0.42              |
| 3:c:5349:ILE:HD11 | 3:c:5375:LEU:O    | 2.19                     | 0.42              |
| 4:d:5014:TRP:CE2  | 16:x:29:ILE:CD1   | 3.03                     | 0.42              |
| 4:d:5048:TRP:CD1  | 18:d:5402:PHO:H13 | 2.54                     | 0.42              |
| 15:n:72:PHE:CD2   | 15:n:76:ARG:CZ    | 3.02                     | 0.42              |
| 1:A:77:ILE:HD12   | 1:A:77:ILE:H      | 1.85                     | 0.42              |
| 1:A:280:VAL:O     | 1:A:283:VAL:N     | 2.51                     | 0.42              |
| 2:B:172:TYR:HE1   | 2:B:283:GLU:OE1   | 2.02                     | 0.42              |
| 2:B:174:LEU:HD11  | 2:B:309:LEU:HD13  | 2.02                     | 0.42              |
| 3:C:97:TRP:HE1    | 3:C:178:LYS:HZ1   | 1.68                     | 0.42              |
| 3:C:106:VAL:HG23  | 3:C:107:ASP:N     | 2.34                     | 0.42              |
| 3:C:157:MET:HE2   | 17:C:507:CLA:HHD  | 2.01                     | 0.42              |
| 17:C:503:CLA:H62  | 17:C:503:CLA:H41  | 1.90                     | 0.42              |
| 17:C:511:CLA:H61  | 17:C:511:CLA:H92  | 1.74                     | 0.42              |
| 1:a:5061:ASP:HB3  | 1:a:5063:ILE:HG12 | 2.01                     | 0.42              |
| 1:a:5119:PHE:O    | 1:a:5123:ALA:N    | 2.45                     | 0.42              |
| 1:a:5125:CYS:SG   | 17:c:5505:CLA:H91 | 2.59                     | 0.42              |
| 1:a:5161:TYR:N    | 1:a:5162:PRO:HD2  | 2.35                     | 0.42              |
| 2:b:5010:THR:O    | 2:b:5013:ILE:N    | 2.50                     | 0.42              |
| 2:b:5172:TYR:HE1  | 2:b:5283:GLU:OE1  | 2.02                     | 0.42              |
| 3:c:5399:ALA:O    | 3:c:5400:PRO:C    | 2.63                     | 0.42              |
| 17:k:5501:CLA:H61 | 17:k:5501:CLA:H92 | 1.74                     | 0.42              |
| 1:A:136:ARG:NH2   | 8:I:27:ASP:OD1    | 2.52                     | 0.42              |
| 2:B:148:LEU:HB2   | 2:B:210:ILE:HD11  | 2.01                     | 0.42              |
| 2:B:368:VAL:CG1   | 2:B:381:ILE:HD12  | 2.49                     | 0.42              |
| 17:C:510:CLA:H2   | 17:C:510:CLA:H61  | 1.63                     | 0.42              |
| 17:C:513:CLA:CAB  | 20:C:515:BCR:H24C | 2.50                     | 0.42              |
| 20:D:407:BCR:H15C | 20:D:407:BCR:H351 | 1.90                     | 0.42              |
| 25:D:410:MGE:H5A1 | 25:D:410:MGE:H2A2 | 1.78                     | 0.42              |
| 1:a:5093:PHE:HA   | 1:a:5113:GLN:NE2  | 2.35                     | 0.42              |
| 2:b:5074:SER:OG   | 2:b:5075:TRP:N    | 2.52                     | 0.42              |
| 2:b:5257:TRP:O    | 2:b:5271:THR:OG1  | 2.32                     | 0.42              |
| 2:b:5461:LEU:HD23 | 2:b:5461:LEU:HA   | 1.87                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 17:b:5612:CLA:HBA1 | 17:b:5612:CLA:H3A  | 1.55                     | 0.42              |
| 3:c:5088:LEU:O     | 3:c:5091:HIS:N     | 2.52                     | 0.42              |
| 3:c:5189:TRP:HB3   | 15:n:76:ARG:CZ     | 2.50                     | 0.42              |
| 4:d:5195:PRO:HD3   | 10:l:5034:TYR:CZ   | 2.55                     | 0.42              |
| 15:n:86:SER:C      | 15:n:89:THR:HG1    | 2.25                     | 0.42              |
| 1:A:135:TYR:CZ     | 8:I:31:ASN:HB3     | 2.55                     | 0.42              |
| 1:A:214:MET:O      | 1:A:217:SER:N      | 2.52                     | 0.42              |
| 1:A:308:ASP:OD2    | 1:A:312:ASN:HB2    | 2.20                     | 0.42              |
| 1:A:317:TRP:HH2    | 4:D:77:ALA:HB3     | 1.85                     | 0.42              |
| 17:A:401:CLA:C1B   | 17:D:404:CLA:HBB1  | 2.49                     | 0.42              |
| 17:B:606:CLA:H41   | 17:B:606:CLA:H62   | 1.44                     | 0.42              |
| 17:B:607:CLA:O2D   | 17:B:607:CLA:H2A   | 2.20                     | 0.42              |
| 17:B:610:CLA:H8    | 17:B:610:CLA:H51   | 1.66                     | 0.42              |
| 17:B:614:CLA:H92   | 17:B:614:CLA:H62   | 1.85                     | 0.42              |
| 17:C:512:CLA:H2A   | 17:C:512:CLA:CED   | 2.50                     | 0.42              |
| 4:D:48:TRP:CD1     | 18:D:402:PHO:H13   | 2.54                     | 0.42              |
| 4:D:279:LEU:HA     | 4:D:279:LEU:HD23   | 1.85                     | 0.42              |
| 25:D:410:MGE:H2    | 25:D:410:MGE:H4    | 1.63                     | 0.42              |
| 2:b:5250:PHE:CD2   | 17:b:5602:CLA:H152 | 2.55                     | 0.42              |
| 17:b:5616:CLA:H141 | 17:b:5616:CLA:H161 | 1.84                     | 0.42              |
| 3:c:5269:GLU:O     | 3:c:5272:LEU:N     | 2.53                     | 0.42              |
| 25:d:5409:MGE:H6B2 | 25:d:5409:MGE:H9B1 | 1.75                     | 0.42              |
| 7:h:5007:LEU:O     | 7:h:5010:ILE:N     | 2.53                     | 0.42              |
| 1:A:286:THR:HB     | 17:A:401:CLA:O1D   | 2.20                     | 0.42              |
| 1:A:300:PHE:CD2    | 3:C:404:LEU:HB2    | 2.55                     | 0.42              |
| 25:A:412:MGE:H211  | 10:L:22:LEU:HG     | 2.02                     | 0.42              |
| 2:B:47:PRO:HB3     | 2:B:78:TRP:CD2     | 2.54                     | 0.42              |
| 3:C:229:ASN:ND2    | 15:N:77:ARG:HB2    | 2.34                     | 0.42              |
| 3:C:457:LYS:HE2    | 4:D:224:GLN:HE21   | 1.85                     | 0.42              |
| 17:C:511:CLA:H72   | 14:Y:35:ILE:CG2    | 2.46                     | 0.42              |
| 4:D:304:ARG:HH11   | 4:D:307:GLU:HB2    | 1.84                     | 0.42              |
| 12:T:1:MET:O       | 12:T:4:ILE:HG22    | 2.20                     | 0.42              |
| 1:a:5140:ARG:HD3   | 1:a:5142:TRP:NE1   | 2.35                     | 0.42              |
| 2:b:5057:ARG:HG2   | 2:b:5331:ASN:ND2   | 2.35                     | 0.42              |
| 2:b:5174:LEU:HD11  | 2:b:5309:LEU:HD13  | 2.02                     | 0.42              |
| 2:b:5453:PHE:HE2   | 25:b:5620:MGE:H102 | 1.85                     | 0.42              |
| 17:b:5605:CLA:H141 | 17:b:5610:CLA:HMA1 | 2.02                     | 0.42              |
| 3:c:5157:MET:HE2   | 17:c:5507:CLA:HHD  | 2.01                     | 0.42              |
| 3:c:5388:GLN:NE2   | 15:n:95:ASN:ND2    | 2.66                     | 0.42              |
| 20:h:5101:BCR:H20C | 20:h:5101:BCR:H361 | 1.89                     | 0.42              |
| 14:Y:22:LEU:HA     | 14:Y:25:ILE:HB     | 2.02                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:X:23:LEU:HA     | 16:X:23:LEU:HD22   | 1.83                     | 0.42              |
| 1:A:40:THR:HG23    | 1:A:41:LEU:N       | 2.35                     | 0.41              |
| 2:B:61:PHE:HB2     | 17:B:607:CLA:HMA3  | 2.02                     | 0.41              |
| 2:B:453:PHE:HE2    | 25:B:619:MGE:H102  | 1.85                     | 0.41              |
| 17:B:612:CLA:H93   | 17:B:612:CLA:H62   | 1.80                     | 0.41              |
| 17:B:612:CLA:H2    | 17:B:612:CLA:H62   | 1.32                     | 0.41              |
| 17:B:613:CLA:H202  | 17:B:613:CLA:H162  | 1.75                     | 0.41              |
| 17:B:615:CLA:H13   | 17:B:615:CLA:H101  | 1.92                     | 0.41              |
| 25:B:619:MGE:H5B2  | 11:M:10:ALA:HB2    | 2.02                     | 0.41              |
| 3:C:76:ILE:HB      | 3:C:84:GLN:NE2     | 2.35                     | 0.41              |
| 17:C:507:CLA:HBD   | 17:C:507:CLA:HAA2  | 2.02                     | 0.41              |
| 4:D:63:LEU:HD12    | 4:D:63:LEU:O       | 2.20                     | 0.41              |
| 7:H:7:LEU:O        | 7:H:10:ILE:N       | 2.53                     | 0.41              |
| 1:a:5215:HIS:NE2   | 24:a:5412:BCT:O2   | 2.52                     | 0.41              |
| 2:b:5073:GLY:HA2   | 2:b:5078:TRP:O     | 2.19                     | 0.41              |
| 2:b:5148:LEU:HB2   | 2:b:5210:ILE:HD11  | 2.01                     | 0.41              |
| 2:b:5151:PHE:HB2   | 2:b:5206:GLY:HA3   | 2.02                     | 0.41              |
| 4:d:5085:MET:CE    | 4:d:5090:LEU:HD21  | 2.50                     | 0.41              |
| 16:x:36:LYS:HG2    | 16:x:36:LYS:HZ2    | 1.78                     | 0.41              |
| 1:A:319:ASP:HA     | 1:A:322:ASN:HB2    | 2.01                     | 0.41              |
| 17:A:405:CLA:C4A   | 17:A:405:CLA:HBA1  | 2.47                     | 0.41              |
| 24:A:411:BCT:O3    | 4:D:214:HIS:NE2    | 2.53                     | 0.41              |
| 2:B:250:PHE:CD2    | 17:B:602:CLA:H152  | 2.55                     | 0.41              |
| 17:B:608:CLA:C1A   | 17:B:608:CLA:CGA   | 2.96                     | 0.41              |
| 3:C:408:GLY:N      | 3:C:418:ASN:HA     | 2.35                     | 0.41              |
| 17:C:501:CLA:C4D   | 17:C:503:CLA:H51   | 2.51                     | 0.41              |
| 17:C:503:CLA:HBA1  | 17:C:503:CLA:HBD   | 2.01                     | 0.41              |
| 4:D:24:ARG:HG2     | 4:D:25:ASP:N       | 2.35                     | 0.41              |
| 4:D:193:LEU:O      | 10:L:34:TYR:OH     | 2.36                     | 0.41              |
| 4:D:232:PHE:CE2    | 23:D:403:SQD:H461  | 2.54                     | 0.41              |
| 20:H:101:BCR:H371  | 20:H:101:BCR:H24C  | 1.75                     | 0.41              |
| 1:a:5059:ASP:OD2   | 1:a:5062:GLY:HA2   | 2.20                     | 0.41              |
| 1:a:5172:MET:HE1   | 17:a:5403:CLA:HMC2 | 2.02                     | 0.41              |
| 1:a:5308:ASP:OD2   | 1:a:5312:ASN:HB2   | 2.20                     | 0.41              |
| 2:b:5215:PHE:CD2   | 2:b:5216:HIS:HD2   | 2.38                     | 0.41              |
| 3:c:5291:TRP:HD1   | 3:c:5292:PHE:CE2   | 2.37                     | 0.41              |
| 4:d:5319:LEU:HD23  | 4:d:5319:LEU:HA    | 1.88                     | 0.41              |
| 25:d:5410:MGE:H2   | 25:d:5410:MGE:H4   | 1.63                     | 0.41              |
| 10:l:5008:GLN:HE21 | 10:l:5009:PRO:HD2  | 1.83                     | 0.41              |
| 15:N:27:THR:N      | 15:N:67:LYS:HG2    | 2.35                     | 0.41              |
| 1:A:172:MET:HE1    | 17:A:402:CLA:HMC2  | 2.02                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:73:GLY:HA2     | 2:B:78:TRP:O       | 2.19                     | 0.41              |
| 20:B:617:BCR:H343  | 20:t:5102:BCR:H382 | 2.01                     | 0.41              |
| 3:C:269:GLU:O      | 3:C:272:LEU:N      | 2.53                     | 0.41              |
| 4:D:176:ALA:HA     | 4:D:179:PHE:CD2    | 2.45                     | 0.41              |
| 25:D:410:MGE:O6D   | 10:L:15:THR:HG21   | 2.20                     | 0.41              |
| 26:D:411:DGD:C1A   | 7:H:50:ASN:HD21    | 2.34                     | 0.41              |
| 1:a:5040:THR:HG23  | 1:a:5041:LEU:N     | 2.35                     | 0.41              |
| 1:a:5224:ILE:HD11  | 1:a:5247:ASN:OD1   | 2.20                     | 0.41              |
| 2:b:5137:LYS:HE3   | 2:b:5217:ILE:HG23  | 2.02                     | 0.41              |
| 17:b:5610:CLA:H101 | 17:b:5615:CLA:HBA2 | 2.02                     | 0.41              |
| 17:b:5613:CLA:H202 | 17:b:5613:CLA:H162 | 1.75                     | 0.41              |
| 20:b:5619:BCR:H15C | 20:b:5619:BCR:H351 | 1.87                     | 0.41              |
| 3:c:5099:VAL:HG23  | 3:c:5100:GLY:N     | 2.35                     | 0.41              |
| 3:c:5218:PHE:HE2   | 25:c:5517:MGE:O1A  | 2.04                     | 0.41              |
| 4:d:5125:PHE:CE2   | 18:d:5402:PHO:HBD  | 2.54                     | 0.41              |
| 10:l:5022:LEU:HG   | 25:l:5101:MGE:H211 | 2.01                     | 0.41              |
| 13:z:5023:VAL:HB   | 13:z:5024:PRO:HD3  | 2.01                     | 0.41              |
| 15:N:33:PHE:CG     | 15:N:81:LEU:HD11   | 2.55                     | 0.41              |
| 15:N:109:LEU:C     | 15:N:114:LYS:HE3   | 2.45                     | 0.41              |
| 15:N:125:GLU:HA    | 15:N:128:LEU:HB3   | 2.02                     | 0.41              |
| 16:X:4:THR:H       | 16:X:7:LEU:HB3     | 1.85                     | 0.41              |
| 2:B:125:ASP:OD1    | 2:B:128:THR:OG1    | 2.31                     | 0.41              |
| 2:B:215:PHE:CD2    | 2:B:216:HIS:HD2    | 2.38                     | 0.41              |
| 2:B:386:ALA:HB1    | 4:D:344:GLU:HB2    | 2.02                     | 0.41              |
| 17:B:607:CLA:H62   | 17:B:607:CLA:H92   | 1.61                     | 0.41              |
| 17:B:613:CLA:H2A   | 17:B:613:CLA:O2A   | 2.19                     | 0.41              |
| 3:C:213:LEU:HB3    | 3:C:224:ILE:HD11   | 2.02                     | 0.41              |
| 25:C:519:MGE:H5A1  | 25:C:519:MGE:H8A2  | 1.95                     | 0.41              |
| 4:D:203:GLY:O      | 4:D:207:GLY:N      | 2.46                     | 0.41              |
| 20:a:5408:BCR:H371 | 20:a:5408:BCR:H24C | 1.83                     | 0.41              |
| 2:b:5166:MET:HG2   | 2:b:5167:TRP:O     | 2.20                     | 0.41              |
| 2:b:5201:HIS:O     | 2:b:5205:ALA:N     | 2.43                     | 0.41              |
| 2:b:5311:PHE:HA    | 2:b:5430:PHE:CZ    | 2.55                     | 0.41              |
| 2:b:5474:LEU:HD13  | 4:d:5134:ARG:HH21  | 1.84                     | 0.41              |
| 3:c:5224:ILE:HD12  | 3:c:5224:ILE:HG23  | 1.82                     | 0.41              |
| 3:c:5226:SER:O     | 3:c:5227:VAL:C     | 2.62                     | 0.41              |
| 3:c:5276:LEU:HD23  | 3:c:5276:LEU:HA    | 1.76                     | 0.41              |
| 17:c:5501:CLA:H72  | 17:c:5501:CLA:H111 | 1.74                     | 0.41              |
| 15:n:27:THR:OG1    | 15:n:70:ASP:OD2    | 2.36                     | 0.41              |
| 15:n:33:PHE:CG     | 15:n:81:LEU:HD11   | 2.55                     | 0.41              |
| 15:n:125:GLU:HA    | 15:n:128:LEU:HB3   | 2.02                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:y:18:VAL:N      | 14:y:21:GLN:CB     | 2.82                     | 0.41              |
| 1:A:59:ASP:OD2     | 1:A:62:GLY:HA2     | 2.20                     | 0.41              |
| 1:A:93:PHE:HA      | 1:A:113:GLN:NE2    | 2.34                     | 0.41              |
| 1:A:97:TRP:HA      | 8:I:1:MET:HE3      | 2.02                     | 0.41              |
| 25:A:412:MGE:H221  | 19:D:406:PQ9:H262  | 2.01                     | 0.41              |
| 2:B:57:ARG:HG2     | 2:B:331:ASN:ND2    | 2.35                     | 0.41              |
| 2:B:166:MET:HG2    | 2:B:167:TRP:O      | 2.20                     | 0.41              |
| 4:D:158:LEU:C      | 4:D:161:PRO:HD2    | 2.46                     | 0.41              |
| 4:D:180:ARG:O      | 4:D:184:PHE:HB2    | 2.21                     | 0.41              |
| 9:K:31:LEU:HB3     | 20:Y:101:BCR:C14   | 2.51                     | 0.41              |
| 22:M:101:LMT:H11   | 22:M:101:LMT:H42   | 1.77                     | 0.41              |
| 3:c:5213:LEU:HB3   | 3:c:5224:ILE:HD11  | 2.02                     | 0.41              |
| 17:c:5501:CLA:C4D  | 17:c:5503:CLA:H51  | 2.51                     | 0.41              |
| 4:d:5180:ARG:O     | 4:d:5184:PHE:HB2   | 2.21                     | 0.41              |
| 25:A:412:MGE:H2A2  | 2:B:5:TRP:CZ2      | 2.56                     | 0.41              |
| 2:B:311:PHE:HA     | 2:B:430:PHE:CZ     | 2.55                     | 0.41              |
| 17:B:605:CLA:H141  | 17:B:610:CLA:HMA1  | 2.02                     | 0.41              |
| 3:C:88:LEU:O       | 3:C:91:HIS:N       | 2.52                     | 0.41              |
| 17:C:513:CLA:H2A   | 17:C:513:CLA:CED   | 2.50                     | 0.41              |
| 1:a:5153:SER:O     | 1:a:5157:VAL:HG12  | 2.20                     | 0.41              |
| 1:a:5286:THR:HB    | 17:a:5402:CLA:O1D  | 2.20                     | 0.41              |
| 1:a:5286:THR:O     | 1:a:5289:GLY:N     | 2.54                     | 0.41              |
| 2:b:5061:PHE:HB2   | 17:b:5607:CLA:HMA3 | 2.02                     | 0.41              |
| 2:b:5183:PRO:HB3   | 2:b:5199:VAL:CG1   | 2.51                     | 0.41              |
| 2:b:5362:PHE:HE2   | 4:d:5334:GLN:HE22  | 1.69                     | 0.41              |
| 2:b:5381:ILE:HG22  | 2:b:5382:PRO:O     | 2.20                     | 0.41              |
| 17:b:5607:CLA:O2D  | 17:b:5607:CLA:H2A  | 2.20                     | 0.41              |
| 17:b:5608:CLA:HBB2 | 4:d:5123:ILE:HG12  | 2.02                     | 0.41              |
| 3:c:5076:ILE:HB    | 3:c:5084:GLN:NE2   | 2.35                     | 0.41              |
| 4:d:5063:LEU:O     | 4:d:5063:LEU:HD12  | 2.20                     | 0.41              |
| 4:d:5152:VAL:HG21  | 4:d:5279:LEU:HD22  | 2.03                     | 0.41              |
| 4:d:5279:LEU:HD11  | 18:d:5402:PHO:HAC2 | 2.01                     | 0.41              |
| 9:k:5043:VAL:CG2   | 14:y:46:LEU:HD13   | 2.50                     | 0.41              |
| 1:A:193:LEU:HD21   | 17:A:401:CLA:HMC2  | 2.01                     | 0.41              |
| 17:B:607:CLA:H3A   | 17:B:607:CLA:HBA2  | 1.51                     | 0.41              |
| 3:C:276:LEU:HD21   | 17:C:508:CLA:CBB   | 2.51                     | 0.41              |
| 4:D:85:MET:CE      | 4:D:90:LEU:HD21    | 2.51                     | 0.41              |
| 17:D:405:CLA:C4A   | 17:D:405:CLA:HBA2  | 2.50                     | 0.41              |
| 1:a:5267:ASN:HB3   | 1:a:5270:SER:HB3   | 2.03                     | 0.41              |
| 2:b:5077:GLY:C     | 2:b:5086:ILE:CD1   | 2.94                     | 0.41              |
| 2:b:5198:VAL:O     | 2:b:5201:HIS:HB3   | 2.20                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 17:b:5614:CLA:H43  | 25:m:5101:MGE:H6A2 | 2.02                     | 0.41              |
| 17:c:5512:CLA:H2A  | 17:c:5512:CLA:CED  | 2.50                     | 0.41              |
| 17:c:5512:CLA:H2A  | 17:c:5512:CLA:HED3 | 2.02                     | 0.41              |
| 4:d:5158:LEU:C     | 4:d:5161:PRO:HD2   | 2.45                     | 0.41              |
| 20:k:5502:BCR:H15C | 20:k:5502:BCR:H351 | 1.91                     | 0.41              |
| 15:n:50:LEU:H      | 15:n:57:LYS:HZ2    | 1.69                     | 0.41              |
| 15:n:73:ALA:HA     | 15:n:76:ARG:NH2    | 2.35                     | 0.41              |
| 1:A:161:TYR:N      | 1:A:162:PRO:HD2    | 2.35                     | 0.41              |
| 1:A:272:HIS:CG     | 4:D:218:VAL:HG11   | 2.55                     | 0.41              |
| 1:A:286:THR:O      | 1:A:289:GLY:N      | 2.54                     | 0.41              |
| 17:A:405:CLA:HBA1  | 17:A:405:CLA:H3A   | 1.64                     | 0.41              |
| 25:A:412:MGE:H8B1  | 4:D:270:PHE:HE1    | 1.86                     | 0.41              |
| 2:B:41:GLU:OE1     | 2:B:60:MET:HA      | 2.21                     | 0.41              |
| 2:B:135:LEU:HD23   | 2:B:237:VAL:HG23   | 2.03                     | 0.41              |
| 20:B:617:BCR:H20C  | 20:B:617:BCR:H361  | 1.81                     | 0.41              |
| 3:C:399:ALA:O      | 3:C:400:PRO:C      | 2.63                     | 0.41              |
| 17:C:501:CLA:H111  | 17:C:501:CLA:H72   | 1.74                     | 0.41              |
| 4:D:89:LEU:HD13    | 7:H:50:ASN:ND2     | 2.35                     | 0.41              |
| 1:a:5143:ILE:H     | 4:d:5220:ASN:HD21  | 1.67                     | 0.41              |
| 17:a:5402:CLA:O1D  | 17:a:5402:CLA:H2A  | 2.21                     | 0.41              |
| 2:b:5069:LEU:HA    | 2:b:5069:LEU:HD23  | 1.87                     | 0.41              |
| 3:c:5199:ILE:HD12  | 3:c:5234:VAL:HG21  | 2.03                     | 0.41              |
| 3:c:5276:LEU:HD21  | 17:c:5508:CLA:CBB  | 2.51                     | 0.41              |
| 3:c:5461:ARG:HH11  | 4:d:5223:PHE:CB    | 2.33                     | 0.41              |
| 17:c:5511:CLA:H2A  | 17:c:5511:CLA:CED  | 2.50                     | 0.41              |
| 4:d:5072:ASN:ND2   | 4:d:5074:LEU:H     | 2.19                     | 0.41              |
| 4:d:5330:ALA:HB3   | 4:d:5331:PRO:HD3   | 2.03                     | 0.41              |
| 14:Y:33:PRO:O      | 14:Y:34:MET:C      | 2.63                     | 0.41              |
| 1:A:61:ASP:HB3     | 1:A:63:ILE:HG12    | 2.01                     | 0.41              |
| 1:A:140:ARG:HD3    | 1:A:142:TRP:NE1    | 2.35                     | 0.41              |
| 1:A:157:VAL:HG21   | 1:A:172:MET:HE3    | 2.03                     | 0.41              |
| 2:B:193:TYR:HA     | 2:B:261:ALA:HB2    | 2.03                     | 0.41              |
| 2:B:383:PHE:CD2    | 2:B:384:ARG:HG2    | 2.55                     | 0.41              |
| 17:B:610:CLA:H101  | 17:B:615:CLA:HBA2  | 2.02                     | 0.41              |
| 3:C:99:VAL:HG23    | 3:C:100:GLY:N      | 2.35                     | 0.41              |
| 3:C:199:ILE:HD12   | 3:C:234:VAL:HG21   | 2.03                     | 0.41              |
| 3:C:298:PRO:HD2    | 3:C:302:TYR:CE2    | 2.56                     | 0.41              |
| 4:D:213:ILE:HD11   | 4:D:253:TRP:CH2    | 2.56                     | 0.41              |
| 4:D:218:VAL:HG23   | 4:D:244:TYR:CD1    | 2.56                     | 0.41              |
| 4:D:288:GLY:O      | 4:D:293:LEU:HB2    | 2.21                     | 0.41              |
| 5:E:63:ILE:CG2     | 5:E:65:LEU:HB2     | 2.51                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:H:101:BCR:H20C  | 20:H:101:BCR:H361  | 1.89                     | 0.41              |
| 9:K:20:PRO:CB      | 14:Y:24:MET:HB2    | 2.48                     | 0.41              |
| 12:T:18:PHE:CB     | 20:T:102:BCR:H10C  | 2.50                     | 0.41              |
| 1:a:5142:TRP:CZ3   | 3:c:5443:TRP:CD1   | 3.09                     | 0.41              |
| 1:a:5172:MET:HE2   | 1:a:5179:THR:HG23  | 2.03                     | 0.41              |
| 1:a:5187:GLN:HE22  | 1:a:5191:ASN:HA    | 1.84                     | 0.41              |
| 1:a:5264:SER:OG    | 19:a:5407:PQ9:O4   | 2.29                     | 0.41              |
| 1:a:5302:PHE:HE2   | 4:d:5072:ASN:HD22  | 1.69                     | 0.41              |
| 17:a:5403:CLA:HED2 | 4:d:5198:MET:SD    | 2.61                     | 0.41              |
| 17:b:5601:CLA:O1D  | 7:h:5041:PHE:HE1   | 2.04                     | 0.41              |
| 17:b:5602:CLA:H92  | 7:h:5046:LEU:HD22  | 2.01                     | 0.41              |
| 17:b:5611:CLA:H161 | 17:b:5611:CLA:H202 | 1.81                     | 0.41              |
| 17:b:5613:CLA:H2A  | 17:b:5613:CLA:O2A  | 2.19                     | 0.41              |
| 3:c:5246:ALA:O     | 3:c:5250:TRP:N     | 2.47                     | 0.41              |
| 3:c:5270:ALA:HB1   | 3:c:5274:TYR:CE2   | 2.56                     | 0.41              |
| 17:c:5505:CLA:H152 | 17:c:5505:CLA:H18  | 1.68                     | 0.41              |
| 4:d:5188:PHE:CE1   | 4:d:5326:ARG:HG2   | 2.56                     | 0.41              |
| 1:A:92:HIS:CE1     | 3:C:220:GLY:HA3    | 2.55                     | 0.41              |
| 1:A:97:TRP:CE2     | 8:I:5:LYS:HG3      | 2.56                     | 0.41              |
| 1:A:225:ARG:HB2    | 2:B:481:GLY:HA3    | 2.02                     | 0.41              |
| 1:A:286:THR:HB     | 17:A:401:CLA:HED2  | 2.03                     | 0.41              |
| 22:A:409:LMT:O6B   | 22:A:409:LMT:O4'   | 2.22                     | 0.41              |
| 2:B:325:PHE:O      | 2:B:327:THR:HG23   | 2.21                     | 0.41              |
| 3:C:78:GLU:OE1     | 3:C:78:GLU:N       | 2.49                     | 0.41              |
| 3:C:139:THR:HG22   | 3:C:141:GLU:H      | 1.87                     | 0.41              |
| 3:C:270:ALA:HB1    | 3:C:274:TYR:CE2    | 2.56                     | 0.41              |
| 4:D:68:LEU:HA      | 6:F:40:MET:SD      | 2.61                     | 0.41              |
| 4:D:330:ALA:HB3    | 4:D:331:PRO:HD3    | 2.03                     | 0.41              |
| 1:a:5133:LEU:HA    | 1:a:5133:LEU:HD12  | 1.89                     | 0.41              |
| 2:b:5041:GLU:OE1   | 2:b:5060:MET:HA    | 2.21                     | 0.41              |
| 20:Y:101:BCR:H24C  | 20:Y:101:BCR:H371  | 1.93                     | 0.41              |
| 16:x:31:ILE:HD12   | 16:x:31:ILE:HA     | 1.83                     | 0.41              |
| 1:A:110:GLY:N      | 1:A:111:PRO:HD2    | 2.36                     | 0.40              |
| 1:A:255:PHE:CD2    | 19:A:406:PQ9:H3    | 2.56                     | 0.40              |
| 1:A:300:PHE:HD2    | 3:C:404:LEU:HB2    | 1.86                     | 0.40              |
| 17:A:405:CLA:H52   | 8:I:9:TYR:HD1      | 1.86                     | 0.40              |
| 2:B:183:PRO:HB3    | 2:B:199:VAL:CG1    | 2.51                     | 0.40              |
| 3:C:408:GLY:H      | 3:C:418:ASN:HA     | 1.87                     | 0.40              |
| 17:C:511:CLA:O2D   | 17:C:511:CLA:H2A   | 2.21                     | 0.40              |
| 10:L:8:GLN:HE21    | 10:L:9:PRO:HD2     | 1.83                     | 0.40              |
| 10:L:14:ARG:NH2    | 23:L:101:SQD:C7    | 2.84                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:a:5110:GLY:N     | 1:a:5111:PRO:HD2   | 2.36                     | 0.40              |
| 2:b:5015:ASP:O     | 2:b:5016:PRO:C     | 2.64                     | 0.40              |
| 20:b:5618:BCR:H351 | 20:b:5618:BCR:H15C | 1.81                     | 0.40              |
| 20:b:5619:BCR:H11C | 20:b:5619:BCR:H341 | 1.92                     | 0.40              |
| 4:d:5288:GLY:O     | 4:d:5293:LEU:HB2   | 2.21                     | 0.40              |
| 25:l:5101:MGE:H122 | 11:m:5018:PRO:HG3  | 2.04                     | 0.40              |
| 13:z:5057:LEU:O    | 13:z:5061:VAL:HG23 | 2.20                     | 0.40              |
| 14:Y:39:LEU:HD22   | 14:Y:39:LEU:HA     | 1.86                     | 0.40              |
| 15:n:49:ALA:O      | 15:n:50:LEU:HD12   | 2.21                     | 0.40              |
| 16:x:21:LEU:HD23   | 16:x:21:LEU:O      | 2.18                     | 0.40              |
| 1:A:206:PHE:O      | 1:A:209:ALA:N      | 2.55                     | 0.40              |
| 2:B:177:SER:HB2    | 2:B:179:GLN:HE22   | 1.86                     | 0.40              |
| 3:C:190:ALA:HB3    | 3:C:194:GLY:H      | 1.86                     | 0.40              |
| 3:C:307:PRO:HA     | 3:C:358:PHE:CE2    | 2.56                     | 0.40              |
| 3:C:466:VAL:HG21   | 4:D:248:THR:HG23   | 2.03                     | 0.40              |
| 20:T:102:BCR:H15C  | 20:T:102:BCR:H351  | 1.85                     | 0.40              |
| 2:b:5024:LEU:HD23  | 2:b:5024:LEU:HA    | 1.94                     | 0.40              |
| 2:b:5331:ASN:HB3   | 2:b:5336:ILE:HD13  | 2.03                     | 0.40              |
| 17:b:5613:CLA:H62  | 17:b:5613:CLA:H101 | 1.68                     | 0.40              |
| 3:c:5199:ILE:HD13  | 3:c:5231:GLU:HG2   | 2.04                     | 0.40              |
| 17:c:5505:CLA:O1D  | 17:c:5505:CLA:H2A  | 2.21                     | 0.40              |
| 4:d:5213:ILE:HD11  | 4:d:5253:TRP:CH2   | 2.56                     | 0.40              |
| 17:k:5501:CLA:H2A  | 17:k:5501:CLA:O2D  | 2.21                     | 0.40              |
| 12:t:5001:MET:O    | 12:t:5004:ILE:HG22 | 2.20                     | 0.40              |
| 14:y:39:LEU:HD22   | 14:y:39:LEU:HA     | 1.66                     | 0.40              |
| 1:A:193:LEU:HD23   | 1:A:193:LEU:HA     | 1.89                     | 0.40              |
| 17:A:401:CLA:O1D   | 17:A:401:CLA:H2A   | 2.20                     | 0.40              |
| 2:B:124:ARG:HG2    | 2:B:131:PRO:HA     | 2.04                     | 0.40              |
| 2:B:151:PHE:HB2    | 2:B:206:GLY:HA3    | 2.02                     | 0.40              |
| 2:B:171:PRO:HD3    | 7:H:63:LYS:HD3     | 2.02                     | 0.40              |
| 2:B:381:ILE:HG12   | 2:B:392:PHE:CE1    | 2.56                     | 0.40              |
| 17:B:603:CLA:H203  | 17:B:609:CLA:H8    | 2.03                     | 0.40              |
| 3:C:294:ASN:ND2    | 3:C:299:SER:OG     | 2.54                     | 0.40              |
| 4:D:72:ASN:ND2     | 4:D:74:LEU:H       | 2.18                     | 0.40              |
| 13:Z:57:LEU:O      | 13:Z:61:VAL:HG23   | 2.20                     | 0.40              |
| 1:a:5255:PHE:CZ    | 19:a:5407:PQ9:H152 | 2.57                     | 0.40              |
| 2:b:5177:SER:HB2   | 2:b:5179:GLN:HE22  | 1.86                     | 0.40              |
| 2:b:5193:TYR:HA    | 2:b:5261:ALA:HB2   | 2.03                     | 0.40              |
| 2:b:5227:LYS:O     | 2:b:5230:ARG:NH1   | 2.54                     | 0.40              |
| 2:b:5381:ILE:HG12  | 2:b:5392:PHE:CE1   | 2.56                     | 0.40              |
| 3:c:5365:TRP:CD1   | 3:c:5365:TRP:H     | 2.40                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:c:5368:PRO:HB2   | 15:n:95:ASN:HD22   | 1.86                     | 0.40              |
| 3:c:5422:PRO:HA    | 3:c:5425:TRP:HD1   | 1.85                     | 0.40              |
| 4:d:5218:VAL:HG23  | 4:d:5244:TYR:CD1   | 2.56                     | 0.40              |
| 4:d:5279:LEU:HA    | 4:d:5279:LEU:HD23  | 1.85                     | 0.40              |
| 15:n:41:ILE:HG12   | 15:n:121:PHE:CD1   | 2.56                     | 0.40              |
| 15:n:109:LEU:O     | 15:n:114:LYS:HE3   | 2.21                     | 0.40              |
| 14:y:18:VAL:CA     | 14:y:21:GLN:HB2    | 2.52                     | 0.40              |
| 3:C:87:ILE:HG23    | 17:C:504:CLA:HMA3  | 2.04                     | 0.40              |
| 3:C:266:TRP:H      | 3:C:266:TRP:CD1    | 2.40                     | 0.40              |
| 7:H:40:VAL:CG2     | 16:X:14:LEU:HD11   | 2.52                     | 0.40              |
| 1:a:5092:HIS:HA    | 3:c:5219:GLY:HA3   | 2.02                     | 0.40              |
| 1:a:5143:ILE:N     | 4:d:5220:ASN:ND2   | 2.68                     | 0.40              |
| 1:a:5147:TYR:O     | 1:a:5150:PRO:HD2   | 2.22                     | 0.40              |
| 1:a:5157:VAL:HG21  | 1:a:5172:MET:HE3   | 2.03                     | 0.40              |
| 2:b:5327:THR:HG21  | 25:b:5620:MGE:H2B2 | 2.02                     | 0.40              |
| 2:b:5346:PHE:O     | 2:b:5354:LEU:N     | 2.48                     | 0.40              |
| 2:b:5440:ASP:OD1   | 2:b:5441:GLY:N     | 2.55                     | 0.40              |
| 17:b:5607:CLA:HBA2 | 17:b:5607:CLA:H3A  | 1.51                     | 0.40              |
| 3:c:5298:PRO:HD2   | 3:c:5302:TYR:CE2   | 2.56                     | 0.40              |
| 3:c:5408:GLY:H     | 3:c:5418:ASN:HA    | 1.87                     | 0.40              |
| 17:c:5503:CLA:H162 | 17:c:5503:CLA:H202 | 1.82                     | 0.40              |
| 15:N:49:ALA:O      | 15:N:50:LEU:HD12   | 2.21                     | 0.40              |
| 1:A:77:ILE:HD11    | 12:T:6:TYR:CD1     | 2.57                     | 0.40              |
| 1:A:187:GLN:HE22   | 1:A:191:ASN:HA     | 1.85                     | 0.40              |
| 1:A:255:PHE:CZ     | 19:A:406:PQ9:H152  | 2.57                     | 0.40              |
| 2:B:327:THR:HG21   | 25:B:619:MGE:H2B2  | 2.02                     | 0.40              |
| 2:B:331:ASN:HB3    | 2:B:336:ILE:HD13   | 2.03                     | 0.40              |
| 3:C:224:ILE:HD12   | 3:C:224:ILE:HG23   | 1.82                     | 0.40              |
| 3:C:269:GLU:O      | 3:C:270:ALA:C      | 2.64                     | 0.40              |
| 4:D:152:VAL:HG21   | 4:D:279:LEU:HD22   | 2.03                     | 0.40              |
| 4:D:213:ILE:HD12   | 4:D:213:ILE:HA     | 1.86                     | 0.40              |
| 4:D:304:ARG:NH1    | 4:D:308:ASP:OD1    | 2.54                     | 0.40              |
| 23:L:101:SQD:H462  | 25:m:5101:MGE:H8B1 | 2.03                     | 0.40              |
| 1:a:5137:LEU:HD23  | 1:a:5137:LEU:HA    | 1.92                     | 0.40              |
| 1:a:5272:HIS:NE2   | 24:a:5412:BCT:C    | 2.84                     | 0.40              |
| 2:b:5340:TRP:HH2   | 2:b:5343:HIS:CD2   | 2.40                     | 0.40              |
| 2:b:5383:PHE:CD2   | 2:b:5384:ARG:HG2   | 2.55                     | 0.40              |
| 3:c:5266:TRP:CD1   | 3:c:5266:TRP:H     | 2.40                     | 0.40              |
| 3:c:5297:TYR:HD1   | 3:c:5302:TYR:CZ    | 2.39                     | 0.40              |
| 4:d:5179:PHE:O     | 4:d:5182:LEU:N     | 2.53                     | 0.40              |
| 4:d:5185:PHE:HB3   | 4:d:5191:TRP:HB2   | 2.04                     | 0.40              |

*Continued on next page...*

Continued from previous page...

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 19:d:5405:PQ9:H262 | 25:l:5101:MGE:H221 | 2.02                     | 0.40              |
| 13:z:5028:ALA:O    | 13:z:5030:PRO:HD3  | 2.22                     | 0.40              |
| 14:Y:43:ARG:NH1    | 14:Y:43:ARG:CB     | 2.73                     | 0.40              |
| 15:N:27:THR:HG21   | 15:N:29:LEU:HD23   | 2.03                     | 0.40              |
| 16:x:23:LEU:HD22   | 16:x:23:LEU:HA     | 1.78                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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     | 322/324 (99%)  | 300 (93%) | 21 (6%)  | 1 (0%)   | 36          | 67  |
| 1   | a     | 320/324 (99%)  | 299 (93%) | 20 (6%)  | 1 (0%)   | 36          | 67  |
| 2   | B     | 482/505 (95%)  | 453 (94%) | 29 (6%)  | 0        | 100         | 100 |
| 2   | b     | 482/505 (95%)  | 452 (94%) | 30 (6%)  | 0        | 100         | 100 |
| 3   | C     | 444/446 (100%) | 408 (92%) | 36 (8%)  | 0        | 100         | 100 |
| 3   | c     | 444/446 (100%) | 408 (92%) | 36 (8%)  | 0        | 100         | 100 |
| 4   | D     | 337/339 (99%)  | 292 (87%) | 45 (13%) | 0        | 100         | 100 |
| 4   | d     | 337/339 (99%)  | 293 (87%) | 44 (13%) | 0        | 100         | 100 |
| 5   | E     | 63/65 (97%)    | 50 (79%)  | 13 (21%) | 0        | 100         | 100 |
| 5   | e     | 63/65 (97%)    | 51 (81%)  | 12 (19%) | 0        | 100         | 100 |
| 6   | F     | 29/31 (94%)    | 23 (79%)  | 6 (21%)  | 0        | 100         | 100 |
| 6   | f     | 26/31 (84%)    | 22 (85%)  | 4 (15%)  | 0        | 100         | 100 |
| 7   | H     | 60/62 (97%)    | 57 (95%)  | 3 (5%)   | 0        | 100         | 100 |
| 7   | h     | 60/62 (97%)    | 57 (95%)  | 3 (5%)   | 0        | 100         | 100 |
| 8   | I     | 32/34 (94%)    | 30 (94%)  | 2 (6%)   | 0        | 100         | 100 |
| 8   | i     | 32/34 (94%)    | 30 (94%)  | 2 (6%)   | 0        | 100         | 100 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 9   | K     | 35/37 (95%)     | 34 (97%)   | 1 (3%)   | 0        | 100         | 100 |
| 9   | k     | 32/37 (86%)     | 31 (97%)   | 1 (3%)   | 0        | 100         | 100 |
| 10  | L     | 35/37 (95%)     | 33 (94%)   | 2 (6%)   | 0        | 100         | 100 |
| 10  | l     | 35/37 (95%)     | 33 (94%)   | 2 (6%)   | 0        | 100         | 100 |
| 11  | M     | 31/33 (94%)     | 30 (97%)   | 1 (3%)   | 0        | 100         | 100 |
| 11  | m     | 31/33 (94%)     | 30 (97%)   | 1 (3%)   | 0        | 100         | 100 |
| 12  | T     | 28/30 (93%)     | 25 (89%)   | 3 (11%)  | 0        | 100         | 100 |
| 12  | t     | 28/30 (93%)     | 25 (89%)   | 3 (11%)  | 0        | 100         | 100 |
| 13  | Z     | 60/62 (97%)     | 57 (95%)   | 3 (5%)   | 0        | 100         | 100 |
| 13  | z     | 60/62 (97%)     | 57 (95%)   | 3 (5%)   | 0        | 100         | 100 |
| 14  | Y     | 27/30 (90%)     | 23 (85%)   | 3 (11%)  | 1 (4%)   | 2           | 21  |
| 14  | y     | 27/30 (90%)     | 24 (89%)   | 2 (7%)   | 1 (4%)   | 2           | 21  |
| 15  | N     | 106/108 (98%)   | 92 (87%)   | 13 (12%) | 1 (1%)   | 14          | 44  |
| 15  | n     | 106/108 (98%)   | 94 (89%)   | 11 (10%) | 1 (1%)   | 14          | 44  |
| 16  | X     | 33/40 (82%)     | 31 (94%)   | 2 (6%)   | 0        | 100         | 100 |
| 16  | x     | 33/40 (82%)     | 31 (94%)   | 2 (6%)   | 0        | 100         | 100 |
| All | All   | 4240/4366 (97%) | 3875 (91%) | 359 (8%) | 6 (0%)   | 49          | 79  |

All (6) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 14  | Y     | 45   | ASN  |
| 14  | y     | 44   | GLY  |
| 1   | A     | 141  | PRO  |
| 1   | a     | 5141 | PRO  |
| 15  | n     | 124  | VAL  |
| 15  | N     | 124  | 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 PDB entries followed by that with respect to all EM entries.

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     | 260/262 (99%)  | 259 (100%) | 1 (0%)   | 84          | 83  |
| 1   | a     | 260/262 (99%)  | 259 (100%) | 1 (0%)   | 84          | 83  |
| 2   | B     | 379/403 (94%)  | 378 (100%) | 1 (0%)   | 86          | 84  |
| 2   | b     | 378/403 (94%)  | 378 (100%) | 0        | 100         | 100 |
| 3   | C     | 340/348 (98%)  | 339 (100%) | 1 (0%)   | 86          | 84  |
| 3   | c     | 340/348 (98%)  | 339 (100%) | 1 (0%)   | 86          | 84  |
| 4   | D     | 273/274 (100%) | 273 (100%) | 0        | 100         | 100 |
| 4   | d     | 272/274 (99%)  | 272 (100%) | 0        | 100         | 100 |
| 5   | E     | 55/57 (96%)    | 55 (100%)  | 0        | 100         | 100 |
| 5   | e     | 55/57 (96%)    | 55 (100%)  | 0        | 100         | 100 |
| 6   | F     | 24/25 (96%)    | 24 (100%)  | 0        | 100         | 100 |
| 6   | f     | 22/25 (88%)    | 22 (100%)  | 0        | 100         | 100 |
| 7   | H     | 50/53 (94%)    | 50 (100%)  | 0        | 100         | 100 |
| 7   | h     | 50/53 (94%)    | 50 (100%)  | 0        | 100         | 100 |
| 8   | I     | 31/31 (100%)   | 31 (100%)  | 0        | 100         | 100 |
| 8   | i     | 31/31 (100%)   | 31 (100%)  | 0        | 100         | 100 |
| 9   | K     | 29/30 (97%)    | 29 (100%)  | 0        | 100         | 100 |
| 9   | k     | 27/30 (90%)    | 27 (100%)  | 0        | 100         | 100 |
| 10  | L     | 34/35 (97%)    | 34 (100%)  | 0        | 100         | 100 |
| 10  | l     | 34/35 (97%)    | 34 (100%)  | 0        | 100         | 100 |
| 11  | M     | 30/30 (100%)   | 30 (100%)  | 0        | 100         | 100 |
| 11  | m     | 30/30 (100%)   | 30 (100%)  | 0        | 100         | 100 |
| 12  | T     | 26/27 (96%)    | 26 (100%)  | 0        | 100         | 100 |
| 12  | t     | 26/27 (96%)    | 25 (96%)   | 1 (4%)   | 29          | 52  |
| 13  | Z     | 43/52 (83%)    | 43 (100%)  | 0        | 100         | 100 |
| 13  | z     | 43/52 (83%)    | 43 (100%)  | 0        | 100         | 100 |
| 14  | Y     | 22/23 (96%)    | 11 (50%)   | 11 (50%) | 0           | 0   |
| 14  | y     | 22/23 (96%)    | 11 (50%)   | 11 (50%) | 0           | 0   |
| 15  | N     | 92/92 (100%)   | 92 (100%)  | 0        | 100         | 100 |
| 15  | n     | 92/92 (100%)   | 91 (99%)   | 1 (1%)   | 65          | 73  |
| 16  | X     | 28/33 (85%)    | 14 (50%)   | 14 (50%) | 0           | 0   |
| 16  | x     | 28/33 (85%)    | 15 (54%)   | 13 (46%) | 0           | 0   |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |
|-----|-------|-----------------|------------|----------|-------------|
| All | All   | 3426/3550 (96%) | 3370 (98%) | 56 (2%)  | 54 68       |

All (56) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 249  | VAL  |
| 2   | B     | 485  | GLU  |
| 3   | C     | 410  | VAL  |
| 1   | a     | 5249 | VAL  |
| 3   | c     | 5410 | VAL  |
| 12  | t     | 5025 | GLU  |
| 14  | Y     | 19   | ILE  |
| 14  | Y     | 22   | LEU  |
| 14  | Y     | 25   | ILE  |
| 14  | Y     | 28   | ILE  |
| 14  | Y     | 30   | ILE  |
| 14  | Y     | 34   | MET  |
| 14  | Y     | 36   | ILE  |
| 14  | Y     | 39   | LEU  |
| 14  | Y     | 42   | ARG  |
| 14  | Y     | 43   | ARG  |
| 14  | Y     | 46   | LEU  |
| 15  | n     | 77   | ARG  |
| 14  | y     | 22   | LEU  |
| 14  | y     | 23   | THR  |
| 14  | y     | 25   | ILE  |
| 14  | y     | 27   | MET  |
| 14  | y     | 34   | MET  |
| 14  | y     | 36   | ILE  |
| 14  | y     | 38   | LEU  |
| 14  | y     | 39   | LEU  |
| 14  | y     | 41   | VAL  |
| 14  | y     | 42   | ARG  |
| 14  | y     | 43   | ARG  |
| 16  | X     | 7    | LEU  |
| 16  | X     | 8    | LYS  |
| 16  | X     | 11   | PHE  |
| 16  | X     | 15   | LEU  |
| 16  | X     | 16   | SER  |
| 16  | X     | 21   | LEU  |
| 16  | X     | 23   | LEU  |
| 16  | X     | 24   | THR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16  | X     | 25  | PHE  |
| 16  | X     | 29  | ILE  |
| 16  | X     | 31  | ILE  |
| 16  | X     | 33  | GLN  |
| 16  | X     | 34  | ILE  |
| 16  | X     | 36  | LYS  |
| 16  | x     | 8   | LYS  |
| 16  | x     | 11  | PHE  |
| 16  | x     | 12  | ILE  |
| 16  | x     | 15  | LEU  |
| 16  | x     | 16  | SER  |
| 16  | x     | 23  | LEU  |
| 16  | x     | 24  | THR  |
| 16  | x     | 25  | PHE  |
| 16  | x     | 29  | ILE  |
| 16  | x     | 31  | ILE  |
| 16  | x     | 34  | ILE  |
| 16  | x     | 36  | LYS  |
| 16  | x     | 37  | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 87  | ASN  |
| 1   | A     | 130 | GLN  |
| 1   | A     | 181 | ASN  |
| 1   | A     | 187 | GLN  |
| 1   | A     | 304 | HIS  |
| 1   | A     | 322 | ASN  |
| 1   | A     | 325 | ASN  |
| 2   | B     | 9   | HIS  |
| 2   | B     | 58  | GLN  |
| 2   | B     | 274 | GLN  |
| 2   | B     | 281 | GLN  |
| 2   | B     | 331 | ASN  |
| 2   | B     | 338 | GLN  |
| 2   | B     | 343 | HIS  |
| 2   | B     | 469 | HIS  |
| 3   | C     | 118 | HIS  |
| 3   | C     | 311 | GLN  |
| 3   | C     | 322 | GLN  |
| 3   | C     | 385 | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | D     | 61   | HIS  |
| 4   | D     | 83   | ASN  |
| 4   | D     | 129  | GLN  |
| 4   | D     | 164  | GLN  |
| 4   | D     | 189  | HIS  |
| 4   | D     | 224  | GLN  |
| 4   | D     | 255  | GLN  |
| 5   | E     | 23   | HIS  |
| 7   | H     | 59   | ASN  |
| 9   | K     | 40   | GLN  |
| 13  | Z     | 58   | ASN  |
| 1   | a     | 5075 | ASN  |
| 1   | a     | 5087 | ASN  |
| 1   | a     | 5092 | HIS  |
| 1   | a     | 5130 | GLN  |
| 1   | a     | 5187 | GLN  |
| 1   | a     | 5322 | ASN  |
| 1   | a     | 5325 | ASN  |
| 2   | b     | 5009 | HIS  |
| 2   | b     | 5058 | GLN  |
| 2   | b     | 5281 | GLN  |
| 2   | b     | 5331 | ASN  |
| 2   | b     | 5338 | GLN  |
| 2   | b     | 5343 | HIS  |
| 2   | b     | 5469 | HIS  |
| 3   | c     | 5056 | HIS  |
| 3   | c     | 5118 | HIS  |
| 3   | c     | 5311 | GLN  |
| 3   | c     | 5382 | ASN  |
| 3   | c     | 5385 | GLN  |
| 4   | d     | 5061 | HIS  |
| 4   | d     | 5083 | ASN  |
| 4   | d     | 5129 | GLN  |
| 4   | d     | 5164 | GLN  |
| 4   | d     | 5189 | HIS  |
| 4   | d     | 5197 | HIS  |
| 4   | d     | 5220 | ASN  |
| 4   | d     | 5301 | GLN  |
| 5   | e     | 5023 | HIS  |
| 5   | e     | 5074 | GLN  |
| 6   | f     | 5024 | HIS  |
| 7   | h     | 5059 | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 9   | k     | 5040 | GLN  |
| 10  | l     | 5004 | ASN  |
| 10  | l     | 5037 | ASN  |
| 11  | m     | 5028 | GLN  |
| 11  | m     | 5032 | GLN  |
| 13  | z     | 5058 | ASN  |
| 14  | Y     | 21   | GLN  |
| 15  | n     | 32   | ASN  |
| 15  | n     | 61   | GLN  |
| 15  | n     | 91   | GLN  |
| 15  | n     | 95   | ASN  |
| 15  | n     | 100  | HIS  |
| 15  | N     | 32   | ASN  |
| 15  | N     | 61   | GLN  |
| 15  | N     | 100  | HIS  |
| 14  | y     | 21   | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 146 ligands modelled in this entry, 6 are monoatomic - leaving 140 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 20  | BCR  | A     | 407  | -    | 41,41,41     | 1.36 | 3 (7%)   | 56,56,56    | 1.37 | 9 (16%)  |
| 17  | CLA  | D     | 404  | 4    | 69,73,73     | 1.32 | 9 (13%)  | 83,113,113  | 1.35 | 7 (8%)   |
| 17  | CLA  | C     | 507  | -    | 69,73,73     | 1.30 | 11 (15%) | 83,113,113  | 1.37 | 9 (10%)  |
| 25  | MGE  | d     | 5408 | -    | 47,47,48     | 0.97 | 2 (4%)   | 55,55,56    | 1.13 | 3 (5%)   |
| 17  | CLA  | c     | 5502 | 17,3 | 64,68,73     | 1.36 | 11 (17%) | 77,107,113  | 1.48 | 9 (11%)  |
| 17  | CLA  | c     | 5512 | 3    | 54,58,73     | 1.42 | 11 (20%) | 65,95,113   | 1.41 | 9 (13%)  |
| 17  | CLA  | B     | 615  | 2    | 69,73,73     | 1.30 | 9 (13%)  | 83,113,113  | 1.39 | 7 (8%)   |
| 25  | MGE  | D     | 410  | 25   | 48,48,48     | 0.92 | 2 (4%)   | 56,56,56    | 1.25 | 4 (7%)   |
| 20  | BCR  | k     | 5502 | -    | 41,41,41     | 1.20 | 3 (7%)   | 56,56,56    | 1.30 | 6 (10%)  |
| 17  | CLA  | C     | 511  | 3    | 69,73,73     | 1.27 | 11 (15%) | 83,113,113  | 1.42 | 7 (8%)   |
| 26  | DGD  | a     | 5411 | -    | 58,58,67     | 0.96 | 3 (5%)   | 72,72,81    | 1.53 | 12 (16%) |
| 20  | BCR  | t     | 5101 | -    | 41,41,41     | 1.39 | 3 (7%)   | 56,56,56    | 1.36 | 10 (17%) |
| 17  | CLA  | b     | 5605 | 2    | 69,73,73     | 1.31 | 12 (17%) | 83,113,113  | 1.41 | 11 (13%) |
| 23  | SQD  | a     | 5401 | -    | 25,26,54     | 1.35 | 4 (16%)  | 34,37,65    | 1.89 | 7 (20%)  |
| 26  | DGD  | C     | 518  | -    | 58,58,67     | 0.96 | 2 (3%)   | 72,72,81    | 1.53 | 12 (16%) |
| 17  | CLA  | C     | 503  | 17,3 | 69,73,73     | 1.28 | 11 (15%) | 83,113,113  | 1.41 | 10 (12%) |
| 26  | DGD  | D     | 411  | 7,4  | 55,55,67     | 1.00 | 3 (5%)   | 69,69,81    | 1.50 | 7 (10%)  |
| 17  | CLA  | a     | 5402 | 1    | 69,73,73     | 1.32 | 10 (14%) | 83,113,113  | 1.34 | 8 (9%)   |
| 25  | MGE  | D     | 408  | -    | 47,47,48     | 0.95 | 2 (4%)   | 55,55,56    | 1.05 | 3 (5%)   |
| 17  | CLA  | b     | 5604 | 2    | 69,73,73     | 1.32 | 10 (14%) | 83,113,113  | 1.42 | 8 (9%)   |
| 20  | BCR  | Y     | 101  | -    | 41,41,41     | 1.17 | 2 (4%)   | 56,56,56    | 1.26 | 5 (8%)   |
| 17  | CLA  | B     | 607  | -    | 69,73,73     | 1.28 | 11 (15%) | 83,113,113  | 1.42 | 7 (8%)   |
| 24  | BCT  | A     | 411  | 28   | 2,3,3        | 1.37 | 0        | 2,3,3       | 4.05 | 2 (100%) |
| 25  | MGE  | l     | 5101 | -    | 48,48,48     | 0.92 | 2 (4%)   | 56,56,56    | 1.23 | 5 (8%)   |
| 20  | BCR  | C     | 516  | -    | 41,41,41     | 1.35 | 4 (9%)   | 56,56,56    | 1.40 | 9 (16%)  |
| 17  | CLA  | a     | 5406 | 1    | 59,63,73     | 1.39 | 10 (16%) | 71,101,113  | 1.41 | 6 (8%)   |
| 17  | CLA  | c     | 5506 | 3    | 69,73,73     | 1.27 | 11 (15%) | 83,113,113  | 1.30 | 7 (8%)   |
| 17  | CLA  | B     | 601  | 20   | 45,49,73     | 1.48 | 9 (20%)  | 54,84,113   | 1.43 | 5 (9%)   |
| 17  | CLA  | B     | 614  | 25,2 | 60,64,73     | 1.37 | 11 (18%) | 72,102,113  | 1.46 | 7 (9%)   |
| 17  | CLA  | c     | 5504 | -    | 50,54,73     | 1.47 | 11 (22%) | 60,90,113   | 1.45 | 6 (10%)  |
| 22  | LMT  | B     | 620  | -    | 36,36,36     | 1.20 | 5 (13%)  | 47,47,47    | 0.95 | 1 (2%)   |
| 23  | SQD  | L     | 101  | -    | 46,47,54     | 1.03 | 6 (13%)  | 55,58,65    | 1.63 | 11 (20%) |
| 18  | PHO  | d     | 5402 | -    | 58,69,69     | 1.88 | 12 (20%) | 56,99,99    | 1.55 | 9 (16%)  |
| 17  | CLA  | b     | 5610 | -    | 69,73,73     | 1.30 | 10 (14%) | 83,113,113  | 1.38 | 10 (12%) |
| 17  | CLA  | B     | 608  | 2    | 69,73,73     | 1.30 | 10 (14%) | 83,113,113  | 1.43 | 9 (10%)  |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 17  | CLA  | C     | 502  | 17,3 | 64,68,73     | 1.36 | 11 (17%) | 77,107,113  | 1.49 | 9 (11%)  |
| 17  | CLA  | d     | 5403 | 4    | 69,73,73     | 1.32 | 9 (13%)  | 83,113,113  | 1.36 | 7 (8%)   |
| 17  | CLA  | c     | 5508 | 3    | 69,73,73     | 1.33 | 11 (15%) | 83,113,113  | 1.46 | 8 (9%)   |
| 22  | LMT  | a     | 5410 | -    | 36,36,36     | 1.19 | 6 (16%)  | 47,47,47    | 1.01 | 1 (2%)   |
| 17  | CLA  | C     | 504  | -    | 50,54,73     | 1.47 | 11 (22%) | 60,90,113   | 1.45 | 6 (10%)  |
| 17  | CLA  | b     | 5603 | 2    | 69,73,73     | 1.30 | 9 (13%)  | 83,113,113  | 1.43 | 7 (8%)   |
| 25  | MGE  | B     | 619  | -    | 48,48,48     | 0.94 | 2 (4%)   | 56,56,56    | 1.14 | 4 (7%)   |
| 20  | BCR  | t     | 5102 | -    | 41,41,41     | 1.29 | 3 (7%)   | 56,56,56    | 1.22 | 7 (12%)  |
| 20  | BCR  | b     | 5619 | -    | 41,41,41     | 1.39 | 3 (7%)   | 56,56,56    | 1.36 | 9 (16%)  |
| 17  | CLA  | a     | 5403 | -    | 69,73,73     | 1.30 | 11 (15%) | 83,113,113  | 1.46 | 8 (9%)   |
| 17  | CLA  | B     | 612  | 2    | 69,73,73     | 1.32 | 9 (13%)  | 83,113,113  | 1.43 | 9 (10%)  |
| 20  | BCR  | B     | 617  | -    | 41,41,41     | 1.41 | 3 (7%)   | 56,56,56    | 1.47 | 10 (17%) |
| 20  | BCR  | d     | 5406 | -    | 41,41,41     | 1.27 | 3 (7%)   | 56,56,56    | 1.28 | 7 (12%)  |
| 17  | CLA  | A     | 402  | -    | 69,73,73     | 1.30 | 12 (17%) | 83,113,113  | 1.46 | 8 (9%)   |
| 26  | DGD  | c     | 5515 | 3    | 54,54,67     | 1.20 | 7 (12%)  | 68,68,81    | 1.43 | 8 (11%)  |
| 17  | CLA  | A     | 401  | 1    | 69,73,73     | 1.32 | 10 (14%) | 83,113,113  | 1.33 | 9 (10%)  |
| 25  | MGE  | d     | 5409 | -    | 41,41,48     | 1.00 | 2 (4%)   | 49,49,56    | 1.44 | 8 (16%)  |
| 17  | CLA  | B     | 604  | 2    | 69,73,73     | 1.32 | 10 (14%) | 83,113,113  | 1.43 | 8 (9%)   |
| 17  | CLA  | d     | 5404 | 4    | 54,58,73     | 1.44 | 11 (20%) | 65,95,113   | 1.42 | 7 (10%)  |
| 17  | CLA  | A     | 403  | -    | 69,73,73     | 1.29 | 11 (15%) | 83,113,113  | 1.38 | 9 (10%)  |
| 26  | DGD  | b     | 5621 | 7,2  | 55,55,67     | 1.00 | 3 (5%)   | 69,69,81    | 1.49 | 7 (10%)  |
| 19  | PQ9  | a     | 5407 | -    | 30,30,45     | 0.79 | 1 (3%)   | 38,39,57    | 1.56 | 10 (26%) |
| 17  | CLA  | b     | 5612 | 2    | 69,73,73     | 1.32 | 9 (13%)  | 83,113,113  | 1.44 | 9 (10%)  |
| 20  | BCR  | b     | 5617 | -    | 41,41,41     | 1.41 | 3 (7%)   | 56,56,56    | 1.47 | 10 (17%) |
| 17  | CLA  | B     | 603  | 2    | 69,73,73     | 1.30 | 9 (13%)  | 83,113,113  | 1.44 | 7 (8%)   |
| 25  | MGE  | d     | 5410 | -    | 48,48,48     | 0.93 | 2 (4%)   | 56,56,56    | 1.25 | 5 (8%)   |
| 20  | BCR  | D     | 407  | -    | 41,41,41     | 1.27 | 3 (7%)   | 56,56,56    | 1.27 | 7 (12%)  |
| 17  | CLA  | C     | 508  | 3    | 69,73,73     | 1.33 | 11 (15%) | 83,113,113  | 1.46 | 8 (9%)   |
| 29  | HEM  | f     | 5101 | -    | 50,50,50     | 1.33 | 4 (8%)   | 66,82,82    | 1.10 | 3 (4%)   |
| 17  | CLA  | C     | 509  | 3    | 51,55,73     | 1.49 | 11 (21%) | 61,91,113   | 1.40 | 8 (13%)  |
| 17  | CLA  | c     | 5503 | 17,3 | 69,73,73     | 1.27 | 11 (15%) | 83,113,113  | 1.41 | 10 (12%) |
| 20  | BCR  | a     | 5408 | -    | 41,41,41     | 1.36 | 4 (9%)   | 56,56,56    | 1.36 | 9 (16%)  |
| 17  | CLA  | B     | 602  | 2    | 69,73,73     | 1.31 | 12 (17%) | 83,113,113  | 1.31 | 7 (8%)   |
| 17  | CLA  | A     | 405  | 1    | 59,63,73     | 1.39 | 10 (16%) | 71,101,113  | 1.41 | 6 (8%)   |
| 17  | CLA  | B     | 609  | 2    | 69,73,73     | 1.28 | 11 (15%) | 83,113,113  | 1.35 | 8 (9%)   |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 22  | LMT  | T     | 101  | 2,12 | 36,36,36     | 1.10 | 4 (11%)  | 47,47,47    | 1.00 | 1 (2%)   |
| 17  | CLA  | b     | 5601 | 20   | 45,49,73     | 1.48 | 8 (17%)  | 54,84,113   | 1.43 | 5 (9%)   |
| 23  | SQD  | l     | 5102 | -    | 46,47,54     | 1.02 | 5 (10%)  | 55,58,65    | 1.72 | 13 (23%) |
| 23  | SQD  | d     | 5407 | -    | 53,54,54     | 0.99 | 5 (9%)   | 62,65,65    | 1.64 | 11 (17%) |
| 17  | CLA  | c     | 5510 | 3    | 69,73,73     | 1.31 | 11 (15%) | 83,113,113  | 1.33 | 8 (9%)   |
| 20  | BCR  | c     | 5513 | -    | 41,41,41     | 1.30 | 2 (4%)   | 56,56,56    | 1.39 | 8 (14%)  |
| 17  | CLA  | D     | 405  | 4    | 54,58,73     | 1.44 | 11 (20%) | 65,95,113   | 1.41 | 7 (10%)  |
| 22  | LMT  | A     | 409  | -    | 36,36,36     | 1.16 | 6 (16%)  | 47,47,47    | 1.11 | 3 (6%)   |
| 25  | MGE  | b     | 5620 | -    | 48,48,48     | 0.94 | 2 (4%)   | 56,56,56    | 1.14 | 4 (7%)   |
| 17  | CLA  | b     | 5614 | 2    | 60,64,73     | 1.37 | 11 (18%) | 72,102,113  | 1.46 | 7 (9%)   |
| 20  | BCR  | B     | 618  | -    | 41,41,41     | 1.31 | 3 (7%)   | 56,56,56    | 1.46 | 9 (16%)  |
| 17  | CLA  | b     | 5606 | -    | 46,50,73     | 1.52 | 11 (23%) | 55,85,113   | 1.66 | 9 (16%)  |
| 17  | CLA  | b     | 5611 | 2    | 69,73,73     | 1.35 | 12 (17%) | 83,113,113  | 1.52 | 8 (9%)   |
| 23  | SQD  | A     | 410  | -    | 25,26,54     | 1.34 | 4 (16%)  | 34,37,65    | 1.83 | 8 (23%)  |
| 19  | PQ9  | d     | 5405 | -    | 45,45,45     | 0.66 | 2 (4%)   | 56,57,57    | 1.84 | 16 (28%) |
| 17  | CLA  | C     | 512  | 3    | 55,59,73     | 1.42 | 11 (20%) | 66,96,113   | 1.43 | 6 (9%)   |
| 17  | CLA  | b     | 5615 | 2    | 69,73,73     | 1.30 | 10 (14%) | 83,113,113  | 1.39 | 7 (8%)   |
| 20  | BCR  | b     | 5618 | -    | 41,41,41     | 1.30 | 3 (7%)   | 56,56,56    | 1.46 | 9 (16%)  |
| 20  | BCR  | C     | 515  | -    | 41,41,41     | 1.27 | 2 (4%)   | 56,56,56    | 1.29 | 8 (14%)  |
| 25  | MGE  | m     | 5101 | -    | 48,48,48     | 0.94 | 2 (4%)   | 56,56,56    | 1.13 | 4 (7%)   |
| 17  | CLA  | B     | 606  | -    | 69,73,73     | 1.27 | 11 (15%) | 83,113,113  | 1.42 | 8 (9%)   |
| 18  | PHO  | D     | 402  | -    | 58,69,69     | 1.88 | 12 (20%) | 56,99,99    | 1.55 | 9 (16%)  |
| 22  | LMT  | M     | 101  | -    | 36,36,36     | 1.26 | 7 (19%)  | 47,47,47    | 1.09 | 1 (2%)   |
| 23  | SQD  | D     | 403  | -    | 53,54,54     | 1.00 | 5 (9%)   | 62,65,65    | 1.54 | 11 (17%) |
| 17  | CLA  | a     | 5404 | -    | 69,73,73     | 1.29 | 11 (15%) | 83,113,113  | 1.37 | 9 (10%)  |
| 26  | DGD  | c     | 5516 | -    | 48,48,67     | 1.02 | 2 (4%)   | 62,62,81    | 1.45 | 7 (11%)  |
| 25  | MGE  | c     | 5517 | -    | 48,48,48     | 0.92 | 2 (4%)   | 56,56,56    | 1.11 | 5 (8%)   |
| 26  | DGD  | C     | 517  | -    | 48,48,67     | 1.03 | 2 (4%)   | 62,62,81    | 1.44 | 7 (11%)  |
| 19  | PQ9  | A     | 406  | -    | 45,45,45     | 0.68 | 1 (2%)   | 56,57,57    | 1.60 | 15 (26%) |
| 25  | MGE  | m     | 5103 | 17   | 48,48,48     | 0.91 | 2 (4%)   | 56,56,56    | 1.03 | 3 (5%)   |
| 24  | BCT  | a     | 5412 | 28   | 2,3,3        | 1.38 | 0        | 2,3,3       | 4.05 | 2 (100%) |
| 21  | LHG  | a     | 5409 | -    | 38,38,48     | 0.76 | 1 (2%)   | 41,44,54    | 1.24 | 5 (12%)  |
| 19  | PQ9  | D     | 406  | -    | 45,45,45     | 0.66 | 2 (4%)   | 56,57,57    | 1.84 | 16 (28%) |
| 17  | CLA  | k     | 5501 | 3    | 69,73,73     | 1.28 | 11 (15%) | 83,113,113  | 1.42 | 7 (8%)   |
| 20  | BCR  | H     | 101  | 17   | 41,41,41     | 1.34 | 3 (7%)   | 56,56,56    | 1.26 | 6 (10%)  |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 17  | CLA  | B     | 605  | 2    | 69,73,73     | 1.31 | 12 (17%) | 83,113,113  | 1.41 | 11 (13%) |
| 17  | CLA  | C     | 513  | 3    | 54,58,73     | 1.42 | 11 (20%) | 65,95,113   | 1.41 | 9 (13%)  |
| 17  | CLA  | B     | 611  | 2    | 69,73,73     | 1.36 | 12 (17%) | 83,113,113  | 1.51 | 8 (9%)   |
| 17  | CLA  | b     | 5608 | 2    | 69,73,73     | 1.29 | 10 (14%) | 83,113,113  | 1.43 | 9 (10%)  |
| 17  | CLA  | C     | 510  | 3    | 69,73,73     | 1.31 | 11 (15%) | 83,113,113  | 1.34 | 7 (8%)   |
| 17  | CLA  | C     | 501  | 3    | 69,73,73     | 1.28 | 11 (15%) | 83,113,113  | 1.39 | 8 (9%)   |
| 20  | BCR  | c     | 5514 | -    | 41,41,41     | 1.35 | 3 (7%)   | 56,56,56    | 1.40 | 9 (16%)  |
| 20  | BCR  | h     | 5101 | 17   | 41,41,41     | 1.35 | 3 (7%)   | 56,56,56    | 1.26 | 6 (10%)  |
| 25  | MGE  | D     | 409  | -    | 41,41,48     | 1.01 | 2 (4%)   | 49,49,56    | 1.44 | 8 (16%)  |
| 17  | CLA  | c     | 5505 | -    | 69,73,73     | 1.25 | 10 (14%) | 83,113,113  | 1.39 | 9 (10%)  |
| 18  | PHO  | a     | 5405 | -    | 58,69,69     | 1.91 | 12 (20%) | 56,99,99    | 1.49 | 7 (12%)  |
| 17  | CLA  | c     | 5501 | 3    | 69,73,73     | 1.29 | 11 (15%) | 83,113,113  | 1.38 | 8 (9%)   |
| 22  | LMT  | m     | 5102 | -    | 36,36,36     | 1.18 | 5 (13%)  | 47,47,47    | 1.10 | 2 (4%)   |
| 17  | CLA  | b     | 5607 | -    | 69,73,73     | 1.28 | 11 (15%) | 83,113,113  | 1.41 | 6 (7%)   |
| 17  | CLA  | C     | 505  | -    | 69,73,73     | 1.25 | 10 (14%) | 83,113,113  | 1.38 | 9 (10%)  |
| 17  | CLA  | C     | 506  | 3    | 69,73,73     | 1.26 | 11 (15%) | 83,113,113  | 1.31 | 7 (8%)   |
| 21  | LHG  | A     | 408  | -    | 38,38,48     | 0.76 | 1 (2%)   | 41,44,54    | 1.25 | 5 (12%)  |
| 17  | CLA  | c     | 5507 | -    | 69,73,73     | 1.30 | 10 (14%) | 83,113,113  | 1.37 | 9 (10%)  |
| 25  | MGE  | C     | 519  | -    | 48,48,48     | 0.92 | 2 (4%)   | 56,56,56    | 1.11 | 5 (8%)   |
| 17  | CLA  | B     | 610  | -    | 69,73,73     | 1.30 | 10 (14%) | 83,113,113  | 1.39 | 9 (10%)  |
| 20  | BCR  | z     | 5101 | -    | 41,41,41     | 1.27 | 2 (4%)   | 56,56,56    | 1.29 | 8 (14%)  |
| 29  | HEM  | F     | 101  | 6    | 50,50,50     | 1.33 | 4 (8%)   | 66,82,82    | 1.09 | 3 (4%)   |
| 25  | MGE  | A     | 412  | 25   | 48,48,48     | 0.91 | 2 (4%)   | 56,56,56    | 1.23 | 5 (8%)   |
| 18  | PHO  | A     | 404  | -    | 58,69,69     | 1.91 | 12 (20%) | 56,99,99    | 1.48 | 7 (12%)  |
| 17  | CLA  | B     | 616  | 2    | 69,73,73     | 1.30 | 12 (17%) | 83,113,113  | 1.38 | 9 (10%)  |
| 20  | BCR  | C     | 514  | -    | 41,41,41     | 1.29 | 3 (7%)   | 56,56,56    | 1.39 | 9 (16%)  |
| 17  | CLA  | c     | 5511 | 3    | 55,59,73     | 1.42 | 11 (20%) | 66,96,113   | 1.43 | 6 (9%)   |
| 17  | CLA  | b     | 5613 | 2    | 69,73,73     | 1.33 | 11 (15%) | 83,113,113  | 1.45 | 9 (10%)  |
| 17  | CLA  | b     | 5609 | 2    | 69,73,73     | 1.28 | 11 (15%) | 83,113,113  | 1.34 | 8 (9%)   |
| 17  | CLA  | b     | 5602 | 2    | 69,73,73     | 1.31 | 12 (17%) | 83,113,113  | 1.32 | 7 (8%)   |
| 26  | DGD  | A     | 413  | 1,3  | 54,54,67     | 1.20 | 7 (12%)  | 68,68,81    | 1.42 | 8 (11%)  |
| 17  | CLA  | B     | 613  | 2    | 69,73,73     | 1.34 | 10 (14%) | 83,113,113  | 1.46 | 10 (12%) |
| 20  | BCR  | T     | 102  | -    | 41,41,41     | 1.17 | 3 (7%)   | 56,56,56    | 1.31 | 7 (12%)  |
| 17  | CLA  | b     | 5616 | 2    | 69,73,73     | 1.31 | 12 (17%) | 83,113,113  | 1.37 | 9 (10%)  |
| 17  | CLA  | c     | 5509 | 3    | 51,55,73     | 1.49 | 11 (21%) | 61,91,113   | 1.39 | 9 (14%)  |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|------|------|---------|---------------|---------|
| 20  | BCR  | A     | 407  | -    | -       | 14/29/63/63   | 0/2/2/2 |
| 17  | CLA  | D     | 404  | 4    | -       | 24/39/115/115 | -       |
| 17  | CLA  | C     | 507  | -    | -       | 16/39/115/115 | -       |
| 25  | MGE  | d     | 5408 | -    | -       | 15/42/62/63   | 0/1/1/1 |
| 17  | CLA  | c     | 5502 | 17,3 | -       | 12/33/109/115 | -       |
| 17  | CLA  | c     | 5512 | 3    | -       | 5/21/97/115   | -       |
| 17  | CLA  | B     | 615  | 2    | -       | 18/39/115/115 | -       |
| 25  | MGE  | D     | 410  | 25   | -       | 17/43/63/63   | 0/1/1/1 |
| 20  | BCR  | k     | 5502 | -    | -       | 15/29/63/63   | 0/2/2/2 |
| 17  | CLA  | C     | 511  | 3    | -       | 16/39/115/115 | -       |
| 26  | DGD  | a     | 5411 | -    | -       | 18/46/86/95   | 0/2/2/2 |
| 20  | BCR  | t     | 5101 | -    | -       | 10/29/63/63   | 0/2/2/2 |
| 17  | CLA  | b     | 5605 | 2    | -       | 20/39/115/115 | -       |
| 23  | SQD  | a     | 5401 | -    | -       | 10/19/39/69   | 0/1/1/1 |
| 26  | DGD  | C     | 518  | -    | -       | 18/46/86/95   | 0/2/2/2 |
| 17  | CLA  | C     | 503  | 17,3 | -       | 22/39/115/115 | -       |
| 26  | DGD  | D     | 411  | 7,4  | -       | 21/43/83/95   | 0/2/2/2 |
| 17  | CLA  | a     | 5402 | 1    | -       | 14/39/115/115 | -       |
| 25  | MGE  | D     | 408  | -    | -       | 9/42/62/63    | 0/1/1/1 |
| 17  | CLA  | b     | 5604 | 2    | -       | 16/39/115/115 | -       |
| 20  | BCR  | Y     | 101  | -    | -       | 11/29/63/63   | 0/2/2/2 |
| 17  | CLA  | B     | 607  | -    | -       | 18/39/115/115 | -       |
| 25  | MGE  | l     | 5101 | -    | -       | 12/43/63/63   | 0/1/1/1 |
| 20  | BCR  | C     | 516  | -    | -       | 19/29/63/63   | 0/2/2/2 |
| 17  | CLA  | a     | 5406 | 1    | -       | 8/27/103/115  | -       |
| 17  | CLA  | c     | 5506 | 3    | -       | 21/39/115/115 | -       |
| 17  | CLA  | B     | 601  | 20   | -       | 2/10/86/115   | -       |
| 17  | CLA  | B     | 614  | 25,2 | -       | 12/29/105/115 | -       |
| 17  | CLA  | c     | 5504 | -    | -       | 11/17/93/115  | -       |
| 22  | LMT  | B     | 620  | -    | -       | 7/21/61/61    | 0/2/2/2 |
| 23  | SQD  | L     | 101  | -    | -       | 23/42/62/69   | 0/1/1/1 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|------|------|---------|---------------|---------|
| 18  | PHO  | d     | 5402 | -    | -       | 12/37/103/103 | 0/5/6/6 |
| 17  | CLA  | b     | 5610 | -    | -       | 15/39/115/115 | -       |
| 17  | CLA  | B     | 608  | 2    | -       | 11/39/115/115 | -       |
| 17  | CLA  | C     | 502  | 17,3 | -       | 12/33/109/115 | -       |
| 17  | CLA  | d     | 5403 | 4    | -       | 24/39/115/115 | -       |
| 17  | CLA  | c     | 5508 | 3    | -       | 15/39/115/115 | -       |
| 22  | LMT  | a     | 5410 | -    | -       | 9/21/61/61    | 0/2/2/2 |
| 17  | CLA  | C     | 504  | -    | -       | 11/17/93/115  | -       |
| 17  | CLA  | b     | 5603 | 2    | -       | 14/39/115/115 | -       |
| 25  | MGE  | B     | 619  | -    | -       | 12/43/63/63   | 0/1/1/1 |
| 20  | BCR  | t     | 5102 | -    | -       | 12/29/63/63   | 0/2/2/2 |
| 20  | BCR  | b     | 5619 | -    | -       | 10/29/63/63   | 0/2/2/2 |
| 17  | CLA  | a     | 5403 | -    | -       | 17/39/115/115 | -       |
| 17  | CLA  | B     | 612  | 2    | -       | 19/39/115/115 | -       |
| 20  | BCR  | B     | 617  | -    | -       | 14/29/63/63   | 0/2/2/2 |
| 20  | BCR  | d     | 5406 | -    | -       | 15/29/63/63   | 0/2/2/2 |
| 17  | CLA  | A     | 402  | -    | -       | 17/39/115/115 | -       |
| 26  | DGD  | c     | 5515 | 3    | -       | 19/42/82/95   | 0/2/2/2 |
| 17  | CLA  | A     | 401  | 1    | -       | 14/39/115/115 | -       |
| 25  | MGE  | d     | 5409 | -    | -       | 12/36/56/63   | 0/1/1/1 |
| 17  | CLA  | B     | 604  | 2    | -       | 16/39/115/115 | -       |
| 17  | CLA  | d     | 5404 | 4    | -       | 11/21/97/115  | -       |
| 17  | CLA  | A     | 403  | -    | -       | 15/39/115/115 | -       |
| 26  | DGD  | b     | 5621 | 7,2  | -       | 21/43/83/95   | 0/2/2/2 |
| 19  | PQ9  | a     | 5407 | -    | -       | 7/23/43/61    | 0/1/1/1 |
| 17  | CLA  | b     | 5612 | 2    | -       | 19/39/115/115 | -       |
| 20  | BCR  | b     | 5617 | -    | -       | 14/29/63/63   | 0/2/2/2 |
| 17  | CLA  | B     | 603  | 2    | -       | 14/39/115/115 | -       |
| 25  | MGE  | d     | 5410 | -    | -       | 14/43/63/63   | 0/1/1/1 |
| 20  | BCR  | D     | 407  | -    | -       | 15/29/63/63   | 0/2/2/2 |
| 17  | CLA  | C     | 508  | 3    | -       | 15/39/115/115 | -       |
| 29  | HEM  | f     | 5101 | -    | -       | 2/14/54/54    | -       |
| 17  | CLA  | C     | 509  | 3    | -       | 6/18/94/115   | -       |
| 17  | CLA  | c     | 5503 | 17,3 | -       | 22/39/115/115 | -       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|------|------|---------|---------------|---------|
| 20  | BCR  | a     | 5408 | -    | -       | 14/29/63/63   | 0/2/2/2 |
| 17  | CLA  | B     | 602  | 2    | -       | 22/39/115/115 | -       |
| 17  | CLA  | A     | 405  | 1    | -       | 8/27/103/115  | -       |
| 17  | CLA  | B     | 609  | 2    | -       | 21/39/115/115 | -       |
| 22  | LMT  | T     | 101  | 2,12 | -       | 10/21/61/61   | 0/2/2/2 |
| 17  | CLA  | b     | 5601 | 20   | -       | 2/10/86/115   | -       |
| 23  | SQD  | l     | 5102 | -    | -       | 15/42/62/69   | 0/1/1/1 |
| 23  | SQD  | d     | 5407 | -    | -       | 14/49/69/69   | 0/1/1/1 |
| 17  | CLA  | c     | 5510 | 3    | -       | 8/39/115/115  | -       |
| 20  | BCR  | c     | 5513 | -    | -       | 13/29/63/63   | 0/2/2/2 |
| 17  | CLA  | D     | 405  | 4    | -       | 11/21/97/115  | -       |
| 22  | LMT  | A     | 409  | -    | -       | 10/21/61/61   | 0/2/2/2 |
| 25  | MGE  | b     | 5620 | -    | -       | 12/43/63/63   | 0/1/1/1 |
| 17  | CLA  | b     | 5614 | 2    | -       | 12/29/105/115 | -       |
| 20  | BCR  | B     | 618  | -    | -       | 16/29/63/63   | 0/2/2/2 |
| 17  | CLA  | b     | 5606 | -    | -       | 6/12/88/115   | -       |
| 17  | CLA  | b     | 5611 | 2    | -       | 12/39/115/115 | -       |
| 23  | SQD  | A     | 410  | -    | -       | 8/19/39/69    | 0/1/1/1 |
| 19  | PQ9  | d     | 5405 | -    | -       | 9/41/61/61    | 0/1/1/1 |
| 17  | CLA  | C     | 512  | 3    | -       | 10/23/99/115  | -       |
| 17  | CLA  | b     | 5615 | 2    | -       | 18/39/115/115 | -       |
| 20  | BCR  | b     | 5618 | -    | -       | 16/29/63/63   | 0/2/2/2 |
| 20  | BCR  | C     | 515  | -    | -       | 21/29/63/63   | 0/2/2/2 |
| 25  | MGE  | m     | 5101 | -    | -       | 8/43/63/63    | 0/1/1/1 |
| 17  | CLA  | B     | 606  | -    | -       | 17/39/115/115 | -       |
| 18  | PHO  | D     | 402  | -    | -       | 12/37/103/103 | 0/5/6/6 |
| 22  | LMT  | M     | 101  | -    | -       | 8/21/61/61    | 0/2/2/2 |
| 23  | SQD  | D     | 403  | -    | -       | 22/49/69/69   | 0/1/1/1 |
| 17  | CLA  | a     | 5404 | -    | -       | 15/39/115/115 | -       |
| 26  | DGD  | c     | 5516 | -    | -       | 17/36/76/95   | 0/2/2/2 |
| 25  | MGE  | c     | 5517 | -    | -       | 11/43/63/63   | 0/1/1/1 |
| 26  | DGD  | C     | 517  | -    | -       | 17/36/76/95   | 0/2/2/2 |
| 19  | PQ9  | A     | 406  | -    | -       | 12/41/61/61   | 0/1/1/1 |
| 25  | MGE  | m     | 5103 | 17   | -       | 21/43/63/63   | 0/1/1/1 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|------|------|---------|---------------|---------|
| 21  | LHG  | a     | 5409 | -    | -       | 22/43/43/53   | -       |
| 19  | PQ9  | D     | 406  | -    | -       | 9/41/61/61    | 0/1/1/1 |
| 17  | CLA  | k     | 5501 | 3    | -       | 16/39/115/115 | -       |
| 20  | BCR  | H     | 101  | 17   | -       | 10/29/63/63   | 0/2/2/2 |
| 17  | CLA  | B     | 605  | 2    | -       | 20/39/115/115 | -       |
| 17  | CLA  | C     | 513  | 3    | -       | 5/21/97/115   | -       |
| 17  | CLA  | B     | 611  | 2    | -       | 12/39/115/115 | -       |
| 17  | CLA  | b     | 5608 | 2    | -       | 11/39/115/115 | -       |
| 17  | CLA  | C     | 510  | 3    | -       | 8/39/115/115  | -       |
| 17  | CLA  | C     | 501  | 3    | -       | 17/39/115/115 | -       |
| 20  | BCR  | c     | 5514 | -    | -       | 19/29/63/63   | 0/2/2/2 |
| 20  | BCR  | h     | 5101 | 17   | -       | 10/29/63/63   | 0/2/2/2 |
| 25  | MGE  | D     | 409  | -    | -       | 16/36/56/63   | 0/1/1/1 |
| 17  | CLA  | c     | 5505 | -    | -       | 23/39/115/115 | -       |
| 18  | PHO  | a     | 5405 | -    | -       | 15/37/103/103 | 0/5/6/6 |
| 17  | CLA  | c     | 5501 | 3    | -       | 17/39/115/115 | -       |
| 22  | LMT  | m     | 5102 | -    | -       | 9/21/61/61    | 0/2/2/2 |
| 17  | CLA  | b     | 5607 | -    | -       | 18/39/115/115 | -       |
| 17  | CLA  | C     | 505  | -    | -       | 23/39/115/115 | -       |
| 17  | CLA  | C     | 506  | 3    | -       | 21/39/115/115 | -       |
| 21  | LHG  | A     | 408  | -    | -       | 22/43/43/53   | -       |
| 17  | CLA  | c     | 5507 | -    | -       | 16/39/115/115 | -       |
| 25  | MGE  | C     | 519  | -    | -       | 11/43/63/63   | 0/1/1/1 |
| 17  | CLA  | B     | 610  | -    | -       | 15/39/115/115 | -       |
| 20  | BCR  | z     | 5101 | -    | -       | 21/29/63/63   | 0/2/2/2 |
| 29  | HEM  | F     | 101  | 6    | -       | 2/14/54/54    | -       |
| 25  | MGE  | A     | 412  | 25   | -       | 12/43/63/63   | 0/1/1/1 |
| 18  | PHO  | A     | 404  | -    | -       | 15/37/103/103 | 0/5/6/6 |
| 17  | CLA  | B     | 616  | 2    | -       | 8/39/115/115  | -       |
| 20  | BCR  | C     | 514  | -    | -       | 12/29/63/63   | 0/2/2/2 |
| 17  | CLA  | c     | 5511 | 3    | -       | 10/23/99/115  | -       |
| 17  | CLA  | b     | 5613 | 2    | -       | 20/39/115/115 | -       |
| 17  | CLA  | b     | 5609 | 2    | -       | 21/39/115/115 | -       |
| 17  | CLA  | b     | 5602 | 2    | -       | 22/39/115/115 | -       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|------|------|---------|---------------|---------|
| 26  | DGD  | A     | 413  | 1,3  | -       | 19/42/82/95   | 0/2/2/2 |
| 17  | CLA  | B     | 613  | 2    | -       | 19/39/115/115 | -       |
| 20  | BCR  | T     | 102  | -    | -       | 12/29/63/63   | 0/2/2/2 |
| 17  | CLA  | b     | 5616 | 2    | -       | 8/39/115/115  | -       |
| 17  | CLA  | c     | 5509 | 3    | -       | 6/18/94/115   | -       |

All (992) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 18  | D     | 402  | PHO  | C1B-C2B | 8.26  | 1.48        | 1.39     |
| 18  | d     | 5402 | PHO  | C1B-C2B | 8.25  | 1.48        | 1.39     |
| 18  | a     | 5405 | PHO  | C1B-C2B | 7.87  | 1.48        | 1.39     |
| 18  | A     | 404  | PHO  | C1B-C2B | 7.86  | 1.48        | 1.39     |
| 18  | A     | 404  | PHO  | C3B-C4B | 6.38  | 1.48        | 1.41     |
| 18  | a     | 5405 | PHO  | C3B-C4B | 6.31  | 1.48        | 1.41     |
| 18  | d     | 5402 | PHO  | C3B-C4B | 5.55  | 1.47        | 1.41     |
| 18  | D     | 402  | PHO  | C3B-C4B | 5.53  | 1.47        | 1.41     |
| 20  | B     | 617  | BCR  | C30-C25 | -4.68 | 1.47        | 1.53     |
| 20  | b     | 5617 | BCR  | C30-C25 | -4.68 | 1.47        | 1.53     |
| 20  | t     | 5101 | BCR  | C30-C25 | -4.51 | 1.47        | 1.53     |
| 20  | h     | 5101 | BCR  | C1-C6   | -4.50 | 1.47        | 1.53     |
| 20  | b     | 5619 | BCR  | C30-C25 | -4.49 | 1.47        | 1.53     |
| 20  | H     | 101  | BCR  | C1-C6   | -4.43 | 1.47        | 1.53     |
| 17  | b     | 5611 | CLA  | C4D-ND  | -4.37 | 1.31        | 1.37     |
| 17  | B     | 611  | CLA  | C4D-ND  | -4.34 | 1.31        | 1.37     |
| 20  | D     | 407  | BCR  | C1-C6   | -4.28 | 1.47        | 1.53     |
| 20  | A     | 407  | BCR  | C30-C25 | -4.26 | 1.47        | 1.53     |
| 20  | a     | 5408 | BCR  | C30-C25 | -4.24 | 1.47        | 1.53     |
| 20  | d     | 5406 | BCR  | C1-C6   | -4.24 | 1.47        | 1.53     |
| 17  | C     | 508  | CLA  | C4D-ND  | -4.22 | 1.31        | 1.37     |
| 17  | b     | 5604 | CLA  | C4D-ND  | -4.21 | 1.31        | 1.37     |
| 20  | t     | 5102 | BCR  | C30-C25 | -4.21 | 1.48        | 1.53     |
| 17  | B     | 604  | CLA  | C4D-ND  | -4.21 | 1.31        | 1.37     |
| 25  | D     | 409  | MGE  | O1G-C1A | 4.20  | 1.45        | 1.33     |
| 17  | b     | 5605 | CLA  | C4D-ND  | -4.20 | 1.31        | 1.37     |
| 25  | b     | 5620 | MGE  | O1G-C1A | 4.20  | 1.45        | 1.33     |
| 17  | C     | 510  | CLA  | C4D-ND  | -4.19 | 1.31        | 1.37     |
| 25  | d     | 5408 | MGE  | O1G-C1A | 4.19  | 1.45        | 1.33     |
| 17  | c     | 5510 | CLA  | C4D-ND  | -4.18 | 1.32        | 1.37     |
| 25  | d     | 5409 | MGE  | O1G-C1A | 4.18  | 1.45        | 1.33     |
| 25  | B     | 619  | MGE  | O1G-C1A | 4.18  | 1.45        | 1.33     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 20  | c     | 5514 | BCR  | C1-C6   | -4.17 | 1.48        | 1.53     |
| 17  | b     | 5615 | CLA  | C4D-ND  | -4.17 | 1.32        | 1.37     |
| 20  | C     | 516  | BCR  | C1-C6   | -4.17 | 1.48        | 1.53     |
| 20  | t     | 5101 | BCR  | C1-C6   | -4.16 | 1.48        | 1.53     |
| 17  | c     | 5508 | CLA  | C4D-ND  | -4.15 | 1.32        | 1.37     |
| 25  | D     | 408  | MGE  | O1G-C1A | 4.15  | 1.45        | 1.33     |
| 17  | A     | 403  | CLA  | C4D-ND  | -4.15 | 1.32        | 1.37     |
| 20  | b     | 5619 | BCR  | C1-C6   | -4.14 | 1.48        | 1.53     |
| 17  | b     | 5612 | CLA  | C4D-ND  | -4.14 | 1.32        | 1.37     |
| 17  | b     | 5616 | CLA  | C4D-ND  | -4.13 | 1.32        | 1.37     |
| 25  | C     | 519  | MGE  | O2G-C1B | 4.13  | 1.45        | 1.34     |
| 17  | B     | 603  | CLA  | C4D-ND  | -4.12 | 1.32        | 1.37     |
| 25  | m     | 5101 | MGE  | O1G-C1A | 4.12  | 1.45        | 1.33     |
| 17  | B     | 605  | CLA  | C4D-ND  | -4.11 | 1.32        | 1.37     |
| 17  | B     | 615  | CLA  | C4D-ND  | -4.11 | 1.32        | 1.37     |
| 25  | d     | 5408 | MGE  | O2G-C1B | 4.11  | 1.45        | 1.34     |
| 17  | b     | 5609 | CLA  | C4D-ND  | -4.11 | 1.32        | 1.37     |
| 17  | c     | 5502 | CLA  | C4D-ND  | -4.11 | 1.32        | 1.37     |
| 25  | m     | 5103 | MGE  | O1G-C1A | 4.10  | 1.45        | 1.33     |
| 17  | b     | 5603 | CLA  | C4D-ND  | -4.10 | 1.32        | 1.37     |
| 25  | C     | 519  | MGE  | O1G-C1A | 4.10  | 1.45        | 1.33     |
| 17  | d     | 5404 | CLA  | C4D-ND  | -4.10 | 1.32        | 1.37     |
| 25  | c     | 5517 | MGE  | O1G-C1A | 4.10  | 1.45        | 1.33     |
| 25  | c     | 5517 | MGE  | O2G-C1B | 4.10  | 1.45        | 1.34     |
| 17  | B     | 610  | CLA  | C4D-ND  | -4.10 | 1.32        | 1.37     |
| 17  | B     | 616  | CLA  | C4D-ND  | -4.10 | 1.32        | 1.37     |
| 17  | B     | 609  | CLA  | C4D-ND  | -4.09 | 1.32        | 1.37     |
| 17  | B     | 613  | CLA  | C4D-ND  | -4.08 | 1.32        | 1.37     |
| 17  | D     | 405  | CLA  | C4D-ND  | -4.08 | 1.32        | 1.37     |
| 17  | a     | 5404 | CLA  | C4D-ND  | -4.08 | 1.32        | 1.37     |
| 25  | l     | 5101 | MGE  | O2G-C1B | 4.08  | 1.45        | 1.34     |
| 17  | B     | 612  | CLA  | C4D-ND  | -4.07 | 1.32        | 1.37     |
| 17  | C     | 502  | CLA  | C4D-ND  | -4.07 | 1.32        | 1.37     |
| 17  | b     | 5610 | CLA  | C4D-ND  | -4.07 | 1.32        | 1.37     |
| 17  | A     | 401  | CLA  | C4D-ND  | -4.06 | 1.32        | 1.37     |
| 17  | C     | 501  | CLA  | C4D-ND  | -4.06 | 1.32        | 1.37     |
| 25  | d     | 5410 | MGE  | O1G-C1A | 4.05  | 1.45        | 1.33     |
| 17  | b     | 5602 | CLA  | C4D-ND  | -4.05 | 1.32        | 1.37     |
| 17  | C     | 507  | CLA  | C4D-ND  | -4.05 | 1.32        | 1.37     |
| 17  | c     | 5512 | CLA  | C4D-ND  | -4.05 | 1.32        | 1.37     |
| 17  | c     | 5507 | CLA  | C4D-ND  | -4.05 | 1.32        | 1.37     |
| 17  | B     | 608  | CLA  | C4D-ND  | -4.05 | 1.32        | 1.37     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 17  | a     | 5402 | CLA  | C4D-ND  | -4.04 | 1.32        | 1.37     |
| 25  | A     | 412  | MGE  | O2G-C1B | 4.04  | 1.45        | 1.34     |
| 17  | C     | 513  | CLA  | C4D-ND  | -4.03 | 1.32        | 1.37     |
| 17  | c     | 5501 | CLA  | C4D-ND  | -4.03 | 1.32        | 1.37     |
| 25  | D     | 410  | MGE  | O1G-C1A | 4.03  | 1.45        | 1.33     |
| 17  | a     | 5403 | CLA  | C4D-ND  | -4.03 | 1.32        | 1.37     |
| 17  | B     | 602  | CLA  | C4D-ND  | -4.02 | 1.32        | 1.37     |
| 17  | A     | 402  | CLA  | C4D-ND  | -4.02 | 1.32        | 1.37     |
| 20  | h     | 5101 | BCR  | C30-C25 | -4.02 | 1.48        | 1.53     |
| 17  | C     | 504  | CLA  | C4D-ND  | -4.01 | 1.32        | 1.37     |
| 17  | C     | 509  | CLA  | C4D-ND  | -4.01 | 1.32        | 1.37     |
| 17  | b     | 5613 | CLA  | C4D-ND  | -4.01 | 1.32        | 1.37     |
| 17  | c     | 5506 | CLA  | C4D-ND  | -4.01 | 1.32        | 1.37     |
| 25  | B     | 619  | MGE  | O2G-C1B | 4.00  | 1.45        | 1.34     |
| 25  | b     | 5620 | MGE  | O2G-C1B | 3.99  | 1.45        | 1.34     |
| 17  | C     | 506  | CLA  | C4D-ND  | -3.98 | 1.32        | 1.37     |
| 17  | c     | 5504 | CLA  | C4D-ND  | -3.98 | 1.32        | 1.37     |
| 17  | A     | 405  | CLA  | C4D-ND  | -3.97 | 1.32        | 1.37     |
| 20  | H     | 101  | BCR  | C30-C25 | -3.96 | 1.48        | 1.53     |
| 25  | l     | 5101 | MGE  | O1G-C1A | 3.95  | 1.44        | 1.33     |
| 20  | c     | 5513 | BCR  | C1-C6   | -3.95 | 1.48        | 1.53     |
| 17  | c     | 5509 | CLA  | C4D-ND  | -3.95 | 1.32        | 1.37     |
| 17  | b     | 5608 | CLA  | C4D-ND  | -3.95 | 1.32        | 1.37     |
| 17  | b     | 5607 | CLA  | C4D-ND  | -3.94 | 1.32        | 1.37     |
| 25  | D     | 408  | MGE  | O2G-C1B | 3.93  | 1.45        | 1.34     |
| 20  | z     | 5101 | BCR  | C1-C6   | -3.93 | 1.48        | 1.53     |
| 17  | d     | 5403 | CLA  | C4D-ND  | -3.93 | 1.32        | 1.37     |
| 17  | a     | 5406 | CLA  | C4D-ND  | -3.92 | 1.32        | 1.37     |
| 20  | A     | 407  | BCR  | C1-C6   | -3.92 | 1.48        | 1.53     |
| 25  | A     | 412  | MGE  | O1G-C1A | 3.92  | 1.44        | 1.33     |
| 17  | b     | 5606 | CLA  | C4D-ND  | -3.91 | 1.32        | 1.37     |
| 20  | C     | 515  | BCR  | C1-C6   | -3.91 | 1.48        | 1.53     |
| 25  | d     | 5409 | MGE  | O2G-C1B | 3.91  | 1.45        | 1.34     |
| 17  | C     | 505  | CLA  | C4D-ND  | -3.90 | 1.32        | 1.37     |
| 17  | c     | 5505 | CLA  | C4D-ND  | -3.90 | 1.32        | 1.37     |
| 20  | a     | 5408 | BCR  | C1-C6   | -3.90 | 1.48        | 1.53     |
| 17  | B     | 614  | CLA  | C4D-ND  | -3.89 | 1.32        | 1.37     |
| 20  | C     | 514  | BCR  | C1-C6   | -3.89 | 1.48        | 1.53     |
| 20  | z     | 5101 | BCR  | C30-C25 | -3.89 | 1.48        | 1.53     |
| 25  | m     | 5103 | MGE  | O2G-C1B | 3.88  | 1.45        | 1.34     |
| 25  | m     | 5101 | MGE  | O2G-C1B | 3.87  | 1.45        | 1.34     |
| 17  | D     | 404  | CLA  | C4D-ND  | -3.87 | 1.32        | 1.37     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 17  | B     | 607  | CLA  | C4D-ND  | -3.86 | 1.32        | 1.37     |
| 20  | C     | 515  | BCR  | C30-C25 | -3.86 | 1.48        | 1.53     |
| 17  | B     | 606  | CLA  | C4D-ND  | -3.84 | 1.32        | 1.37     |
| 17  | c     | 5511 | CLA  | C4D-ND  | -3.83 | 1.32        | 1.37     |
| 25  | D     | 409  | MGE  | O2G-C1B | 3.82  | 1.45        | 1.34     |
| 17  | b     | 5614 | CLA  | C4D-ND  | -3.81 | 1.32        | 1.37     |
| 17  | C     | 512  | CLA  | C4D-ND  | -3.79 | 1.32        | 1.37     |
| 25  | d     | 5410 | MGE  | O2G-C1B | 3.79  | 1.45        | 1.34     |
| 17  | C     | 511  | CLA  | C4D-ND  | -3.78 | 1.32        | 1.37     |
| 20  | b     | 5618 | BCR  | C30-C25 | -3.77 | 1.48        | 1.53     |
| 20  | b     | 5617 | BCR  | C1-C6   | -3.76 | 1.48        | 1.53     |
| 20  | B     | 618  | BCR  | C30-C25 | -3.74 | 1.48        | 1.53     |
| 20  | t     | 5102 | BCR  | C1-C6   | -3.74 | 1.48        | 1.53     |
| 17  | k     | 5501 | CLA  | C4D-ND  | -3.74 | 1.32        | 1.37     |
| 20  | B     | 617  | BCR  | C1-C6   | -3.72 | 1.48        | 1.53     |
| 17  | C     | 503  | CLA  | C4D-ND  | -3.72 | 1.32        | 1.37     |
| 20  | C     | 514  | BCR  | C30-C25 | -3.71 | 1.48        | 1.53     |
| 25  | D     | 410  | MGE  | O2G-C1B | 3.71  | 1.44        | 1.34     |
| 20  | c     | 5513 | BCR  | C30-C25 | -3.70 | 1.48        | 1.53     |
| 20  | c     | 5514 | BCR  | C30-C25 | -3.69 | 1.48        | 1.53     |
| 20  | C     | 516  | BCR  | C30-C25 | -3.68 | 1.48        | 1.53     |
| 17  | c     | 5503 | CLA  | C4D-ND  | -3.67 | 1.32        | 1.37     |
| 20  | k     | 5502 | BCR  | C1-C6   | -3.66 | 1.48        | 1.53     |
| 20  | B     | 618  | BCR  | C1-C6   | -3.52 | 1.48        | 1.53     |
| 20  | b     | 5618 | BCR  | C1-C6   | -3.47 | 1.49        | 1.53     |
| 20  | T     | 102  | BCR  | C1-C6   | -3.40 | 1.49        | 1.53     |
| 17  | d     | 5403 | CLA  | MG-NB   | -3.39 | 1.99        | 2.05     |
| 17  | D     | 404  | CLA  | MG-NB   | -3.38 | 1.99        | 2.05     |
| 18  | a     | 5405 | PHO  | C3B-C2B | -3.36 | 1.35        | 1.40     |
| 18  | A     | 404  | PHO  | C3B-C2B | -3.36 | 1.35        | 1.40     |
| 20  | Y     | 101  | BCR  | C1-C6   | -3.34 | 1.49        | 1.53     |
| 17  | B     | 601  | CLA  | C4D-ND  | -3.32 | 1.33        | 1.37     |
| 17  | b     | 5601 | CLA  | C4D-ND  | -3.30 | 1.33        | 1.37     |
| 17  | B     | 613  | CLA  | MG-NB   | -3.27 | 1.99        | 2.05     |
| 17  | A     | 401  | CLA  | MG-NB   | -3.26 | 1.99        | 2.05     |
| 20  | d     | 5406 | BCR  | C30-C25 | -3.26 | 1.49        | 1.53     |
| 17  | a     | 5402 | CLA  | MG-NB   | -3.25 | 1.99        | 2.05     |
| 20  | D     | 407  | BCR  | C30-C25 | -3.25 | 1.49        | 1.53     |
| 17  | b     | 5613 | CLA  | MG-NB   | -3.25 | 1.99        | 2.05     |
| 17  | b     | 5601 | CLA  | C1D-ND  | 3.24  | 1.41        | 1.37     |
| 17  | b     | 5603 | CLA  | MG-NB   | -3.24 | 1.99        | 2.05     |
| 17  | b     | 5608 | CLA  | MG-NB   | -3.23 | 1.99        | 2.05     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 17  | B     | 608  | CLA  | MG-NB   | -3.23 | 1.99        | 2.05     |
| 20  | Y     | 101  | BCR  | C30-C25 | -3.22 | 1.49        | 1.53     |
| 17  | B     | 601  | CLA  | C1D-ND  | 3.22  | 1.41        | 1.37     |
| 17  | B     | 603  | CLA  | MG-NB   | -3.21 | 1.99        | 2.05     |
| 17  | b     | 5611 | CLA  | CMC-C2C | -3.20 | 1.44        | 1.50     |
| 23  | a     | 5401 | SQD  | O47-C7  | 3.20  | 1.42        | 1.35     |
| 20  | k     | 5502 | BCR  | C30-C25 | -3.19 | 1.49        | 1.53     |
| 18  | d     | 5402 | PHO  | CAC-C3C | -3.19 | 1.45        | 1.51     |
| 18  | D     | 402  | PHO  | CAC-C3C | -3.18 | 1.45        | 1.51     |
| 17  | b     | 5612 | CLA  | MG-NB   | -3.18 | 1.99        | 2.05     |
| 17  | B     | 611  | CLA  | CMC-C2C | -3.18 | 1.44        | 1.50     |
| 17  | B     | 612  | CLA  | MG-NB   | -3.17 | 1.99        | 2.05     |
| 29  | F     | 101  | HEM  | FE-ND   | 3.16  | 2.04        | 1.94     |
| 17  | B     | 604  | CLA  | MG-NB   | -3.15 | 1.99        | 2.05     |
| 29  | f     | 5101 | HEM  | FE-ND   | 3.15  | 2.04        | 1.94     |
| 23  | A     | 410  | SQD  | O47-C7  | 3.14  | 1.42        | 1.35     |
| 17  | b     | 5604 | CLA  | MG-NB   | -3.13 | 1.99        | 2.05     |
| 17  | b     | 5610 | CLA  | MG-NB   | -3.13 | 1.99        | 2.05     |
| 17  | B     | 610  | CLA  | MG-NB   | -3.12 | 1.99        | 2.05     |
| 17  | C     | 508  | CLA  | MG-NB   | -3.12 | 1.99        | 2.05     |
| 17  | B     | 615  | CLA  | MG-NB   | -3.11 | 1.99        | 2.05     |
| 17  | C     | 502  | CLA  | MG-NB   | -3.11 | 1.99        | 2.05     |
| 17  | b     | 5615 | CLA  | MG-NB   | -3.11 | 1.99        | 2.05     |
| 17  | c     | 5510 | CLA  | MG-NB   | -3.10 | 1.99        | 2.05     |
| 23  | D     | 403  | SQD  | O48-C23 | 3.09  | 1.42        | 1.33     |
| 17  | c     | 5508 | CLA  | MG-NB   | -3.09 | 1.99        | 2.05     |
| 17  | k     | 5501 | CLA  | MG-NB   | -3.07 | 1.99        | 2.05     |
| 17  | c     | 5502 | CLA  | MG-NB   | -3.07 | 1.99        | 2.05     |
| 17  | c     | 5507 | CLA  | MG-NB   | -3.07 | 1.99        | 2.05     |
| 17  | c     | 5509 | CLA  | MG-NB   | -3.06 | 1.99        | 2.05     |
| 26  | D     | 411  | DGD  | O1G-C1G | -3.06 | 1.38        | 1.45     |
| 17  | C     | 507  | CLA  | MG-NB   | -3.06 | 1.99        | 2.05     |
| 17  | C     | 508  | CLA  | CMC-C2C | -3.06 | 1.44        | 1.50     |
| 17  | B     | 616  | CLA  | MG-NB   | -3.05 | 1.99        | 2.05     |
| 18  | A     | 404  | PHO  | CAC-C3C | -3.05 | 1.46        | 1.51     |
| 17  | C     | 511  | CLA  | MG-NB   | -3.05 | 1.99        | 2.05     |
| 23  | d     | 5407 | SQD  | O48-C23 | 3.05  | 1.42        | 1.33     |
| 17  | C     | 510  | CLA  | MG-NB   | -3.05 | 1.99        | 2.05     |
| 20  | T     | 102  | BCR  | C30-C25 | -3.05 | 1.49        | 1.53     |
| 17  | b     | 5614 | CLA  | MG-NB   | -3.04 | 1.99        | 2.05     |
| 17  | C     | 505  | CLA  | MG-NB   | -3.04 | 1.99        | 2.05     |
| 17  | C     | 502  | CLA  | C1D-ND  | 3.03  | 1.41        | 1.37     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 26  | b     | 5621 | DGD  | O1G-C1G | -3.03 | 1.38        | 1.45     |
| 17  | a     | 5404 | CLA  | MG-NB   | -3.03 | 1.99        | 2.05     |
| 17  | c     | 5508 | CLA  | CMC-C2C | -3.03 | 1.44        | 1.50     |
| 17  | B     | 614  | CLA  | MG-NB   | -3.03 | 1.99        | 2.05     |
| 17  | b     | 5606 | CLA  | MG-NB   | -3.03 | 1.99        | 2.05     |
| 17  | A     | 403  | CLA  | MG-NB   | -3.02 | 1.99        | 2.05     |
| 18  | a     | 5405 | PHO  | CAC-C3C | -3.02 | 1.46        | 1.51     |
| 17  | D     | 405  | CLA  | MG-NB   | -3.02 | 1.99        | 2.05     |
| 17  | C     | 509  | CLA  | MG-NB   | -3.01 | 1.99        | 2.05     |
| 17  | c     | 5502 | CLA  | C1D-ND  | 3.01  | 1.41        | 1.37     |
| 17  | b     | 5616 | CLA  | MG-NB   | -3.01 | 1.99        | 2.05     |
| 17  | d     | 5404 | CLA  | MG-NB   | -3.00 | 1.99        | 2.05     |
| 17  | B     | 606  | CLA  | MG-NB   | -3.00 | 1.99        | 2.05     |
| 17  | c     | 5505 | CLA  | MG-NB   | -3.00 | 1.99        | 2.05     |
| 26  | c     | 5515 | DGD  | O1G-C1G | -2.99 | 1.38        | 1.45     |
| 18  | A     | 404  | PHO  | CMC-C2C | -2.99 | 1.45        | 1.50     |
| 17  | C     | 503  | CLA  | MG-NB   | -2.99 | 1.99        | 2.05     |
| 18  | a     | 5405 | PHO  | CMC-C2C | -2.98 | 1.45        | 1.50     |
| 22  | B     | 620  | LMT  | O3'-C3' | -2.98 | 1.36        | 1.43     |
| 17  | c     | 5503 | CLA  | MG-NB   | -2.97 | 1.99        | 2.05     |
| 26  | A     | 413  | DGD  | O1G-C1G | -2.97 | 1.38        | 1.45     |
| 17  | b     | 5607 | CLA  | MG-NB   | -2.97 | 1.99        | 2.05     |
| 17  | D     | 404  | CLA  | CMD-C2D | -2.97 | 1.44        | 1.50     |
| 18  | a     | 5405 | PHO  | C1D-C2D | 2.97  | 1.42        | 1.39     |
| 18  | D     | 402  | PHO  | C3B-C2B | -2.96 | 1.36        | 1.40     |
| 17  | d     | 5403 | CLA  | CMD-C2D | -2.96 | 1.44        | 1.50     |
| 17  | A     | 402  | CLA  | MG-NB   | -2.96 | 1.99        | 2.05     |
| 18  | d     | 5402 | PHO  | C3B-C2B | -2.96 | 1.36        | 1.40     |
| 23  | L     | 101  | SQD  | O48-C23 | 2.95  | 1.42        | 1.33     |
| 17  | b     | 5602 | CLA  | MG-NB   | -2.95 | 1.99        | 2.05     |
| 18  | D     | 402  | PHO  | CMC-C2C | -2.95 | 1.45        | 1.50     |
| 23  | l     | 5102 | SQD  | O48-C23 | 2.94  | 1.41        | 1.33     |
| 17  | c     | 5506 | CLA  | MG-NB   | -2.94 | 2.00        | 2.05     |
| 17  | B     | 604  | CLA  | C1B-NB  | -2.94 | 1.34        | 1.37     |
| 17  | B     | 602  | CLA  | MG-NB   | -2.94 | 2.00        | 2.05     |
| 17  | B     | 605  | CLA  | MG-NB   | -2.94 | 2.00        | 2.05     |
| 17  | C     | 512  | CLA  | C1D-ND  | 2.94  | 1.41        | 1.37     |
| 18  | A     | 404  | PHO  | C1D-C2D | 2.93  | 1.42        | 1.39     |
| 29  | f     | 5101 | HEM  | CAC-C3C | 2.93  | 1.55        | 1.47     |
| 17  | B     | 607  | CLA  | MG-NB   | -2.92 | 2.00        | 2.05     |
| 29  | F     | 101  | HEM  | CAC-C3C | 2.92  | 1.55        | 1.47     |
| 17  | b     | 5611 | CLA  | MG-NB   | -2.92 | 2.00        | 2.05     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 18  | d     | 5402 | PHO  | CMC-C2C | -2.92 | 1.45        | 1.50     |
| 17  | C     | 512  | CLA  | MG-NB   | -2.92 | 2.00        | 2.05     |
| 17  | a     | 5403 | CLA  | MG-NB   | -2.91 | 2.00        | 2.05     |
| 17  | b     | 5603 | CLA  | C1B-NB  | -2.91 | 1.34        | 1.37     |
| 17  | b     | 5605 | CLA  | MG-NB   | -2.91 | 2.00        | 2.05     |
| 17  | B     | 611  | CLA  | MG-NB   | -2.90 | 2.00        | 2.05     |
| 18  | a     | 5405 | PHO  | CMD-C2D | -2.90 | 1.45        | 1.51     |
| 17  | C     | 511  | CLA  | C1D-ND  | 2.90  | 1.41        | 1.37     |
| 17  | c     | 5511 | CLA  | MG-NB   | -2.89 | 2.00        | 2.05     |
| 17  | b     | 5604 | CLA  | C1B-NB  | -2.89 | 1.34        | 1.37     |
| 17  | c     | 5501 | CLA  | MG-NB   | -2.88 | 2.00        | 2.05     |
| 17  | B     | 603  | CLA  | C1B-NB  | -2.88 | 1.34        | 1.37     |
| 17  | C     | 506  | CLA  | MG-NB   | -2.88 | 2.00        | 2.05     |
| 17  | c     | 5512 | CLA  | MG-NB   | -2.88 | 2.00        | 2.05     |
| 18  | A     | 404  | PHO  | CMD-C2D | -2.88 | 1.45        | 1.51     |
| 17  | k     | 5501 | CLA  | C1D-ND  | 2.88  | 1.41        | 1.37     |
| 17  | B     | 612  | CLA  | C1B-NB  | -2.87 | 1.34        | 1.37     |
| 17  | C     | 501  | CLA  | MG-NB   | -2.87 | 2.00        | 2.05     |
| 17  | b     | 5612 | CLA  | C1B-NB  | -2.87 | 1.34        | 1.37     |
| 17  | c     | 5511 | CLA  | C1D-ND  | 2.87  | 1.41        | 1.37     |
| 17  | B     | 613  | CLA  | C1B-NB  | -2.87 | 1.34        | 1.37     |
| 17  | a     | 5406 | CLA  | MG-NB   | -2.87 | 2.00        | 2.05     |
| 17  | c     | 5501 | CLA  | C1D-ND  | 2.87  | 1.41        | 1.37     |
| 17  | A     | 405  | CLA  | MG-NB   | -2.86 | 2.00        | 2.05     |
| 18  | a     | 5405 | PHO  | CMB-C2B | -2.86 | 1.45        | 1.51     |
| 17  | a     | 5406 | CLA  | C1D-ND  | 2.85  | 1.41        | 1.37     |
| 17  | b     | 5613 | CLA  | C1B-NB  | -2.85 | 1.34        | 1.37     |
| 18  | A     | 404  | PHO  | C4D-ND  | -2.85 | 1.34        | 1.38     |
| 18  | D     | 402  | PHO  | C4D-ND  | -2.84 | 1.34        | 1.38     |
| 17  | C     | 501  | CLA  | C1D-ND  | 2.84  | 1.41        | 1.37     |
| 17  | C     | 513  | CLA  | MG-NB   | -2.84 | 2.00        | 2.05     |
| 29  | F     | 101  | HEM  | CAB-C3B | 2.83  | 1.55        | 1.47     |
| 18  | a     | 5405 | PHO  | C4D-ND  | -2.83 | 1.34        | 1.38     |
| 23  | l     | 5102 | SQD  | O47-C7  | 2.83  | 1.42        | 1.34     |
| 18  | D     | 402  | PHO  | CMB-C2B | -2.83 | 1.45        | 1.51     |
| 29  | f     | 5101 | HEM  | CAB-C3B | 2.83  | 1.55        | 1.47     |
| 17  | c     | 5504 | CLA  | MG-NB   | -2.82 | 2.00        | 2.05     |
| 18  | A     | 404  | PHO  | CMB-C2B | -2.82 | 1.45        | 1.51     |
| 18  | d     | 5402 | PHO  | C4D-ND  | -2.82 | 1.34        | 1.38     |
| 17  | C     | 509  | CLA  | C1D-ND  | 2.82  | 1.41        | 1.37     |
| 17  | A     | 405  | CLA  | C1D-ND  | 2.82  | 1.41        | 1.37     |
| 17  | b     | 5601 | CLA  | C3B-C4B | 2.81  | 1.49        | 1.42     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 17  | a     | 5403 | CLA  | C1D-ND  | 2.81  | 1.41        | 1.37     |
| 17  | C     | 503  | CLA  | C1D-ND  | 2.81  | 1.41        | 1.37     |
| 18  | d     | 5402 | PHO  | CMB-C2B | -2.81 | 1.45        | 1.51     |
| 17  | B     | 602  | CLA  | C1D-ND  | 2.81  | 1.41        | 1.37     |
| 17  | c     | 5512 | CLA  | C1D-ND  | 2.80  | 1.41        | 1.37     |
| 17  | B     | 601  | CLA  | C3B-C4B | 2.80  | 1.49        | 1.42     |
| 17  | b     | 5609 | CLA  | MG-NB   | -2.80 | 2.00        | 2.05     |
| 17  | A     | 403  | CLA  | C1D-ND  | 2.79  | 1.41        | 1.37     |
| 17  | b     | 5608 | CLA  | C1B-NB  | -2.79 | 1.34        | 1.37     |
| 17  | C     | 504  | CLA  | MG-NB   | -2.78 | 2.00        | 2.05     |
| 22  | B     | 620  | LMT  | O2'-C2' | -2.78 | 1.36        | 1.43     |
| 17  | c     | 5503 | CLA  | C1D-ND  | 2.78  | 1.41        | 1.37     |
| 17  | B     | 609  | CLA  | MG-NB   | -2.77 | 2.00        | 2.05     |
| 17  | c     | 5509 | CLA  | C1D-ND  | 2.77  | 1.41        | 1.37     |
| 17  | a     | 5402 | CLA  | MG-ND   | -2.77 | 2.00        | 2.05     |
| 22  | M     | 101  | LMT  | O2B-C2B | -2.77 | 1.36        | 1.43     |
| 18  | D     | 402  | PHO  | C1D-C2D | 2.77  | 1.42        | 1.39     |
| 17  | a     | 5404 | CLA  | C1D-ND  | 2.77  | 1.41        | 1.37     |
| 17  | b     | 5607 | CLA  | C1D-ND  | 2.77  | 1.41        | 1.37     |
| 17  | c     | 5504 | CLA  | C1D-ND  | 2.76  | 1.41        | 1.37     |
| 17  | A     | 402  | CLA  | C1D-ND  | 2.76  | 1.41        | 1.37     |
| 23  | d     | 5407 | SQD  | O47-C7  | 2.76  | 1.42        | 1.34     |
| 23  | D     | 403  | SQD  | O47-C7  | 2.76  | 1.42        | 1.34     |
| 17  | C     | 504  | CLA  | C1D-ND  | 2.76  | 1.41        | 1.37     |
| 22  | B     | 620  | LMT  | O2B-C2B | -2.75 | 1.36        | 1.43     |
| 17  | B     | 608  | CLA  | C1B-NB  | -2.75 | 1.34        | 1.37     |
| 18  | A     | 404  | PHO  | CBD-CGD | -2.75 | 1.48        | 1.52     |
| 17  | C     | 513  | CLA  | C1D-ND  | 2.75  | 1.41        | 1.37     |
| 21  | A     | 408  | LHG  | O7-C5   | -2.75 | 1.39        | 1.46     |
| 22  | T     | 101  | LMT  | O3'-C3' | -2.75 | 1.36        | 1.43     |
| 18  | D     | 402  | PHO  | CMD-C2D | -2.75 | 1.45        | 1.51     |
| 17  | B     | 607  | CLA  | C1D-ND  | 2.75  | 1.41        | 1.37     |
| 17  | C     | 510  | CLA  | C1D-ND  | 2.75  | 1.41        | 1.37     |
| 21  | a     | 5409 | LHG  | O7-C5   | -2.74 | 1.39        | 1.46     |
| 18  | d     | 5402 | PHO  | CBD-CGD | -2.74 | 1.48        | 1.52     |
| 17  | b     | 5602 | CLA  | C1D-ND  | 2.74  | 1.41        | 1.37     |
| 17  | A     | 401  | CLA  | MG-ND   | -2.74 | 2.00        | 2.05     |
| 18  | D     | 402  | PHO  | CBD-CGD | -2.74 | 1.48        | 1.52     |
| 17  | c     | 5510 | CLA  | C1D-ND  | 2.74  | 1.41        | 1.37     |
| 18  | d     | 5402 | PHO  | CMD-C2D | -2.73 | 1.46        | 1.51     |
| 17  | B     | 616  | CLA  | C1D-ND  | 2.73  | 1.41        | 1.37     |
| 17  | D     | 404  | CLA  | MG-ND   | -2.73 | 2.00        | 2.05     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 17  | b     | 5606 | CLA  | C1D-ND  | 2.72  | 1.41        | 1.37     |
| 17  | B     | 604  | CLA  | MG-ND   | -2.72 | 2.00        | 2.05     |
| 17  | D     | 405  | CLA  | C1D-ND  | 2.72  | 1.41        | 1.37     |
| 17  | d     | 5404 | CLA  | C1D-ND  | 2.71  | 1.41        | 1.37     |
| 18  | a     | 5405 | PHO  | CBD-CGD | -2.71 | 1.48        | 1.52     |
| 17  | B     | 608  | CLA  | MG-ND   | -2.71 | 2.00        | 2.05     |
| 17  | d     | 5403 | CLA  | MG-ND   | -2.71 | 2.00        | 2.05     |
| 17  | B     | 602  | CLA  | MG-ND   | -2.71 | 2.00        | 2.05     |
| 17  | b     | 5604 | CLA  | MG-ND   | -2.70 | 2.00        | 2.05     |
| 29  | f     | 5101 | HEM  | FE-NB   | 2.69  | 2.03        | 1.94     |
| 17  | b     | 5609 | CLA  | C4B-NB  | 2.69  | 1.41        | 1.37     |
| 17  | B     | 611  | CLA  | CMB-C2B | -2.69 | 1.45        | 1.50     |
| 17  | C     | 507  | CLA  | C1D-ND  | 2.69  | 1.41        | 1.37     |
| 22  | M     | 101  | LMT  | O3'-C3' | -2.69 | 1.36        | 1.43     |
| 17  | b     | 5608 | CLA  | MG-ND   | -2.69 | 2.00        | 2.05     |
| 17  | B     | 609  | CLA  | C3B-C4B | 2.68  | 1.49        | 1.42     |
| 17  | b     | 5616 | CLA  | C1D-ND  | 2.68  | 1.41        | 1.37     |
| 17  | B     | 606  | CLA  | C1D-ND  | 2.68  | 1.41        | 1.37     |
| 17  | a     | 5406 | CLA  | C3B-C4B | 2.68  | 1.49        | 1.42     |
| 17  | b     | 5613 | CLA  | MG-ND   | -2.68 | 2.00        | 2.05     |
| 17  | c     | 5507 | CLA  | C1D-ND  | 2.68  | 1.41        | 1.37     |
| 17  | b     | 5611 | CLA  | CMB-C2B | -2.68 | 1.45        | 1.50     |
| 17  | b     | 5602 | CLA  | MG-ND   | -2.67 | 2.00        | 2.05     |
| 17  | B     | 613  | CLA  | MG-ND   | -2.67 | 2.00        | 2.05     |
| 17  | B     | 604  | CLA  | CMB-C2B | -2.67 | 1.45        | 1.50     |
| 17  | b     | 5604 | CLA  | CMB-C2B | -2.67 | 1.45        | 1.50     |
| 17  | A     | 405  | CLA  | C3B-C4B | 2.66  | 1.49        | 1.42     |
| 17  | b     | 5615 | CLA  | C1B-NB  | -2.66 | 1.34        | 1.37     |
| 17  | D     | 404  | CLA  | CMB-C2B | -2.66 | 1.45        | 1.50     |
| 17  | B     | 612  | CLA  | CMD-C2D | -2.66 | 1.45        | 1.50     |
| 17  | C     | 507  | CLA  | MG-ND   | -2.66 | 2.00        | 2.05     |
| 17  | C     | 503  | CLA  | CMD-C2D | -2.66 | 1.45        | 1.50     |
| 17  | B     | 608  | CLA  | CMB-C2B | -2.66 | 1.45        | 1.50     |
| 17  | b     | 5608 | CLA  | CMB-C2B | -2.66 | 1.45        | 1.50     |
| 29  | F     | 101  | HEM  | FE-NB   | 2.65  | 2.03        | 1.94     |
| 17  | c     | 5507 | CLA  | MG-ND   | -2.65 | 2.00        | 2.05     |
| 18  | d     | 5402 | PHO  | C1D-C2D | 2.65  | 1.42        | 1.39     |
| 17  | b     | 5609 | CLA  | C1D-ND  | 2.65  | 1.41        | 1.37     |
| 17  | D     | 404  | CLA  | C1B-NB  | -2.64 | 1.34        | 1.37     |
| 17  | b     | 5609 | CLA  | C3B-C4B | 2.64  | 1.48        | 1.42     |
| 17  | C     | 508  | CLA  | MG-ND   | -2.64 | 2.00        | 2.05     |
| 18  | d     | 5402 | PHO  | C4D-CHA | 2.63  | 1.43        | 1.39     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 17  | B     | 610  | CLA  | MG-ND   | -2.63 | 2.00        | 2.05     |
| 17  | B     | 613  | CLA  | CMD-C2D | -2.63 | 1.45        | 1.50     |
| 17  | b     | 5610 | CLA  | MG-ND   | -2.63 | 2.00        | 2.05     |
| 17  | d     | 5403 | CLA  | CMB-C2B | -2.63 | 1.45        | 1.50     |
| 17  | B     | 607  | CLA  | C1B-NB  | -2.62 | 1.34        | 1.37     |
| 22  | A     | 409  | LMT  | O3'-C3' | -2.62 | 1.36        | 1.43     |
| 17  | B     | 612  | CLA  | MG-ND   | -2.62 | 2.00        | 2.05     |
| 18  | D     | 402  | PHO  | C4D-CHA | 2.62  | 1.43        | 1.39     |
| 17  | b     | 5612 | CLA  | C1D-ND  | 2.62  | 1.41        | 1.37     |
| 17  | b     | 5611 | CLA  | CMD-C2D | -2.62 | 1.45        | 1.50     |
| 17  | a     | 5403 | CLA  | CMB-C2B | -2.62 | 1.45        | 1.50     |
| 17  | c     | 5508 | CLA  | MG-ND   | -2.62 | 2.00        | 2.05     |
| 17  | c     | 5509 | CLA  | CMD-C2D | -2.62 | 1.45        | 1.50     |
| 22  | a     | 5410 | LMT  | O3'-C3' | -2.61 | 1.36        | 1.43     |
| 22  | m     | 5102 | LMT  | O3'-C3' | -2.61 | 1.36        | 1.43     |
| 17  | B     | 611  | CLA  | CMD-C2D | -2.61 | 1.45        | 1.50     |
| 18  | A     | 404  | PHO  | C3B-CAB | -2.61 | 1.42        | 1.47     |
| 22  | a     | 5410 | LMT  | O2'-C2' | -2.61 | 1.36        | 1.43     |
| 17  | c     | 5503 | CLA  | CMD-C2D | -2.60 | 1.45        | 1.50     |
| 17  | B     | 615  | CLA  | C1B-NB  | -2.60 | 1.34        | 1.37     |
| 17  | b     | 5616 | CLA  | C1B-NB  | -2.60 | 1.34        | 1.37     |
| 17  | b     | 5612 | CLA  | CMD-C2D | -2.60 | 1.45        | 1.50     |
| 17  | b     | 5616 | CLA  | CMC-C2C | -2.60 | 1.45        | 1.50     |
| 17  | a     | 5404 | CLA  | MG-ND   | -2.60 | 2.00        | 2.05     |
| 17  | B     | 614  | CLA  | C1D-ND  | 2.60  | 1.41        | 1.37     |
| 18  | a     | 5405 | PHO  | C4D-CHA | 2.60  | 1.43        | 1.39     |
| 17  | b     | 5612 | CLA  | MG-ND   | -2.59 | 2.00        | 2.05     |
| 17  | C     | 508  | CLA  | C1D-ND  | 2.59  | 1.41        | 1.37     |
| 17  | b     | 5613 | CLA  | CMD-C2D | -2.59 | 1.45        | 1.50     |
| 17  | A     | 403  | CLA  | MG-ND   | -2.59 | 2.00        | 2.05     |
| 17  | C     | 509  | CLA  | CMD-C2D | -2.59 | 1.45        | 1.50     |
| 17  | d     | 5403 | CLA  | C1B-NB  | -2.59 | 1.34        | 1.37     |
| 17  | C     | 506  | CLA  | C1D-ND  | 2.59  | 1.41        | 1.37     |
| 17  | B     | 611  | CLA  | C1B-NB  | -2.58 | 1.34        | 1.37     |
| 17  | c     | 5505 | CLA  | MG-ND   | -2.58 | 2.00        | 2.05     |
| 17  | B     | 609  | CLA  | C1D-ND  | 2.58  | 1.41        | 1.37     |
| 17  | B     | 609  | CLA  | C4B-NB  | 2.58  | 1.41        | 1.37     |
| 17  | b     | 5614 | CLA  | C1D-ND  | 2.58  | 1.41        | 1.37     |
| 22  | m     | 5102 | LMT  | O2B-C2B | -2.58 | 1.36        | 1.43     |
| 17  | b     | 5610 | CLA  | CMD-C2D | -2.57 | 1.45        | 1.50     |
| 17  | A     | 401  | CLA  | CMD-C2D | -2.57 | 1.45        | 1.50     |
| 17  | a     | 5402 | CLA  | C1D-ND  | 2.57  | 1.40        | 1.37     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 18  | a     | 5405 | PHO  | C3B-CAB | -2.57 | 1.42        | 1.47     |
| 17  | B     | 612  | CLA  | C1D-ND  | 2.57  | 1.40        | 1.37     |
| 17  | B     | 616  | CLA  | CMC-C2C | -2.57 | 1.45        | 1.50     |
| 17  | c     | 5506 | CLA  | C1D-ND  | 2.57  | 1.40        | 1.37     |
| 17  | B     | 613  | CLA  | CMB-C2B | -2.57 | 1.45        | 1.50     |
| 17  | b     | 5603 | CLA  | C1D-ND  | 2.57  | 1.40        | 1.37     |
| 17  | C     | 505  | CLA  | MG-ND   | -2.56 | 2.00        | 2.05     |
| 22  | M     | 101  | LMT  | O2'-C2' | -2.56 | 1.36        | 1.43     |
| 17  | A     | 402  | CLA  | CMB-C2B | -2.56 | 1.45        | 1.50     |
| 17  | a     | 5406 | CLA  | CMB-C2B | -2.56 | 1.45        | 1.50     |
| 17  | A     | 401  | CLA  | CMB-C2B | -2.56 | 1.45        | 1.50     |
| 17  | C     | 509  | CLA  | C1B-NB  | -2.56 | 1.34        | 1.37     |
| 17  | C     | 507  | CLA  | C1B-NB  | -2.55 | 1.34        | 1.37     |
| 17  | B     | 605  | CLA  | C1D-ND  | 2.55  | 1.40        | 1.37     |
| 17  | B     | 616  | CLA  | C1B-NB  | -2.55 | 1.34        | 1.37     |
| 17  | C     | 509  | CLA  | MG-ND   | -2.55 | 2.00        | 2.05     |
| 17  | a     | 5402 | CLA  | CMD-C2D | -2.55 | 1.45        | 1.50     |
| 26  | c     | 5515 | DGD  | O6D-C5D | -2.55 | 1.38        | 1.44     |
| 17  | B     | 603  | CLA  | C1D-ND  | 2.55  | 1.40        | 1.37     |
| 17  | b     | 5613 | CLA  | CMB-C2B | -2.55 | 1.45        | 1.50     |
| 17  | B     | 607  | CLA  | CMC-C2C | -2.55 | 1.45        | 1.50     |
| 26  | A     | 413  | DGD  | O6D-C5D | -2.54 | 1.38        | 1.44     |
| 17  | b     | 5606 | CLA  | C1B-NB  | -2.54 | 1.34        | 1.37     |
| 17  | b     | 5607 | CLA  | C1B-NB  | -2.54 | 1.34        | 1.37     |
| 17  | c     | 5509 | CLA  | C1B-NB  | -2.54 | 1.34        | 1.37     |
| 17  | b     | 5614 | CLA  | CMD-C2D | -2.54 | 1.45        | 1.50     |
| 17  | b     | 5603 | CLA  | MG-ND   | -2.54 | 2.00        | 2.05     |
| 17  | B     | 610  | CLA  | CMD-C2D | -2.54 | 1.45        | 1.50     |
| 17  | c     | 5508 | CLA  | C1D-ND  | 2.54  | 1.40        | 1.37     |
| 17  | b     | 5607 | CLA  | CMC-C2C | -2.54 | 1.45        | 1.50     |
| 17  | C     | 502  | CLA  | CMB-C2B | -2.54 | 1.45        | 1.50     |
| 17  | B     | 614  | CLA  | CMD-C2D | -2.53 | 1.45        | 1.50     |
| 17  | b     | 5610 | CLA  | C1D-ND  | 2.53  | 1.40        | 1.37     |
| 17  | b     | 5611 | CLA  | C1B-NB  | -2.53 | 1.34        | 1.37     |
| 17  | c     | 5507 | CLA  | C1B-NB  | -2.53 | 1.34        | 1.37     |
| 17  | a     | 5402 | CLA  | CMB-C2B | -2.53 | 1.45        | 1.50     |
| 17  | A     | 403  | CLA  | CMD-C2D | -2.53 | 1.45        | 1.50     |
| 17  | B     | 603  | CLA  | CMB-C2B | -2.53 | 1.45        | 1.50     |
| 17  | c     | 5511 | CLA  | C3B-C4B | 2.53  | 1.48        | 1.42     |
| 17  | b     | 5606 | CLA  | CMD-C2D | -2.52 | 1.45        | 1.50     |
| 18  | A     | 404  | PHO  | C4D-CHA | 2.52  | 1.43        | 1.39     |
| 17  | b     | 5615 | CLA  | CMB-C2B | -2.52 | 1.45        | 1.50     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 17  | c     | 5502 | CLA  | CMB-C2B | -2.52 | 1.45        | 1.50     |
| 17  | B     | 615  | CLA  | CMB-C2B | -2.52 | 1.45        | 1.50     |
| 17  | A     | 402  | CLA  | C1B-NB  | -2.52 | 1.34        | 1.37     |
| 17  | c     | 5507 | CLA  | CMD-C2D | -2.52 | 1.45        | 1.50     |
| 17  | a     | 5403 | CLA  | MG-ND   | -2.52 | 2.00        | 2.05     |
| 17  | A     | 405  | CLA  | CMB-C2B | -2.52 | 1.45        | 1.50     |
| 17  | b     | 5602 | CLA  | C1B-NB  | -2.52 | 1.34        | 1.37     |
| 17  | b     | 5604 | CLA  | CMD-C2D | -2.52 | 1.45        | 1.50     |
| 19  | A     | 406  | PQ9  | C10-C5  | 2.51  | 1.48        | 1.35     |
| 17  | B     | 603  | CLA  | MG-ND   | -2.51 | 2.00        | 2.05     |
| 19  | a     | 5407 | PQ9  | C10-C5  | 2.51  | 1.48        | 1.35     |
| 17  | C     | 512  | CLA  | C3B-C4B | 2.51  | 1.48        | 1.42     |
| 17  | C     | 513  | CLA  | C3B-C4B | 2.51  | 1.48        | 1.42     |
| 17  | B     | 604  | CLA  | CMD-C2D | -2.50 | 1.45        | 1.50     |
| 17  | b     | 5603 | CLA  | CMB-C2B | -2.50 | 1.45        | 1.50     |
| 17  | b     | 5601 | CLA  | C4B-NB  | 2.50  | 1.40        | 1.37     |
| 17  | c     | 5506 | CLA  | C1B-NB  | -2.50 | 1.34        | 1.37     |
| 17  | B     | 610  | CLA  | C1D-ND  | 2.50  | 1.40        | 1.37     |
| 22  | m     | 5102 | LMT  | O3B-C3B | -2.50 | 1.37        | 1.43     |
| 17  | c     | 5509 | CLA  | MG-ND   | -2.50 | 2.00        | 2.05     |
| 17  | b     | 5605 | CLA  | C1D-ND  | 2.50  | 1.40        | 1.37     |
| 17  | B     | 606  | CLA  | C1B-NB  | -2.50 | 1.34        | 1.37     |
| 17  | c     | 5512 | CLA  | C3B-C4B | 2.49  | 1.48        | 1.42     |
| 17  | b     | 5608 | CLA  | C1D-ND  | 2.49  | 1.40        | 1.37     |
| 17  | B     | 607  | CLA  | CMD-C2D | -2.49 | 1.45        | 1.50     |
| 17  | A     | 405  | CLA  | CMD-C2D | -2.49 | 1.45        | 1.50     |
| 17  | a     | 5404 | CLA  | CMD-C2D | -2.49 | 1.45        | 1.50     |
| 17  | a     | 5406 | CLA  | CMD-C2D | -2.49 | 1.45        | 1.50     |
| 17  | B     | 615  | CLA  | MG-ND   | -2.49 | 2.00        | 2.05     |
| 22  | M     | 101  | LMT  | O3B-C3B | -2.49 | 1.37        | 1.43     |
| 17  | A     | 401  | CLA  | C1D-ND  | 2.49  | 1.40        | 1.37     |
| 17  | B     | 614  | CLA  | MG-ND   | -2.49 | 2.00        | 2.05     |
| 17  | b     | 5615 | CLA  | MG-ND   | -2.49 | 2.00        | 2.05     |
| 17  | B     | 606  | CLA  | CMD-C2D | -2.49 | 1.45        | 1.50     |
| 17  | B     | 608  | CLA  | CMD-C2D | -2.49 | 1.45        | 1.50     |
| 17  | D     | 404  | CLA  | CMC-C2C | -2.49 | 1.45        | 1.50     |
| 17  | B     | 602  | CLA  | C1B-NB  | -2.48 | 1.34        | 1.37     |
| 22  | A     | 409  | LMT  | O2'-C2' | -2.48 | 1.37        | 1.43     |
| 17  | B     | 614  | CLA  | C1B-NB  | -2.48 | 1.34        | 1.37     |
| 17  | b     | 5614 | CLA  | MG-ND   | -2.48 | 2.00        | 2.05     |
| 17  | c     | 5509 | CLA  | CMB-C2B | -2.48 | 1.45        | 1.50     |
| 17  | c     | 5504 | CLA  | C4B-NB  | 2.48  | 1.40        | 1.37     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 17  | c     | 5505 | CLA  | CMD-C2D | -2.48 | 1.45        | 1.50     |
| 17  | C     | 504  | CLA  | C4B-NB  | 2.48  | 1.40        | 1.37     |
| 17  | c     | 5502 | CLA  | CMC-C2C | -2.48 | 1.45        | 1.50     |
| 17  | B     | 610  | CLA  | CMC-C2C | -2.48 | 1.45        | 1.50     |
| 17  | B     | 608  | CLA  | C1D-ND  | 2.48  | 1.40        | 1.37     |
| 17  | c     | 5507 | CLA  | CMB-C2B | -2.47 | 1.45        | 1.50     |
| 17  | b     | 5608 | CLA  | CMD-C2D | -2.47 | 1.45        | 1.50     |
| 17  | C     | 506  | CLA  | C1B-NB  | -2.47 | 1.34        | 1.37     |
| 17  | B     | 601  | CLA  | C4B-NB  | 2.47  | 1.40        | 1.37     |
| 17  | c     | 5506 | CLA  | CMB-C2B | -2.47 | 1.45        | 1.50     |
| 17  | b     | 5616 | CLA  | MG-ND   | -2.47 | 2.00        | 2.05     |
| 17  | C     | 507  | CLA  | CMD-C2D | -2.47 | 1.45        | 1.50     |
| 17  | A     | 402  | CLA  | MG-ND   | -2.47 | 2.00        | 2.05     |
| 17  | C     | 506  | CLA  | CMB-C2B | -2.47 | 1.45        | 1.50     |
| 17  | B     | 615  | CLA  | C1D-ND  | 2.47  | 1.40        | 1.37     |
| 17  | b     | 5601 | CLA  | MG-NB   | -2.47 | 2.00        | 2.05     |
| 17  | a     | 5402 | CLA  | CMC-C2C | -2.46 | 1.45        | 1.50     |
| 17  | b     | 5603 | CLA  | CMD-C2D | -2.46 | 1.45        | 1.50     |
| 17  | B     | 610  | CLA  | CMB-C2B | -2.46 | 1.45        | 1.50     |
| 17  | B     | 616  | CLA  | MG-ND   | -2.46 | 2.00        | 2.05     |
| 17  | b     | 5607 | CLA  | CMD-C2D | -2.46 | 1.45        | 1.50     |
| 17  | b     | 5610 | CLA  | CMC-C2C | -2.46 | 1.45        | 1.50     |
| 17  | b     | 5613 | CLA  | CMC-C2C | -2.46 | 1.45        | 1.50     |
| 17  | b     | 5614 | CLA  | CMB-C2B | -2.46 | 1.45        | 1.50     |
| 17  | k     | 5501 | CLA  | MG-ND   | -2.46 | 2.00        | 2.05     |
| 17  | b     | 5602 | CLA  | CMD-C2D | -2.46 | 1.45        | 1.50     |
| 17  | b     | 5616 | CLA  | CMB-C2B | -2.46 | 1.45        | 1.50     |
| 17  | d     | 5404 | CLA  | MG-ND   | -2.45 | 2.00        | 2.05     |
| 17  | C     | 510  | CLA  | MG-ND   | -2.45 | 2.00        | 2.05     |
| 17  | C     | 511  | CLA  | MG-ND   | -2.45 | 2.00        | 2.05     |
| 17  | B     | 605  | CLA  | C1B-NB  | -2.45 | 1.34        | 1.37     |
| 17  | b     | 5610 | CLA  | CMB-C2B | -2.45 | 1.45        | 1.50     |
| 17  | B     | 601  | CLA  | MG-NB   | -2.45 | 2.00        | 2.05     |
| 17  | B     | 611  | CLA  | MG-ND   | -2.45 | 2.00        | 2.05     |
| 17  | C     | 511  | CLA  | C1B-NB  | -2.45 | 1.34        | 1.37     |
| 17  | a     | 5406 | CLA  | C1B-NB  | -2.45 | 1.34        | 1.37     |
| 17  | A     | 401  | CLA  | CMC-C2C | -2.45 | 1.45        | 1.50     |
| 17  | a     | 5403 | CLA  | C1B-NB  | -2.45 | 1.34        | 1.37     |
| 17  | C     | 507  | CLA  | CMB-C2B | -2.45 | 1.45        | 1.50     |
| 17  | B     | 603  | CLA  | CMD-C2D | -2.45 | 1.45        | 1.50     |
| 17  | A     | 402  | CLA  | CMD-C2D | -2.45 | 1.45        | 1.50     |
| 17  | C     | 506  | CLA  | MG-ND   | -2.45 | 2.00        | 2.05     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 17  | C     | 508  | CLA  | CMB-C2B | -2.45 | 1.45        | 1.50     |
| 17  | D     | 405  | CLA  | MG-ND   | -2.44 | 2.00        | 2.05     |
| 22  | m     | 5102 | LMT  | O2'-C2' | -2.44 | 1.37        | 1.43     |
| 17  | C     | 509  | CLA  | CMB-C2B | -2.44 | 1.45        | 1.50     |
| 17  | c     | 5508 | CLA  | C1B-NB  | -2.44 | 1.34        | 1.37     |
| 17  | B     | 605  | CLA  | MG-ND   | -2.44 | 2.00        | 2.05     |
| 17  | B     | 612  | CLA  | CMC-C2C | -2.44 | 1.45        | 1.50     |
| 17  | B     | 608  | CLA  | CMC-C2C | -2.44 | 1.45        | 1.50     |
| 17  | B     | 607  | CLA  | MG-ND   | -2.44 | 2.01        | 2.05     |
| 23  | L     | 101  | SQD  | O47-C7  | 2.44  | 1.41        | 1.34     |
| 17  | B     | 605  | CLA  | CMB-C2B | -2.44 | 1.45        | 1.50     |
| 17  | b     | 5615 | CLA  | C1D-ND  | 2.44  | 1.40        | 1.37     |
| 17  | a     | 5403 | CLA  | CMD-C2D | -2.44 | 1.45        | 1.50     |
| 17  | A     | 405  | CLA  | CMC-C2C | -2.44 | 1.45        | 1.50     |
| 17  | B     | 614  | CLA  | CMB-C2B | -2.44 | 1.45        | 1.50     |
| 17  | C     | 505  | CLA  | CMD-C2D | -2.44 | 1.45        | 1.50     |
| 17  | b     | 5605 | CLA  | CMB-C2B | -2.44 | 1.45        | 1.50     |
| 22  | T     | 101  | LMT  | O3B-C3B | -2.44 | 1.37        | 1.43     |
| 17  | B     | 613  | CLA  | CMC-C2C | -2.43 | 1.45        | 1.50     |
| 17  | B     | 605  | CLA  | CMD-C2D | -2.43 | 1.45        | 1.50     |
| 17  | d     | 5403 | CLA  | CMC-C2C | -2.43 | 1.45        | 1.50     |
| 17  | c     | 5510 | CLA  | MG-ND   | -2.43 | 2.01        | 2.05     |
| 17  | B     | 604  | CLA  | C1D-ND  | 2.43  | 1.40        | 1.37     |
| 17  | C     | 502  | CLA  | CMC-C2C | -2.43 | 1.45        | 1.50     |
| 17  | b     | 5604 | CLA  | C1D-ND  | 2.43  | 1.40        | 1.37     |
| 17  | a     | 5406 | CLA  | CMC-C2C | -2.43 | 1.45        | 1.50     |
| 17  | a     | 5406 | CLA  | C4B-NB  | 2.43  | 1.40        | 1.37     |
| 17  | B     | 612  | CLA  | CMB-C2B | -2.43 | 1.45        | 1.50     |
| 17  | c     | 5508 | CLA  | CMD-C2D | -2.43 | 1.45        | 1.50     |
| 17  | k     | 5501 | CLA  | C1B-NB  | -2.43 | 1.34        | 1.37     |
| 17  | C     | 508  | CLA  | CMD-C2D | -2.43 | 1.45        | 1.50     |
| 17  | C     | 508  | CLA  | C1B-NB  | -2.43 | 1.34        | 1.37     |
| 17  | c     | 5511 | CLA  | MG-ND   | -2.43 | 2.01        | 2.05     |
| 17  | b     | 5605 | CLA  | C1B-NB  | -2.42 | 1.34        | 1.37     |
| 17  | b     | 5612 | CLA  | CMC-C2C | -2.42 | 1.45        | 1.50     |
| 17  | c     | 5508 | CLA  | CMB-C2B | -2.42 | 1.45        | 1.50     |
| 17  | b     | 5605 | CLA  | CMD-C2D | -2.42 | 1.45        | 1.50     |
| 23  | d     | 5407 | SQD  | O2-C2   | -2.42 | 1.37        | 1.43     |
| 17  | b     | 5612 | CLA  | CMB-C2B | -2.42 | 1.45        | 1.50     |
| 17  | B     | 611  | CLA  | C1D-ND  | 2.42  | 1.40        | 1.37     |
| 17  | b     | 5605 | CLA  | MG-ND   | -2.41 | 2.01        | 2.05     |
| 22  | B     | 620  | LMT  | O3B-C3B | -2.41 | 1.37        | 1.43     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 17  | A     | 405  | CLA  | C1B-NB  | -2.41 | 1.34        | 1.37     |
| 17  | B     | 616  | CLA  | CMB-C2B | -2.41 | 1.45        | 1.50     |
| 17  | B     | 615  | CLA  | CMC-C2C | -2.41 | 1.45        | 1.50     |
| 17  | b     | 5615 | CLA  | CMC-C2C | -2.41 | 1.45        | 1.50     |
| 17  | b     | 5607 | CLA  | MG-ND   | -2.41 | 2.01        | 2.05     |
| 17  | b     | 5602 | CLA  | CMB-C2B | -2.41 | 1.45        | 1.50     |
| 17  | B     | 602  | CLA  | CMD-C2D | -2.41 | 1.45        | 1.50     |
| 17  | C     | 505  | CLA  | C1D-ND  | 2.41  | 1.40        | 1.37     |
| 17  | c     | 5506 | CLA  | MG-ND   | -2.41 | 2.01        | 2.05     |
| 17  | C     | 512  | CLA  | MG-ND   | -2.41 | 2.01        | 2.05     |
| 17  | d     | 5404 | CLA  | CMB-C2B | -2.40 | 1.45        | 1.50     |
| 17  | b     | 5609 | CLA  | CMB-C2B | -2.40 | 1.45        | 1.50     |
| 17  | B     | 605  | CLA  | C4B-NB  | 2.40  | 1.40        | 1.37     |
| 17  | B     | 609  | CLA  | CMB-C2B | -2.40 | 1.45        | 1.50     |
| 17  | c     | 5507 | CLA  | CMC-C2C | -2.40 | 1.45        | 1.50     |
| 26  | c     | 5515 | DGD  | O6E-C5E | -2.40 | 1.38        | 1.44     |
| 17  | c     | 5505 | CLA  | C4B-NB  | 2.40  | 1.40        | 1.37     |
| 26  | A     | 413  | DGD  | O6E-C5E | -2.39 | 1.38        | 1.44     |
| 17  | c     | 5509 | CLA  | CMC-C2C | -2.39 | 1.45        | 1.50     |
| 17  | C     | 507  | CLA  | CMC-C2C | -2.39 | 1.45        | 1.50     |
| 17  | C     | 511  | CLA  | CMC-C2C | -2.39 | 1.45        | 1.50     |
| 17  | k     | 5501 | CLA  | CMB-C2B | -2.39 | 1.45        | 1.50     |
| 17  | C     | 509  | CLA  | CMC-C2C | -2.39 | 1.45        | 1.50     |
| 17  | D     | 405  | CLA  | CMB-C2B | -2.39 | 1.45        | 1.50     |
| 17  | B     | 606  | CLA  | MG-ND   | -2.39 | 2.01        | 2.05     |
| 17  | c     | 5501 | CLA  | MG-ND   | -2.39 | 2.01        | 2.05     |
| 17  | C     | 510  | CLA  | C1B-NB  | -2.39 | 1.34        | 1.37     |
| 17  | c     | 5510 | CLA  | CMD-C2D | -2.38 | 1.45        | 1.50     |
| 17  | A     | 405  | CLA  | C4B-NB  | 2.38  | 1.40        | 1.37     |
| 17  | c     | 5505 | CLA  | C1D-ND  | 2.38  | 1.40        | 1.37     |
| 17  | b     | 5606 | CLA  | CMB-C2B | -2.38 | 1.45        | 1.50     |
| 17  | d     | 5404 | CLA  | CMD-C2D | -2.38 | 1.45        | 1.50     |
| 17  | C     | 513  | CLA  | MG-ND   | -2.38 | 2.01        | 2.05     |
| 17  | C     | 506  | CLA  | C3B-C4B | 2.38  | 1.48        | 1.42     |
| 17  | B     | 606  | CLA  | CMB-C2B | -2.38 | 1.45        | 1.50     |
| 17  | C     | 513  | CLA  | C1B-NB  | -2.38 | 1.34        | 1.37     |
| 17  | D     | 405  | CLA  | CMD-C2D | -2.38 | 1.45        | 1.50     |
| 17  | c     | 5501 | CLA  | CMC-C2C | -2.38 | 1.45        | 1.50     |
| 17  | c     | 5506 | CLA  | CMD-C2D | -2.38 | 1.45        | 1.50     |
| 17  | C     | 512  | CLA  | C4B-NB  | 2.38  | 1.40        | 1.37     |
| 17  | c     | 5506 | CLA  | C4B-NB  | 2.38  | 1.40        | 1.37     |
| 17  | b     | 5615 | CLA  | CMD-C2D | -2.38 | 1.45        | 1.50     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 26  | A     | 413  | DGD  | O2G-C2G | -2.38 | 1.40        | 1.46     |
| 17  | B     | 615  | CLA  | CMD-C2D | -2.38 | 1.45        | 1.50     |
| 17  | c     | 5512 | CLA  | C4B-NB  | 2.38  | 1.40        | 1.37     |
| 17  | C     | 505  | CLA  | C4B-NB  | 2.38  | 1.40        | 1.37     |
| 22  | a     | 5410 | LMT  | O3B-C3B | -2.37 | 1.37        | 1.43     |
| 17  | C     | 510  | CLA  | CMB-C2B | -2.37 | 1.45        | 1.50     |
| 17  | k     | 5501 | CLA  | CMC-C2C | -2.37 | 1.45        | 1.50     |
| 17  | c     | 5512 | CLA  | MG-ND   | -2.37 | 2.01        | 2.05     |
| 17  | C     | 501  | CLA  | MG-ND   | -2.37 | 2.01        | 2.05     |
| 17  | B     | 602  | CLA  | CMB-C2B | -2.37 | 1.45        | 1.50     |
| 17  | k     | 5501 | CLA  | CMD-C2D | -2.37 | 1.45        | 1.50     |
| 17  | b     | 5603 | CLA  | CMC-C2C | -2.37 | 1.45        | 1.50     |
| 17  | c     | 5511 | CLA  | CMD-C2D | -2.37 | 1.45        | 1.50     |
| 17  | C     | 511  | CLA  | CMD-C2D | -2.36 | 1.45        | 1.50     |
| 17  | b     | 5606 | CLA  | MG-ND   | -2.36 | 2.01        | 2.05     |
| 17  | C     | 506  | CLA  | CMD-C2D | -2.36 | 1.45        | 1.50     |
| 17  | b     | 5610 | CLA  | C1B-NB  | -2.36 | 1.34        | 1.37     |
| 17  | C     | 512  | CLA  | CMD-C2D | -2.36 | 1.45        | 1.50     |
| 17  | C     | 510  | CLA  | CMD-C2D | -2.36 | 1.45        | 1.50     |
| 17  | b     | 5611 | CLA  | MG-ND   | -2.36 | 2.01        | 2.05     |
| 17  | b     | 5608 | CLA  | CMC-C2C | -2.36 | 1.45        | 1.50     |
| 17  | B     | 602  | CLA  | C3B-C4B | 2.35  | 1.48        | 1.42     |
| 17  | B     | 610  | CLA  | C1B-NB  | -2.35 | 1.34        | 1.37     |
| 17  | B     | 603  | CLA  | CMC-C2C | -2.35 | 1.45        | 1.50     |
| 17  | a     | 5404 | CLA  | C1B-NB  | -2.35 | 1.34        | 1.37     |
| 17  | b     | 5605 | CLA  | C4B-NB  | 2.35  | 1.40        | 1.37     |
| 17  | c     | 5511 | CLA  | C4B-NB  | 2.35  | 1.40        | 1.37     |
| 26  | c     | 5515 | DGD  | O2G-C2G | -2.35 | 1.40        | 1.46     |
| 17  | C     | 505  | CLA  | C3B-C4B | 2.35  | 1.48        | 1.42     |
| 22  | A     | 409  | LMT  | O3B-C3B | -2.35 | 1.37        | 1.43     |
| 17  | C     | 502  | CLA  | C1B-NB  | -2.35 | 1.34        | 1.37     |
| 17  | b     | 5614 | CLA  | C1B-NB  | -2.34 | 1.34        | 1.37     |
| 17  | C     | 511  | CLA  | CMB-C2B | -2.34 | 1.45        | 1.50     |
| 17  | c     | 5505 | CLA  | C3B-C4B | 2.34  | 1.48        | 1.42     |
| 17  | a     | 5404 | CLA  | CMB-C2B | -2.34 | 1.45        | 1.50     |
| 17  | c     | 5504 | CLA  | C3B-C4B | 2.34  | 1.48        | 1.42     |
| 17  | C     | 501  | CLA  | CMC-C2C | -2.34 | 1.45        | 1.50     |
| 17  | b     | 5602 | CLA  | C3B-C4B | 2.34  | 1.48        | 1.42     |
| 17  | c     | 5510 | CLA  | CMB-C2B | -2.34 | 1.45        | 1.50     |
| 17  | D     | 405  | CLA  | C3B-C4B | 2.34  | 1.48        | 1.42     |
| 17  | B     | 602  | CLA  | CMC-C2C | -2.34 | 1.45        | 1.50     |
| 17  | B     | 608  | CLA  | C4B-NB  | 2.34  | 1.40        | 1.37     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 17  | c     | 5506 | CLA  | C3B-C4B | 2.34  | 1.48        | 1.42     |
| 17  | b     | 5604 | CLA  | CMC-C2C | -2.34 | 1.45        | 1.50     |
| 17  | b     | 5616 | CLA  | CMD-C2D | -2.34 | 1.45        | 1.50     |
| 17  | c     | 5504 | CLA  | CMD-C2D | -2.34 | 1.45        | 1.50     |
| 17  | C     | 504  | CLA  | CMD-C2D | -2.33 | 1.45        | 1.50     |
| 17  | d     | 5404 | CLA  | C3B-C4B | 2.33  | 1.48        | 1.42     |
| 17  | B     | 609  | CLA  | MG-ND   | -2.33 | 2.01        | 2.05     |
| 17  | b     | 5609 | CLA  | MG-ND   | -2.33 | 2.01        | 2.05     |
| 17  | b     | 5602 | CLA  | CMC-C2C | -2.33 | 1.45        | 1.50     |
| 17  | C     | 504  | CLA  | C3B-C4B | 2.33  | 1.48        | 1.42     |
| 17  | B     | 616  | CLA  | CMD-C2D | -2.33 | 1.45        | 1.50     |
| 17  | c     | 5502 | CLA  | C1B-C2B | 2.33  | 1.48        | 1.43     |
| 17  | A     | 405  | CLA  | MG-ND   | -2.33 | 2.01        | 2.05     |
| 17  | c     | 5502 | CLA  | MG-ND   | -2.33 | 2.01        | 2.05     |
| 17  | A     | 403  | CLA  | CMB-C2B | -2.33 | 1.45        | 1.50     |
| 18  | d     | 5402 | PHO  | C3B-CAB | -2.33 | 1.43        | 1.47     |
| 17  | b     | 5611 | CLA  | C1D-ND  | 2.33  | 1.40        | 1.37     |
| 17  | a     | 5406 | CLA  | MG-ND   | -2.32 | 2.01        | 2.05     |
| 17  | A     | 403  | CLA  | C1B-NB  | -2.32 | 1.34        | 1.37     |
| 17  | c     | 5504 | CLA  | CMC-C2C | -2.32 | 1.45        | 1.50     |
| 17  | C     | 505  | CLA  | CMB-C2B | -2.32 | 1.45        | 1.50     |
| 17  | C     | 513  | CLA  | C4B-NB  | 2.32  | 1.40        | 1.37     |
| 17  | C     | 504  | CLA  | CMB-C2B | -2.32 | 1.45        | 1.50     |
| 17  | C     | 502  | CLA  | C1B-C2B | 2.32  | 1.48        | 1.43     |
| 23  | D     | 403  | SQD  | O2-C2   | -2.31 | 1.37        | 1.43     |
| 17  | B     | 602  | CLA  | C1B-C2B | 2.31  | 1.48        | 1.43     |
| 17  | C     | 504  | CLA  | MG-ND   | -2.31 | 2.01        | 2.05     |
| 17  | c     | 5512 | CLA  | C1B-NB  | -2.31 | 1.34        | 1.37     |
| 17  | B     | 610  | CLA  | C3B-C4B | 2.31  | 1.48        | 1.42     |
| 17  | B     | 605  | CLA  | CMC-C2C | -2.31 | 1.45        | 1.50     |
| 17  | C     | 510  | CLA  | C4B-NB  | 2.31  | 1.40        | 1.37     |
| 17  | C     | 504  | CLA  | CMC-C2C | -2.30 | 1.45        | 1.50     |
| 17  | c     | 5501 | CLA  | CMB-C2B | -2.30 | 1.45        | 1.50     |
| 17  | c     | 5504 | CLA  | CMB-C2B | -2.30 | 1.45        | 1.50     |
| 17  | k     | 5501 | CLA  | C4B-NB  | 2.30  | 1.40        | 1.37     |
| 17  | c     | 5505 | CLA  | CMB-C2B | -2.30 | 1.45        | 1.50     |
| 17  | C     | 506  | CLA  | C4B-NB  | 2.30  | 1.40        | 1.37     |
| 17  | C     | 505  | CLA  | CMC-C2C | -2.30 | 1.45        | 1.50     |
| 17  | B     | 604  | CLA  | CMC-C2C | -2.30 | 1.45        | 1.50     |
| 17  | D     | 404  | CLA  | C1D-ND  | 2.30  | 1.40        | 1.37     |
| 17  | C     | 502  | CLA  | CMD-C2D | -2.30 | 1.45        | 1.50     |
| 17  | b     | 5602 | CLA  | C1B-C2B | 2.30  | 1.48        | 1.43     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 17  | B     | 609  | CLA  | CMC-C2C | -2.30 | 1.45        | 1.50     |
| 17  | b     | 5610 | CLA  | C3B-C4B | 2.30  | 1.48        | 1.42     |
| 17  | c     | 5502 | CLA  | C1B-NB  | -2.30 | 1.35        | 1.37     |
| 17  | c     | 5502 | CLA  | CMD-C2D | -2.30 | 1.45        | 1.50     |
| 26  | C     | 517  | DGD  | O1G-C1G | -2.30 | 1.39        | 1.45     |
| 17  | c     | 5505 | CLA  | CMC-C2C | -2.30 | 1.45        | 1.50     |
| 17  | C     | 502  | CLA  | MG-ND   | -2.29 | 2.01        | 2.05     |
| 17  | b     | 5606 | CLA  | CMC-C2C | -2.29 | 1.45        | 1.50     |
| 17  | b     | 5613 | CLA  | C1D-ND  | 2.29  | 1.40        | 1.37     |
| 17  | b     | 5609 | CLA  | CMC-C2C | -2.29 | 1.45        | 1.50     |
| 22  | M     | 101  | LMT  | O1'-C1' | -2.29 | 1.36        | 1.40     |
| 17  | C     | 501  | CLA  | CMB-C2B | -2.29 | 1.45        | 1.50     |
| 18  | D     | 402  | PHO  | C3B-CAB | -2.29 | 1.43        | 1.47     |
| 17  | c     | 5510 | CLA  | C1B-NB  | -2.29 | 1.35        | 1.37     |
| 17  | c     | 5511 | CLA  | CMB-C2B | -2.28 | 1.46        | 1.50     |
| 17  | C     | 503  | CLA  | C3B-C4B | 2.28  | 1.48        | 1.42     |
| 22  | a     | 5410 | LMT  | O2B-C2B | -2.28 | 1.37        | 1.43     |
| 17  | c     | 5504 | CLA  | MG-ND   | -2.28 | 2.01        | 2.05     |
| 17  | c     | 5501 | CLA  | C4B-NB  | 2.28  | 1.40        | 1.37     |
| 17  | c     | 5510 | CLA  | CMC-C2C | -2.28 | 1.46        | 1.50     |
| 17  | B     | 609  | CLA  | CMD-C2D | -2.28 | 1.46        | 1.50     |
| 17  | c     | 5510 | CLA  | C4B-NB  | 2.28  | 1.40        | 1.37     |
| 17  | B     | 613  | CLA  | CAA-C2A | -2.27 | 1.49        | 1.54     |
| 17  | B     | 601  | CLA  | C1B-C2B | 2.27  | 1.48        | 1.43     |
| 17  | B     | 607  | CLA  | C3B-C4B | 2.27  | 1.48        | 1.42     |
| 17  | C     | 501  | CLA  | C1B-C2B | 2.27  | 1.48        | 1.43     |
| 17  | a     | 5402 | CLA  | C1B-NB  | -2.27 | 1.35        | 1.37     |
| 17  | b     | 5601 | CLA  | CMD-C2D | -2.27 | 1.46        | 1.50     |
| 26  | C     | 517  | DGD  | O2G-C2G | -2.27 | 1.40        | 1.46     |
| 17  | A     | 401  | CLA  | C1B-NB  | -2.27 | 1.35        | 1.37     |
| 17  | C     | 510  | CLA  | CMC-C2C | -2.26 | 1.46        | 1.50     |
| 22  | M     | 101  | LMT  | O4'-C4B | -2.26 | 1.37        | 1.43     |
| 17  | D     | 405  | CLA  | CMC-C2C | -2.26 | 1.46        | 1.50     |
| 17  | C     | 511  | CLA  | C4B-NB  | 2.26  | 1.40        | 1.37     |
| 17  | d     | 5403 | CLA  | C1D-ND  | 2.26  | 1.40        | 1.37     |
| 26  | c     | 5516 | DGD  | O1G-C1G | -2.26 | 1.40        | 1.45     |
| 17  | B     | 613  | CLA  | C1D-ND  | 2.26  | 1.40        | 1.37     |
| 26  | c     | 5516 | DGD  | O2G-C2G | -2.26 | 1.41        | 1.46     |
| 17  | c     | 5501 | CLA  | CMD-C2D | -2.26 | 1.46        | 1.50     |
| 17  | c     | 5511 | CLA  | C1B-NB  | -2.26 | 1.35        | 1.37     |
| 17  | b     | 5613 | CLA  | CAA-C2A | -2.25 | 1.49        | 1.54     |
| 17  | b     | 5607 | CLA  | C3B-C4B | 2.25  | 1.48        | 1.42     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 23  | D     | 403  | SQD  | O3-C3   | -2.25 | 1.37        | 1.43     |
| 17  | b     | 5605 | CLA  | CMC-C2C | -2.25 | 1.46        | 1.50     |
| 17  | b     | 5606 | CLA  | C4B-NB  | 2.25  | 1.40        | 1.37     |
| 17  | b     | 5614 | CLA  | CMC-C2C | -2.25 | 1.46        | 1.50     |
| 17  | b     | 5601 | CLA  | C1B-C2B | 2.25  | 1.48        | 1.43     |
| 17  | A     | 403  | CLA  | CMC-C2C | -2.24 | 1.46        | 1.50     |
| 17  | B     | 601  | CLA  | CMD-C2D | -2.24 | 1.46        | 1.50     |
| 17  | C     | 508  | CLA  | C4B-NB  | 2.24  | 1.40        | 1.37     |
| 17  | c     | 5501 | CLA  | C1B-C2B | 2.24  | 1.48        | 1.43     |
| 17  | b     | 5607 | CLA  | C4B-NB  | 2.24  | 1.40        | 1.37     |
| 17  | c     | 5503 | CLA  | CMB-C2B | -2.24 | 1.46        | 1.50     |
| 17  | k     | 5501 | CLA  | C3B-C4B | 2.24  | 1.48        | 1.42     |
| 17  | B     | 606  | CLA  | C4B-NB  | 2.24  | 1.40        | 1.37     |
| 17  | C     | 512  | CLA  | CMB-C2B | -2.24 | 1.46        | 1.50     |
| 17  | B     | 607  | CLA  | CMB-C2B | -2.24 | 1.46        | 1.50     |
| 17  | B     | 607  | CLA  | C4B-NB  | 2.24  | 1.40        | 1.37     |
| 17  | B     | 606  | CLA  | CMC-C2C | -2.23 | 1.46        | 1.50     |
| 17  | b     | 5607 | CLA  | CMB-C2B | -2.23 | 1.46        | 1.50     |
| 17  | C     | 503  | CLA  | MG-ND   | -2.23 | 2.01        | 2.05     |
| 17  | B     | 616  | CLA  | C4B-NB  | 2.23  | 1.40        | 1.37     |
| 17  | B     | 614  | CLA  | CMC-C2C | -2.23 | 1.46        | 1.50     |
| 17  | c     | 5506 | CLA  | CMC-C2C | -2.23 | 1.46        | 1.50     |
| 19  | D     | 406  | PQ9  | C10-C5  | 2.23  | 1.47        | 1.35     |
| 17  | C     | 509  | CLA  | C4B-NB  | 2.23  | 1.40        | 1.37     |
| 17  | C     | 503  | CLA  | C1B-NB  | -2.23 | 1.35        | 1.37     |
| 17  | c     | 5503 | CLA  | MG-ND   | -2.23 | 2.01        | 2.05     |
| 17  | c     | 5511 | CLA  | C1B-C2B | 2.23  | 1.48        | 1.43     |
| 17  | C     | 512  | CLA  | C1B-NB  | -2.23 | 1.35        | 1.37     |
| 19  | d     | 5405 | PQ9  | C3-C4   | -2.23 | 1.38        | 1.44     |
| 20  | A     | 407  | BCR  | C33-C5  | -2.23 | 1.47        | 1.50     |
| 17  | C     | 503  | CLA  | CMB-C2B | -2.23 | 1.46        | 1.50     |
| 17  | b     | 5609 | CLA  | CMD-C2D | -2.23 | 1.46        | 1.50     |
| 17  | c     | 5503 | CLA  | C3B-C4B | 2.23  | 1.48        | 1.42     |
| 17  | C     | 513  | CLA  | CMC-C2C | -2.23 | 1.46        | 1.50     |
| 19  | D     | 406  | PQ9  | C3-C4   | -2.22 | 1.38        | 1.44     |
| 17  | C     | 510  | CLA  | C3B-C4B | 2.22  | 1.48        | 1.42     |
| 17  | a     | 5404 | CLA  | CMC-C2C | -2.22 | 1.46        | 1.50     |
| 17  | d     | 5404 | CLA  | CMC-C2C | -2.22 | 1.46        | 1.50     |
| 17  | C     | 513  | CLA  | C1B-C2B | 2.22  | 1.48        | 1.43     |
| 17  | c     | 5504 | CLA  | C1B-C2B | 2.22  | 1.48        | 1.43     |
| 17  | C     | 504  | CLA  | C1B-C2B | 2.22  | 1.48        | 1.43     |
| 17  | C     | 501  | CLA  | CMD-C2D | -2.22 | 1.46        | 1.50     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 17  | c     | 5512 | CLA  | C1B-C2B | 2.22  | 1.48        | 1.43     |
| 17  | C     | 506  | CLA  | CMC-C2C | -2.22 | 1.46        | 1.50     |
| 23  | A     | 410  | SQD  | O3-C3   | -2.21 | 1.37        | 1.43     |
| 17  | c     | 5503 | CLA  | C4B-NB  | 2.21  | 1.40        | 1.37     |
| 17  | c     | 5509 | CLA  | C4B-NB  | 2.21  | 1.40        | 1.37     |
| 17  | A     | 402  | CLA  | C4B-NB  | 2.21  | 1.40        | 1.37     |
| 19  | d     | 5405 | PQ9  | C10-C5  | 2.21  | 1.46        | 1.35     |
| 17  | a     | 5403 | CLA  | C4B-NB  | 2.21  | 1.40        | 1.37     |
| 17  | c     | 5503 | CLA  | C1B-NB  | -2.21 | 1.35        | 1.37     |
| 26  | c     | 5515 | DGD  | O3E-C3E | -2.21 | 1.37        | 1.43     |
| 17  | b     | 5616 | CLA  | C4B-NB  | 2.21  | 1.40        | 1.37     |
| 17  | D     | 405  | CLA  | C1B-NB  | -2.21 | 1.35        | 1.37     |
| 17  | c     | 5503 | CLA  | C1B-C2B | 2.20  | 1.48        | 1.43     |
| 17  | C     | 511  | CLA  | C3B-C4B | 2.20  | 1.47        | 1.42     |
| 17  | c     | 5512 | CLA  | CMC-C2C | -2.20 | 1.46        | 1.50     |
| 26  | A     | 413  | DGD  | O3E-C3E | -2.20 | 1.37        | 1.43     |
| 17  | B     | 607  | CLA  | C1B-C2B | 2.20  | 1.48        | 1.43     |
| 17  | C     | 509  | CLA  | C3B-C4B | 2.20  | 1.47        | 1.42     |
| 17  | b     | 5611 | CLA  | C3B-C4B | 2.20  | 1.47        | 1.42     |
| 17  | c     | 5508 | CLA  | C4B-NB  | 2.20  | 1.40        | 1.37     |
| 20  | h     | 5101 | BCR  | C33-C5  | -2.20 | 1.47        | 1.50     |
| 17  | B     | 613  | CLA  | CAC-C3C | -2.20 | 1.45        | 1.51     |
| 23  | d     | 5407 | SQD  | O3-C3   | -2.19 | 1.37        | 1.43     |
| 17  | C     | 503  | CLA  | C1B-C2B | 2.19  | 1.48        | 1.43     |
| 17  | c     | 5509 | CLA  | C3B-C4B | 2.19  | 1.47        | 1.42     |
| 20  | H     | 101  | BCR  | C33-C5  | -2.19 | 1.47        | 1.50     |
| 17  | b     | 5605 | CLA  | CAC-C3C | -2.19 | 1.45        | 1.51     |
| 17  | b     | 5613 | CLA  | CAC-C3C | -2.19 | 1.45        | 1.51     |
| 17  | b     | 5614 | CLA  | C3B-C4B | 2.19  | 1.47        | 1.42     |
| 17  | B     | 610  | CLA  | C4B-NB  | 2.18  | 1.40        | 1.37     |
| 20  | a     | 5408 | BCR  | C33-C5  | -2.18 | 1.47        | 1.50     |
| 17  | b     | 5604 | CLA  | CAC-C3C | -2.18 | 1.45        | 1.51     |
| 23  | A     | 410  | SQD  | O2-C2   | -2.18 | 1.37        | 1.43     |
| 23  | a     | 5401 | SQD  | O3-C3   | -2.18 | 1.37        | 1.43     |
| 17  | B     | 604  | CLA  | CAC-C3C | -2.18 | 1.45        | 1.51     |
| 17  | B     | 605  | CLA  | CAC-C3C | -2.18 | 1.45        | 1.51     |
| 17  | B     | 611  | CLA  | CAC-C3C | -2.18 | 1.45        | 1.51     |
| 17  | B     | 616  | CLA  | C3B-C4B | 2.18  | 1.47        | 1.42     |
| 17  | B     | 611  | CLA  | C3B-C4B | 2.18  | 1.47        | 1.42     |
| 26  | a     | 5411 | DGD  | O5D-C6D | -2.18 | 1.39        | 1.43     |
| 26  | D     | 411  | DGD  | O2G-C2G | -2.18 | 1.41        | 1.46     |
| 17  | C     | 507  | CLA  | C3B-C4B | 2.18  | 1.47        | 1.42     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 17  | C     | 501  | CLA  | C4B-NB  | 2.18  | 1.40        | 1.37     |
| 17  | b     | 5610 | CLA  | C4B-NB  | 2.18  | 1.40        | 1.37     |
| 17  | B     | 609  | CLA  | C1B-C2B | 2.18  | 1.48        | 1.43     |
| 17  | C     | 512  | CLA  | C1B-C2B | 2.18  | 1.48        | 1.43     |
| 17  | B     | 614  | CLA  | C3B-C4B | 2.17  | 1.47        | 1.42     |
| 26  | D     | 411  | DGD  | O6D-C5D | -2.17 | 1.39        | 1.44     |
| 17  | C     | 503  | CLA  | CMC-C2C | -2.17 | 1.46        | 1.50     |
| 17  | c     | 5510 | CLA  | C3B-C4B | 2.17  | 1.47        | 1.42     |
| 23  | a     | 5401 | SQD  | O4-C4   | -2.17 | 1.37        | 1.43     |
| 17  | a     | 5404 | CLA  | C4B-NB  | 2.17  | 1.40        | 1.37     |
| 17  | C     | 513  | CLA  | CMB-C2B | -2.17 | 1.46        | 1.50     |
| 17  | A     | 401  | CLA  | CAA-C2A | -2.17 | 1.50        | 1.54     |
| 23  | a     | 5401 | SQD  | O2-C2   | -2.17 | 1.37        | 1.43     |
| 17  | b     | 5608 | CLA  | C4B-NB  | 2.17  | 1.40        | 1.37     |
| 17  | C     | 503  | CLA  | C4B-NB  | 2.17  | 1.40        | 1.37     |
| 17  | d     | 5404 | CLA  | C1B-NB  | -2.16 | 1.35        | 1.37     |
| 22  | A     | 409  | LMT  | O4'-C4B | -2.16 | 1.37        | 1.43     |
| 17  | b     | 5607 | CLA  | C1B-C2B | 2.16  | 1.48        | 1.43     |
| 17  | c     | 5512 | CLA  | CMB-C2B | -2.16 | 1.46        | 1.50     |
| 17  | b     | 5605 | CLA  | C3B-C4B | 2.16  | 1.47        | 1.42     |
| 17  | B     | 605  | CLA  | C3B-C4B | 2.16  | 1.47        | 1.42     |
| 17  | A     | 402  | CLA  | CMC-C2C | -2.16 | 1.46        | 1.50     |
| 17  | B     | 605  | CLA  | C1B-C2B | 2.16  | 1.48        | 1.43     |
| 17  | c     | 5507 | CLA  | C3B-C4B | 2.16  | 1.47        | 1.42     |
| 26  | b     | 5621 | DGD  | O2G-C2G | -2.16 | 1.41        | 1.46     |
| 17  | d     | 5403 | CLA  | C3B-C4B | 2.15  | 1.47        | 1.42     |
| 22  | T     | 101  | LMT  | O4'-C4B | -2.15 | 1.37        | 1.43     |
| 17  | b     | 5611 | CLA  | CAC-C3C | -2.15 | 1.45        | 1.51     |
| 17  | b     | 5609 | CLA  | C1B-C2B | 2.15  | 1.48        | 1.43     |
| 26  | C     | 518  | DGD  | O5D-C6D | -2.15 | 1.39        | 1.43     |
| 17  | a     | 5403 | CLA  | CMC-C2C | -2.15 | 1.46        | 1.50     |
| 26  | b     | 5621 | DGD  | O6D-C5D | -2.15 | 1.39        | 1.44     |
| 17  | b     | 5605 | CLA  | C1B-C2B | 2.15  | 1.48        | 1.43     |
| 17  | C     | 512  | CLA  | CMC-C2C | -2.14 | 1.46        | 1.50     |
| 17  | c     | 5503 | CLA  | CMC-C2C | -2.14 | 1.46        | 1.50     |
| 17  | b     | 5616 | CLA  | C3B-C4B | 2.14  | 1.47        | 1.42     |
| 23  | A     | 410  | SQD  | O4-C4   | -2.14 | 1.37        | 1.43     |
| 23  | L     | 101  | SQD  | O2-C2   | -2.14 | 1.37        | 1.43     |
| 17  | B     | 606  | CLA  | C3B-C4B | 2.14  | 1.47        | 1.42     |
| 17  | C     | 501  | CLA  | C1B-NB  | -2.14 | 1.35        | 1.37     |
| 17  | c     | 5509 | CLA  | C1B-C2B | 2.14  | 1.48        | 1.43     |
| 17  | c     | 5511 | CLA  | CMC-C2C | -2.14 | 1.46        | 1.50     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 20  | t     | 5102 | BCR  | C33-C5  | -2.13 | 1.47        | 1.50     |
| 17  | B     | 614  | CLA  | C4B-NB  | 2.13  | 1.40        | 1.37     |
| 17  | c     | 5504 | CLA  | C1B-NB  | -2.13 | 1.35        | 1.37     |
| 23  | L     | 101  | SQD  | O47-C45 | -2.13 | 1.41        | 1.46     |
| 17  | A     | 403  | CLA  | C4B-NB  | 2.13  | 1.40        | 1.37     |
| 17  | C     | 510  | CLA  | C1B-C2B | 2.13  | 1.48        | 1.43     |
| 23  | D     | 403  | SQD  | O4-C4   | -2.12 | 1.38        | 1.43     |
| 17  | c     | 5501 | CLA  | C1B-NB  | -2.12 | 1.35        | 1.37     |
| 17  | D     | 404  | CLA  | C3B-C4B | 2.12  | 1.47        | 1.42     |
| 23  | d     | 5407 | SQD  | O4-C4   | -2.12 | 1.38        | 1.43     |
| 17  | B     | 614  | CLA  | C1B-C2B | 2.12  | 1.48        | 1.43     |
| 23  | L     | 101  | SQD  | O4-C4   | -2.12 | 1.38        | 1.43     |
| 17  | b     | 5601 | CLA  | MG-ND   | -2.12 | 2.01        | 2.05     |
| 23  | l     | 5102 | SQD  | O4-C4   | -2.12 | 1.38        | 1.43     |
| 26  | A     | 413  | DGD  | O4D-C4D | -2.11 | 1.38        | 1.43     |
| 17  | k     | 5501 | CLA  | C1B-C2B | 2.11  | 1.48        | 1.43     |
| 17  | C     | 509  | CLA  | C1B-C2B | 2.11  | 1.48        | 1.43     |
| 17  | B     | 612  | CLA  | C3B-C4B | 2.11  | 1.47        | 1.42     |
| 17  | B     | 601  | CLA  | MG-ND   | -2.11 | 2.01        | 2.05     |
| 26  | C     | 518  | DGD  | O2G-C2G | -2.11 | 1.41        | 1.46     |
| 17  | b     | 5614 | CLA  | C4B-NB  | 2.11  | 1.40        | 1.37     |
| 17  | b     | 5614 | CLA  | C1B-C2B | 2.11  | 1.48        | 1.43     |
| 17  | a     | 5402 | CLA  | CAA-C2A | -2.11 | 1.50        | 1.54     |
| 23  | L     | 101  | SQD  | O3-C3   | -2.11 | 1.38        | 1.43     |
| 17  | C     | 504  | CLA  | C1B-NB  | -2.11 | 1.35        | 1.37     |
| 17  | b     | 5612 | CLA  | C3B-C4B | 2.10  | 1.47        | 1.42     |
| 23  | l     | 5102 | SQD  | O3-C3   | -2.10 | 1.38        | 1.43     |
| 17  | b     | 5606 | CLA  | C3B-C4B | 2.10  | 1.47        | 1.42     |
| 22  | B     | 620  | LMT  | O4'-C4B | -2.10 | 1.38        | 1.43     |
| 17  | c     | 5501 | CLA  | C3B-C4B | 2.10  | 1.47        | 1.42     |
| 20  | b     | 5618 | BCR  | C38-C26 | -2.10 | 1.47        | 1.50     |
| 26  | a     | 5411 | DGD  | O2G-C2G | -2.10 | 1.41        | 1.46     |
| 17  | C     | 502  | CLA  | C4B-NB  | 2.10  | 1.40        | 1.37     |
| 17  | C     | 513  | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 17  | b     | 5602 | CLA  | C4B-NB  | 2.10  | 1.40        | 1.37     |
| 17  | c     | 5508 | CLA  | CAC-C3C | -2.09 | 1.45        | 1.51     |
| 17  | a     | 5402 | CLA  | C3B-C4B | 2.09  | 1.47        | 1.42     |
| 17  | C     | 511  | CLA  | C1B-C2B | 2.09  | 1.48        | 1.43     |
| 17  | a     | 5403 | CLA  | C1B-C2B | 2.09  | 1.48        | 1.43     |
| 17  | C     | 508  | CLA  | CAC-C3C | -2.09 | 1.45        | 1.51     |
| 22  | a     | 5410 | LMT  | O4'-C4B | -2.09 | 1.38        | 1.43     |
| 17  | b     | 5606 | CLA  | C1B-C2B | 2.09  | 1.48        | 1.43     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 17  | c     | 5512 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 17  | B     | 608  | CLA  | C3B-C4B | 2.09  | 1.47        | 1.42     |
| 20  | D     | 407  | BCR  | C33-C5  | -2.09 | 1.47        | 1.50     |
| 17  | b     | 5608 | CLA  | C3B-C4B | 2.09  | 1.47        | 1.42     |
| 17  | B     | 604  | CLA  | C4B-NB  | 2.09  | 1.40        | 1.37     |
| 17  | C     | 506  | CLA  | C1B-C2B | 2.08  | 1.48        | 1.43     |
| 17  | A     | 401  | CLA  | C3B-C4B | 2.08  | 1.47        | 1.42     |
| 17  | A     | 402  | CLA  | C1B-C2B | 2.08  | 1.48        | 1.43     |
| 20  | B     | 618  | BCR  | C38-C26 | -2.08 | 1.47        | 1.50     |
| 17  | c     | 5507 | CLA  | C1B-C2B | 2.08  | 1.48        | 1.43     |
| 17  | C     | 501  | CLA  | C3B-C4B | 2.08  | 1.47        | 1.42     |
| 17  | B     | 611  | CLA  | C4B-NB  | 2.08  | 1.40        | 1.37     |
| 17  | c     | 5505 | CLA  | C1B-NB  | -2.08 | 1.35        | 1.37     |
| 17  | B     | 606  | CLA  | C1B-C2B | 2.08  | 1.48        | 1.43     |
| 26  | c     | 5515 | DGD  | O4D-C4D | -2.08 | 1.38        | 1.43     |
| 17  | d     | 5404 | CLA  | C4B-NB  | 2.08  | 1.40        | 1.37     |
| 17  | b     | 5611 | CLA  | C4B-NB  | 2.07  | 1.40        | 1.37     |
| 17  | c     | 5510 | CLA  | C1B-C2B | 2.07  | 1.48        | 1.43     |
| 17  | c     | 5506 | CLA  | C1B-C2B | 2.07  | 1.48        | 1.43     |
| 17  | b     | 5616 | CLA  | C1B-C2B | 2.07  | 1.48        | 1.43     |
| 22  | a     | 5410 | LMT  | O1'-C1' | -2.07 | 1.36        | 1.40     |
| 17  | A     | 403  | CLA  | C3B-C4B | 2.07  | 1.47        | 1.42     |
| 17  | C     | 508  | CLA  | C3B-C4B | 2.06  | 1.47        | 1.42     |
| 17  | c     | 5508 | CLA  | C3B-C4B | 2.06  | 1.47        | 1.42     |
| 22  | M     | 101  | LMT  | O5'-C5' | -2.06 | 1.39        | 1.44     |
| 17  | B     | 602  | CLA  | C4B-NB  | 2.06  | 1.40        | 1.37     |
| 17  | C     | 505  | CLA  | C1B-NB  | -2.05 | 1.35        | 1.37     |
| 17  | b     | 5604 | CLA  | C4B-NB  | 2.05  | 1.40        | 1.37     |
| 20  | d     | 5406 | BCR  | C33-C5  | -2.05 | 1.47        | 1.50     |
| 17  | b     | 5616 | CLA  | CAC-C3C | -2.05 | 1.45        | 1.51     |
| 20  | t     | 5101 | BCR  | C33-C5  | -2.05 | 1.47        | 1.50     |
| 17  | B     | 609  | CLA  | C1B-NB  | -2.05 | 1.35        | 1.37     |
| 17  | D     | 405  | CLA  | C4B-NB  | 2.05  | 1.40        | 1.37     |
| 17  | c     | 5502 | CLA  | C4B-NB  | 2.05  | 1.40        | 1.37     |
| 20  | a     | 5408 | BCR  | C38-C26 | -2.05 | 1.47        | 1.50     |
| 20  | c     | 5514 | BCR  | C38-C26 | -2.05 | 1.47        | 1.50     |
| 17  | C     | 507  | CLA  | C1B-C2B | 2.05  | 1.48        | 1.43     |
| 17  | a     | 5404 | CLA  | C3B-C4B | 2.05  | 1.47        | 1.42     |
| 20  | C     | 516  | BCR  | C33-C5  | -2.04 | 1.47        | 1.50     |
| 17  | b     | 5615 | CLA  | C3B-C4B | 2.04  | 1.47        | 1.42     |
| 22  | m     | 5102 | LMT  | O5'-C5' | -2.04 | 1.39        | 1.44     |
| 23  | l     | 5102 | SQD  | O2-C2   | -2.04 | 1.38        | 1.43     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 26  | a     | 5411 | DGD  | O1G-C1G | -2.04 | 1.40        | 1.45     |
| 20  | C     | 516  | BCR  | C38-C26 | -2.04 | 1.47        | 1.50     |
| 20  | C     | 514  | BCR  | C33-C5  | -2.04 | 1.47        | 1.50     |
| 22  | T     | 101  | LMT  | O2B-C2B | -2.03 | 1.38        | 1.43     |
| 17  | c     | 5502 | CLA  | C3B-C4B | 2.03  | 1.47        | 1.42     |
| 17  | B     | 616  | CLA  | C1B-C2B | 2.03  | 1.48        | 1.43     |
| 17  | A     | 402  | CLA  | C3B-C4B | 2.03  | 1.47        | 1.42     |
| 20  | b     | 5619 | BCR  | C33-C5  | -2.03 | 1.47        | 1.50     |
| 17  | b     | 5611 | CLA  | CAA-C2A | -2.03 | 1.50        | 1.54     |
| 17  | d     | 5404 | CLA  | C1B-C2B | 2.03  | 1.48        | 1.43     |
| 17  | a     | 5403 | CLA  | CHC-C4B | -2.03 | 1.34        | 1.39     |
| 17  | B     | 616  | CLA  | CAC-C3C | -2.03 | 1.45        | 1.51     |
| 17  | B     | 611  | CLA  | CAA-C2A | -2.02 | 1.50        | 1.54     |
| 17  | A     | 402  | CLA  | CHC-C4B | -2.02 | 1.34        | 1.39     |
| 17  | D     | 405  | CLA  | C1B-C2B | 2.02  | 1.48        | 1.43     |
| 17  | A     | 403  | CLA  | C1B-C2B | 2.02  | 1.48        | 1.43     |
| 20  | B     | 617  | BCR  | C38-C26 | -2.02 | 1.47        | 1.50     |
| 17  | B     | 615  | CLA  | C3B-C4B | 2.02  | 1.47        | 1.42     |
| 17  | B     | 602  | CLA  | CAC-C3C | -2.02 | 1.45        | 1.51     |
| 17  | b     | 5615 | CLA  | C4B-NB  | 2.02  | 1.40        | 1.37     |
| 17  | B     | 603  | CLA  | CAC-C3C | -2.02 | 1.45        | 1.51     |
| 17  | C     | 502  | CLA  | C3B-C4B | 2.02  | 1.47        | 1.42     |
| 17  | b     | 5609 | CLA  | C1B-NB  | -2.02 | 1.35        | 1.37     |
| 17  | b     | 5613 | CLA  | C3B-C4B | 2.01  | 1.47        | 1.42     |
| 22  | A     | 409  | LMT  | O2B-C2B | -2.01 | 1.38        | 1.43     |
| 17  | B     | 601  | CLA  | C1B-NB  | -2.01 | 1.35        | 1.37     |
| 20  | b     | 5617 | BCR  | C33-C5  | -2.01 | 1.47        | 1.50     |
| 20  | T     | 102  | BCR  | C33-C5  | -2.01 | 1.47        | 1.50     |
| 17  | C     | 507  | CLA  | CHC-C4B | -2.01 | 1.34        | 1.39     |
| 17  | b     | 5603 | CLA  | CAC-C3C | -2.01 | 1.46        | 1.51     |
| 20  | k     | 5502 | BCR  | C33-C5  | -2.01 | 1.47        | 1.50     |
| 26  | A     | 413  | DGD  | O4E-C4E | -2.01 | 1.38        | 1.43     |
| 17  | a     | 5404 | CLA  | C1B-C2B | 2.01  | 1.48        | 1.43     |
| 22  | A     | 409  | LMT  | O1'-C1' | -2.01 | 1.36        | 1.40     |
| 17  | b     | 5602 | CLA  | CAC-C3C | -2.00 | 1.46        | 1.51     |
| 26  | c     | 5515 | DGD  | O4E-C4E | -2.00 | 1.38        | 1.43     |

All (1047) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|------|-------------|----------|
| 17  | a     | 5403 | CLA  | C4A-NA-C1A | 7.84 | 110.23      | 106.71   |
| 17  | A     | 402  | CLA  | C4A-NA-C1A | 7.73 | 110.18      | 106.71   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms      | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|------|-------------|----------|
| 17  | C     | 508  | CLA  | C4A-NA-C1A | 7.56 | 110.11      | 106.71   |
| 17  | c     | 5508 | CLA  | C4A-NA-C1A | 7.56 | 110.11      | 106.71   |
| 17  | b     | 5611 | CLA  | C4A-NA-C1A | 7.46 | 110.06      | 106.71   |
| 17  | B     | 607  | CLA  | C4A-NA-C1A | 7.43 | 110.05      | 106.71   |
| 17  | b     | 5607 | CLA  | C4A-NA-C1A | 7.38 | 110.02      | 106.71   |
| 17  | B     | 611  | CLA  | C4A-NA-C1A | 7.34 | 110.00      | 106.71   |
| 17  | C     | 511  | CLA  | C4A-NA-C1A | 7.32 | 110.00      | 106.71   |
| 17  | k     | 5501 | CLA  | C4A-NA-C1A | 7.25 | 109.96      | 106.71   |
| 17  | b     | 5615 | CLA  | C4A-NA-C1A | 7.24 | 109.96      | 106.71   |
| 17  | B     | 615  | CLA  | C4A-NA-C1A | 7.22 | 109.95      | 106.71   |
| 17  | b     | 5606 | CLA  | C4A-NA-C1A | 7.16 | 109.93      | 106.71   |
| 17  | A     | 405  | CLA  | C4A-NA-C1A | 7.06 | 109.88      | 106.71   |
| 17  | a     | 5406 | CLA  | C4A-NA-C1A | 7.06 | 109.88      | 106.71   |
| 17  | b     | 5614 | CLA  | C4A-NA-C1A | 7.06 | 109.88      | 106.71   |
| 17  | B     | 606  | CLA  | C4A-NA-C1A | 7.04 | 109.87      | 106.71   |
| 17  | C     | 501  | CLA  | C4A-NA-C1A | 7.04 | 109.87      | 106.71   |
| 17  | B     | 614  | CLA  | C4A-NA-C1A | 7.02 | 109.86      | 106.71   |
| 17  | B     | 613  | CLA  | C4A-NA-C1A | 6.99 | 109.85      | 106.71   |
| 17  | b     | 5612 | CLA  | C4A-NA-C1A | 6.96 | 109.83      | 106.71   |
| 17  | C     | 503  | CLA  | C4A-NA-C1A | 6.93 | 109.82      | 106.71   |
| 17  | c     | 5501 | CLA  | C4A-NA-C1A | 6.92 | 109.82      | 106.71   |
| 17  | c     | 5503 | CLA  | C4A-NA-C1A | 6.91 | 109.81      | 106.71   |
| 17  | A     | 403  | CLA  | C4A-NA-C1A | 6.89 | 109.80      | 106.71   |
| 17  | B     | 612  | CLA  | C4A-NA-C1A | 6.88 | 109.80      | 106.71   |
| 17  | b     | 5603 | CLA  | C4A-NA-C1A | 6.83 | 109.78      | 106.71   |
| 17  | B     | 603  | CLA  | C4A-NA-C1A | 6.82 | 109.77      | 106.71   |
| 17  | b     | 5613 | CLA  | C4A-NA-C1A | 6.79 | 109.76      | 106.71   |
| 17  | B     | 604  | CLA  | C4A-NA-C1A | 6.78 | 109.75      | 106.71   |
| 17  | B     | 610  | CLA  | C4A-NA-C1A | 6.73 | 109.73      | 106.71   |
| 17  | b     | 5604 | CLA  | C4A-NA-C1A | 6.72 | 109.72      | 106.71   |
| 17  | a     | 5404 | CLA  | C4A-NA-C1A | 6.71 | 109.72      | 106.71   |
| 17  | C     | 502  | CLA  | C4A-NA-C1A | 6.67 | 109.70      | 106.71   |
| 17  | b     | 5610 | CLA  | C4A-NA-C1A | 6.62 | 109.68      | 106.71   |
| 17  | b     | 5605 | CLA  | C4A-NA-C1A | 6.60 | 109.67      | 106.71   |
| 17  | b     | 5609 | CLA  | C4A-NA-C1A | 6.60 | 109.67      | 106.71   |
| 17  | B     | 609  | CLA  | C4A-NA-C1A | 6.59 | 109.67      | 106.71   |
| 17  | c     | 5502 | CLA  | C4A-NA-C1A | 6.59 | 109.67      | 106.71   |
| 17  | b     | 5602 | CLA  | C4A-NA-C1A | 6.54 | 109.65      | 106.71   |
| 17  | B     | 605  | CLA  | C4A-NA-C1A | 6.53 | 109.64      | 106.71   |
| 17  | c     | 5511 | CLA  | C4A-NA-C1A | 6.51 | 109.63      | 106.71   |
| 17  | C     | 506  | CLA  | C4A-NA-C1A | 6.50 | 109.63      | 106.71   |
| 17  | B     | 602  | CLA  | C4A-NA-C1A | 6.49 | 109.62      | 106.71   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | C     | 512  | CLA  | C4A-NA-C1A  | 6.47  | 109.61      | 106.71   |
| 17  | C     | 504  | CLA  | C4A-NA-C1A  | 6.45  | 109.61      | 106.71   |
| 17  | c     | 5504 | CLA  | C4A-NA-C1A  | 6.40  | 109.58      | 106.71   |
| 17  | c     | 5506 | CLA  | C4A-NA-C1A  | 6.39  | 109.58      | 106.71   |
| 17  | B     | 616  | CLA  | C4A-NA-C1A  | 6.37  | 109.57      | 106.71   |
| 17  | B     | 608  | CLA  | C4A-NA-C1A  | 6.35  | 109.56      | 106.71   |
| 17  | b     | 5608 | CLA  | C4A-NA-C1A  | 6.33  | 109.55      | 106.71   |
| 17  | d     | 5404 | CLA  | C4A-NA-C1A  | 6.32  | 109.55      | 106.71   |
| 17  | D     | 405  | CLA  | C4A-NA-C1A  | 6.31  | 109.54      | 106.71   |
| 17  | b     | 5616 | CLA  | C4A-NA-C1A  | 6.25  | 109.52      | 106.71   |
| 17  | C     | 510  | CLA  | C4A-NA-C1A  | 6.01  | 109.41      | 106.71   |
| 18  | a     | 5405 | PHO  | C4D-CHA-CBD | -5.99 | 105.81      | 108.52   |
| 17  | C     | 513  | CLA  | C4A-NA-C1A  | 5.98  | 109.40      | 106.71   |
| 17  | c     | 5512 | CLA  | C4A-NA-C1A  | 5.98  | 109.40      | 106.71   |
| 17  | c     | 5510 | CLA  | C4A-NA-C1A  | 5.91  | 109.36      | 106.71   |
| 18  | d     | 5402 | PHO  | C4D-CHA-CBD | -5.87 | 105.86      | 108.52   |
| 17  | C     | 507  | CLA  | C4A-NA-C1A  | 5.86  | 109.34      | 106.71   |
| 17  | c     | 5507 | CLA  | C4A-NA-C1A  | 5.83  | 109.33      | 106.71   |
| 18  | A     | 404  | PHO  | C4D-CHA-CBD | -5.82 | 105.88      | 108.52   |
| 18  | D     | 402  | PHO  | C4D-CHA-CBD | -5.79 | 105.90      | 108.52   |
| 17  | C     | 509  | CLA  | C4A-NA-C1A  | 5.59  | 109.22      | 106.71   |
| 17  | d     | 5403 | CLA  | C4A-NA-C1A  | 5.54  | 109.20      | 106.71   |
| 17  | c     | 5509 | CLA  | C4A-NA-C1A  | 5.52  | 109.19      | 106.71   |
| 17  | B     | 601  | CLA  | C4A-NA-C1A  | 5.50  | 109.18      | 106.71   |
| 17  | b     | 5601 | CLA  | C4A-NA-C1A  | 5.50  | 109.18      | 106.71   |
| 19  | d     | 5405 | PQ9  | C11-C12-C13 | -5.46 | 117.71      | 126.79   |
| 26  | b     | 5621 | DGD  | O3G-C3G-C2G | -5.46 | 97.73       | 110.90   |
| 17  | D     | 404  | CLA  | C4A-NA-C1A  | 5.45  | 109.16      | 106.71   |
| 26  | D     | 411  | DGD  | O3G-C3G-C2G | -5.45 | 97.75       | 110.90   |
| 19  | D     | 406  | PQ9  | C11-C12-C13 | -5.42 | 117.77      | 126.79   |
| 17  | c     | 5505 | CLA  | C4A-NA-C1A  | 5.36  | 109.11      | 106.71   |
| 17  | a     | 5402 | CLA  | C4A-NA-C1A  | 5.33  | 109.10      | 106.71   |
| 17  | A     | 401  | CLA  | C4A-NA-C1A  | 5.30  | 109.09      | 106.71   |
| 17  | C     | 505  | CLA  | C4A-NA-C1A  | 5.25  | 109.07      | 106.71   |
| 24  | A     | 411  | BCT  | O2-C-O1     | 5.06  | 132.66      | 119.55   |
| 24  | a     | 5412 | BCT  | O2-C-O1     | 5.05  | 132.66      | 119.55   |
| 23  | a     | 5401 | SQD  | O47-C7-C8   | 4.99  | 120.28      | 111.09   |
| 23  | A     | 410  | SQD  | O47-C7-C8   | 4.90  | 120.10      | 111.09   |
| 25  | d     | 5408 | MGE  | O2G-C1B-C2B | 4.79  | 121.83      | 111.50   |
| 17  | c     | 5502 | CLA  | C6-C5-C3    | -4.74 | 101.02      | 113.45   |
| 23  | l     | 5102 | SQD  | O7-S-C6     | 4.74  | 112.57      | 106.94   |
| 17  | C     | 502  | CLA  | C6-C5-C3    | -4.72 | 101.07      | 113.45   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23  | d     | 5407 | SQD  | O5-C5-C4    | 4.63  | 118.11      | 109.69   |
| 26  | c     | 5516 | DGD  | O3G-C3G-C2G | -4.62 | 99.75       | 110.90   |
| 26  | C     | 517  | DGD  | O3G-C3G-C2G | -4.61 | 99.78       | 110.90   |
| 23  | L     | 101  | SQD  | O8-S-C6     | 4.58  | 113.04      | 105.74   |
| 25  | B     | 619  | MGE  | O2G-C1B-C2B | 4.44  | 121.08      | 111.50   |
| 25  | b     | 5620 | MGE  | O2G-C1B-C2B | 4.44  | 121.08      | 111.50   |
| 25  | d     | 5410 | MGE  | O2G-C1B-C2B | 4.44  | 121.07      | 111.50   |
| 25  | D     | 410  | MGE  | O2G-C1B-C2B | 4.44  | 121.07      | 111.50   |
| 26  | a     | 5411 | DGD  | O3G-C3G-C2G | -4.44 | 100.20      | 110.90   |
| 25  | D     | 409  | MGE  | C3G-O3G-C1D | -4.42 | 105.10      | 113.74   |
| 26  | C     | 518  | DGD  | O3G-C3G-C2G | -4.40 | 100.27      | 110.90   |
| 23  | l     | 5102 | SQD  | O47-C7-C8   | 4.36  | 120.91      | 111.50   |
| 21  | A     | 408  | LHG  | O4-P-O5     | 4.29  | 133.45      | 112.24   |
| 21  | a     | 5409 | LHG  | O4-P-O5     | 4.29  | 133.45      | 112.24   |
| 20  | b     | 5618 | BCR  | C15-C14-C13 | -4.24 | 121.25      | 127.31   |
| 20  | B     | 618  | BCR  | C15-C14-C13 | -4.24 | 121.26      | 127.31   |
| 25  | D     | 409  | MGE  | O2G-C1B-C2B | 4.20  | 120.56      | 111.50   |
| 23  | L     | 101  | SQD  | O47-C7-C8   | 4.19  | 120.53      | 111.50   |
| 20  | b     | 5618 | BCR  | C15-C16-C17 | -4.12 | 115.03      | 123.47   |
| 23  | l     | 5102 | SQD  | O9-S-C6     | 4.11  | 111.83      | 106.94   |
| 20  | B     | 618  | BCR  | C15-C16-C17 | -4.10 | 115.07      | 123.47   |
| 25  | D     | 408  | MGE  | O2G-C1B-C2B | 4.08  | 120.29      | 111.50   |
| 25  | A     | 412  | MGE  | O2G-C1B-C2B | 4.02  | 120.17      | 111.50   |
| 25  | l     | 5101 | MGE  | O2G-C1B-C2B | 4.01  | 120.14      | 111.50   |
| 25  | D     | 410  | MGE  | C2G-O2G-C1B | -4.00 | 107.94      | 117.79   |
| 25  | d     | 5409 | MGE  | O2G-C1B-C2B | 3.89  | 119.88      | 111.50   |
| 26  | b     | 5621 | DGD  | O6D-C1D-O3G | -3.88 | 100.78      | 109.97   |
| 26  | D     | 411  | DGD  | O6D-C1D-O3G | -3.88 | 100.79      | 109.97   |
| 25  | d     | 5409 | MGE  | C3G-O3G-C1D | -3.86 | 106.20      | 113.74   |
| 23  | d     | 5407 | SQD  | O47-C7-C8   | 3.86  | 119.82      | 111.50   |
| 23  | d     | 5407 | SQD  | O7-S-C6     | 3.86  | 111.53      | 106.94   |
| 23  | D     | 403  | SQD  | O7-S-C6     | 3.82  | 111.48      | 106.94   |
| 25  | C     | 519  | MGE  | O2G-C1B-C2B | 3.80  | 119.69      | 111.50   |
| 25  | d     | 5410 | MGE  | C2G-O2G-C1B | -3.80 | 108.44      | 117.79   |
| 25  | c     | 5517 | MGE  | O2G-C1B-C2B | 3.80  | 119.68      | 111.50   |
| 23  | A     | 410  | SQD  | O7-S-C6     | 3.79  | 111.45      | 106.94   |
| 25  | m     | 5103 | MGE  | O2G-C1B-C2B | 3.79  | 119.67      | 111.50   |
| 25  | m     | 5101 | MGE  | O2G-C1B-C2B | 3.79  | 119.67      | 111.50   |
| 23  | l     | 5102 | SQD  | O9-S-O7     | -3.78 | 100.85      | 113.95   |
| 17  | C     | 505  | CLA  | CAA-C2A-C3A | -3.78 | 102.42      | 112.78   |
| 17  | c     | 5505 | CLA  | CAA-C2A-C3A | -3.77 | 102.45      | 112.78   |
| 20  | c     | 5513 | BCR  | C15-C16-C17 | -3.77 | 115.75      | 123.47   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23  | a     | 5401 | SQD  | O9-S-O7     | -3.77 | 100.91      | 113.95   |
| 20  | t     | 5101 | BCR  | C24-C23-C22 | -3.77 | 120.54      | 126.23   |
| 20  | b     | 5619 | BCR  | C24-C23-C22 | -3.77 | 120.55      | 126.23   |
| 20  | C     | 514  | BCR  | C15-C16-C17 | -3.76 | 115.78      | 123.47   |
| 19  | A     | 406  | PQ9  | C11-C2-C1   | 3.69  | 119.87      | 116.88   |
| 23  | L     | 101  | SQD  | O9-S-O7     | -3.66 | 101.27      | 113.95   |
| 23  | A     | 410  | SQD  | O9-S-O7     | -3.65 | 101.31      | 113.95   |
| 26  | C     | 518  | DGD  | O6D-C1D-O3G | -3.64 | 101.34      | 109.97   |
| 26  | a     | 5411 | DGD  | O6D-C1D-O3G | -3.64 | 101.34      | 109.97   |
| 23  | D     | 403  | SQD  | O5-C5-C4    | 3.61  | 116.25      | 109.69   |
| 23  | D     | 403  | SQD  | O47-C7-C8   | 3.60  | 119.26      | 111.50   |
| 19  | a     | 5407 | PQ9  | C11-C2-C1   | 3.60  | 119.80      | 116.88   |
| 20  | b     | 5617 | BCR  | C15-C16-C17 | -3.59 | 116.13      | 123.47   |
| 20  | B     | 617  | BCR  | C15-C16-C17 | -3.58 | 116.15      | 123.47   |
| 17  | D     | 404  | CLA  | C3B-C4B-NB  | -3.56 | 107.22      | 110.52   |
| 23  | d     | 5407 | SQD  | C3-C4-C5    | 3.56  | 116.58      | 110.24   |
| 17  | d     | 5403 | CLA  | C3B-C4B-NB  | -3.56 | 107.22      | 110.52   |
| 25  | A     | 412  | MGE  | C3G-O3G-C1D | -3.55 | 106.80      | 113.74   |
| 25  | l     | 5101 | MGE  | C3G-O3G-C1D | -3.55 | 106.80      | 113.74   |
| 22  | M     | 101  | LMT  | C1'-O5'-C5' | -3.53 | 106.75      | 113.69   |
| 17  | a     | 5402 | CLA  | C3B-C4B-NB  | -3.53 | 107.24      | 110.52   |
| 17  | B     | 609  | CLA  | C3B-C4B-NB  | -3.53 | 107.24      | 110.52   |
| 17  | A     | 401  | CLA  | C3B-C4B-NB  | -3.51 | 107.26      | 110.52   |
| 19  | d     | 5405 | PQ9  | C19-C18-C20 | 3.51  | 121.17      | 115.27   |
| 19  | D     | 406  | PQ9  | C19-C18-C20 | 3.50  | 121.16      | 115.27   |
| 17  | b     | 5609 | CLA  | C3B-C4B-NB  | -3.50 | 107.27      | 110.52   |
| 26  | c     | 5515 | DGD  | O6D-C1D-O3G | -3.49 | 101.70      | 109.97   |
| 26  | A     | 413  | DGD  | O6D-C1D-O3G | -3.48 | 101.72      | 109.97   |
| 17  | C     | 510  | CLA  | C3B-C4B-NB  | -3.45 | 107.31      | 110.52   |
| 20  | C     | 516  | BCR  | C15-C16-C17 | -3.44 | 116.42      | 123.47   |
| 20  | c     | 5514 | BCR  | C15-C16-C17 | -3.44 | 116.43      | 123.47   |
| 23  | a     | 5401 | SQD  | O7-S-C6     | 3.43  | 111.02      | 106.94   |
| 23  | d     | 5407 | SQD  | O9-S-O7     | -3.43 | 102.06      | 113.95   |
| 18  | d     | 5402 | PHO  | CBC-CAC-C3C | -3.43 | 107.86      | 112.88   |
| 22  | A     | 409  | LMT  | C1'-O5'-C5' | -3.42 | 106.97      | 113.69   |
| 26  | c     | 5516 | DGD  | O6D-C1D-O3G | -3.42 | 101.87      | 109.97   |
| 18  | D     | 402  | PHO  | CBC-CAC-C3C | -3.42 | 107.87      | 112.88   |
| 23  | D     | 403  | SQD  | O9-S-O7     | -3.41 | 102.14      | 113.95   |
| 26  | C     | 517  | DGD  | O6D-C1D-O3G | -3.40 | 101.93      | 109.97   |
| 20  | b     | 5617 | BCR  | C15-C14-C13 | -3.39 | 122.47      | 127.31   |
| 25  | d     | 5409 | MGE  | O1G-C1A-C2A | 3.39  | 122.56      | 111.91   |
| 22  | m     | 5102 | LMT  | C1'-O5'-C5' | -3.39 | 107.04      | 113.69   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 26  | a     | 5411 | DGD  | O5D-C6D-C5D | -3.38 | 102.79      | 109.05   |
| 19  | D     | 406  | PQ9  | C36-C37-C38 | -3.38 | 119.52      | 127.66   |
| 20  | B     | 617  | BCR  | C15-C14-C13 | -3.38 | 122.49      | 127.31   |
| 26  | C     | 518  | DGD  | O5D-C6D-C5D | -3.38 | 102.79      | 109.05   |
| 19  | d     | 5405 | PQ9  | C36-C37-C38 | -3.38 | 119.53      | 127.66   |
| 17  | c     | 5510 | CLA  | C3B-C4B-NB  | -3.37 | 107.39      | 110.52   |
| 20  | d     | 5406 | BCR  | C24-C23-C22 | -3.36 | 121.16      | 126.23   |
| 23  | L     | 101  | SQD  | O6-C1-C2    | 3.35  | 113.54      | 108.30   |
| 26  | C     | 517  | DGD  | O5D-C6D-C5D | -3.35 | 102.84      | 109.05   |
| 18  | D     | 402  | PHO  | C2B-C1B-NB  | -3.35 | 107.21      | 109.53   |
| 26  | c     | 5516 | DGD  | O5D-C6D-C5D | -3.35 | 102.84      | 109.05   |
| 20  | D     | 407  | BCR  | C24-C23-C22 | -3.34 | 121.19      | 126.23   |
| 17  | b     | 5611 | CLA  | C3B-C4B-NB  | -3.33 | 107.42      | 110.52   |
| 17  | a     | 5406 | CLA  | C3B-C4B-NB  | -3.33 | 107.43      | 110.52   |
| 23  | a     | 5401 | SQD  | O9-S-C6     | 3.33  | 110.89      | 106.94   |
| 25  | D     | 409  | MGE  | O1G-C1A-C2A | 3.32  | 122.33      | 111.91   |
| 17  | B     | 608  | CLA  | C3B-C4B-NB  | -3.31 | 107.44      | 110.52   |
| 18  | d     | 5402 | PHO  | C2B-C1B-NB  | -3.31 | 107.24      | 109.53   |
| 23  | l     | 5102 | SQD  | O5-C5-C4    | 3.30  | 115.69      | 109.69   |
| 17  | b     | 5608 | CLA  | C3B-C4B-NB  | -3.30 | 107.45      | 110.52   |
| 17  | c     | 5508 | CLA  | C1-C2-C3    | -3.28 | 120.37      | 126.04   |
| 17  | B     | 611  | CLA  | C3B-C4B-NB  | -3.28 | 107.48      | 110.52   |
| 18  | A     | 404  | PHO  | C2B-C1B-NB  | -3.27 | 107.27      | 109.53   |
| 18  | D     | 402  | PHO  | C1C-C2C-C3C | -3.27 | 105.89      | 108.61   |
| 17  | C     | 508  | CLA  | C1-C2-C3    | -3.27 | 120.40      | 126.04   |
| 17  | b     | 5609 | CLA  | C1-C2-C3    | -3.25 | 120.42      | 126.04   |
| 20  | k     | 5502 | BCR  | C24-C23-C22 | -3.25 | 121.33      | 126.23   |
| 17  | A     | 405  | CLA  | C3B-C4B-NB  | -3.25 | 107.50      | 110.52   |
| 17  | d     | 5404 | CLA  | C3B-C4B-NB  | -3.24 | 107.50      | 110.52   |
| 17  | B     | 609  | CLA  | C1-C2-C3    | -3.24 | 120.43      | 126.04   |
| 17  | b     | 5613 | CLA  | C3B-C4B-NB  | -3.24 | 107.51      | 110.52   |
| 20  | Y     | 101  | BCR  | C24-C23-C22 | -3.23 | 121.35      | 126.23   |
| 17  | b     | 5608 | CLA  | C1-C2-C3    | -3.22 | 120.47      | 126.04   |
| 19  | D     | 406  | PQ9  | C24-C23-C25 | 3.22  | 120.69      | 115.27   |
| 19  | d     | 5405 | PQ9  | C24-C23-C25 | 3.22  | 120.69      | 115.27   |
| 17  | B     | 608  | CLA  | C1-C2-C3    | -3.22 | 120.47      | 126.04   |
| 17  | C     | 503  | CLA  | C1-C2-C3    | -3.22 | 120.48      | 126.04   |
| 18  | a     | 5405 | PHO  | C2B-C1B-NB  | -3.22 | 107.31      | 109.53   |
| 17  | c     | 5503 | CLA  | C1-C2-C3    | -3.21 | 120.49      | 126.04   |
| 23  | l     | 5102 | SQD  | C1-O5-C5    | 3.21  | 119.99      | 113.69   |
| 20  | A     | 407  | BCR  | C15-C16-C17 | -3.21 | 116.91      | 123.47   |
| 17  | B     | 603  | CLA  | C3B-C4B-NB  | -3.21 | 107.54      | 110.52   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | D     | 405  | CLA  | C3B-C4B-NB  | -3.20 | 107.54      | 110.52   |
| 20  | a     | 5408 | BCR  | C15-C16-C17 | -3.20 | 116.92      | 123.47   |
| 25  | B     | 619  | MGE  | C2G-O2G-C1B | -3.20 | 109.92      | 117.79   |
| 23  | d     | 5407 | SQD  | C4-C3-C2    | 3.19  | 116.39      | 110.82   |
| 25  | b     | 5620 | MGE  | C2G-O2G-C1B | -3.18 | 109.95      | 117.79   |
| 17  | B     | 613  | CLA  | C3B-C4B-NB  | -3.18 | 107.57      | 110.52   |
| 23  | A     | 410  | SQD  | O8-S-C6     | 3.18  | 110.80      | 105.74   |
| 23  | A     | 410  | SQD  | C44-O6-C1   | 3.18  | 119.94      | 113.74   |
| 20  | H     | 101  | BCR  | C24-C23-C22 | -3.17 | 121.44      | 126.23   |
| 20  | z     | 5101 | BCR  | C15-C16-C17 | -3.17 | 116.97      | 123.47   |
| 18  | d     | 5402 | PHO  | C1C-C2C-C3C | -3.17 | 105.97      | 108.61   |
| 17  | b     | 5615 | CLA  | C3B-C4B-NB  | -3.16 | 107.58      | 110.52   |
| 20  | C     | 515  | BCR  | C15-C16-C17 | -3.16 | 117.00      | 123.47   |
| 17  | B     | 615  | CLA  | C3B-C4B-NB  | -3.16 | 107.59      | 110.52   |
| 23  | L     | 101  | SQD  | O9-S-C6     | 3.16  | 110.69      | 106.94   |
| 20  | h     | 5101 | BCR  | C24-C23-C22 | -3.15 | 121.47      | 126.23   |
| 17  | B     | 614  | CLA  | C3B-C4B-NB  | -3.15 | 107.59      | 110.52   |
| 26  | C     | 518  | DGD  | CDB-CCB-CBB | -3.14 | 98.48       | 114.42   |
| 17  | b     | 5614 | CLA  | C3B-C4B-NB  | -3.14 | 107.60      | 110.52   |
| 23  | d     | 5407 | SQD  | O8-S-C6     | 3.14  | 110.74      | 105.74   |
| 26  | a     | 5411 | DGD  | CDB-CCB-CBB | -3.14 | 98.50       | 114.42   |
| 19  | d     | 5405 | PQ9  | C31-C32-C33 | -3.13 | 120.13      | 127.66   |
| 17  | B     | 606  | CLA  | O2D-CGD-O1D | -3.12 | 117.73      | 123.84   |
| 19  | A     | 406  | PQ9  | C34-C33-C35 | 3.12  | 120.51      | 115.27   |
| 17  | b     | 5603 | CLA  | C3B-C4B-NB  | -3.12 | 107.62      | 110.52   |
| 17  | k     | 5501 | CLA  | C3B-C4B-NB  | -3.12 | 107.62      | 110.52   |
| 23  | a     | 5401 | SQD  | O8-S-C6     | 3.12  | 110.70      | 105.74   |
| 17  | b     | 5606 | CLA  | O2D-CGD-O1D | -3.11 | 117.75      | 123.84   |
| 19  | D     | 406  | PQ9  | C31-C32-C33 | -3.11 | 120.18      | 127.66   |
| 17  | B     | 606  | CLA  | C3B-C4B-NB  | -3.10 | 107.64      | 110.52   |
| 20  | c     | 5513 | BCR  | C15-C14-C13 | -3.09 | 122.89      | 127.31   |
| 17  | C     | 511  | CLA  | C3B-C4B-NB  | -3.09 | 107.65      | 110.52   |
| 17  | b     | 5610 | CLA  | C3B-C4B-NB  | -3.08 | 107.65      | 110.52   |
| 23  | a     | 5401 | SQD  | C44-O6-C1   | 3.08  | 119.75      | 113.74   |
| 17  | c     | 5511 | CLA  | C3B-C4B-NB  | -3.08 | 107.66      | 110.52   |
| 23  | A     | 410  | SQD  | O9-S-C6     | 3.08  | 110.60      | 106.94   |
| 20  | k     | 5502 | BCR  | C15-C16-C17 | -3.07 | 117.18      | 123.47   |
| 19  | D     | 406  | PQ9  | C21-C22-C23 | -3.07 | 120.27      | 127.66   |
| 20  | C     | 514  | BCR  | C15-C14-C13 | -3.07 | 122.93      | 127.31   |
| 17  | B     | 610  | CLA  | C3B-C4B-NB  | -3.06 | 107.67      | 110.52   |
| 19  | d     | 5405 | PQ9  | C21-C22-C23 | -3.06 | 120.29      | 127.66   |
| 17  | b     | 5606 | CLA  | C3B-C4B-NB  | -3.06 | 107.68      | 110.52   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | C     | 512  | CLA  | C3B-C4B-NB  | -3.05 | 107.68      | 110.52   |
| 17  | c     | 5503 | CLA  | C3B-C4B-NB  | -3.05 | 107.68      | 110.52   |
| 20  | b     | 5618 | BCR  | C35-C13-C14 | -3.04 | 118.66      | 122.92   |
| 17  | C     | 503  | CLA  | C3B-C4B-NB  | -3.04 | 107.70      | 110.52   |
| 20  | B     | 618  | BCR  | C35-C13-C14 | -3.03 | 118.68      | 122.92   |
| 17  | b     | 5611 | CLA  | C1-C2-C3    | -3.02 | 120.82      | 126.04   |
| 17  | c     | 5508 | CLA  | C3B-C4B-NB  | -3.01 | 107.72      | 110.52   |
| 17  | B     | 611  | CLA  | C1-C2-C3    | -3.00 | 120.85      | 126.04   |
| 20  | a     | 5408 | BCR  | C15-C14-C13 | -3.00 | 123.03      | 127.31   |
| 17  | C     | 504  | CLA  | C3B-C4B-NB  | -3.00 | 107.74      | 110.52   |
| 20  | Y     | 101  | BCR  | C15-C16-C17 | -2.99 | 117.35      | 123.47   |
| 26  | D     | 411  | DGD  | C3D-C4D-C5D | -2.98 | 104.93      | 110.24   |
| 17  | c     | 5504 | CLA  | C3B-C4B-NB  | -2.98 | 107.75      | 110.52   |
| 23  | D     | 403  | SQD  | C4-C3-C2    | 2.97  | 116.02      | 110.82   |
| 23  | D     | 403  | SQD  | O8-S-C6     | 2.97  | 110.48      | 105.74   |
| 17  | C     | 508  | CLA  | C3B-C4B-NB  | -2.97 | 107.76      | 110.52   |
| 17  | B     | 613  | CLA  | CHB-C4A-NA  | 2.97  | 128.61      | 124.51   |
| 20  | A     | 407  | BCR  | C15-C14-C13 | -2.96 | 123.08      | 127.31   |
| 25  | A     | 412  | MGE  | O1G-C1A-C2A | 2.96  | 121.18      | 111.91   |
| 26  | a     | 5411 | DGD  | O6E-C1E-O5D | -2.95 | 102.98      | 109.97   |
| 26  | C     | 518  | DGD  | O6E-C1E-O5D | -2.95 | 102.98      | 109.97   |
| 17  | b     | 5608 | CLA  | CHB-C1B-NB  | 2.95  | 127.38      | 124.26   |
| 26  | b     | 5621 | DGD  | C3D-C4D-C5D | -2.95 | 104.98      | 110.24   |
| 20  | h     | 5101 | BCR  | C7-C8-C9    | -2.94 | 121.79      | 126.23   |
| 25  | l     | 5101 | MGE  | O1G-C1A-C2A | 2.93  | 121.11      | 111.91   |
| 17  | b     | 5612 | CLA  | CHB-C4A-NA  | 2.93  | 128.57      | 124.51   |
| 17  | B     | 603  | CLA  | O2D-CGD-O1D | -2.93 | 118.11      | 123.84   |
| 17  | B     | 608  | CLA  | CHB-C1B-NB  | 2.93  | 127.35      | 124.26   |
| 20  | H     | 101  | BCR  | C7-C8-C9    | -2.93 | 121.81      | 126.23   |
| 17  | B     | 604  | CLA  | CHB-C1B-NB  | 2.92  | 127.35      | 124.26   |
| 17  | B     | 604  | CLA  | C3B-C4B-NB  | -2.92 | 107.81      | 110.52   |
| 18  | A     | 404  | PHO  | C1C-C2C-C3C | -2.92 | 106.18      | 108.61   |
| 17  | c     | 5502 | CLA  | C4-C3-C5    | 2.92  | 120.18      | 115.27   |
| 17  | B     | 612  | CLA  | CHB-C4A-NA  | 2.91  | 128.53      | 124.51   |
| 17  | b     | 5613 | CLA  | CHB-C4A-NA  | 2.90  | 128.53      | 124.51   |
| 17  | b     | 5603 | CLA  | O2D-CGD-O1D | -2.90 | 118.17      | 123.84   |
| 19  | D     | 406  | PQ9  | C6-C5-C4    | 2.90  | 120.91      | 114.99   |
| 25  | m     | 5101 | MGE  | C2G-O2G-C1B | -2.90 | 110.66      | 117.79   |
| 17  | C     | 505  | CLA  | O2D-CGD-O1D | -2.90 | 118.18      | 123.84   |
| 17  | b     | 5604 | CLA  | C3B-C4B-NB  | -2.90 | 107.83      | 110.52   |
| 17  | b     | 5612 | CLA  | C3B-C4B-NB  | -2.90 | 107.83      | 110.52   |
| 17  | c     | 5505 | CLA  | O2D-CGD-O1D | -2.89 | 118.18      | 123.84   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | b     | 5604 | CLA  | CHB-C1B-NB  | 2.89  | 127.32      | 124.26   |
| 25  | D     | 408  | MGE  | C2G-O2G-C1B | -2.89 | 110.67      | 117.79   |
| 19  | d     | 5405 | PQ9  | C6-C5-C4    | 2.89  | 120.90      | 114.99   |
| 25  | c     | 5517 | MGE  | C3G-O3G-C1D | -2.89 | 108.10      | 113.74   |
| 17  | B     | 616  | CLA  | C3B-C4B-NB  | -2.89 | 107.84      | 110.52   |
| 17  | C     | 502  | CLA  | C4-C3-C5    | 2.88  | 120.12      | 115.27   |
| 17  | B     | 612  | CLA  | C3B-C4B-NB  | -2.88 | 107.84      | 110.52   |
| 17  | C     | 506  | CLA  | C3B-C4B-NB  | -2.88 | 107.84      | 110.52   |
| 17  | c     | 5506 | CLA  | C3B-C4B-NB  | -2.88 | 107.84      | 110.52   |
| 25  | C     | 519  | MGE  | C3G-O3G-C1D | -2.88 | 108.12      | 113.74   |
| 17  | c     | 5511 | CLA  | O2D-CGD-O1D | -2.87 | 118.22      | 123.84   |
| 20  | T     | 102  | BCR  | C15-C16-C17 | -2.87 | 117.59      | 123.47   |
| 17  | c     | 5508 | CLA  | CHB-C4A-NA  | 2.87  | 128.48      | 124.51   |
| 17  | C     | 508  | CLA  | CHB-C4A-NA  | 2.87  | 128.48      | 124.51   |
| 20  | C     | 514  | BCR  | C33-C5-C6   | -2.87 | 121.31      | 124.53   |
| 17  | B     | 602  | CLA  | C3B-C4B-NB  | -2.87 | 107.86      | 110.52   |
| 17  | B     | 608  | CLA  | CMB-C2B-C1B | -2.86 | 121.01      | 125.37   |
| 26  | a     | 5411 | DGD  | C1D-C2D-C3D | -2.86 | 104.04      | 110.00   |
| 17  | C     | 509  | CLA  | C3B-C4B-NB  | -2.86 | 107.86      | 110.52   |
| 17  | a     | 5403 | CLA  | CHB-C4A-NA  | 2.86  | 128.46      | 124.51   |
| 17  | b     | 5611 | CLA  | CHB-C4A-NA  | 2.86  | 128.46      | 124.51   |
| 23  | d     | 5407 | SQD  | O48-C23-C24 | 2.86  | 120.87      | 111.91   |
| 19  | A     | 406  | PQ9  | C26-C27-C28 | -2.86 | 120.78      | 127.66   |
| 17  | b     | 5602 | CLA  | C3B-C4B-NB  | -2.86 | 107.87      | 110.52   |
| 17  | b     | 5608 | CLA  | CMB-C2B-C1B | -2.85 | 121.02      | 125.37   |
| 17  | C     | 512  | CLA  | O2D-CGD-O1D | -2.85 | 118.26      | 123.84   |
| 19  | A     | 406  | PQ9  | C11-C12-C13 | -2.85 | 122.04      | 126.79   |
| 26  | C     | 518  | DGD  | C1D-C2D-C3D | -2.85 | 104.05      | 110.00   |
| 26  | c     | 5515 | DGD  | O6D-C5D-C6D | -2.85 | 100.91      | 106.67   |
| 23  | D     | 403  | SQD  | C3-C4-C5    | 2.85  | 115.33      | 110.24   |
| 25  | m     | 5101 | MGE  | O1G-C1A-C2A | 2.85  | 120.85      | 111.91   |
| 17  | B     | 605  | CLA  | CHB-C4A-NA  | 2.84  | 128.44      | 124.51   |
| 17  | b     | 5605 | CLA  | CHB-C4A-NA  | 2.84  | 128.44      | 124.51   |
| 22  | B     | 620  | LMT  | C3'-C4'-C5' | -2.84 | 104.41      | 110.93   |
| 17  | b     | 5602 | CLA  | O2D-CGD-O1D | -2.84 | 118.28      | 123.84   |
| 18  | a     | 5405 | PHO  | C1C-C2C-C3C | -2.84 | 106.25      | 108.61   |
| 26  | A     | 413  | DGD  | O6D-C5D-C6D | -2.84 | 100.93      | 106.67   |
| 17  | A     | 405  | CLA  | CHB-C4A-NA  | 2.84  | 128.44      | 124.51   |
| 17  | c     | 5509 | CLA  | C3B-C4B-NB  | -2.84 | 107.88      | 110.52   |
| 20  | B     | 617  | BCR  | C11-C10-C9  | -2.84 | 123.26      | 127.31   |
| 18  | A     | 404  | PHO  | O1D-CGD-CBD | 2.83  | 129.46      | 124.74   |
| 17  | C     | 511  | CLA  | CHB-C4A-NA  | 2.83  | 128.42      | 124.51   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | A     | 402  | CLA  | CHB-C4A-NA  | 2.83  | 128.42      | 124.51   |
| 19  | a     | 5407 | PQ9  | C11-C12-C13 | -2.83 | 122.08      | 126.79   |
| 17  | k     | 5501 | CLA  | CHB-C4A-NA  | 2.82  | 128.42      | 124.51   |
| 17  | B     | 602  | CLA  | O2D-CGD-O1D | -2.82 | 118.32      | 123.84   |
| 20  | b     | 5617 | BCR  | C35-C13-C14 | -2.82 | 118.97      | 122.92   |
| 20  | b     | 5617 | BCR  | C11-C10-C9  | -2.82 | 123.28      | 127.31   |
| 17  | C     | 507  | CLA  | C3B-C4B-NB  | -2.82 | 107.90      | 110.52   |
| 17  | b     | 5616 | CLA  | C3B-C4B-NB  | -2.82 | 107.90      | 110.52   |
| 20  | B     | 617  | BCR  | C7-C8-C9    | -2.82 | 121.98      | 126.23   |
| 25  | C     | 519  | MGE  | O1G-C1A-C2A | 2.81  | 120.74      | 111.91   |
| 17  | B     | 607  | CLA  | CHB-C4A-NA  | 2.81  | 128.40      | 124.51   |
| 25  | c     | 5517 | MGE  | O1G-C1A-C2A | 2.81  | 120.72      | 111.91   |
| 17  | A     | 402  | CLA  | O2D-CGD-O1D | -2.81 | 118.35      | 123.84   |
| 17  | b     | 5604 | CLA  | C1-C2-C3    | -2.81 | 121.19      | 126.04   |
| 20  | B     | 617  | BCR  | C35-C13-C14 | -2.80 | 119.00      | 122.92   |
| 18  | a     | 5405 | PHO  | O1D-CGD-CBD | 2.80  | 129.41      | 124.74   |
| 20  | b     | 5617 | BCR  | C7-C8-C9    | -2.80 | 122.01      | 126.23   |
| 17  | a     | 5403 | CLA  | O2D-CGD-O1D | -2.79 | 118.38      | 123.84   |
| 17  | B     | 611  | CLA  | CHB-C4A-NA  | 2.79  | 128.38      | 124.51   |
| 17  | c     | 5507 | CLA  | CAC-C3C-C4C | 2.79  | 128.43      | 124.81   |
| 17  | B     | 605  | CLA  | C3B-C4B-NB  | -2.79 | 107.92      | 110.52   |
| 17  | a     | 5406 | CLA  | CHB-C4A-NA  | 2.79  | 128.37      | 124.51   |
| 17  | B     | 604  | CLA  | C1-C2-C3    | -2.79 | 121.22      | 126.04   |
| 17  | C     | 507  | CLA  | CAC-C3C-C4C | 2.79  | 128.43      | 124.81   |
| 23  | D     | 403  | SQD  | O6-C1-C2    | 2.79  | 112.66      | 108.30   |
| 20  | c     | 5513 | BCR  | C33-C5-C6   | -2.79 | 121.40      | 124.53   |
| 17  | b     | 5607 | CLA  | CHB-C4A-NA  | 2.79  | 128.37      | 124.51   |
| 17  | c     | 5507 | CLA  | C3B-C4B-NB  | -2.78 | 107.93      | 110.52   |
| 17  | b     | 5605 | CLA  | C3B-C4B-NB  | -2.78 | 107.93      | 110.52   |
| 17  | B     | 610  | CLA  | CHB-C4A-NA  | 2.78  | 128.36      | 124.51   |
| 17  | B     | 607  | CLA  | O2D-CGD-O1D | -2.77 | 118.42      | 123.84   |
| 17  | b     | 5601 | CLA  | CAA-C2A-C3A | -2.77 | 109.63      | 116.10   |
| 25  | D     | 409  | MGE  | C2G-O2G-C1B | -2.77 | 110.97      | 117.79   |
| 17  | B     | 601  | CLA  | CAA-C2A-C3A | -2.77 | 109.64      | 116.10   |
| 17  | C     | 505  | CLA  | O2A-CGA-O1A | -2.76 | 116.61      | 123.59   |
| 17  | c     | 5505 | CLA  | O2A-CGA-O1A | -2.76 | 116.61      | 123.59   |
| 19  | a     | 5407 | PQ9  | C14-C13-C15 | 2.76  | 119.92      | 115.27   |
| 25  | D     | 409  | MGE  | O3G-C1D-C2D | 2.76  | 112.61      | 108.30   |
| 19  | A     | 406  | PQ9  | C39-C38-C40 | 2.76  | 119.91      | 115.27   |
| 26  | A     | 413  | DGD  | O3G-C3G-C2G | -2.75 | 104.25      | 110.90   |
| 17  | b     | 5610 | CLA  | CHB-C4A-NA  | 2.75  | 128.32      | 124.51   |
| 20  | D     | 407  | BCR  | C15-C14-C13 | -2.75 | 123.38      | 127.31   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 20  | b     | 5618 | BCR  | C27-C26-C25 | 2.75  | 126.73      | 122.73   |
| 17  | B     | 608  | CLA  | O2D-CGD-O1D | -2.75 | 118.46      | 123.84   |
| 20  | B     | 618  | BCR  | C27-C26-C25 | 2.75  | 126.72      | 122.73   |
| 26  | c     | 5515 | DGD  | O3G-C3G-C2G | -2.75 | 104.27      | 110.90   |
| 20  | T     | 102  | BCR  | C27-C26-C25 | 2.75  | 126.72      | 122.73   |
| 17  | b     | 5607 | CLA  | O2D-CGD-O1D | -2.74 | 118.47      | 123.84   |
| 19  | A     | 406  | PQ9  | C14-C13-C15 | 2.74  | 119.89      | 115.27   |
| 17  | d     | 5403 | CLA  | O2D-CGD-O1D | -2.74 | 118.48      | 123.84   |
| 20  | d     | 5406 | BCR  | C33-C5-C6   | -2.74 | 121.46      | 124.53   |
| 20  | d     | 5406 | BCR  | C15-C14-C13 | -2.73 | 123.42      | 127.31   |
| 22  | a     | 5410 | LMT  | C1'-O5'-C5' | -2.72 | 108.34      | 113.69   |
| 17  | b     | 5608 | CLA  | O2D-CGD-O1D | -2.72 | 118.51      | 123.84   |
| 17  | b     | 5604 | CLA  | O2A-CGA-O1A | -2.72 | 116.72      | 123.59   |
| 17  | B     | 604  | CLA  | O2A-CGA-O1A | -2.72 | 116.72      | 123.59   |
| 17  | B     | 612  | CLA  | O2D-CGD-O1D | -2.72 | 118.52      | 123.84   |
| 19  | A     | 406  | PQ9  | C11-C2-C3   | -2.72 | 119.72      | 123.30   |
| 19  | a     | 5407 | PQ9  | C11-C2-C3   | -2.72 | 119.73      | 123.30   |
| 17  | C     | 505  | CLA  | C3B-C4B-NB  | -2.71 | 108.00      | 110.52   |
| 17  | C     | 511  | CLA  | O2D-CGD-O1D | -2.71 | 118.54      | 123.84   |
| 24  | a     | 5412 | BCT  | O3-C-O1     | -2.71 | 112.52      | 119.55   |
| 20  | t     | 5101 | BCR  | C11-C10-C9  | -2.71 | 123.45      | 127.31   |
| 20  | D     | 407  | BCR  | C33-C5-C6   | -2.71 | 121.49      | 124.53   |
| 17  | D     | 404  | CLA  | O2D-CGD-O1D | -2.71 | 118.55      | 123.84   |
| 17  | B     | 614  | CLA  | O2D-CGD-O1D | -2.70 | 118.55      | 123.84   |
| 24  | A     | 411  | BCT  | O3-C-O1     | -2.70 | 112.54      | 119.55   |
| 25  | B     | 619  | MGE  | O1G-C1A-C2A | 2.70  | 120.38      | 111.91   |
| 23  | l     | 5102 | SQD  | O48-C23-C24 | 2.70  | 120.38      | 111.91   |
| 17  | k     | 5501 | CLA  | O2D-CGD-O1D | -2.70 | 118.56      | 123.84   |
| 17  | C     | 501  | CLA  | O2D-CGD-O1D | -2.70 | 118.57      | 123.84   |
| 20  | c     | 5514 | BCR  | C15-C14-C13 | -2.70 | 123.46      | 127.31   |
| 17  | b     | 5612 | CLA  | O2D-CGD-O1D | -2.69 | 118.57      | 123.84   |
| 25  | d     | 5410 | MGE  | O1G-C1A-C2A | 2.69  | 120.36      | 111.91   |
| 17  | c     | 5505 | CLA  | C3B-C4B-NB  | -2.69 | 108.02      | 110.52   |
| 25  | b     | 5620 | MGE  | O1G-C1A-C2A | 2.69  | 120.34      | 111.91   |
| 26  | C     | 517  | DGD  | C3D-C4D-C5D | -2.69 | 105.45      | 110.24   |
| 20  | C     | 516  | BCR  | C15-C14-C13 | -2.68 | 123.48      | 127.31   |
| 25  | d     | 5409 | MGE  | C3G-C2G-C1G | -2.68 | 105.44      | 111.79   |
| 19  | D     | 406  | PQ9  | C26-C27-C28 | -2.68 | 121.20      | 127.66   |
| 20  | b     | 5619 | BCR  | C11-C10-C9  | -2.68 | 123.48      | 127.31   |
| 19  | d     | 5405 | PQ9  | C26-C27-C28 | -2.68 | 121.20      | 127.66   |
| 20  | A     | 407  | BCR  | C24-C23-C22 | -2.68 | 122.19      | 126.23   |
| 25  | d     | 5408 | MGE  | O1G-C1A-C2A | 2.68  | 120.31      | 111.91   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | A     | 403  | CLA  | O2D-CGD-O1D | -2.68 | 118.61      | 123.84   |
| 26  | A     | 413  | DGD  | O3E-C3E-C2E | -2.68 | 104.16      | 110.35   |
| 17  | a     | 5404 | CLA  | O2D-CGD-O1D | -2.67 | 118.61      | 123.84   |
| 17  | d     | 5403 | CLA  | C2D-C1D-ND  | -2.67 | 108.13      | 110.10   |
| 17  | B     | 606  | CLA  | CHB-C4A-NA  | 2.67  | 128.21      | 124.51   |
| 17  | b     | 5606 | CLA  | CHB-C4A-NA  | 2.67  | 128.21      | 124.51   |
| 20  | h     | 5101 | BCR  | C33-C5-C6   | -2.67 | 121.53      | 124.53   |
| 17  | c     | 5501 | CLA  | O2D-CGD-O1D | -2.67 | 118.61      | 123.84   |
| 17  | b     | 5614 | CLA  | CHB-C4A-NA  | 2.67  | 128.21      | 124.51   |
| 17  | C     | 510  | CLA  | CHB-C1B-NB  | 2.67  | 127.08      | 124.26   |
| 17  | b     | 5614 | CLA  | O2D-CGD-O1D | -2.67 | 118.62      | 123.84   |
| 17  | C     | 501  | CLA  | CHB-C4A-NA  | 2.67  | 128.20      | 124.51   |
| 19  | A     | 406  | PQ9  | C19-C18-C20 | 2.67  | 119.76      | 115.27   |
| 26  | c     | 5515 | DGD  | O3E-C3E-C2E | -2.67 | 104.18      | 110.35   |
| 17  | c     | 5507 | CLA  | O2D-CGD-O1D | -2.66 | 118.63      | 123.84   |
| 26  | c     | 5516 | DGD  | C3D-C4D-C5D | -2.66 | 105.49      | 110.24   |
| 23  | D     | 403  | SQD  | O48-C23-C24 | 2.66  | 120.27      | 111.91   |
| 20  | H     | 101  | BCR  | C33-C5-C6   | -2.66 | 121.54      | 124.53   |
| 19  | a     | 5407 | PQ9  | C19-C18-C20 | 2.66  | 119.75      | 115.27   |
| 17  | C     | 507  | CLA  | O2D-CGD-O1D | -2.66 | 118.64      | 123.84   |
| 17  | c     | 5503 | CLA  | CAA-C2A-C3A | -2.66 | 105.50      | 112.78   |
| 19  | a     | 5407 | PQ9  | C6-C5-C4    | 2.65  | 120.41      | 114.99   |
| 17  | D     | 404  | CLA  | C2D-C1D-ND  | -2.65 | 108.15      | 110.10   |
| 17  | B     | 608  | CLA  | CHB-C4A-NA  | 2.65  | 128.18      | 124.51   |
| 17  | A     | 405  | CLA  | O2D-CGD-O1D | -2.65 | 118.66      | 123.84   |
| 19  | A     | 406  | PQ9  | C6-C5-C4    | 2.65  | 120.41      | 114.99   |
| 19  | d     | 5405 | PQ9  | C39-C38-C40 | 2.65  | 119.72      | 115.27   |
| 17  | C     | 503  | CLA  | CAA-C2A-C3A | -2.65 | 105.53      | 112.78   |
| 17  | B     | 614  | CLA  | CHB-C4A-NA  | 2.65  | 128.17      | 124.51   |
| 19  | D     | 406  | PQ9  | C39-C38-C40 | 2.65  | 119.72      | 115.27   |
| 18  | a     | 5405 | PHO  | CMB-C2B-C3B | 2.64  | 129.62      | 124.68   |
| 20  | a     | 5408 | BCR  | C24-C23-C22 | -2.64 | 122.24      | 126.23   |
| 20  | t     | 5102 | BCR  | C27-C26-C25 | 2.64  | 126.56      | 122.73   |
| 17  | C     | 509  | CLA  | O2A-CGA-O1A | -2.64 | 116.94      | 123.59   |
| 17  | c     | 5509 | CLA  | O2A-CGA-O1A | -2.64 | 116.94      | 123.59   |
| 17  | c     | 5501 | CLA  | CHB-C4A-NA  | 2.64  | 128.16      | 124.51   |
| 17  | B     | 613  | CLA  | O2D-CGD-O1D | -2.63 | 118.70      | 123.84   |
| 17  | b     | 5616 | CLA  | O2D-CGD-O1D | -2.63 | 118.70      | 123.84   |
| 20  | h     | 5101 | BCR  | C27-C26-C25 | 2.63  | 126.55      | 122.73   |
| 20  | C     | 514  | BCR  | C24-C23-C22 | -2.63 | 122.26      | 126.23   |
| 17  | B     | 611  | CLA  | O2D-CGD-O1D | -2.63 | 118.70      | 123.84   |
| 18  | A     | 404  | PHO  | CMB-C2B-C3B | 2.63  | 129.59      | 124.68   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | b     | 5613 | CLA  | O2D-CGD-O1D | -2.62 | 118.71      | 123.84   |
| 17  | B     | 616  | CLA  | O2D-CGD-O1D | -2.62 | 118.72      | 123.84   |
| 20  | H     | 101  | BCR  | C27-C26-C25 | 2.62  | 126.53      | 122.73   |
| 17  | a     | 5406 | CLA  | O2D-CGD-O1D | -2.62 | 118.72      | 123.84   |
| 20  | t     | 5101 | BCR  | C33-C5-C6   | -2.62 | 121.59      | 124.53   |
| 20  | t     | 5102 | BCR  | C33-C5-C6   | -2.62 | 121.59      | 124.53   |
| 18  | d     | 5402 | PHO  | CMB-C2B-C3B | 2.62  | 129.57      | 124.68   |
| 22  | m     | 5102 | LMT  | C3B-C4B-C5B | -2.61 | 105.58      | 110.24   |
| 17  | B     | 607  | CLA  | C3B-C4B-NB  | -2.61 | 108.09      | 110.52   |
| 17  | b     | 5608 | CLA  | CHC-C4B-NB  | 2.61  | 127.02      | 124.26   |
| 19  | D     | 406  | PQ9  | C29-C28-C30 | 2.61  | 119.66      | 115.27   |
| 17  | b     | 5610 | CLA  | CHB-C1B-NB  | 2.61  | 127.02      | 124.26   |
| 17  | b     | 5608 | CLA  | CHB-C4A-NA  | 2.61  | 128.12      | 124.51   |
| 17  | C     | 502  | CLA  | C3B-C4B-NB  | -2.61 | 108.09      | 110.52   |
| 17  | b     | 5607 | CLA  | C3B-C4B-NB  | -2.61 | 108.10      | 110.52   |
| 20  | a     | 5408 | BCR  | C33-C5-C6   | -2.61 | 121.60      | 124.53   |
| 17  | b     | 5611 | CLA  | O2D-CGD-O1D | -2.61 | 118.74      | 123.84   |
| 17  | c     | 5502 | CLA  | C3B-C4B-NB  | -2.61 | 108.10      | 110.52   |
| 20  | c     | 5513 | BCR  | C24-C23-C22 | -2.61 | 122.30      | 126.23   |
| 17  | c     | 5510 | CLA  | CHB-C1B-NB  | 2.60  | 127.01      | 124.26   |
| 17  | b     | 5606 | CLA  | CAA-C2A-C3A | -2.60 | 107.76      | 114.26   |
| 17  | a     | 5402 | CLA  | CAA-C2A-C1A | -2.60 | 103.46      | 111.97   |
| 26  | c     | 5516 | DGD  | C4E-C3E-C2E | -2.60 | 106.29      | 110.82   |
| 18  | D     | 402  | PHO  | CMB-C2B-C3B | 2.60  | 129.53      | 124.68   |
| 17  | A     | 401  | CLA  | CAA-C2A-C1A | -2.59 | 103.48      | 111.97   |
| 17  | b     | 5616 | CLA  | CHB-C1B-NB  | 2.59  | 127.00      | 124.26   |
| 23  | d     | 5407 | SQD  | O6-C1-C2    | 2.59  | 112.34      | 108.30   |
| 17  | B     | 610  | CLA  | CHB-C1B-NB  | 2.59  | 127.00      | 124.26   |
| 17  | C     | 513  | CLA  | C3B-C4B-NB  | -2.59 | 108.11      | 110.52   |
| 17  | b     | 5615 | CLA  | CHB-C1B-NB  | 2.59  | 126.99      | 124.26   |
| 20  | A     | 407  | BCR  | C33-C5-C6   | -2.58 | 121.63      | 124.53   |
| 17  | d     | 5404 | CLA  | CHB-C4A-NA  | 2.58  | 128.08      | 124.51   |
| 19  | d     | 5405 | PQ9  | C29-C28-C30 | 2.58  | 119.61      | 115.27   |
| 20  | C     | 515  | BCR  | C33-C5-C6   | -2.58 | 121.63      | 124.53   |
| 20  | t     | 5101 | BCR  | C27-C26-C25 | 2.58  | 126.47      | 122.73   |
| 20  | b     | 5619 | BCR  | C33-C5-C6   | -2.57 | 121.64      | 124.53   |
| 20  | k     | 5502 | BCR  | C33-C5-C6   | -2.57 | 121.64      | 124.53   |
| 18  | d     | 5402 | PHO  | C1-C2-C3    | -2.57 | 121.60      | 126.04   |
| 17  | B     | 616  | CLA  | CHB-C1B-NB  | 2.57  | 126.98      | 124.26   |
| 17  | C     | 504  | CLA  | O2D-CGD-O1D | -2.57 | 118.81      | 123.84   |
| 17  | D     | 404  | CLA  | CHB-C1B-NB  | 2.57  | 126.98      | 124.26   |
| 26  | C     | 517  | DGD  | C4E-C3E-C2E | -2.57 | 106.34      | 110.82   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | c     | 5501 | CLA  | C3B-C4B-NB  | -2.57 | 108.13      | 110.52   |
| 17  | c     | 5504 | CLA  | O2D-CGD-O1D | -2.57 | 118.82      | 123.84   |
| 17  | c     | 5512 | CLA  | C3B-C4B-NB  | -2.56 | 108.14      | 110.52   |
| 17  | A     | 403  | CLA  | CHB-C4A-NA  | 2.56  | 128.06      | 124.51   |
| 20  | b     | 5619 | BCR  | C27-C26-C25 | 2.56  | 126.45      | 122.73   |
| 17  | B     | 615  | CLA  | CHB-C1B-NB  | 2.56  | 126.96      | 124.26   |
| 18  | d     | 5402 | PHO  | O2D-CGD-O1D | -2.55 | 118.85      | 123.84   |
| 17  | D     | 405  | CLA  | CHB-C4A-NA  | 2.55  | 128.04      | 124.51   |
| 23  | l     | 5102 | SQD  | C4-C3-C2    | 2.55  | 115.27      | 110.82   |
| 20  | c     | 5514 | BCR  | C7-C8-C9    | -2.55 | 122.39      | 126.23   |
| 23  | L     | 101  | SQD  | C4-C3-C2    | 2.55  | 115.27      | 110.82   |
| 20  | z     | 5101 | BCR  | C33-C5-C6   | -2.54 | 121.67      | 124.53   |
| 18  | D     | 402  | PHO  | O2D-CGD-O1D | -2.54 | 118.86      | 123.84   |
| 18  | D     | 402  | PHO  | C1-C2-C3    | -2.54 | 121.64      | 126.04   |
| 17  | b     | 5615 | CLA  | CHB-C4A-NA  | 2.54  | 128.03      | 124.51   |
| 17  | b     | 5609 | CLA  | CHB-C4A-NA  | 2.54  | 128.02      | 124.51   |
| 26  | c     | 5516 | DGD  | C3G-C2G-C1G | -2.54 | 105.78      | 111.79   |
| 23  | L     | 101  | SQD  | O48-C23-O10 | -2.54 | 117.19      | 123.59   |
| 17  | B     | 608  | CLA  | CHC-C4B-NB  | 2.53  | 126.94      | 124.26   |
| 17  | a     | 5406 | CLA  | CHB-C1B-NB  | 2.53  | 126.94      | 124.26   |
| 26  | C     | 518  | DGD  | C3G-C2G-C1G | -2.53 | 105.80      | 111.79   |
| 17  | C     | 501  | CLA  | C3B-C4B-NB  | -2.53 | 108.17      | 110.52   |
| 26  | C     | 517  | DGD  | C3G-C2G-C1G | -2.53 | 105.81      | 111.79   |
| 26  | a     | 5411 | DGD  | C3G-C2G-C1G | -2.53 | 105.81      | 111.79   |
| 17  | d     | 5403 | CLA  | CHB-C1B-NB  | 2.52  | 126.93      | 124.26   |
| 17  | a     | 5404 | CLA  | CHB-C4A-NA  | 2.52  | 128.00      | 124.51   |
| 20  | C     | 516  | BCR  | C7-C8-C9    | -2.52 | 122.43      | 126.23   |
| 17  | A     | 405  | CLA  | CHB-C1B-NB  | 2.52  | 126.92      | 124.26   |
| 20  | C     | 516  | BCR  | C11-C10-C9  | -2.52 | 123.72      | 127.31   |
| 17  | B     | 609  | CLA  | CHB-C4A-NA  | 2.52  | 127.99      | 124.51   |
| 17  | B     | 616  | CLA  | CHB-C4A-NA  | 2.51  | 127.99      | 124.51   |
| 17  | b     | 5616 | CLA  | CHB-C4A-NA  | 2.51  | 127.99      | 124.51   |
| 20  | c     | 5514 | BCR  | C11-C10-C9  | -2.51 | 123.72      | 127.31   |
| 17  | C     | 502  | CLA  | CHB-C4A-NA  | 2.51  | 127.99      | 124.51   |
| 17  | B     | 605  | CLA  | C1-C2-C3    | -2.51 | 121.70      | 126.04   |
| 17  | B     | 615  | CLA  | CHC-C4B-NB  | 2.51  | 126.91      | 124.26   |
| 20  | A     | 407  | BCR  | C27-C26-C25 | 2.51  | 126.37      | 122.73   |
| 17  | B     | 601  | CLA  | C2A-C1A-CHA | 2.50  | 128.22      | 123.85   |
| 20  | C     | 515  | BCR  | C15-C14-C13 | -2.50 | 123.74      | 127.31   |
| 23  | l     | 5102 | SQD  | C44-O6-C1   | 2.50  | 118.63      | 113.74   |
| 17  | C     | 506  | CLA  | O2D-CGD-O1D | -2.50 | 118.94      | 123.84   |
| 17  | C     | 501  | CLA  | C1-C2-C3    | -2.50 | 121.72      | 126.04   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 20  | c     | 5514 | BCR  | C33-C5-C6   | -2.50 | 121.72      | 124.53   |
| 17  | c     | 5506 | CLA  | O2D-CGD-O1D | -2.50 | 118.95      | 123.84   |
| 17  | b     | 5601 | CLA  | C2A-C1A-CHA | 2.50  | 128.21      | 123.85   |
| 20  | b     | 5617 | BCR  | C27-C26-C25 | 2.50  | 126.36      | 122.73   |
| 23  | L     | 101  | SQD  | O7-S-C6     | 2.50  | 109.91      | 106.94   |
| 26  | b     | 5621 | DGD  | C4E-C3E-C2E | -2.50 | 106.47      | 110.82   |
| 17  | B     | 615  | CLA  | CHB-C4A-NA  | 2.49  | 127.96      | 124.51   |
| 26  | D     | 411  | DGD  | C4E-C3E-C2E | -2.49 | 106.48      | 110.82   |
| 17  | c     | 5511 | CLA  | CHB-C4A-NA  | 2.49  | 127.95      | 124.51   |
| 17  | A     | 403  | CLA  | C3B-C4B-NB  | -2.49 | 108.21      | 110.52   |
| 17  | c     | 5502 | CLA  | CHB-C4A-NA  | 2.48  | 127.94      | 124.51   |
| 20  | z     | 5101 | BCR  | C27-C26-C25 | 2.48  | 126.33      | 122.73   |
| 17  | C     | 501  | CLA  | O2A-CGA-O1A | -2.48 | 117.33      | 123.59   |
| 20  | z     | 5101 | BCR  | C15-C14-C13 | -2.48 | 123.77      | 127.31   |
| 17  | b     | 5605 | CLA  | O2D-CGD-O1D | -2.48 | 118.99      | 123.84   |
| 17  | C     | 506  | CLA  | CHB-C4A-NA  | 2.48  | 127.94      | 124.51   |
| 23  | L     | 101  | SQD  | C44-O6-C1   | 2.47  | 118.57      | 113.74   |
| 17  | A     | 403  | CLA  | CHB-C1B-NB  | 2.47  | 126.88      | 124.26   |
| 17  | b     | 5605 | CLA  | C1-C2-C3    | -2.47 | 121.77      | 126.04   |
| 17  | b     | 5604 | CLA  | O2D-CGD-O1D | -2.47 | 119.00      | 123.84   |
| 17  | B     | 605  | CLA  | O2D-CGD-O1D | -2.47 | 119.01      | 123.84   |
| 17  | c     | 5501 | CLA  | O2A-CGA-O1A | -2.47 | 117.36      | 123.59   |
| 17  | B     | 603  | CLA  | CHB-C1B-NB  | 2.47  | 126.87      | 124.26   |
| 17  | a     | 5404 | CLA  | C3B-C4B-NB  | -2.47 | 108.22      | 110.52   |
| 17  | B     | 605  | CLA  | CHD-C1D-ND  | -2.47 | 122.18      | 124.45   |
| 17  | c     | 5501 | CLA  | C1-C2-C3    | -2.47 | 121.77      | 126.04   |
| 17  | C     | 511  | CLA  | CHB-C1B-NB  | 2.47  | 126.87      | 124.26   |
| 17  | C     | 512  | CLA  | CHB-C4A-NA  | 2.47  | 127.92      | 124.51   |
| 17  | a     | 5403 | CLA  | C1-C2-C3    | -2.47 | 121.78      | 126.04   |
| 23  | d     | 5407 | SQD  | C44-O6-C1   | 2.46  | 118.55      | 113.74   |
| 25  | D     | 408  | MGE  | O1G-C1A-C2A | 2.46  | 119.64      | 111.91   |
| 17  | c     | 5507 | CLA  | CHB-C1B-NB  | 2.46  | 126.86      | 124.26   |
| 17  | A     | 401  | CLA  | CHB-C1B-NB  | 2.46  | 126.86      | 124.26   |
| 17  | b     | 5615 | CLA  | CHC-C4B-NB  | 2.46  | 126.86      | 124.26   |
| 17  | A     | 402  | CLA  | C1-C2-C3    | -2.46 | 121.79      | 126.04   |
| 19  | A     | 406  | PQ9  | C31-C32-C33 | -2.46 | 121.74      | 127.66   |
| 17  | C     | 507  | CLA  | CHB-C1B-NB  | 2.46  | 126.86      | 124.26   |
| 17  | a     | 5404 | CLA  | CHB-C1B-NB  | 2.46  | 126.86      | 124.26   |
| 20  | C     | 515  | BCR  | C11-C10-C9  | -2.46 | 123.80      | 127.31   |
| 17  | c     | 5506 | CLA  | CHB-C4A-NA  | 2.46  | 127.91      | 124.51   |
| 17  | k     | 5501 | CLA  | CHB-C1B-NB  | 2.46  | 126.86      | 124.26   |
| 17  | c     | 5508 | CLA  | CHC-C4B-NB  | 2.46  | 126.86      | 124.26   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 20  | B     | 617  | BCR  | C27-C26-C25 | 2.45  | 126.29      | 122.73   |
| 20  | a     | 5408 | BCR  | C27-C26-C25 | 2.45  | 126.29      | 122.73   |
| 17  | B     | 604  | CLA  | O2D-CGD-O1D | -2.45 | 119.05      | 123.84   |
| 17  | d     | 5404 | CLA  | O2D-CGD-O1D | -2.45 | 119.05      | 123.84   |
| 19  | d     | 5405 | PQ9  | C16-C17-C18 | -2.45 | 121.76      | 127.66   |
| 17  | C     | 509  | CLA  | O2D-CGD-O1D | -2.45 | 119.06      | 123.84   |
| 17  | a     | 5402 | CLA  | CHB-C1B-NB  | 2.44  | 126.84      | 124.26   |
| 17  | b     | 5603 | CLA  | CHB-C1B-NB  | 2.44  | 126.84      | 124.26   |
| 17  | B     | 603  | CLA  | CHC-C4B-NB  | 2.44  | 126.84      | 124.26   |
| 21  | A     | 408  | LHG  | O8-C23-C24  | 2.44  | 119.57      | 111.91   |
| 20  | C     | 516  | BCR  | C33-C5-C6   | -2.44 | 121.79      | 124.53   |
| 17  | b     | 5606 | CLA  | O2D-CGD-CBD | 2.44  | 115.61      | 111.27   |
| 20  | D     | 407  | BCR  | C15-C16-C17 | -2.44 | 118.47      | 123.47   |
| 20  | z     | 5101 | BCR  | C11-C10-C9  | -2.44 | 123.83      | 127.31   |
| 19  | A     | 406  | PQ9  | C29-C28-C30 | 2.44  | 119.38      | 115.27   |
| 26  | c     | 5515 | DGD  | O2D-C2D-C1D | -2.44 | 104.12      | 110.05   |
| 17  | c     | 5503 | CLA  | CHB-C1B-NB  | 2.44  | 126.84      | 124.26   |
| 19  | D     | 406  | PQ9  | C16-C17-C18 | -2.44 | 121.79      | 127.66   |
| 20  | d     | 5406 | BCR  | C27-C26-C25 | 2.44  | 126.27      | 122.73   |
| 17  | D     | 405  | CLA  | O2D-CGD-O1D | -2.44 | 119.08      | 123.84   |
| 26  | A     | 413  | DGD  | O2D-C2D-C1D | -2.43 | 104.13      | 110.05   |
| 23  | D     | 403  | SQD  | O9-S-C6     | 2.43  | 109.83      | 106.94   |
| 17  | B     | 606  | CLA  | O2D-CGD-CBD | 2.43  | 115.59      | 111.27   |
| 20  | C     | 515  | BCR  | C27-C26-C25 | 2.43  | 126.26      | 122.73   |
| 17  | C     | 513  | CLA  | C1-C2-C3    | -2.43 | 122.82      | 126.75   |
| 17  | C     | 508  | CLA  | CHC-C4B-NB  | 2.43  | 126.83      | 124.26   |
| 21  | a     | 5409 | LHG  | O8-C23-C24  | 2.43  | 119.54      | 111.91   |
| 17  | c     | 5511 | CLA  | CHB-C1B-NB  | 2.43  | 126.83      | 124.26   |
| 17  | C     | 507  | CLA  | CHB-C4A-NA  | 2.43  | 127.87      | 124.51   |
| 17  | C     | 501  | CLA  | CHC-C4B-NB  | 2.43  | 126.83      | 124.26   |
| 17  | c     | 5509 | CLA  | O2D-CGD-O1D | -2.43 | 119.09      | 123.84   |
| 25  | d     | 5409 | MGE  | O6D-C5D-C4D | 2.43  | 114.10      | 109.69   |
| 17  | b     | 5605 | CLA  | CHD-C1D-ND  | -2.43 | 122.22      | 124.45   |
| 17  | C     | 503  | CLA  | CHB-C1B-NB  | 2.43  | 126.83      | 124.26   |
| 20  | T     | 102  | BCR  | C15-C14-C13 | -2.42 | 123.85      | 127.31   |
| 17  | c     | 5512 | CLA  | C1-C2-C3    | -2.42 | 122.83      | 126.75   |
| 17  | b     | 5615 | CLA  | O2A-CGA-O1A | -2.42 | 117.48      | 123.59   |
| 20  | d     | 5406 | BCR  | C15-C16-C17 | -2.42 | 118.52      | 123.47   |
| 17  | C     | 505  | CLA  | CAC-C3C-C4C | 2.42  | 127.95      | 124.81   |
| 17  | D     | 405  | CLA  | C1-C2-C3    | -2.42 | 122.84      | 126.75   |
| 17  | c     | 5501 | CLA  | CHC-C4B-NB  | 2.42  | 126.82      | 124.26   |
| 17  | c     | 5505 | CLA  | CAC-C3C-C4C | 2.42  | 127.94      | 124.81   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | B     | 615  | CLA  | O2A-CGA-O1A | -2.41 | 117.50      | 123.59   |
| 20  | t     | 5101 | BCR  | C8-C7-C6    | -2.41 | 120.43      | 127.20   |
| 20  | b     | 5617 | BCR  | C33-C5-C6   | -2.41 | 121.82      | 124.53   |
| 17  | c     | 5507 | CLA  | CHB-C4A-NA  | 2.41  | 127.84      | 124.51   |
| 17  | B     | 609  | CLA  | CHB-C1B-NB  | 2.41  | 126.81      | 124.26   |
| 17  | D     | 405  | CLA  | CHB-C1B-NB  | 2.41  | 126.80      | 124.26   |
| 23  | L     | 101  | SQD  | O48-C23-C24 | 2.40  | 119.45      | 111.91   |
| 17  | B     | 606  | CLA  | CHB-C1B-NB  | 2.40  | 126.80      | 124.26   |
| 17  | d     | 5404 | CLA  | C1-C2-C3    | -2.40 | 122.86      | 126.75   |
| 17  | c     | 5508 | CLA  | O2D-CGD-O1D | -2.40 | 119.14      | 123.84   |
| 17  | c     | 5509 | CLA  | CHB-C4A-NA  | 2.40  | 127.83      | 124.51   |
| 17  | C     | 508  | CLA  | O2D-CGD-O1D | -2.40 | 119.14      | 123.84   |
| 20  | b     | 5619 | BCR  | C8-C7-C6    | -2.40 | 120.46      | 127.20   |
| 17  | b     | 5609 | CLA  | CHD-C1D-ND  | -2.40 | 122.25      | 124.45   |
| 17  | b     | 5606 | CLA  | CHC-C4B-NB  | 2.40  | 126.79      | 124.26   |
| 17  | B     | 604  | CLA  | CHB-C4A-NA  | 2.40  | 127.83      | 124.51   |
| 17  | b     | 5604 | CLA  | CHB-C4A-NA  | 2.40  | 127.83      | 124.51   |
| 17  | B     | 610  | CLA  | O2D-CGD-O1D | -2.40 | 119.15      | 123.84   |
| 20  | D     | 407  | BCR  | C27-C26-C25 | 2.40  | 126.21      | 122.73   |
| 20  | t     | 5102 | BCR  | C15-C14-C13 | -2.39 | 123.89      | 127.31   |
| 17  | b     | 5606 | CLA  | CHB-C1B-NB  | 2.39  | 126.79      | 124.26   |
| 17  | b     | 5611 | CLA  | CHB-C1B-NB  | 2.39  | 126.79      | 124.26   |
| 17  | B     | 606  | CLA  | CHC-C4B-NB  | 2.39  | 126.79      | 124.26   |
| 20  | B     | 617  | BCR  | C33-C5-C6   | -2.39 | 121.84      | 124.53   |
| 17  | B     | 611  | CLA  | CHB-C1B-NB  | 2.39  | 126.79      | 124.26   |
| 17  | c     | 5505 | CLA  | CHB-C4A-NA  | 2.39  | 127.81      | 124.51   |
| 17  | b     | 5610 | CLA  | O2D-CGD-O1D | -2.39 | 119.17      | 123.84   |
| 17  | C     | 503  | CLA  | CHB-C4A-NA  | 2.38  | 127.81      | 124.51   |
| 17  | b     | 5603 | CLA  | CHC-C4B-NB  | 2.38  | 126.78      | 124.26   |
| 17  | C     | 509  | CLA  | CHB-C4A-NA  | 2.38  | 127.81      | 124.51   |
| 17  | B     | 609  | CLA  | CHD-C1D-ND  | -2.38 | 122.27      | 124.45   |
| 20  | b     | 5618 | BCR  | C24-C23-C22 | -2.38 | 122.64      | 126.23   |
| 17  | d     | 5403 | CLA  | CHB-C4A-NA  | 2.38  | 127.80      | 124.51   |
| 20  | C     | 514  | BCR  | C27-C26-C25 | 2.38  | 126.19      | 122.73   |
| 17  | B     | 603  | CLA  | CHB-C4A-NA  | 2.38  | 127.80      | 124.51   |
| 17  | C     | 512  | CLA  | CHB-C1B-NB  | 2.37  | 126.77      | 124.26   |
| 17  | c     | 5512 | CLA  | O2D-CGD-O1D | -2.37 | 119.20      | 123.84   |
| 20  | c     | 5513 | BCR  | C7-C8-C9    | -2.37 | 122.65      | 126.23   |
| 17  | c     | 5502 | CLA  | CHC-C4B-NB  | 2.37  | 126.77      | 124.26   |
| 20  | D     | 407  | BCR  | C7-C8-C9    | -2.37 | 122.66      | 126.23   |
| 29  | f     | 5101 | HEM  | CHC-C1C-NC  | 2.37  | 127.00      | 124.44   |
| 17  | b     | 5603 | CLA  | O2A-CGA-O1A | -2.37 | 117.61      | 123.59   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | d     | 5404 | CLA  | CHB-C1B-NB  | 2.37  | 126.76      | 124.26   |
| 17  | B     | 603  | CLA  | O2A-CGA-O1A | -2.37 | 117.62      | 123.59   |
| 25  | m     | 5103 | MGE  | O1G-C1A-C2A | 2.37  | 119.33      | 111.91   |
| 20  | c     | 5513 | BCR  | C27-C26-C25 | 2.37  | 126.17      | 122.73   |
| 17  | c     | 5503 | CLA  | CHB-C4A-NA  | 2.36  | 127.78      | 124.51   |
| 17  | C     | 502  | CLA  | CHC-C4B-NB  | 2.36  | 126.76      | 124.26   |
| 18  | A     | 404  | PHO  | O2D-CGD-O1D | -2.36 | 119.22      | 123.84   |
| 17  | C     | 513  | CLA  | O2D-CGD-O1D | -2.36 | 119.22      | 123.84   |
| 17  | D     | 404  | CLA  | CHB-C4A-NA  | 2.36  | 127.78      | 124.51   |
| 18  | a     | 5405 | PHO  | O2D-CGD-O1D | -2.36 | 119.22      | 123.84   |
| 25  | D     | 410  | MGE  | O1G-C1A-C2A | 2.36  | 119.31      | 111.91   |
| 20  | t     | 5101 | BCR  | C38-C26-C25 | -2.36 | 121.88      | 124.53   |
| 19  | A     | 406  | PQ9  | C45-C43-C44 | 2.36  | 119.81      | 114.60   |
| 20  | h     | 5101 | BCR  | C16-C15-C14 | -2.36 | 118.64      | 123.47   |
| 20  | b     | 5619 | BCR  | C38-C26-C25 | -2.36 | 121.88      | 124.53   |
| 18  | d     | 5402 | PHO  | O1D-CGD-CBD | 2.36  | 128.66      | 124.74   |
| 17  | b     | 5609 | CLA  | CHB-C1B-NB  | 2.36  | 126.75      | 124.26   |
| 20  | H     | 101  | BCR  | C16-C15-C14 | -2.35 | 118.65      | 123.47   |
| 20  | C     | 514  | BCR  | C7-C8-C9    | -2.35 | 122.68      | 126.23   |
| 17  | C     | 505  | CLA  | CHB-C4A-NA  | 2.35  | 127.77      | 124.51   |
| 17  | b     | 5603 | CLA  | CHB-C4A-NA  | 2.35  | 127.76      | 124.51   |
| 20  | B     | 618  | BCR  | C24-C23-C22 | -2.35 | 122.69      | 126.23   |
| 17  | b     | 5605 | CLA  | CHB-C1B-NB  | 2.35  | 126.74      | 124.26   |
| 20  | c     | 5514 | BCR  | C24-C23-C22 | -2.34 | 122.69      | 126.23   |
| 20  | d     | 5406 | BCR  | C7-C8-C9    | -2.34 | 122.70      | 126.23   |
| 26  | C     | 518  | DGD  | C6D-O5D-C1E | 2.34  | 118.31      | 113.74   |
| 26  | a     | 5411 | DGD  | C6D-O5D-C1E | 2.34  | 118.31      | 113.74   |
| 25  | l     | 5101 | MGE  | C2G-O2G-C1B | -2.34 | 112.04      | 117.79   |
| 25  | A     | 412  | MGE  | C2G-O2G-C1B | -2.34 | 112.04      | 117.79   |
| 17  | b     | 5601 | CLA  | O2D-CGD-O1D | -2.34 | 119.27      | 123.84   |
| 17  | B     | 605  | CLA  | CHB-C1B-NB  | 2.33  | 126.72      | 124.26   |
| 17  | A     | 403  | CLA  | C1-C2-C3    | -2.33 | 122.01      | 126.04   |
| 20  | t     | 5101 | BCR  | C15-C14-C13 | -2.33 | 123.99      | 127.31   |
| 17  | B     | 601  | CLA  | O2D-CGD-O1D | -2.33 | 119.29      | 123.84   |
| 17  | a     | 5404 | CLA  | C1-C2-C3    | -2.32 | 122.02      | 126.04   |
| 17  | C     | 503  | CLA  | O2A-CGA-O1A | -2.32 | 117.73      | 123.59   |
| 20  | C     | 516  | BCR  | C24-C23-C22 | -2.32 | 122.72      | 126.23   |
| 17  | B     | 610  | CLA  | O2A-CGA-O1A | -2.32 | 117.73      | 123.59   |
| 18  | D     | 402  | PHO  | O1D-CGD-CBD | 2.32  | 128.60      | 124.74   |
| 17  | c     | 5504 | CLA  | CHD-C1D-ND  | -2.32 | 122.32      | 124.45   |
| 17  | c     | 5503 | CLA  | O2A-CGA-O1A | -2.32 | 117.74      | 123.59   |
| 17  | B     | 611  | CLA  | O2A-CGA-O1A | -2.31 | 117.75      | 123.59   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | b     | 5615 | CLA  | C1-C2-C3    | -2.31 | 122.04      | 126.04   |
| 20  | b     | 5619 | BCR  | C15-C14-C13 | -2.31 | 124.01      | 127.31   |
| 17  | C     | 504  | CLA  | CHD-C1D-ND  | -2.31 | 122.33      | 124.45   |
| 17  | B     | 613  | CLA  | CAA-CBA-CGA | -2.31 | 106.49      | 113.25   |
| 23  | l     | 5102 | SQD  | C3-C4-C5    | 2.31  | 114.36      | 110.24   |
| 21  | A     | 408  | LHG  | C27-C26-C25 | -2.31 | 102.69      | 114.42   |
| 17  | a     | 5402 | CLA  | CHC-C4B-NB  | 2.31  | 126.70      | 124.26   |
| 17  | A     | 401  | CLA  | CAA-CBA-CGA | -2.31 | 106.50      | 113.25   |
| 21  | a     | 5409 | LHG  | C27-C26-C25 | -2.31 | 102.70      | 114.42   |
| 22  | T     | 101  | LMT  | C3'-C4'-C5' | -2.31 | 105.63      | 110.93   |
| 17  | B     | 610  | CLA  | CMB-C2B-C1B | -2.31 | 121.85      | 125.37   |
| 23  | D     | 403  | SQD  | C44-O6-C1   | 2.31  | 118.25      | 113.74   |
| 29  | F     | 101  | HEM  | CHC-C1C-NC  | 2.31  | 126.93      | 124.44   |
| 17  | C     | 513  | CLA  | O2A-CGA-O1A | -2.30 | 117.78      | 123.59   |
| 17  | C     | 510  | CLA  | CHB-C4A-NA  | 2.30  | 127.70      | 124.51   |
| 20  | C     | 515  | BCR  | C24-C23-C22 | -2.30 | 122.76      | 126.23   |
| 20  | A     | 407  | BCR  | C2-C1-C6    | 2.30  | 114.02      | 110.48   |
| 20  | Y     | 101  | BCR  | C27-C26-C25 | 2.30  | 126.07      | 122.73   |
| 23  | L     | 101  | SQD  | O5-C5-C4    | 2.30  | 113.87      | 109.69   |
| 17  | b     | 5610 | CLA  | CMB-C2B-C1B | -2.30 | 121.87      | 125.37   |
| 17  | C     | 508  | CLA  | CHB-C1B-NB  | 2.30  | 126.69      | 124.26   |
| 17  | b     | 5611 | CLA  | O2A-CGA-O1A | -2.30 | 117.80      | 123.59   |
| 17  | c     | 5508 | CLA  | CHB-C1B-NB  | 2.30  | 126.69      | 124.26   |
| 17  | b     | 5610 | CLA  | O2A-CGA-O1A | -2.30 | 117.80      | 123.59   |
| 23  | a     | 5401 | SQD  | O5-C5-C4    | 2.29  | 113.86      | 109.69   |
| 20  | a     | 5408 | BCR  | C2-C1-C6    | 2.29  | 114.01      | 110.48   |
| 17  | a     | 5402 | CLA  | CAA-CBA-CGA | -2.29 | 106.56      | 113.25   |
| 17  | b     | 5613 | CLA  | CAA-CBA-CGA | -2.29 | 106.56      | 113.25   |
| 17  | b     | 5613 | CLA  | C1-C2-C3    | -2.29 | 122.08      | 126.04   |
| 26  | C     | 518  | DGD  | CBB-CAB-C9B | -2.29 | 102.80      | 114.42   |
| 26  | a     | 5411 | DGD  | CBB-CAB-C9B | -2.29 | 102.80      | 114.42   |
| 20  | T     | 102  | BCR  | C40-C30-C25 | 2.29  | 114.01      | 110.30   |
| 17  | b     | 5613 | CLA  | C2D-C1D-ND  | -2.29 | 108.42      | 110.10   |
| 17  | C     | 513  | CLA  | CHB-C4A-NA  | 2.29  | 127.67      | 124.51   |
| 17  | c     | 5512 | CLA  | O2A-CGA-O1A | -2.28 | 117.83      | 123.59   |
| 17  | C     | 509  | CLA  | CHC-C4B-NB  | 2.28  | 126.67      | 124.26   |
| 17  | B     | 609  | CLA  | O2D-CGD-O1D | -2.28 | 119.38      | 123.84   |
| 26  | C     | 518  | DGD  | O6D-C5D-C6D | -2.28 | 102.07      | 106.67   |
| 17  | B     | 613  | CLA  | C1-C2-C3    | -2.28 | 122.11      | 126.04   |
| 17  | B     | 602  | CLA  | CHB-C4A-NA  | 2.27  | 127.66      | 124.51   |
| 17  | A     | 401  | CLA  | CHC-C4B-NB  | 2.27  | 126.66      | 124.26   |
| 19  | D     | 406  | PQ9  | C41-C42-C43 | -2.27 | 119.99      | 127.75   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 20  | Y     | 101  | BCR  | C33-C5-C6   | -2.27 | 121.98      | 124.53   |
| 20  | z     | 5101 | BCR  | C24-C23-C22 | -2.27 | 122.80      | 126.23   |
| 17  | c     | 5512 | CLA  | CHB-C4A-NA  | 2.27  | 127.65      | 124.51   |
| 19  | d     | 5405 | PQ9  | C41-C42-C43 | -2.27 | 120.00      | 127.75   |
| 17  | C     | 508  | CLA  | O2A-CGA-O1A | -2.27 | 117.87      | 123.59   |
| 20  | T     | 102  | BCR  | C30-C25-C26 | -2.27 | 119.42      | 122.61   |
| 17  | B     | 613  | CLA  | CHB-C1B-NB  | 2.27  | 126.66      | 124.26   |
| 29  | f     | 5101 | HEM  | C4C-NC-C1C  | 2.26  | 107.56      | 105.35   |
| 17  | A     | 402  | CLA  | C3B-C4B-NB  | -2.26 | 108.42      | 110.52   |
| 26  | b     | 5621 | DGD  | C3G-C2G-C1G | -2.26 | 106.44      | 111.79   |
| 17  | b     | 5602 | CLA  | CHB-C4A-NA  | 2.26  | 127.64      | 124.51   |
| 17  | c     | 5504 | CLA  | CHB-C4A-NA  | 2.26  | 127.64      | 124.51   |
| 17  | B     | 615  | CLA  | C1-C2-C3    | -2.26 | 122.14      | 126.04   |
| 29  | f     | 5101 | HEM  | C4D-ND-C1D  | 2.26  | 107.41      | 105.07   |
| 25  | d     | 5408 | MGE  | C2G-O2G-C1B | -2.26 | 112.23      | 117.79   |
| 17  | C     | 503  | CLA  | CHC-C4B-NB  | 2.26  | 126.65      | 124.26   |
| 25  | d     | 5410 | MGE  | O2G-C1B-O1B | -2.26 | 118.25      | 123.70   |
| 17  | b     | 5612 | CLA  | CMB-C2B-C1B | -2.26 | 121.93      | 125.37   |
| 17  | C     | 511  | CLA  | C1-C2-C3    | -2.26 | 122.14      | 126.04   |
| 17  | B     | 614  | CLA  | CHB-C1B-NB  | 2.26  | 126.64      | 124.26   |
| 17  | A     | 403  | CLA  | CHC-C4B-NB  | 2.25  | 126.64      | 124.26   |
| 17  | c     | 5509 | CLA  | CHC-C4B-NB  | 2.25  | 126.64      | 124.26   |
| 20  | b     | 5617 | BCR  | C20-C21-C22 | -2.25 | 124.09      | 127.31   |
| 17  | C     | 505  | CLA  | CHC-C4B-NB  | 2.25  | 126.64      | 124.26   |
| 26  | D     | 411  | DGD  | C3G-C2G-C1G | -2.25 | 106.46      | 111.79   |
| 17  | B     | 604  | CLA  | CHC-C4B-NB  | 2.25  | 126.64      | 124.26   |
| 17  | C     | 504  | CLA  | CHB-C4A-NA  | 2.25  | 127.63      | 124.51   |
| 17  | b     | 5613 | CLA  | CHB-C1B-NB  | 2.25  | 126.64      | 124.26   |
| 20  | B     | 617  | BCR  | C20-C21-C22 | -2.25 | 124.10      | 127.31   |
| 19  | A     | 406  | PQ9  | C36-C37-C38 | -2.25 | 122.25      | 127.66   |
| 17  | B     | 602  | CLA  | C2D-C1D-ND  | -2.25 | 108.45      | 110.10   |
| 17  | b     | 5614 | CLA  | CHB-C1B-NB  | 2.25  | 126.63      | 124.26   |
| 25  | m     | 5101 | MGE  | C3G-O3G-C1D | -2.25 | 109.35      | 113.74   |
| 20  | C     | 514  | BCR  | C11-C10-C9  | -2.24 | 124.11      | 127.31   |
| 20  | k     | 5502 | BCR  | C27-C26-C25 | 2.24  | 125.98      | 122.73   |
| 20  | z     | 5101 | BCR  | C8-C7-C6    | -2.24 | 120.91      | 127.20   |
| 17  | b     | 5609 | CLA  | O2D-CGD-O1D | -2.24 | 119.46      | 123.84   |
| 26  | a     | 5411 | DGD  | O6D-C5D-C6D | -2.24 | 102.14      | 106.67   |
| 17  | C     | 506  | CLA  | CHB-C1B-NB  | 2.24  | 126.63      | 124.26   |
| 25  | D     | 409  | MGE  | C3G-C2G-C1G | -2.24 | 106.49      | 111.79   |
| 17  | c     | 5508 | CLA  | O2A-CGA-O1A | -2.24 | 117.94      | 123.59   |
| 17  | b     | 5604 | CLA  | CHC-C4B-NB  | 2.24  | 126.63      | 124.26   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | C     | 503  | CLA  | O2D-CGD-O1D | -2.24 | 119.46      | 123.84   |
| 17  | c     | 5510 | CLA  | CHB-C4A-NA  | 2.23  | 127.60      | 124.51   |
| 17  | k     | 5501 | CLA  | C1-C2-C3    | -2.23 | 122.18      | 126.04   |
| 17  | A     | 402  | CLA  | CHB-C1B-NB  | 2.23  | 126.62      | 124.26   |
| 17  | B     | 613  | CLA  | C2D-C1D-ND  | -2.23 | 108.46      | 110.10   |
| 26  | c     | 5515 | DGD  | O6E-C1E-O5D | -2.23 | 104.69      | 109.97   |
| 20  | C     | 515  | BCR  | C8-C7-C6    | -2.23 | 120.94      | 127.20   |
| 17  | c     | 5506 | CLA  | CHB-C1B-NB  | 2.23  | 126.62      | 124.26   |
| 17  | a     | 5403 | CLA  | C3B-C4B-NB  | -2.22 | 108.45      | 110.52   |
| 17  | c     | 5505 | CLA  | CHB-C1B-NB  | 2.22  | 126.61      | 124.26   |
| 17  | C     | 510  | CLA  | O2A-CGA-O1A | -2.22 | 117.99      | 123.59   |
| 17  | B     | 614  | CLA  | C1-C2-C3    | -2.22 | 122.21      | 126.04   |
| 17  | c     | 5505 | CLA  | CHC-C4B-NB  | 2.22  | 126.61      | 124.26   |
| 17  | B     | 612  | CLA  | CMB-C2B-C1B | -2.22 | 121.99      | 125.37   |
| 17  | b     | 5609 | CLA  | O2A-CGA-O1A | -2.22 | 118.00      | 123.59   |
| 17  | a     | 5404 | CLA  | C2D-C1D-ND  | -2.22 | 108.47      | 110.10   |
| 17  | a     | 5404 | CLA  | CHC-C4B-NB  | 2.22  | 126.60      | 124.26   |
| 17  | c     | 5503 | CLA  | O2D-CGD-O1D | -2.22 | 119.50      | 123.84   |
| 20  | c     | 5513 | BCR  | C11-C10-C9  | -2.22 | 124.15      | 127.31   |
| 17  | B     | 609  | CLA  | O2A-CGA-O1A | -2.21 | 118.00      | 123.59   |
| 29  | F     | 101  | HEM  | C4D-ND-C1D  | 2.21  | 107.36      | 105.07   |
| 17  | C     | 513  | CLA  | CHB-C1B-NB  | 2.21  | 126.60      | 124.26   |
| 17  | B     | 605  | CLA  | CHC-C4B-NB  | 2.21  | 126.60      | 124.26   |
| 17  | b     | 5616 | CLA  | CMB-C2B-C1B | -2.21 | 122.00      | 125.37   |
| 17  | c     | 5506 | CLA  | CAA-C2A-C3A | -2.21 | 106.72      | 112.78   |
| 17  | b     | 5608 | CLA  | CMB-C2B-C3B | 2.21  | 131.94      | 126.59   |
| 17  | c     | 5510 | CLA  | O2A-CGA-O1A | -2.21 | 118.01      | 123.59   |
| 26  | A     | 413  | DGD  | O6E-C1E-O5D | -2.21 | 104.74      | 109.97   |
| 17  | a     | 5403 | CLA  | CHB-C1B-NB  | 2.21  | 126.60      | 124.26   |
| 17  | b     | 5614 | CLA  | C1-C2-C3    | -2.21 | 122.23      | 126.04   |
| 17  | b     | 5602 | CLA  | C2D-C1D-ND  | -2.21 | 108.48      | 110.10   |
| 17  | b     | 5605 | CLA  | CHC-C4B-NB  | 2.20  | 126.59      | 124.26   |
| 17  | b     | 5612 | CLA  | CHB-C1B-NB  | 2.20  | 126.59      | 124.26   |
| 17  | A     | 402  | CLA  | CHC-C4B-NB  | 2.20  | 126.59      | 124.26   |
| 19  | d     | 5405 | PQ9  | C14-C13-C15 | 2.20  | 118.98      | 115.27   |
| 17  | a     | 5402 | CLA  | CAA-C2A-C3A | -2.20 | 106.75      | 112.78   |
| 23  | A     | 410  | SQD  | O5-C5-C4    | 2.20  | 113.69      | 109.69   |
| 29  | F     | 101  | HEM  | C4C-NC-C1C  | 2.20  | 107.50      | 105.35   |
| 20  | t     | 5101 | BCR  | C16-C15-C14 | -2.20 | 118.97      | 123.47   |
| 17  | B     | 616  | CLA  | CMB-C2B-C1B | -2.20 | 122.02      | 125.37   |
| 17  | c     | 5503 | CLA  | CHC-C4B-NB  | 2.20  | 126.58      | 124.26   |
| 17  | C     | 506  | CLA  | CAA-C2A-C3A | -2.20 | 106.77      | 112.78   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 19  | a     | 5407 | PQ9  | C24-C23-C25 | 2.19  | 118.96      | 115.27   |
| 17  | b     | 5614 | CLA  | CHC-C4B-NB  | 2.19  | 126.58      | 124.26   |
| 19  | a     | 5407 | PQ9  | C16-C17-C18 | -2.19 | 122.38      | 127.66   |
| 20  | b     | 5619 | BCR  | C16-C15-C14 | -2.19 | 118.99      | 123.47   |
| 17  | B     | 608  | CLA  | CMB-C2B-C3B | 2.19  | 131.89      | 126.59   |
| 19  | A     | 406  | PQ9  | C24-C23-C25 | 2.19  | 118.95      | 115.27   |
| 20  | C     | 515  | BCR  | C35-C13-C14 | -2.19 | 119.86      | 122.92   |
| 20  | t     | 5102 | BCR  | C30-C25-C26 | -2.19 | 119.53      | 122.61   |
| 17  | B     | 614  | CLA  | CHC-C4B-NB  | 2.19  | 126.57      | 124.26   |
| 20  | T     | 102  | BCR  | C33-C5-C6   | -2.19 | 122.07      | 124.53   |
| 20  | c     | 5514 | BCR  | C28-C27-C26 | -2.19 | 110.17      | 114.08   |
| 17  | C     | 502  | CLA  | CHB-C1B-NB  | 2.18  | 126.57      | 124.26   |
| 17  | C     | 513  | CLA  | CHC-C4B-NB  | 2.18  | 126.56      | 124.26   |
| 20  | z     | 5101 | BCR  | C35-C13-C14 | -2.18 | 119.87      | 122.92   |
| 19  | D     | 406  | PQ9  | C34-C33-C35 | 2.18  | 118.94      | 115.27   |
| 19  | A     | 406  | PQ9  | C16-C17-C18 | -2.18 | 122.42      | 127.66   |
| 18  | a     | 5405 | PHO  | CMA-C3A-C4A | -2.18 | 109.61      | 114.38   |
| 25  | b     | 5620 | MGE  | O2G-C1B-O1B | -2.18 | 118.44      | 123.70   |
| 23  | l     | 5102 | SQD  | O5-C1-C2    | 2.18  | 114.95      | 110.35   |
| 25  | B     | 619  | MGE  | O2G-C1B-O1B | -2.17 | 118.45      | 123.70   |
| 17  | A     | 403  | CLA  | C2D-C1D-ND  | -2.17 | 108.50      | 110.10   |
| 17  | C     | 511  | CLA  | CHC-C4B-NB  | 2.17  | 126.55      | 124.26   |
| 17  | c     | 5512 | CLA  | CHB-C1B-NB  | 2.17  | 126.55      | 124.26   |
| 17  | A     | 401  | CLA  | CAA-C2A-C3A | -2.17 | 106.84      | 112.78   |
| 17  | c     | 5502 | CLA  | CHB-C1B-NB  | 2.17  | 126.55      | 124.26   |
| 19  | d     | 5405 | PQ9  | C34-C33-C35 | 2.17  | 118.92      | 115.27   |
| 19  | a     | 5407 | PQ9  | C30-C28-C29 | 2.17  | 119.39      | 114.60   |
| 19  | D     | 406  | PQ9  | C14-C13-C15 | 2.17  | 118.92      | 115.27   |
| 26  | c     | 5515 | DGD  | C5B-C4B-C3B | -2.17 | 103.43      | 114.42   |
| 17  | C     | 509  | CLA  | CHB-C1B-NB  | 2.17  | 126.55      | 124.26   |
| 20  | t     | 5102 | BCR  | C35-C13-C14 | -2.17 | 119.89      | 122.92   |
| 17  | a     | 5403 | CLA  | CHC-C4B-NB  | 2.16  | 126.55      | 124.26   |
| 25  | C     | 519  | MGE  | C2G-O2G-C1B | -2.16 | 112.47      | 117.79   |
| 20  | C     | 516  | BCR  | C28-C27-C26 | -2.16 | 110.22      | 114.08   |
| 20  | b     | 5618 | BCR  | C33-C5-C6   | -2.16 | 122.10      | 124.53   |
| 17  | k     | 5501 | CLA  | CHC-C4B-NB  | 2.16  | 126.54      | 124.26   |
| 26  | A     | 413  | DGD  | C5B-C4B-C3B | -2.16 | 103.46      | 114.42   |
| 17  | C     | 510  | CLA  | CHC-C4B-NB  | 2.16  | 126.54      | 124.26   |
| 25  | c     | 5517 | MGE  | C2G-O2G-C1B | -2.16 | 112.48      | 117.79   |
| 20  | Y     | 101  | BCR  | C15-C14-C13 | -2.16 | 124.23      | 127.31   |
| 18  | A     | 404  | PHO  | CMA-C3A-C4A | -2.16 | 109.65      | 114.38   |
| 20  | b     | 5619 | BCR  | C15-C16-C17 | -2.16 | 119.06      | 123.47   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 20  | b     | 5618 | BCR  | C8-C7-C6    | -2.16 | 121.15      | 127.20   |
| 20  | B     | 618  | BCR  | C2-C1-C6    | 2.16  | 113.80      | 110.48   |
| 17  | C     | 505  | CLA  | CHB-C1B-NB  | 2.15  | 126.54      | 124.26   |
| 17  | B     | 616  | CLA  | CHC-C4B-NB  | 2.15  | 126.54      | 124.26   |
| 17  | c     | 5512 | CLA  | CHC-C4B-NB  | 2.15  | 126.54      | 124.26   |
| 17  | B     | 606  | CLA  | C1-C2-C3    | -2.15 | 122.32      | 126.04   |
| 17  | c     | 5509 | CLA  | CHB-C1B-NB  | 2.15  | 126.53      | 124.26   |
| 17  | B     | 612  | CLA  | O2A-CGA-O1A | -2.15 | 118.17      | 123.59   |
| 20  | B     | 618  | BCR  | C33-C5-C6   | -2.15 | 122.12      | 124.53   |
| 25  | d     | 5409 | MGE  | C1D-C2D-C3D | -2.15 | 105.52      | 110.00   |
| 17  | b     | 5612 | CLA  | O2A-CGA-O1A | -2.15 | 118.18      | 123.59   |
| 17  | b     | 5616 | CLA  | CHC-C4B-NB  | 2.14  | 126.53      | 124.26   |
| 17  | B     | 612  | CLA  | CHB-C1B-NB  | 2.14  | 126.53      | 124.26   |
| 20  | B     | 618  | BCR  | C8-C7-C6    | -2.14 | 121.19      | 127.20   |
| 20  | T     | 102  | BCR  | C38-C26-C25 | -2.14 | 122.12      | 124.53   |
| 20  | t     | 5101 | BCR  | C15-C16-C17 | -2.14 | 119.09      | 123.47   |
| 25  | c     | 5517 | MGE  | O1G-C1A-O1A | -2.14 | 118.20      | 123.59   |
| 17  | c     | 5507 | CLA  | C3C-C4C-NC  | -2.13 | 108.18      | 110.57   |
| 25  | C     | 519  | MGE  | O1G-C1A-O1A | -2.13 | 118.21      | 123.59   |
| 20  | b     | 5618 | BCR  | C2-C1-C6    | 2.13  | 113.77      | 110.48   |
| 17  | C     | 513  | CLA  | CHD-C1D-ND  | -2.13 | 122.50      | 124.45   |
| 17  | b     | 5607 | CLA  | CHC-C4B-NB  | 2.13  | 126.51      | 124.26   |
| 20  | k     | 5502 | BCR  | C7-C8-C9    | -2.13 | 123.02      | 126.23   |
| 19  | d     | 5405 | PQ9  | C45-C43-C44 | 2.13  | 119.30      | 114.60   |
| 19  | D     | 406  | PQ9  | C45-C43-C44 | 2.13  | 119.30      | 114.60   |
| 20  | h     | 5101 | BCR  | C30-C25-C26 | -2.13 | 119.62      | 122.61   |
| 17  | c     | 5512 | CLA  | CHD-C1D-ND  | -2.13 | 122.50      | 124.45   |
| 17  | B     | 607  | CLA  | CHC-C4B-NB  | 2.12  | 126.50      | 124.26   |
| 17  | C     | 507  | CLA  | C3C-C4C-NC  | -2.12 | 108.19      | 110.57   |
| 25  | l     | 5101 | MGE  | O1G-C1A-O1A | -2.12 | 118.24      | 123.59   |
| 17  | b     | 5611 | CLA  | CAA-C2A-C3A | -2.12 | 106.97      | 112.78   |
| 20  | b     | 5617 | BCR  | C24-C23-C22 | -2.12 | 123.03      | 126.23   |
| 20  | A     | 407  | BCR  | C38-C26-C25 | -2.12 | 122.15      | 124.53   |
| 25  | d     | 5409 | MGE  | C2G-O2G-C1B | -2.12 | 112.58      | 117.79   |
| 22  | A     | 409  | LMT  | O5B-C5B-C4B | 2.12  | 113.54      | 109.69   |
| 17  | B     | 607  | CLA  | CAA-CBA-CGA | -2.11 | 107.08      | 113.25   |
| 17  | b     | 5607 | CLA  | CAA-CBA-CGA | -2.11 | 107.08      | 113.25   |
| 17  | d     | 5404 | CLA  | O2A-CGA-O1A | -2.11 | 118.26      | 123.59   |
| 25  | A     | 412  | MGE  | O1G-C1A-O1A | -2.11 | 118.26      | 123.59   |
| 17  | D     | 405  | CLA  | O2A-CGA-O1A | -2.11 | 118.27      | 123.59   |
| 17  | B     | 611  | CLA  | CAA-C2A-C3A | -2.11 | 107.00      | 112.78   |
| 17  | b     | 5612 | CLA  | CMB-C2B-C3B | 2.11  | 131.69      | 126.59   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | c     | 5502 | CLA  | C6-C7-C8    | -2.11 | 109.11      | 115.92   |
| 21  | A     | 408  | LHG  | C5-O7-C7    | -2.11 | 112.60      | 117.79   |
| 25  | d     | 5409 | MGE  | O1G-C1A-O1A | -2.11 | 118.27      | 123.59   |
| 20  | B     | 617  | BCR  | C24-C23-C22 | -2.11 | 123.05      | 126.23   |
| 20  | A     | 407  | BCR  | C8-C7-C6    | -2.11 | 121.29      | 127.20   |
| 17  | c     | 5507 | CLA  | CHC-C4B-NB  | 2.10  | 126.48      | 124.26   |
| 17  | c     | 5510 | CLA  | CHC-C4B-NB  | 2.10  | 126.48      | 124.26   |
| 17  | C     | 502  | CLA  | C6-C7-C8    | -2.10 | 109.12      | 115.92   |
| 21  | a     | 5409 | LHG  | C5-O7-C7    | -2.10 | 112.61      | 117.79   |
| 26  | c     | 5516 | DGD  | O2D-C2D-C1D | -2.10 | 104.94      | 110.05   |
| 20  | H     | 101  | BCR  | C30-C25-C26 | -2.10 | 119.65      | 122.61   |
| 17  | b     | 5610 | CLA  | C2D-C1D-ND  | -2.10 | 108.55      | 110.10   |
| 20  | a     | 5408 | BCR  | C38-C26-C25 | -2.10 | 122.17      | 124.53   |
| 23  | l     | 5102 | SQD  | O8-S-C6     | 2.10  | 109.08      | 105.74   |
| 18  | D     | 402  | PHO  | O2A-CGA-O1A | -2.10 | 118.30      | 123.59   |
| 17  | B     | 612  | CLA  | C11-C10-C8  | -2.10 | 109.14      | 115.92   |
| 18  | d     | 5402 | PHO  | O2A-CGA-O1A | -2.10 | 118.30      | 123.59   |
| 26  | C     | 517  | DGD  | O2D-C2D-C1D | -2.10 | 104.96      | 110.05   |
| 17  | C     | 510  | CLA  | C16-C15-C13 | -2.10 | 109.15      | 115.92   |
| 23  | A     | 410  | SQD  | O6-C1-C2    | 2.09  | 111.57      | 108.30   |
| 20  | b     | 5617 | BCR  | C2-C1-C6    | 2.09  | 113.70      | 110.48   |
| 17  | C     | 507  | CLA  | CHC-C4B-NB  | 2.09  | 126.47      | 124.26   |
| 17  | b     | 5606 | CLA  | CAA-C2A-C1A | -2.09 | 107.51      | 112.14   |
| 17  | b     | 5612 | CLA  | C11-C10-C8  | -2.09 | 109.16      | 115.92   |
| 17  | B     | 612  | CLA  | CMB-C2B-C3B | 2.09  | 131.65      | 126.59   |
| 17  | c     | 5510 | CLA  | C16-C15-C13 | -2.09 | 109.17      | 115.92   |
| 17  | B     | 601  | CLA  | C3B-C4B-NB  | -2.09 | 108.58      | 110.52   |
| 17  | B     | 616  | CLA  | O2D-CGD-CBD | 2.09  | 114.97      | 111.27   |
| 17  | C     | 512  | CLA  | O2D-CGD-CBD | 2.09  | 114.97      | 111.27   |
| 25  | D     | 410  | MGE  | O2G-C1B-O1B | -2.08 | 118.67      | 123.70   |
| 22  | A     | 409  | LMT  | C3'-C4'-C5' | -2.08 | 106.15      | 110.93   |
| 26  | D     | 411  | DGD  | O3E-C3E-C2E | -2.08 | 105.54      | 110.35   |
| 17  | c     | 5511 | CLA  | O2D-CGD-CBD | 2.08  | 114.96      | 111.27   |
| 17  | c     | 5502 | CLA  | O2D-CGD-O1D | -2.08 | 119.78      | 123.84   |
| 25  | d     | 5410 | MGE  | C4D-C3D-C2D | -2.08 | 107.20      | 110.82   |
| 17  | C     | 501  | CLA  | CHD-C1D-ND  | -2.07 | 122.55      | 124.45   |
| 20  | a     | 5408 | BCR  | C8-C7-C6    | -2.07 | 121.38      | 127.20   |
| 17  | B     | 602  | CLA  | CHB-C1B-NB  | 2.07  | 126.45      | 124.26   |
| 17  | b     | 5601 | CLA  | C3B-C4B-NB  | -2.07 | 108.59      | 110.52   |
| 20  | a     | 5408 | BCR  | C11-C10-C9  | -2.07 | 124.36      | 127.31   |
| 17  | C     | 502  | CLA  | O2D-CGD-O1D | -2.07 | 119.79      | 123.84   |
| 26  | b     | 5621 | DGD  | O3E-C3E-C2E | -2.07 | 105.57      | 110.35   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 26  | b     | 5621 | DGD  | C5B-C4B-C3B | -2.06 | 103.95      | 114.42   |
| 26  | C     | 518  | DGD  | C5B-C4B-C3B | -2.06 | 103.96      | 114.42   |
| 20  | A     | 407  | BCR  | C11-C10-C9  | -2.06 | 124.37      | 127.31   |
| 26  | C     | 518  | DGD  | CAB-C9B-C8B | -2.06 | 103.96      | 114.42   |
| 17  | b     | 5616 | CLA  | O2D-CGD-CBD | 2.06  | 114.93      | 111.27   |
| 20  | B     | 617  | BCR  | C2-C1-C6    | 2.06  | 113.65      | 110.48   |
| 26  | a     | 5411 | DGD  | CAB-C9B-C8B | -2.06 | 103.99      | 114.42   |
| 17  | b     | 5613 | CLA  | CHC-C4B-NB  | 2.05  | 126.43      | 124.26   |
| 26  | D     | 411  | DGD  | C5B-C4B-C3B | -2.05 | 104.00      | 114.42   |
| 23  | l     | 5102 | SQD  | O47-C7-O49  | -2.05 | 118.74      | 123.70   |
| 17  | C     | 506  | CLA  | O1D-CGD-CBD | 2.05  | 128.68      | 124.48   |
| 17  | c     | 5503 | CLA  | CHD-C1D-ND  | -2.05 | 122.57      | 124.45   |
| 17  | a     | 5404 | CLA  | CAA-C2A-C3A | -2.05 | 107.16      | 112.78   |
| 20  | b     | 5618 | BCR  | C38-C26-C25 | -2.05 | 122.22      | 124.53   |
| 17  | A     | 405  | CLA  | O2A-CGA-O1A | -2.05 | 118.42      | 123.59   |
| 17  | B     | 605  | CLA  | O2A-CGA-O1A | -2.05 | 118.42      | 123.59   |
| 26  | a     | 5411 | DGD  | C5B-C4B-C3B | -2.05 | 104.02      | 114.42   |
| 17  | b     | 5602 | CLA  | O2A-CGA-O1A | -2.05 | 118.42      | 123.59   |
| 20  | c     | 5513 | BCR  | C20-C21-C22 | -2.05 | 124.39      | 127.31   |
| 20  | C     | 516  | BCR  | C8-C7-C6    | -2.05 | 121.45      | 127.20   |
| 17  | A     | 403  | CLA  | CAA-C2A-C3A | -2.05 | 107.17      | 112.78   |
| 17  | b     | 5602 | CLA  | CHB-C1B-NB  | 2.05  | 126.42      | 124.26   |
| 17  | a     | 5406 | CLA  | O2A-CGA-O1A | -2.05 | 118.42      | 123.59   |
| 20  | B     | 618  | BCR  | C38-C26-C25 | -2.05 | 122.23      | 124.53   |
| 19  | D     | 406  | PQ9  | C11-C2-C1   | 2.05  | 118.54      | 116.88   |
| 17  | c     | 5506 | CLA  | O1D-CGD-CBD | 2.04  | 128.67      | 124.48   |
| 17  | B     | 602  | CLA  | O2A-CGA-O1A | -2.04 | 118.43      | 123.59   |
| 20  | d     | 5406 | BCR  | C38-C26-C25 | -2.04 | 122.23      | 124.53   |
| 17  | a     | 5402 | CLA  | CHB-C4A-NA  | 2.04  | 127.33      | 124.51   |
| 17  | C     | 503  | CLA  | CHD-C1D-ND  | -2.04 | 122.58      | 124.45   |
| 19  | a     | 5407 | PQ9  | C26-C27-C28 | -2.04 | 120.79      | 127.75   |
| 20  | C     | 516  | BCR  | C27-C26-C25 | 2.04  | 125.69      | 122.73   |
| 17  | B     | 616  | CLA  | CAA-C2A-C3A | -2.04 | 107.20      | 112.78   |
| 20  | C     | 514  | BCR  | C20-C21-C22 | -2.04 | 124.40      | 127.31   |
| 17  | C     | 509  | CLA  | C2D-C1D-ND  | -2.04 | 108.60      | 110.10   |
| 17  | c     | 5507 | CLA  | CHC-C1C-NC  | 2.04  | 127.29      | 124.20   |
| 25  | D     | 409  | MGE  | O1G-C1A-O1A | -2.04 | 118.45      | 123.59   |
| 17  | c     | 5504 | CLA  | CHB-C1B-NB  | 2.04  | 126.41      | 124.26   |
| 26  | c     | 5515 | DGD  | O4D-C4D-C5D | -2.03 | 104.25      | 109.30   |
| 20  | c     | 5514 | BCR  | C8-C7-C6    | -2.03 | 121.49      | 127.20   |
| 23  | d     | 5407 | SQD  | O9-S-C6     | 2.03  | 109.35      | 106.94   |
| 20  | t     | 5102 | BCR  | C11-C10-C9  | -2.03 | 124.41      | 127.31   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 20  | t     | 5102 | BCR  | C15-C16-C17 | -2.03 | 119.31      | 123.47   |
| 17  | b     | 5610 | CLA  | CMB-C2B-C3B | 2.03  | 131.51      | 126.59   |
| 17  | a     | 5403 | CLA  | CAA-C2A-C3A | -2.03 | 107.22      | 112.78   |
| 17  | b     | 5616 | CLA  | CAA-C2A-C3A | -2.03 | 107.22      | 112.78   |
| 17  | c     | 5501 | CLA  | CHD-C1D-ND  | -2.03 | 122.59      | 124.45   |
| 17  | B     | 610  | CLA  | CMB-C2B-C3B | 2.03  | 131.50      | 126.59   |
| 17  | b     | 5605 | CLA  | C11-C10-C8  | -2.02 | 109.38      | 115.92   |
| 20  | t     | 5101 | BCR  | C20-C21-C22 | -2.02 | 124.42      | 127.31   |
| 20  | D     | 407  | BCR  | C38-C26-C25 | -2.02 | 122.26      | 124.53   |
| 17  | A     | 401  | CLA  | CHB-C4A-NA  | 2.02  | 127.31      | 124.51   |
| 17  | d     | 5403 | CLA  | C1-C2-C3    | -2.02 | 122.55      | 126.04   |
| 17  | B     | 605  | CLA  | C3C-C4C-NC  | -2.02 | 108.31      | 110.57   |
| 17  | B     | 610  | CLA  | C2D-C1D-ND  | -2.02 | 108.61      | 110.10   |
| 20  | C     | 514  | BCR  | C35-C13-C14 | -2.02 | 120.09      | 122.92   |
| 17  | B     | 613  | CLA  | CHC-C4B-NB  | 2.02  | 126.39      | 124.26   |
| 17  | B     | 607  | CLA  | CHB-C1B-NB  | 2.02  | 126.39      | 124.26   |
| 17  | C     | 504  | CLA  | CHB-C1B-NB  | 2.02  | 126.39      | 124.26   |
| 21  | A     | 408  | LHG  | O8-C6-C5    | -2.02 | 102.56      | 108.43   |
| 17  | A     | 402  | CLA  | CAA-C2A-C3A | -2.02 | 107.25      | 112.78   |
| 20  | c     | 5514 | BCR  | C27-C26-C25 | 2.02  | 125.66      | 122.73   |
| 17  | b     | 5605 | CLA  | C3C-C4C-NC  | -2.02 | 108.31      | 110.57   |
| 25  | m     | 5103 | MGE  | C3G-O3G-C1D | -2.02 | 109.80      | 113.74   |
| 17  | C     | 507  | CLA  | CHC-C1C-NC  | 2.02  | 127.26      | 124.20   |
| 26  | A     | 413  | DGD  | O4D-C4D-C5D | -2.01 | 104.29      | 109.30   |
| 17  | c     | 5509 | CLA  | CHA-C1A-NA  | -2.01 | 121.78      | 126.40   |
| 17  | B     | 613  | CLA  | C3C-C4C-NC  | -2.01 | 108.31      | 110.57   |
| 25  | D     | 409  | MGE  | O2G-C1B-O1B | -2.01 | 118.84      | 123.70   |
| 17  | B     | 605  | CLA  | C11-C10-C8  | -2.01 | 109.42      | 115.92   |
| 19  | d     | 5405 | PQ9  | C11-C2-C1   | 2.01  | 118.51      | 116.88   |
| 17  | b     | 5610 | CLA  | CHC-C4B-NB  | 2.01  | 126.39      | 124.26   |
| 17  | A     | 401  | CLA  | C1-C2-C3    | -2.01 | 122.57      | 126.04   |
| 21  | a     | 5409 | LHG  | O8-C6-C5    | -2.01 | 102.59      | 108.43   |
| 17  | c     | 5510 | CLA  | O2D-CGD-O1D | -2.01 | 119.91      | 123.84   |
| 17  | b     | 5605 | CLA  | O2A-CGA-O1A | -2.01 | 118.52      | 123.59   |
| 17  | c     | 5509 | CLA  | C2D-C1D-ND  | -2.01 | 108.62      | 110.10   |
| 17  | D     | 404  | CLA  | C1-C2-C3    | -2.00 | 122.58      | 126.04   |
| 20  | k     | 5502 | BCR  | C15-C14-C13 | -2.00 | 124.45      | 127.31   |

There are no chirality outliers.

All (1949) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 17  | A     | 402 | CLA  | C2B-C3B-CAB-CBB |
| 17  | A     | 403 | CLA  | CHA-CBD-CGD-O1D |
| 17  | A     | 403 | CLA  | CHA-CBD-CGD-O2D |
| 17  | B     | 602 | CLA  | C2-C3-C5-C6     |
| 17  | B     | 602 | CLA  | C4-C3-C5-C6     |
| 17  | B     | 603 | CLA  | CBD-CGD-O2D-CED |
| 17  | B     | 604 | CLA  | CHA-CBD-CGD-O1D |
| 17  | B     | 604 | CLA  | CHA-CBD-CGD-O2D |
| 17  | B     | 605 | CLA  | CHA-CBD-CGD-O1D |
| 17  | B     | 605 | CLA  | CHA-CBD-CGD-O2D |
| 17  | B     | 605 | CLA  | C14-C13-C15-C16 |
| 17  | B     | 606 | CLA  | C1A-C2A-CAA-CBA |
| 17  | B     | 606 | CLA  | C3A-C2A-CAA-CBA |
| 17  | B     | 606 | CLA  | C4-C3-C5-C6     |
| 17  | B     | 607 | CLA  | CAD-CBD-CGD-O2D |
| 17  | B     | 607 | CLA  | C2-C3-C5-C6     |
| 17  | B     | 607 | CLA  | C4-C3-C5-C6     |
| 17  | B     | 608 | CLA  | C1A-C2A-CAA-CBA |
| 17  | B     | 609 | CLA  | C1A-C2A-CAA-CBA |
| 17  | B     | 609 | CLA  | C3A-C2A-CAA-CBA |
| 17  | B     | 609 | CLA  | CHA-CBD-CGD-O1D |
| 17  | B     | 609 | CLA  | CHA-CBD-CGD-O2D |
| 17  | B     | 609 | CLA  | CAD-CBD-CGD-O1D |
| 17  | B     | 609 | CLA  | CAD-CBD-CGD-O2D |
| 17  | B     | 609 | CLA  | CBD-CGD-O2D-CED |
| 17  | B     | 609 | CLA  | C11-C10-C8-C9   |
| 17  | B     | 612 | CLA  | C1A-C2A-CAA-CBA |
| 17  | B     | 612 | CLA  | C3A-C2A-CAA-CBA |
| 17  | B     | 615 | CLA  | CHA-CBD-CGD-O1D |
| 17  | B     | 615 | CLA  | CHA-CBD-CGD-O2D |
| 17  | B     | 615 | CLA  | CBD-CGD-O2D-CED |
| 17  | B     | 616 | CLA  | C1A-C2A-CAA-CBA |
| 17  | B     | 616 | CLA  | C3A-C2A-CAA-CBA |
| 17  | C     | 502 | CLA  | C4B-C3B-CAB-CBB |
| 17  | C     | 503 | CLA  | C1A-C2A-CAA-CBA |
| 17  | C     | 503 | CLA  | C2B-C3B-CAB-CBB |
| 17  | C     | 503 | CLA  | C4B-C3B-CAB-CBB |
| 17  | C     | 503 | CLA  | C2-C3-C5-C6     |
| 17  | C     | 503 | CLA  | C4-C3-C5-C6     |
| 17  | C     | 504 | CLA  | CBA-CGA-O2A-C1  |
| 17  | C     | 504 | CLA  | O1A-CGA-O2A-C1  |
| 17  | C     | 505 | CLA  | CAD-CBD-CGD-O1D |
| 17  | C     | 506 | CLA  | C1A-C2A-CAA-CBA |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | C     | 507  | CLA  | CHA-CBD-CGD-O1D |
| 17  | C     | 507  | CLA  | CHA-CBD-CGD-O2D |
| 17  | C     | 508  | CLA  | C2B-C3B-CAB-CBB |
| 17  | C     | 508  | CLA  | C4B-C3B-CAB-CBB |
| 17  | C     | 510  | CLA  | CBD-CGD-O2D-CED |
| 17  | C     | 513  | CLA  | CHA-CBD-CGD-O1D |
| 17  | C     | 513  | CLA  | CHA-CBD-CGD-O2D |
| 17  | D     | 404  | CLA  | C1A-C2A-CAA-CBA |
| 17  | D     | 405  | CLA  | C1A-C2A-CAA-CBA |
| 17  | D     | 405  | CLA  | C3A-C2A-CAA-CBA |
| 17  | D     | 405  | CLA  | CBD-CGD-O2D-CED |
| 17  | a     | 5403 | CLA  | C2B-C3B-CAB-CBB |
| 17  | a     | 5404 | CLA  | CHA-CBD-CGD-O1D |
| 17  | a     | 5404 | CLA  | CHA-CBD-CGD-O2D |
| 17  | b     | 5602 | CLA  | C2-C3-C5-C6     |
| 17  | b     | 5602 | CLA  | C4-C3-C5-C6     |
| 17  | b     | 5603 | CLA  | CBD-CGD-O2D-CED |
| 17  | b     | 5604 | CLA  | CHA-CBD-CGD-O1D |
| 17  | b     | 5604 | CLA  | CHA-CBD-CGD-O2D |
| 17  | b     | 5605 | CLA  | CHA-CBD-CGD-O1D |
| 17  | b     | 5605 | CLA  | CHA-CBD-CGD-O2D |
| 17  | b     | 5605 | CLA  | C14-C13-C15-C16 |
| 17  | b     | 5606 | CLA  | C1A-C2A-CAA-CBA |
| 17  | b     | 5606 | CLA  | C3A-C2A-CAA-CBA |
| 17  | b     | 5607 | CLA  | CAD-CBD-CGD-O2D |
| 17  | b     | 5607 | CLA  | C2-C3-C5-C6     |
| 17  | b     | 5607 | CLA  | C4-C3-C5-C6     |
| 17  | b     | 5608 | CLA  | C1A-C2A-CAA-CBA |
| 17  | b     | 5609 | CLA  | C1A-C2A-CAA-CBA |
| 17  | b     | 5609 | CLA  | C3A-C2A-CAA-CBA |
| 17  | b     | 5609 | CLA  | CHA-CBD-CGD-O1D |
| 17  | b     | 5609 | CLA  | CHA-CBD-CGD-O2D |
| 17  | b     | 5609 | CLA  | CAD-CBD-CGD-O1D |
| 17  | b     | 5609 | CLA  | CAD-CBD-CGD-O2D |
| 17  | b     | 5609 | CLA  | CBD-CGD-O2D-CED |
| 17  | b     | 5609 | CLA  | C11-C10-C8-C9   |
| 17  | b     | 5612 | CLA  | C1A-C2A-CAA-CBA |
| 17  | b     | 5612 | CLA  | C3A-C2A-CAA-CBA |
| 17  | b     | 5615 | CLA  | CHA-CBD-CGD-O1D |
| 17  | b     | 5615 | CLA  | CHA-CBD-CGD-O2D |
| 17  | b     | 5615 | CLA  | CBD-CGD-O2D-CED |
| 17  | b     | 5616 | CLA  | C1A-C2A-CAA-CBA |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | b     | 5616 | CLA  | C3A-C2A-CAA-CBA |
| 17  | c     | 5502 | CLA  | C4B-C3B-CAB-CBB |
| 17  | c     | 5503 | CLA  | C1A-C2A-CAA-CBA |
| 17  | c     | 5503 | CLA  | C2B-C3B-CAB-CBB |
| 17  | c     | 5503 | CLA  | C4B-C3B-CAB-CBB |
| 17  | c     | 5503 | CLA  | C2-C3-C5-C6     |
| 17  | c     | 5503 | CLA  | C4-C3-C5-C6     |
| 17  | c     | 5504 | CLA  | CBA-CGA-O2A-C1  |
| 17  | c     | 5504 | CLA  | O1A-CGA-O2A-C1  |
| 17  | c     | 5505 | CLA  | CAD-CBD-CGD-O1D |
| 17  | c     | 5506 | CLA  | C1A-C2A-CAA-CBA |
| 17  | c     | 5507 | CLA  | CHA-CBD-CGD-O1D |
| 17  | c     | 5507 | CLA  | CHA-CBD-CGD-O2D |
| 17  | c     | 5508 | CLA  | C2B-C3B-CAB-CBB |
| 17  | c     | 5508 | CLA  | C4B-C3B-CAB-CBB |
| 17  | c     | 5510 | CLA  | CBD-CGD-O2D-CED |
| 17  | c     | 5512 | CLA  | CHA-CBD-CGD-O1D |
| 17  | c     | 5512 | CLA  | CHA-CBD-CGD-O2D |
| 17  | d     | 5403 | CLA  | C1A-C2A-CAA-CBA |
| 17  | d     | 5404 | CLA  | C1A-C2A-CAA-CBA |
| 17  | d     | 5404 | CLA  | C3A-C2A-CAA-CBA |
| 17  | d     | 5404 | CLA  | CBD-CGD-O2D-CED |
| 18  | D     | 402  | PHO  | C1A-C2A-CAA-CBA |
| 18  | D     | 402  | PHO  | C3A-C2A-CAA-CBA |
| 18  | D     | 402  | PHO  | CBD-CGD-O2D-CED |
| 18  | d     | 5402 | PHO  | C1A-C2A-CAA-CBA |
| 18  | d     | 5402 | PHO  | C3A-C2A-CAA-CBA |
| 18  | d     | 5402 | PHO  | CBD-CGD-O2D-CED |
| 19  | A     | 406  | PQ9  | C19-C18-C20-C21 |
| 19  | A     | 406  | PQ9  | C18-C20-C21-C22 |
| 19  | A     | 406  | PQ9  | C23-C25-C26-C27 |
| 19  | A     | 406  | PQ9  | C27-C28-C30-C31 |
| 19  | A     | 406  | PQ9  | C29-C28-C30-C31 |
| 19  | A     | 406  | PQ9  | C34-C33-C35-C36 |
| 19  | D     | 406  | PQ9  | C24-C23-C25-C26 |
| 19  | D     | 406  | PQ9  | C34-C33-C35-C36 |
| 19  | a     | 5407 | PQ9  | C19-C18-C20-C21 |
| 19  | a     | 5407 | PQ9  | C18-C20-C21-C22 |
| 19  | a     | 5407 | PQ9  | C23-C25-C26-C27 |
| 19  | d     | 5405 | PQ9  | C24-C23-C25-C26 |
| 19  | d     | 5405 | PQ9  | C34-C33-C35-C36 |
| 20  | A     | 407  | BCR  | C1-C6-C7-C8     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 20  | A     | 407 | BCR  | C9-C10-C11-C12  |
| 20  | A     | 407 | BCR  | C11-C12-C13-C35 |
| 20  | A     | 407 | BCR  | C18-C19-C20-C21 |
| 20  | B     | 617 | BCR  | C11-C12-C13-C35 |
| 20  | B     | 617 | BCR  | C14-C15-C16-C17 |
| 20  | B     | 617 | BCR  | C21-C22-C23-C24 |
| 20  | B     | 617 | BCR  | C37-C22-C23-C24 |
| 20  | B     | 618 | BCR  | C11-C10-C9-C8   |
| 20  | B     | 618 | BCR  | C10-C11-C12-C13 |
| 20  | B     | 618 | BCR  | C21-C22-C23-C24 |
| 20  | B     | 618 | BCR  | C37-C22-C23-C24 |
| 20  | C     | 514 | BCR  | C7-C8-C9-C34    |
| 20  | C     | 514 | BCR  | C14-C15-C16-C17 |
| 20  | C     | 515 | BCR  | C1-C6-C7-C8     |
| 20  | C     | 515 | BCR  | C6-C7-C8-C9     |
| 20  | C     | 515 | BCR  | C11-C10-C9-C8   |
| 20  | C     | 515 | BCR  | C11-C12-C13-C14 |
| 20  | C     | 515 | BCR  | C11-C12-C13-C35 |
| 20  | C     | 515 | BCR  | C12-C13-C14-C15 |
| 20  | C     | 515 | BCR  | C14-C15-C16-C17 |
| 20  | C     | 515 | BCR  | C16-C17-C18-C19 |
| 20  | C     | 515 | BCR  | C16-C17-C18-C36 |
| 20  | C     | 515 | BCR  | C18-C19-C20-C21 |
| 20  | C     | 515 | BCR  | C22-C23-C24-C25 |
| 20  | C     | 516 | BCR  | C6-C7-C8-C9     |
| 20  | C     | 516 | BCR  | C7-C8-C9-C34    |
| 20  | C     | 516 | BCR  | C10-C11-C12-C13 |
| 20  | C     | 516 | BCR  | C11-C12-C13-C35 |
| 20  | C     | 516 | BCR  | C12-C13-C14-C15 |
| 20  | C     | 516 | BCR  | C35-C13-C14-C15 |
| 20  | C     | 516 | BCR  | C20-C21-C22-C37 |
| 20  | C     | 516 | BCR  | C21-C22-C23-C24 |
| 20  | C     | 516 | BCR  | C22-C23-C24-C25 |
| 20  | D     | 407 | BCR  | C7-C8-C9-C10    |
| 20  | D     | 407 | BCR  | C11-C12-C13-C35 |
| 20  | D     | 407 | BCR  | C23-C24-C25-C30 |
| 20  | H     | 101 | BCR  | C6-C7-C8-C9     |
| 20  | H     | 101 | BCR  | C16-C17-C18-C19 |
| 20  | H     | 101 | BCR  | C16-C17-C18-C36 |
| 20  | T     | 102 | BCR  | C16-C17-C18-C19 |
| 20  | T     | 102 | BCR  | C16-C17-C18-C36 |
| 20  | T     | 102 | BCR  | C23-C24-C25-C26 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 20  | T     | 102  | BCR  | C23-C24-C25-C30 |
| 20  | a     | 5408 | BCR  | C1-C6-C7-C8     |
| 20  | a     | 5408 | BCR  | C9-C10-C11-C12  |
| 20  | a     | 5408 | BCR  | C11-C12-C13-C35 |
| 20  | a     | 5408 | BCR  | C18-C19-C20-C21 |
| 20  | b     | 5617 | BCR  | C11-C12-C13-C35 |
| 20  | b     | 5617 | BCR  | C14-C15-C16-C17 |
| 20  | b     | 5617 | BCR  | C21-C22-C23-C24 |
| 20  | b     | 5617 | BCR  | C37-C22-C23-C24 |
| 20  | b     | 5618 | BCR  | C11-C10-C9-C8   |
| 20  | b     | 5618 | BCR  | C10-C11-C12-C13 |
| 20  | b     | 5618 | BCR  | C21-C22-C23-C24 |
| 20  | b     | 5618 | BCR  | C37-C22-C23-C24 |
| 20  | b     | 5619 | BCR  | C1-C6-C7-C8     |
| 20  | b     | 5619 | BCR  | C6-C7-C8-C9     |
| 20  | b     | 5619 | BCR  | C7-C8-C9-C34    |
| 20  | b     | 5619 | BCR  | C22-C23-C24-C25 |
| 20  | c     | 5513 | BCR  | C7-C8-C9-C34    |
| 20  | c     | 5513 | BCR  | C14-C15-C16-C17 |
| 20  | c     | 5514 | BCR  | C6-C7-C8-C9     |
| 20  | c     | 5514 | BCR  | C7-C8-C9-C34    |
| 20  | c     | 5514 | BCR  | C10-C11-C12-C13 |
| 20  | c     | 5514 | BCR  | C11-C12-C13-C35 |
| 20  | c     | 5514 | BCR  | C12-C13-C14-C15 |
| 20  | c     | 5514 | BCR  | C35-C13-C14-C15 |
| 20  | c     | 5514 | BCR  | C20-C21-C22-C37 |
| 20  | c     | 5514 | BCR  | C21-C22-C23-C24 |
| 20  | c     | 5514 | BCR  | C22-C23-C24-C25 |
| 20  | d     | 5406 | BCR  | C7-C8-C9-C10    |
| 20  | d     | 5406 | BCR  | C11-C12-C13-C35 |
| 20  | d     | 5406 | BCR  | C23-C24-C25-C30 |
| 20  | h     | 5101 | BCR  | C6-C7-C8-C9     |
| 20  | h     | 5101 | BCR  | C16-C17-C18-C19 |
| 20  | h     | 5101 | BCR  | C16-C17-C18-C36 |
| 20  | k     | 5502 | BCR  | C6-C7-C8-C9     |
| 20  | k     | 5502 | BCR  | C14-C15-C16-C17 |
| 20  | k     | 5502 | BCR  | C18-C19-C20-C21 |
| 20  | k     | 5502 | BCR  | C19-C20-C21-C22 |
| 20  | k     | 5502 | BCR  | C20-C21-C22-C37 |
| 20  | k     | 5502 | BCR  | C21-C22-C23-C24 |
| 20  | k     | 5502 | BCR  | C22-C23-C24-C25 |
| 20  | t     | 5101 | BCR  | C1-C6-C7-C8     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 20  | t     | 5101 | BCR  | C6-C7-C8-C9     |
| 20  | t     | 5101 | BCR  | C7-C8-C9-C34    |
| 20  | t     | 5101 | BCR  | C22-C23-C24-C25 |
| 20  | t     | 5102 | BCR  | C1-C6-C7-C8     |
| 20  | t     | 5102 | BCR  | C9-C10-C11-C12  |
| 20  | t     | 5102 | BCR  | C14-C15-C16-C17 |
| 20  | t     | 5102 | BCR  | C16-C17-C18-C36 |
| 20  | t     | 5102 | BCR  | C21-C22-C23-C24 |
| 20  | t     | 5102 | BCR  | C37-C22-C23-C24 |
| 20  | t     | 5102 | BCR  | C22-C23-C24-C25 |
| 20  | z     | 5101 | BCR  | C1-C6-C7-C8     |
| 20  | z     | 5101 | BCR  | C6-C7-C8-C9     |
| 20  | z     | 5101 | BCR  | C11-C10-C9-C8   |
| 20  | z     | 5101 | BCR  | C11-C12-C13-C14 |
| 20  | z     | 5101 | BCR  | C11-C12-C13-C35 |
| 20  | z     | 5101 | BCR  | C12-C13-C14-C15 |
| 20  | z     | 5101 | BCR  | C14-C15-C16-C17 |
| 20  | z     | 5101 | BCR  | C16-C17-C18-C19 |
| 20  | z     | 5101 | BCR  | C16-C17-C18-C36 |
| 20  | z     | 5101 | BCR  | C18-C19-C20-C21 |
| 20  | z     | 5101 | BCR  | C22-C23-C24-C25 |
| 20  | Y     | 101  | BCR  | C11-C12-C13-C14 |
| 20  | Y     | 101  | BCR  | C11-C12-C13-C35 |
| 20  | Y     | 101  | BCR  | C14-C15-C16-C17 |
| 20  | Y     | 101  | BCR  | C17-C18-C19-C20 |
| 20  | Y     | 101  | BCR  | C18-C19-C20-C21 |
| 20  | Y     | 101  | BCR  | C22-C23-C24-C25 |
| 21  | A     | 408  | LHG  | O1-C1-C2-C3     |
| 21  | A     | 408  | LHG  | C3-O3-P-O4      |
| 21  | A     | 408  | LHG  | C3-O3-P-O5      |
| 21  | A     | 408  | LHG  | C4-O6-P-O3      |
| 21  | A     | 408  | LHG  | C4-O6-P-O4      |
| 21  | A     | 408  | LHG  | C4-O6-P-O5      |
| 21  | a     | 5409 | LHG  | O1-C1-C2-C3     |
| 21  | a     | 5409 | LHG  | C3-O3-P-O4      |
| 21  | a     | 5409 | LHG  | C3-O3-P-O5      |
| 21  | a     | 5409 | LHG  | C4-O6-P-O3      |
| 21  | a     | 5409 | LHG  | C4-O6-P-O4      |
| 21  | a     | 5409 | LHG  | C4-O6-P-O5      |
| 22  | A     | 409  | LMT  | C2'-C1'-O1'-C1  |
| 22  | A     | 409  | LMT  | O5'-C1'-O1'-C1  |
| 22  | B     | 620  | LMT  | C2'-C1'-O1'-C1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | B     | 620  | LMT  | O5'-C1'-O1'-C1  |
| 22  | m     | 5102 | LMT  | C2'-C1'-O1'-C1  |
| 22  | m     | 5102 | LMT  | O5'-C1'-O1'-C1  |
| 23  | A     | 410  | SQD  | O5-C5-C6-S      |
| 23  | D     | 403  | SQD  | O5-C5-C6-S      |
| 23  | L     | 101  | SQD  | O47-C45-C46-O48 |
| 23  | L     | 101  | SQD  | O49-C7-O47-C45  |
| 23  | L     | 101  | SQD  | C5-C6-S-O7      |
| 23  | L     | 101  | SQD  | C5-C6-S-O8      |
| 23  | L     | 101  | SQD  | C5-C6-S-O9      |
| 23  | a     | 5401 | SQD  | C8-C7-O47-C45   |
| 23  | a     | 5401 | SQD  | O5-C5-C6-S      |
| 23  | a     | 5401 | SQD  | C5-C6-S-O7      |
| 23  | a     | 5401 | SQD  | C5-C6-S-O8      |
| 23  | a     | 5401 | SQD  | C5-C6-S-O9      |
| 23  | d     | 5407 | SQD  | O5-C1-O6-C44    |
| 23  | d     | 5407 | SQD  | O5-C5-C6-S      |
| 23  | l     | 5102 | SQD  | O5-C1-O6-C44    |
| 23  | l     | 5102 | SQD  | O5-C5-C6-S      |
| 25  | C     | 519  | MGE  | O2G-C2G-C3G-O3G |
| 25  | D     | 409  | MGE  | O2G-C2G-C3G-O3G |
| 25  | D     | 410  | MGE  | O6D-C1D-O3G-C3G |
| 25  | c     | 5517 | MGE  | O2G-C2G-C3G-O3G |
| 25  | d     | 5410 | MGE  | O6D-C1D-O3G-C3G |
| 25  | m     | 5103 | MGE  | C2B-C1B-O2G-C2G |
| 25  | m     | 5103 | MGE  | O6D-C1D-O3G-C3G |
| 26  | A     | 413  | DGD  | C2D-C1D-O3G-C3G |
| 26  | A     | 413  | DGD  | O6D-C1D-O3G-C3G |
| 26  | A     | 413  | DGD  | O6E-C1E-O5D-C6D |
| 26  | C     | 517  | DGD  | C2E-C1E-O5D-C6D |
| 26  | C     | 517  | DGD  | O6E-C1E-O5D-C6D |
| 26  | C     | 518  | DGD  | O2G-C2G-C3G-O3G |
| 26  | C     | 518  | DGD  | O6E-C1E-O5D-C6D |
| 26  | D     | 411  | DGD  | O1G-C1G-C2G-O2G |
| 26  | D     | 411  | DGD  | C2D-C1D-O3G-C3G |
| 26  | D     | 411  | DGD  | O6D-C1D-O3G-C3G |
| 26  | D     | 411  | DGD  | C2E-C1E-O5D-C6D |
| 26  | D     | 411  | DGD  | O6E-C1E-O5D-C6D |
| 26  | a     | 5411 | DGD  | O2G-C2G-C3G-O3G |
| 26  | a     | 5411 | DGD  | O6E-C1E-O5D-C6D |
| 26  | b     | 5621 | DGD  | O1G-C1G-C2G-O2G |
| 26  | b     | 5621 | DGD  | C2D-C1D-O3G-C3G |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 26  | b     | 5621 | DGD  | O6D-C1D-O3G-C3G |
| 26  | b     | 5621 | DGD  | C2E-C1E-O5D-C6D |
| 26  | b     | 5621 | DGD  | O6E-C1E-O5D-C6D |
| 26  | c     | 5515 | DGD  | C2D-C1D-O3G-C3G |
| 26  | c     | 5515 | DGD  | O6D-C1D-O3G-C3G |
| 26  | c     | 5515 | DGD  | O6E-C1E-O5D-C6D |
| 26  | c     | 5516 | DGD  | C2E-C1E-O5D-C6D |
| 26  | c     | 5516 | DGD  | O6E-C1E-O5D-C6D |
| 17  | B     | 607  | CLA  | O1D-CGD-O2D-CED |
| 17  | B     | 609  | CLA  | O1D-CGD-O2D-CED |
| 17  | B     | 611  | CLA  | O1D-CGD-O2D-CED |
| 17  | B     | 613  | CLA  | O1D-CGD-O2D-CED |
| 17  | B     | 615  | CLA  | O1D-CGD-O2D-CED |
| 17  | C     | 511  | CLA  | O1D-CGD-O2D-CED |
| 17  | b     | 5607 | CLA  | O1D-CGD-O2D-CED |
| 17  | b     | 5609 | CLA  | O1D-CGD-O2D-CED |
| 17  | b     | 5611 | CLA  | O1D-CGD-O2D-CED |
| 17  | b     | 5615 | CLA  | O1D-CGD-O2D-CED |
| 17  | k     | 5501 | CLA  | O1D-CGD-O2D-CED |
| 23  | a     | 5401 | SQD  | O49-C7-O47-C45  |
| 17  | C     | 502  | CLA  | O1D-CGD-O2D-CED |
| 17  | b     | 5613 | CLA  | O1D-CGD-O2D-CED |
| 17  | c     | 5502 | CLA  | O1D-CGD-O2D-CED |
| 17  | A     | 405  | CLA  | CBD-CGD-O2D-CED |
| 17  | B     | 605  | CLA  | CBD-CGD-O2D-CED |
| 17  | B     | 606  | CLA  | CBD-CGD-O2D-CED |
| 17  | B     | 607  | CLA  | CBD-CGD-O2D-CED |
| 17  | B     | 611  | CLA  | CBD-CGD-O2D-CED |
| 17  | B     | 613  | CLA  | CBD-CGD-O2D-CED |
| 17  | B     | 614  | CLA  | CBD-CGD-O2D-CED |
| 17  | B     | 616  | CLA  | CBD-CGD-O2D-CED |
| 17  | C     | 501  | CLA  | CBD-CGD-O2D-CED |
| 17  | C     | 502  | CLA  | CBD-CGD-O2D-CED |
| 17  | C     | 503  | CLA  | CBD-CGD-O2D-CED |
| 17  | C     | 506  | CLA  | CBD-CGD-O2D-CED |
| 17  | C     | 507  | CLA  | CBD-CGD-O2D-CED |
| 17  | C     | 509  | CLA  | CBD-CGD-O2D-CED |
| 17  | C     | 511  | CLA  | CBD-CGD-O2D-CED |
| 17  | C     | 512  | CLA  | CBD-CGD-O2D-CED |
| 17  | a     | 5406 | CLA  | CBD-CGD-O2D-CED |
| 17  | b     | 5605 | CLA  | CBD-CGD-O2D-CED |
| 17  | b     | 5606 | CLA  | CBD-CGD-O2D-CED |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | b     | 5607 | CLA  | CBD-CGD-O2D-CED |
| 17  | b     | 5611 | CLA  | CBD-CGD-O2D-CED |
| 17  | b     | 5613 | CLA  | CBD-CGD-O2D-CED |
| 17  | b     | 5614 | CLA  | CBD-CGD-O2D-CED |
| 17  | b     | 5616 | CLA  | CBD-CGD-O2D-CED |
| 17  | c     | 5501 | CLA  | CBD-CGD-O2D-CED |
| 17  | c     | 5502 | CLA  | CBD-CGD-O2D-CED |
| 17  | c     | 5503 | CLA  | CBD-CGD-O2D-CED |
| 17  | c     | 5506 | CLA  | CBD-CGD-O2D-CED |
| 17  | c     | 5507 | CLA  | CBD-CGD-O2D-CED |
| 17  | c     | 5509 | CLA  | CBD-CGD-O2D-CED |
| 17  | c     | 5511 | CLA  | CBD-CGD-O2D-CED |
| 17  | k     | 5501 | CLA  | CBD-CGD-O2D-CED |
| 22  | T     | 101  | LMT  | O5B-C1B-O1B-C4' |
| 22  | T     | 101  | LMT  | C4B-C5B-C6B-O6B |
| 17  | C     | 501  | CLA  | O1D-CGD-O2D-CED |
| 17  | c     | 5501 | CLA  | O1D-CGD-O2D-CED |
| 17  | B     | 603  | CLA  | O1D-CGD-O2D-CED |
| 17  | C     | 509  | CLA  | O1D-CGD-O2D-CED |
| 17  | C     | 510  | CLA  | O1D-CGD-O2D-CED |
| 17  | b     | 5603 | CLA  | O1D-CGD-O2D-CED |
| 17  | c     | 5509 | CLA  | O1D-CGD-O2D-CED |
| 17  | c     | 5510 | CLA  | O1D-CGD-O2D-CED |
| 18  | D     | 402  | PHO  | O1D-CGD-O2D-CED |
| 18  | d     | 5402 | PHO  | O1D-CGD-O2D-CED |
| 17  | B     | 602  | CLA  | CBD-CGD-O2D-CED |
| 17  | B     | 604  | CLA  | CBD-CGD-O2D-CED |
| 17  | C     | 508  | CLA  | CBD-CGD-O2D-CED |
| 17  | b     | 5602 | CLA  | CBD-CGD-O2D-CED |
| 17  | b     | 5604 | CLA  | CBD-CGD-O2D-CED |
| 17  | c     | 5508 | CLA  | CBD-CGD-O2D-CED |
| 17  | C     | 507  | CLA  | O1A-CGA-O2A-C1  |
| 17  | D     | 405  | CLA  | O1A-CGA-O2A-C1  |
| 17  | c     | 5507 | CLA  | O1A-CGA-O2A-C1  |
| 17  | d     | 5404 | CLA  | O1A-CGA-O2A-C1  |
| 23  | L     | 101  | SQD  | O10-C23-O48-C46 |
| 25  | D     | 409  | MGE  | C4D-C5D-C6D-O5D |
| 17  | D     | 405  | CLA  | O1D-CGD-O2D-CED |
| 17  | d     | 5404 | CLA  | O1D-CGD-O2D-CED |
| 22  | T     | 101  | LMT  | C2B-C1B-O1B-C4' |
| 17  | A     | 401  | CLA  | CBD-CGD-O2D-CED |
| 17  | a     | 5402 | CLA  | CBD-CGD-O2D-CED |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 25  | m     | 5103 | MGE  | O1B-C1B-O2G-C2G |
| 26  | A     | 413  | DGD  | O1B-C1B-O2G-C2G |
| 26  | C     | 517  | DGD  | O1B-C1B-O2G-C2G |
| 26  | c     | 5515 | DGD  | O1B-C1B-O2G-C2G |
| 26  | c     | 5516 | DGD  | O1B-C1B-O2G-C2G |
| 17  | B     | 602  | CLA  | C3-C5-C6-C7     |
| 17  | B     | 606  | CLA  | C3-C5-C6-C7     |
| 17  | B     | 608  | CLA  | C3-C5-C6-C7     |
| 17  | B     | 614  | CLA  | C3-C5-C6-C7     |
| 17  | b     | 5602 | CLA  | C3-C5-C6-C7     |
| 17  | b     | 5608 | CLA  | C3-C5-C6-C7     |
| 17  | b     | 5614 | CLA  | C3-C5-C6-C7     |
| 17  | C     | 507  | CLA  | CBA-CGA-O2A-C1  |
| 17  | D     | 405  | CLA  | CBA-CGA-O2A-C1  |
| 17  | c     | 5507 | CLA  | CBA-CGA-O2A-C1  |
| 17  | d     | 5404 | CLA  | CBA-CGA-O2A-C1  |
| 26  | C     | 518  | DGD  | C2A-C1A-O1G-C1G |
| 26  | a     | 5411 | DGD  | C2A-C1A-O1G-C1G |
| 23  | L     | 101  | SQD  | C8-C7-O47-C45   |
| 17  | c     | 5505 | CLA  | C2C-C3C-CAC-CBC |
| 17  | B     | 606  | CLA  | C2-C3-C5-C6     |
| 19  | A     | 406  | PQ9  | C17-C18-C20-C21 |
| 19  | A     | 406  | PQ9  | C32-C33-C35-C36 |
| 19  | D     | 406  | PQ9  | C32-C33-C35-C36 |
| 19  | a     | 5407 | PQ9  | C17-C18-C20-C21 |
| 19  | d     | 5405 | PQ9  | C32-C33-C35-C36 |
| 17  | B     | 601  | CLA  | CBD-CGD-O2D-CED |
| 17  | C     | 513  | CLA  | CBD-CGD-O2D-CED |
| 17  | b     | 5601 | CLA  | CBD-CGD-O2D-CED |
| 17  | c     | 5512 | CLA  | CBD-CGD-O2D-CED |
| 17  | B     | 602  | CLA  | C2A-CAA-CBA-CGA |
| 17  | C     | 508  | CLA  | C2A-CAA-CBA-CGA |
| 17  | b     | 5602 | CLA  | C2A-CAA-CBA-CGA |
| 17  | c     | 5508 | CLA  | C2A-CAA-CBA-CGA |
| 17  | C     | 506  | CLA  | O1D-CGD-O2D-CED |
| 17  | c     | 5506 | CLA  | O1D-CGD-O2D-CED |
| 17  | C     | 505  | CLA  | C2C-C3C-CAC-CBC |
| 17  | A     | 402  | CLA  | C3-C5-C6-C7     |
| 17  | B     | 612  | CLA  | C3-C5-C6-C7     |
| 17  | C     | 505  | CLA  | C3-C5-C6-C7     |
| 17  | a     | 5403 | CLA  | C3-C5-C6-C7     |
| 17  | b     | 5612 | CLA  | C3-C5-C6-C7     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | c     | 5505 | CLA  | C3-C5-C6-C7     |
| 23  | L     | 101  | SQD  | C24-C23-O48-C46 |
| 26  | D     | 411  | DGD  | C4D-C5D-C6D-O5D |
| 26  | b     | 5621 | DGD  | C4D-C5D-C6D-O5D |
| 17  | B     | 605  | CLA  | O1D-CGD-O2D-CED |
| 17  | b     | 5605 | CLA  | O1D-CGD-O2D-CED |
| 25  | D     | 409  | MGE  | O6D-C5D-C6D-O5D |
| 23  | a     | 5401 | SQD  | C24-C23-O48-C46 |
| 20  | A     | 407  | BCR  | C13-C14-C15-C16 |
| 20  | C     | 514  | BCR  | C9-C10-C11-C12  |
| 20  | C     | 515  | BCR  | C19-C20-C21-C22 |
| 20  | D     | 407  | BCR  | C9-C10-C11-C12  |
| 20  | T     | 102  | BCR  | C9-C10-C11-C12  |
| 20  | a     | 5408 | BCR  | C13-C14-C15-C16 |
| 20  | c     | 5513 | BCR  | C9-C10-C11-C12  |
| 20  | d     | 5406 | BCR  | C9-C10-C11-C12  |
| 20  | t     | 5102 | BCR  | C15-C16-C17-C18 |
| 20  | z     | 5101 | BCR  | C19-C20-C21-C22 |
| 20  | Y     | 101  | BCR  | C19-C20-C21-C22 |
| 22  | A     | 409  | LMT  | O5B-C5B-C6B-O6B |
| 22  | B     | 620  | LMT  | O5'-C5'-C6'-O6' |
| 22  | A     | 409  | LMT  | C4B-C5B-C6B-O6B |
| 17  | C     | 504  | CLA  | CBD-CGD-O2D-CED |
| 17  | D     | 404  | CLA  | CBD-CGD-O2D-CED |
| 17  | c     | 5504 | CLA  | CBD-CGD-O2D-CED |
| 17  | d     | 5403 | CLA  | CBD-CGD-O2D-CED |
| 17  | A     | 405  | CLA  | O1D-CGD-O2D-CED |
| 17  | B     | 614  | CLA  | O1D-CGD-O2D-CED |
| 17  | a     | 5406 | CLA  | O1D-CGD-O2D-CED |
| 17  | b     | 5614 | CLA  | O1D-CGD-O2D-CED |
| 22  | T     | 101  | LMT  | O5B-C5B-C6B-O6B |
| 22  | a     | 5410 | LMT  | O5'-C5'-C6'-O6' |
| 22  | m     | 5102 | LMT  | O5B-C5B-C6B-O6B |
| 22  | m     | 5102 | LMT  | C4B-C5B-C6B-O6B |
| 17  | c     | 5503 | CLA  | O1D-CGD-O2D-CED |
| 25  | D     | 409  | MGE  | C2B-C1B-O2G-C2G |
| 17  | C     | 503  | CLA  | O1D-CGD-O2D-CED |
| 22  | M     | 101  | LMT  | O5B-C5B-C6B-O6B |
| 17  | C     | 507  | CLA  | O1D-CGD-O2D-CED |
| 17  | c     | 5507 | CLA  | O1D-CGD-O2D-CED |
| 22  | T     | 101  | LMT  | O5'-C5'-C6'-O6' |
| 17  | b     | 5616 | CLA  | O1D-CGD-O2D-CED |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | C     | 505  | CLA  | C5-C6-C7-C8     |
| 17  | c     | 5505 | CLA  | C5-C6-C7-C8     |
| 17  | A     | 403  | CLA  | C3-C5-C6-C7     |
| 17  | a     | 5404 | CLA  | C3-C5-C6-C7     |
| 23  | a     | 5401 | SQD  | O10-C23-O48-C46 |
| 17  | B     | 616  | CLA  | O1D-CGD-O2D-CED |
| 26  | C     | 518  | DGD  | O6E-C5E-C6E-O5E |
| 26  | a     | 5411 | DGD  | O6E-C5E-C6E-O5E |
| 17  | B     | 605  | CLA  | C4-C3-C5-C6     |
| 17  | D     | 404  | CLA  | C4-C3-C5-C6     |
| 17  | b     | 5605 | CLA  | C4-C3-C5-C6     |
| 17  | d     | 5403 | CLA  | C4-C3-C5-C6     |
| 19  | A     | 406  | PQ9  | C14-C13-C15-C16 |
| 19  | D     | 406  | PQ9  | C19-C18-C20-C21 |
| 19  | a     | 5407 | PQ9  | C14-C13-C15-C16 |
| 19  | d     | 5405 | PQ9  | C19-C18-C20-C21 |
| 17  | B     | 605  | CLA  | C2-C3-C5-C6     |
| 17  | D     | 404  | CLA  | C2-C3-C5-C6     |
| 17  | b     | 5605 | CLA  | C2-C3-C5-C6     |
| 17  | d     | 5403 | CLA  | C2-C3-C5-C6     |
| 19  | A     | 406  | PQ9  | C12-C13-C15-C16 |
| 19  | D     | 406  | PQ9  | C17-C18-C20-C21 |
| 19  | D     | 406  | PQ9  | C22-C23-C25-C26 |
| 19  | a     | 5407 | PQ9  | C12-C13-C15-C16 |
| 19  | d     | 5405 | PQ9  | C17-C18-C20-C21 |
| 19  | d     | 5405 | PQ9  | C22-C23-C25-C26 |
| 26  | D     | 411  | DGD  | O6D-C5D-C6D-O5D |
| 26  | b     | 5621 | DGD  | O6D-C5D-C6D-O5D |
| 17  | B     | 606  | CLA  | C2A-CAA-CBA-CGA |
| 17  | C     | 509  | CLA  | C2A-CAA-CBA-CGA |
| 17  | c     | 5509 | CLA  | C2A-CAA-CBA-CGA |
| 22  | M     | 101  | LMT  | O5'-C1'-O1'-C1  |
| 23  | D     | 403  | SQD  | O5-C1-O6-C44    |
| 19  | A     | 406  | PQ9  | C38-C40-C41-C42 |
| 17  | B     | 606  | CLA  | O1D-CGD-O2D-CED |
| 17  | C     | 512  | CLA  | O1D-CGD-O2D-CED |
| 17  | b     | 5606 | CLA  | O1D-CGD-O2D-CED |
| 17  | c     | 5511 | CLA  | O1D-CGD-O2D-CED |
| 17  | C     | 505  | CLA  | C4C-C3C-CAC-CBC |
| 17  | c     | 5505 | CLA  | C4C-C3C-CAC-CBC |
| 17  | C     | 508  | CLA  | O1D-CGD-O2D-CED |
| 17  | c     | 5508 | CLA  | O1D-CGD-O2D-CED |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | A     | 401  | CLA  | CBA-CGA-O2A-C1  |
| 17  | B     | 607  | CLA  | CBA-CGA-O2A-C1  |
| 17  | C     | 506  | CLA  | CBA-CGA-O2A-C1  |
| 17  | a     | 5402 | CLA  | CBA-CGA-O2A-C1  |
| 17  | b     | 5607 | CLA  | CBA-CGA-O2A-C1  |
| 17  | c     | 5506 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 620  | LMT  | C4'-C5'-C6'-O6' |
| 20  | B     | 617  | BCR  | C9-C10-C11-C12  |
| 20  | C     | 516  | BCR  | C9-C10-C11-C12  |
| 20  | C     | 516  | BCR  | C13-C14-C15-C16 |
| 20  | b     | 5617 | BCR  | C9-C10-C11-C12  |
| 20  | c     | 5514 | BCR  | C9-C10-C11-C12  |
| 20  | c     | 5514 | BCR  | C13-C14-C15-C16 |
| 22  | M     | 101  | LMT  | O5'-C5'-C6'-O6' |
| 26  | C     | 518  | DGD  | O1A-C1A-O1G-C1G |
| 26  | a     | 5411 | DGD  | O1A-C1A-O1G-C1G |
| 17  | C     | 503  | CLA  | C10-C11-C12-C13 |
| 17  | c     | 5503 | CLA  | C10-C11-C12-C13 |
| 23  | A     | 410  | SQD  | C2-C1-O6-C44    |
| 26  | C     | 518  | DGD  | C2E-C1E-O5D-C6D |
| 26  | a     | 5411 | DGD  | C2E-C1E-O5D-C6D |
| 23  | l     | 5102 | SQD  | O47-C45-C46-O48 |
| 17  | B     | 607  | CLA  | O1A-CGA-O2A-C1  |
| 17  | b     | 5607 | CLA  | O1A-CGA-O2A-C1  |
| 17  | B     | 603  | CLA  | C4-C3-C5-C6     |
| 17  | b     | 5603 | CLA  | C4-C3-C5-C6     |
| 17  | B     | 604  | CLA  | C14-C13-C15-C16 |
| 17  | C     | 501  | CLA  | C11-C12-C13-C14 |
| 17  | C     | 506  | CLA  | C11-C10-C8-C9   |
| 17  | C     | 507  | CLA  | C11-C10-C8-C9   |
| 17  | C     | 508  | CLA  | C11-C10-C8-C9   |
| 17  | C     | 511  | CLA  | C6-C7-C8-C9     |
| 17  | D     | 404  | CLA  | C6-C7-C8-C9     |
| 17  | b     | 5604 | CLA  | C14-C13-C15-C16 |
| 17  | c     | 5501 | CLA  | C11-C12-C13-C14 |
| 17  | c     | 5506 | CLA  | C11-C10-C8-C9   |
| 17  | c     | 5507 | CLA  | C11-C10-C8-C9   |
| 17  | c     | 5508 | CLA  | C11-C10-C8-C9   |
| 17  | d     | 5403 | CLA  | C6-C7-C8-C9     |
| 17  | k     | 5501 | CLA  | C6-C7-C8-C9     |
| 18  | A     | 404  | PHO  | C11-C10-C8-C9   |
| 18  | a     | 5405 | PHO  | C11-C10-C8-C9   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | B     | 602  | CLA  | O1D-CGD-O2D-CED |
| 17  | b     | 5602 | CLA  | O1D-CGD-O2D-CED |
| 17  | A     | 403  | CLA  | CBD-CGD-O2D-CED |
| 17  | a     | 5404 | CLA  | CBD-CGD-O2D-CED |
| 17  | C     | 510  | CLA  | C15-C16-C17-C18 |
| 17  | c     | 5510 | CLA  | C15-C16-C17-C18 |
| 17  | A     | 405  | CLA  | C2A-CAA-CBA-CGA |
| 17  | a     | 5406 | CLA  | C2A-CAA-CBA-CGA |
| 20  | C     | 515  | BCR  | C7-C8-C9-C34    |
| 20  | D     | 407  | BCR  | C7-C8-C9-C34    |
| 20  | d     | 5406 | BCR  | C7-C8-C9-C34    |
| 20  | z     | 5101 | BCR  | C7-C8-C9-C34    |
| 20  | A     | 407  | BCR  | C11-C12-C13-C14 |
| 20  | C     | 515  | BCR  | C7-C8-C9-C10    |
| 20  | T     | 102  | BCR  | C7-C8-C9-C10    |
| 20  | a     | 5408 | BCR  | C11-C12-C13-C14 |
| 20  | z     | 5101 | BCR  | C7-C8-C9-C10    |
| 25  | D     | 409  | MGE  | O1B-C1B-O2G-C2G |
| 23  | d     | 5407 | SQD  | C8-C7-O47-C45   |
| 23  | L     | 101  | SQD  | C9-C10-C11-C12  |
| 25  | d     | 5409 | MGE  | C1B-C2B-C3B-C4B |
| 25  | m     | 5103 | MGE  | C1A-C2A-C3A-C4A |
| 17  | C     | 506  | CLA  | C15-C16-C17-C18 |
| 17  | c     | 5506 | CLA  | C15-C16-C17-C18 |
| 22  | m     | 5102 | LMT  | O5'-C5'-C6'-O6' |
| 22  | a     | 5410 | LMT  | C4'-C5'-C6'-O6' |
| 17  | A     | 402  | CLA  | C15-C16-C17-C18 |
| 17  | B     | 609  | CLA  | C10-C11-C12-C13 |
| 17  | B     | 609  | CLA  | C13-C15-C16-C17 |
| 17  | C     | 505  | CLA  | C13-C15-C16-C17 |
| 17  | D     | 404  | CLA  | C13-C15-C16-C17 |
| 17  | a     | 5403 | CLA  | C15-C16-C17-C18 |
| 17  | c     | 5505 | CLA  | C13-C15-C16-C17 |
| 17  | d     | 5403 | CLA  | C13-C15-C16-C17 |
| 18  | D     | 402  | PHO  | C5-C6-C7-C8     |
| 18  | d     | 5402 | PHO  | C5-C6-C7-C8     |
| 17  | A     | 401  | CLA  | O1A-CGA-O2A-C1  |
| 17  | a     | 5402 | CLA  | O1A-CGA-O2A-C1  |
| 17  | A     | 402  | CLA  | C5-C6-C7-C8     |
| 17  | A     | 403  | CLA  | C8-C10-C11-C12  |
| 17  | A     | 405  | CLA  | C5-C6-C7-C8     |
| 17  | C     | 508  | CLA  | C10-C11-C12-C13 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | C     | 511  | CLA  | C10-C11-C12-C13 |
| 17  | a     | 5403 | CLA  | C5-C6-C7-C8     |
| 17  | a     | 5404 | CLA  | C8-C10-C11-C12  |
| 17  | a     | 5406 | CLA  | C5-C6-C7-C8     |
| 17  | b     | 5609 | CLA  | C10-C11-C12-C13 |
| 17  | b     | 5609 | CLA  | C13-C15-C16-C17 |
| 17  | c     | 5508 | CLA  | C10-C11-C12-C13 |
| 17  | k     | 5501 | CLA  | C10-C11-C12-C13 |
| 23  | A     | 410  | SQD  | O10-C23-O48-C46 |
| 17  | C     | 506  | CLA  | O1A-CGA-O2A-C1  |
| 17  | c     | 5506 | CLA  | O1A-CGA-O2A-C1  |
| 21  | A     | 408  | LHG  | C23-C24-C25-C26 |
| 21  | a     | 5409 | LHG  | C23-C24-C25-C26 |
| 25  | D     | 409  | MGE  | C1B-C2B-C3B-C4B |
| 17  | B     | 611  | CLA  | C13-C15-C16-C17 |
| 17  | b     | 5611 | CLA  | C13-C15-C16-C17 |
| 25  | d     | 5410 | MGE  | C2A-C3A-C4A-C5A |
| 17  | B     | 603  | CLA  | C10-C11-C12-C13 |
| 17  | B     | 611  | CLA  | C15-C16-C17-C18 |
| 17  | D     | 404  | CLA  | C15-C16-C17-C18 |
| 17  | b     | 5603 | CLA  | C10-C11-C12-C13 |
| 17  | b     | 5611 | CLA  | C15-C16-C17-C18 |
| 17  | d     | 5403 | CLA  | C15-C16-C17-C18 |
| 18  | D     | 402  | PHO  | C15-C16-C17-C18 |
| 18  | d     | 5402 | PHO  | C15-C16-C17-C18 |
| 25  | A     | 412  | MGE  | C1A-C2A-C3A-C4A |
| 25  | A     | 412  | MGE  | C1B-C2B-C3B-C4B |
| 25  | l     | 5101 | MGE  | C1A-C2A-C3A-C4A |
| 25  | l     | 5101 | MGE  | C1B-C2B-C3B-C4B |
| 17  | B     | 612  | CLA  | CBD-CGD-O2D-CED |
| 17  | b     | 5612 | CLA  | CBD-CGD-O2D-CED |
| 26  | A     | 413  | DGD  | C2B-C1B-O2G-C2G |
| 26  | c     | 5515 | DGD  | C2B-C1B-O2G-C2G |
| 17  | B     | 601  | CLA  | O1D-CGD-O2D-CED |
| 17  | b     | 5601 | CLA  | O1D-CGD-O2D-CED |
| 17  | B     | 606  | CLA  | C12-C13-C15-C16 |
| 17  | B     | 612  | CLA  | C11-C10-C8-C7   |
| 17  | C     | 503  | CLA  | C12-C13-C15-C16 |
| 17  | b     | 5612 | CLA  | C11-C10-C8-C7   |
| 17  | c     | 5503 | CLA  | C12-C13-C15-C16 |
| 18  | A     | 404  | PHO  | C11-C10-C8-C7   |
| 18  | A     | 404  | PHO  | C12-C13-C15-C16 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 18  | a     | 5405 | PHO  | C11-C10-C8-C7   |
| 18  | a     | 5405 | PHO  | C12-C13-C15-C16 |
| 20  | k     | 5502 | BCR  | C9-C10-C11-C12  |
| 17  | A     | 401  | CLA  | O1D-CGD-O2D-CED |
| 17  | a     | 5402 | CLA  | O1D-CGD-O2D-CED |
| 17  | b     | 5604 | CLA  | O1D-CGD-O2D-CED |
| 17  | B     | 611  | CLA  | C5-C6-C7-C8     |
| 17  | b     | 5611 | CLA  | C5-C6-C7-C8     |
| 22  | M     | 101  | LMT  | O1'-C1-C2-C3    |
| 20  | T     | 102  | BCR  | C22-C23-C24-C25 |
| 17  | B     | 610  | CLA  | C15-C16-C17-C18 |
| 17  | b     | 5610 | CLA  | C15-C16-C17-C18 |
| 17  | B     | 604  | CLA  | O1D-CGD-O2D-CED |
| 19  | A     | 406  | PQ9  | C13-C15-C16-C17 |
| 19  | D     | 406  | PQ9  | C13-C15-C16-C17 |
| 19  | a     | 5407 | PQ9  | C13-C15-C16-C17 |
| 19  | d     | 5405 | PQ9  | C13-C15-C16-C17 |
| 23  | L     | 101  | SQD  | C14-C15-C16-C17 |
| 20  | B     | 617  | BCR  | C10-C11-C12-C13 |
| 20  | B     | 618  | BCR  | C18-C19-C20-C21 |
| 20  | D     | 407  | BCR  | C10-C11-C12-C13 |
| 20  | H     | 101  | BCR  | C18-C19-C20-C21 |
| 20  | b     | 5617 | BCR  | C10-C11-C12-C13 |
| 20  | b     | 5618 | BCR  | C18-C19-C20-C21 |
| 20  | d     | 5406 | BCR  | C10-C11-C12-C13 |
| 20  | h     | 5101 | BCR  | C18-C19-C20-C21 |
| 20  | k     | 5502 | BCR  | C10-C11-C12-C13 |
| 17  | A     | 401  | CLA  | C13-C15-C16-C17 |
| 17  | a     | 5402 | CLA  | C13-C15-C16-C17 |
| 23  | l     | 5102 | SQD  | C23-C24-C25-C26 |
| 17  | A     | 401  | CLA  | C5-C6-C7-C8     |
| 17  | B     | 602  | CLA  | C15-C16-C17-C18 |
| 17  | B     | 612  | CLA  | C10-C11-C12-C13 |
| 17  | B     | 616  | CLA  | C13-C15-C16-C17 |
| 17  | C     | 508  | CLA  | C15-C16-C17-C18 |
| 17  | a     | 5402 | CLA  | C5-C6-C7-C8     |
| 17  | b     | 5602 | CLA  | C15-C16-C17-C18 |
| 17  | b     | 5612 | CLA  | C10-C11-C12-C13 |
| 17  | b     | 5616 | CLA  | C13-C15-C16-C17 |
| 17  | c     | 5508 | CLA  | C15-C16-C17-C18 |
| 26  | C     | 517  | DGD  | C2B-C1B-O2G-C2G |
| 26  | c     | 5516 | DGD  | C2B-C1B-O2G-C2G |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 21  | A     | 408  | LHG  | C3-O3-P-O6      |
| 21  | a     | 5409 | LHG  | C3-O3-P-O6      |
| 17  | C     | 506  | CLA  | C3-C5-C6-C7     |
| 17  | c     | 5506 | CLA  | C3-C5-C6-C7     |
| 23  | D     | 403  | SQD  | C24-C23-O48-C46 |
| 25  | D     | 410  | MGE  | C1B-C2B-C3B-C4B |
| 17  | B     | 614  | CLA  | C2A-CAA-CBA-CGA |
| 17  | b     | 5614 | CLA  | C2A-CAA-CBA-CGA |
| 17  | B     | 605  | CLA  | CBA-CGA-O2A-C1  |
| 17  | C     | 512  | CLA  | CBA-CGA-O2A-C1  |
| 17  | b     | 5605 | CLA  | CBA-CGA-O2A-C1  |
| 17  | c     | 5511 | CLA  | CBA-CGA-O2A-C1  |
| 23  | l     | 5102 | SQD  | C24-C25-C26-C27 |
| 23  | D     | 403  | SQD  | C8-C7-O47-C45   |
| 25  | D     | 410  | MGE  | C2B-C1B-O2G-C2G |
| 25  | d     | 5408 | MGE  | C2B-C1B-O2G-C2G |
| 25  | d     | 5410 | MGE  | C2B-C1B-O2G-C2G |
| 20  | A     | 407  | BCR  | C11-C10-C9-C34  |
| 20  | A     | 407  | BCR  | C16-C17-C18-C36 |
| 20  | B     | 618  | BCR  | C11-C10-C9-C34  |
| 20  | C     | 515  | BCR  | C11-C10-C9-C34  |
| 20  | D     | 407  | BCR  | C35-C13-C14-C15 |
| 20  | H     | 101  | BCR  | C20-C21-C22-C37 |
| 20  | T     | 102  | BCR  | C20-C21-C22-C37 |
| 20  | a     | 5408 | BCR  | C11-C10-C9-C34  |
| 20  | a     | 5408 | BCR  | C16-C17-C18-C36 |
| 20  | b     | 5618 | BCR  | C11-C10-C9-C34  |
| 20  | d     | 5406 | BCR  | C35-C13-C14-C15 |
| 20  | h     | 5101 | BCR  | C20-C21-C22-C37 |
| 20  | z     | 5101 | BCR  | C11-C10-C9-C34  |
| 20  | Y     | 101  | BCR  | C20-C21-C22-C37 |
| 22  | B     | 620  | LMT  | C4-C5-C6-C7     |
| 26  | A     | 413  | DGD  | C4A-C5A-C6A-C7A |
| 26  | C     | 517  | DGD  | C8A-C9A-CAA-CBA |
| 26  | c     | 5515 | DGD  | C4A-C5A-C6A-C7A |
| 26  | c     | 5516 | DGD  | C8A-C9A-CAA-CBA |
| 26  | C     | 518  | DGD  | C5A-C6A-C7A-C8A |
| 26  | a     | 5411 | DGD  | C5A-C6A-C7A-C8A |
| 17  | C     | 513  | CLA  | O1D-CGD-O2D-CED |
| 17  | c     | 5512 | CLA  | O1D-CGD-O2D-CED |
| 25  | C     | 519  | MGE  | O6D-C5D-C6D-O5D |
| 25  | D     | 410  | MGE  | O1B-C1B-O2G-C2G |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 25  | d     | 5408 | MGE  | O1B-C1B-O2G-C2G |
| 25  | d     | 5410 | MGE  | O1B-C1B-O2G-C2G |
| 26  | A     | 413  | DGD  | O1A-C1A-O1G-C1G |
| 17  | D     | 404  | CLA  | O1D-CGD-O2D-CED |
| 17  | d     | 5403 | CLA  | O1D-CGD-O2D-CED |
| 25  | D     | 410  | MGE  | C2B-C3B-C4B-C5B |
| 17  | B     | 605  | CLA  | C3-C5-C6-C7     |
| 17  | b     | 5605 | CLA  | C3-C5-C6-C7     |
| 25  | c     | 5517 | MGE  | O6D-C5D-C6D-O5D |
| 17  | C     | 504  | CLA  | O1D-CGD-O2D-CED |
| 17  | c     | 5504 | CLA  | O1D-CGD-O2D-CED |
| 20  | B     | 618  | BCR  | C12-C13-C14-C15 |
| 20  | C     | 514  | BCR  | C16-C17-C18-C19 |
| 20  | C     | 516  | BCR  | C20-C21-C22-C23 |
| 20  | T     | 102  | BCR  | C20-C21-C22-C23 |
| 20  | b     | 5618 | BCR  | C12-C13-C14-C15 |
| 20  | c     | 5513 | BCR  | C16-C17-C18-C19 |
| 20  | c     | 5514 | BCR  | C20-C21-C22-C23 |
| 20  | k     | 5502 | BCR  | C20-C21-C22-C23 |
| 20  | t     | 5102 | BCR  | C12-C13-C14-C15 |
| 23  | L     | 101  | SQD  | C2-C1-O6-C44    |
| 23  | l     | 5102 | SQD  | C27-C28-C29-C30 |
| 17  | A     | 402  | CLA  | C8-C10-C11-C12  |
| 17  | B     | 605  | CLA  | C8-C10-C11-C12  |
| 17  | a     | 5403 | CLA  | C8-C10-C11-C12  |
| 17  | b     | 5605 | CLA  | C8-C10-C11-C12  |
| 26  | c     | 5515 | DGD  | O1A-C1A-O1G-C1G |
| 17  | A     | 403  | CLA  | C16-C17-C18-C19 |
| 17  | B     | 609  | CLA  | C16-C17-C18-C20 |
| 17  | a     | 5404 | CLA  | C16-C17-C18-C19 |
| 17  | b     | 5609 | CLA  | C16-C17-C18-C20 |
| 22  | A     | 409  | LMT  | C5'-C4'-O1B-C1B |
| 23  | D     | 403  | SQD  | C15-C16-C17-C18 |
| 26  | A     | 413  | DGD  | C3A-C4A-C5A-C6A |
| 26  | c     | 5515 | DGD  | C3A-C4A-C5A-C6A |
| 17  | B     | 602  | CLA  | C6-C7-C8-C9     |
| 17  | b     | 5602 | CLA  | C6-C7-C8-C9     |
| 26  | C     | 517  | DGD  | C1A-C2A-C3A-C4A |
| 26  | c     | 5516 | DGD  | C1A-C2A-C3A-C4A |
| 23  | D     | 403  | SQD  | C17-C18-C19-C20 |
| 25  | D     | 409  | MGE  | C9B-CAB-CBB-CCB |
| 25  | m     | 5103 | MGE  | C2A-C3A-C4A-C5A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 26  | A     | 413  | DGD  | C2B-C3B-C4B-C5B |
| 26  | C     | 517  | DGD  | C2A-C3A-C4A-C5A |
| 26  | D     | 411  | DGD  | C2A-C3A-C4A-C5A |
| 26  | b     | 5621 | DGD  | C2A-C3A-C4A-C5A |
| 26  | c     | 5515 | DGD  | C2B-C3B-C4B-C5B |
| 26  | c     | 5516 | DGD  | C2A-C3A-C4A-C5A |
| 17  | C     | 503  | CLA  | C13-C15-C16-C17 |
| 17  | c     | 5503 | CLA  | C13-C15-C16-C17 |
| 17  | B     | 610  | CLA  | C2A-CAA-CBA-CGA |
| 17  | b     | 5610 | CLA  | C2A-CAA-CBA-CGA |
| 26  | A     | 413  | DGD  | C4D-C5D-C6D-O5D |
| 26  | c     | 5515 | DGD  | C4D-C5D-C6D-O5D |
| 20  | T     | 102  | BCR  | C7-C8-C9-C34    |
| 20  | B     | 617  | BCR  | C7-C8-C9-C10    |
| 20  | B     | 617  | BCR  | C11-C12-C13-C14 |
| 20  | C     | 514  | BCR  | C7-C8-C9-C10    |
| 20  | C     | 516  | BCR  | C7-C8-C9-C10    |
| 20  | b     | 5617 | BCR  | C7-C8-C9-C10    |
| 20  | b     | 5617 | BCR  | C11-C12-C13-C14 |
| 20  | c     | 5513 | BCR  | C7-C8-C9-C10    |
| 20  | c     | 5514 | BCR  | C7-C8-C9-C10    |
| 17  | D     | 404  | CLA  | C3-C5-C6-C7     |
| 17  | d     | 5403 | CLA  | C3-C5-C6-C7     |
| 23  | D     | 403  | SQD  | C34-C35-C36-C37 |
| 25  | d     | 5409 | MGE  | C9B-CAB-CBB-CCB |
| 23  | d     | 5407 | SQD  | C11-C12-C13-C14 |
| 26  | C     | 518  | DGD  | C6A-C7A-C8A-C9A |
| 26  | D     | 411  | DGD  | C4A-C5A-C6A-C7A |
| 26  | a     | 5411 | DGD  | C6A-C7A-C8A-C9A |
| 26  | b     | 5621 | DGD  | C4A-C5A-C6A-C7A |
| 17  | A     | 402  | CLA  | C4B-C3B-CAB-CBB |
| 17  | A     | 403  | CLA  | C4B-C3B-CAB-CBB |
| 17  | B     | 605  | CLA  | C4B-C3B-CAB-CBB |
| 17  | C     | 501  | CLA  | C4B-C3B-CAB-CBB |
| 17  | a     | 5403 | CLA  | C4B-C3B-CAB-CBB |
| 17  | a     | 5404 | CLA  | C4B-C3B-CAB-CBB |
| 17  | b     | 5605 | CLA  | C4B-C3B-CAB-CBB |
| 17  | c     | 5501 | CLA  | C4B-C3B-CAB-CBB |
| 17  | B     | 606  | CLA  | C16-C17-C18-C19 |
| 18  | A     | 404  | PHO  | C16-C17-C18-C19 |
| 18  | a     | 5405 | PHO  | C16-C17-C18-C19 |
| 23  | L     | 101  | SQD  | O5-C1-O6-C44    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | B     | 615  | CLA  | C5-C6-C7-C8     |
| 17  | C     | 506  | CLA  | C13-C15-C16-C17 |
| 17  | D     | 404  | CLA  | C5-C6-C7-C8     |
| 17  | b     | 5615 | CLA  | C5-C6-C7-C8     |
| 17  | c     | 5506 | CLA  | C13-C15-C16-C17 |
| 17  | d     | 5403 | CLA  | C5-C6-C7-C8     |
| 22  | a     | 5410 | LMT  | C4-C5-C6-C7     |
| 26  | A     | 413  | DGD  | C3B-C4B-C5B-C6B |
| 26  | C     | 518  | DGD  | C2B-C3B-C4B-C5B |
| 26  | a     | 5411 | DGD  | C2B-C3B-C4B-C5B |
| 26  | c     | 5515 | DGD  | C3B-C4B-C5B-C6B |
| 23  | D     | 403  | SQD  | C27-C28-C29-C30 |
| 23  | L     | 101  | SQD  | C25-C26-C27-C28 |
| 17  | B     | 605  | CLA  | O1A-CGA-O2A-C1  |
| 17  | b     | 5605 | CLA  | O1A-CGA-O2A-C1  |
| 17  | B     | 613  | CLA  | CBA-CGA-O2A-C1  |
| 17  | b     | 5613 | CLA  | CBA-CGA-O2A-C1  |
| 23  | d     | 5407 | SQD  | C24-C25-C26-C27 |
| 17  | C     | 503  | CLA  | C3A-C2A-CAA-CBA |
| 17  | C     | 512  | CLA  | C3A-C2A-CAA-CBA |
| 17  | D     | 404  | CLA  | C3A-C2A-CAA-CBA |
| 17  | c     | 5503 | CLA  | C3A-C2A-CAA-CBA |
| 17  | c     | 5511 | CLA  | C3A-C2A-CAA-CBA |
| 17  | d     | 5403 | CLA  | C3A-C2A-CAA-CBA |
| 22  | T     | 101  | LMT  | C2-C1-O1'-C1'   |
| 23  | D     | 403  | SQD  | C11-C12-C13-C14 |
| 17  | A     | 403  | CLA  | C16-C17-C18-C20 |
| 17  | B     | 606  | CLA  | C16-C17-C18-C20 |
| 17  | a     | 5404 | CLA  | C16-C17-C18-C20 |
| 18  | A     | 404  | PHO  | C16-C17-C18-C20 |
| 18  | a     | 5405 | PHO  | C16-C17-C18-C20 |
| 25  | d     | 5408 | MGE  | C7A-C8A-C9A-CAA |
| 21  | A     | 408  | LHG  | C4-C5-C6-O8     |
| 21  | a     | 5409 | LHG  | C4-C5-C6-O8     |
| 23  | L     | 101  | SQD  | O6-C44-C45-C46  |
| 25  | D     | 409  | MGE  | O1G-C1G-C2G-C3G |
| 25  | d     | 5409 | MGE  | C1G-C2G-C3G-O3G |
| 25  | d     | 5410 | MGE  | O1G-C1G-C2G-C3G |
| 17  | B     | 608  | CLA  | CBD-CGD-O2D-CED |
| 17  | b     | 5608 | CLA  | CBD-CGD-O2D-CED |
| 21  | A     | 408  | LHG  | C25-C26-C27-C28 |
| 21  | a     | 5409 | LHG  | C25-C26-C27-C28 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 26  | A     | 413  | DGD  | C6A-C7A-C8A-C9A |
| 26  | C     | 518  | DGD  | C4A-C5A-C6A-C7A |
| 26  | a     | 5411 | DGD  | C4A-C5A-C6A-C7A |
| 26  | c     | 5515 | DGD  | C6A-C7A-C8A-C9A |
| 20  | B     | 618  | BCR  | C14-C15-C16-C17 |
| 20  | b     | 5618 | BCR  | C14-C15-C16-C17 |
| 17  | C     | 508  | CLA  | C3-C5-C6-C7     |
| 17  | c     | 5508 | CLA  | C3-C5-C6-C7     |
| 25  | D     | 409  | MGE  | C2B-C3B-C4B-C5B |
| 17  | B     | 611  | CLA  | CBA-CGA-O2A-C1  |
| 17  | b     | 5611 | CLA  | CBA-CGA-O2A-C1  |
| 26  | C     | 518  | DGD  | C4E-C5E-C6E-O5E |
| 26  | a     | 5411 | DGD  | C4E-C5E-C6E-O5E |
| 25  | A     | 412  | MGE  | C2B-C1B-O2G-C2G |
| 25  | l     | 5101 | MGE  | C2B-C1B-O2G-C2G |
| 26  | C     | 518  | DGD  | C2B-C1B-O2G-C2G |
| 26  | a     | 5411 | DGD  | C2B-C1B-O2G-C2G |
| 22  | M     | 101  | LMT  | C4B-C5B-C6B-O6B |
| 21  | A     | 408  | LHG  | O1-C1-C2-O2     |
| 21  | a     | 5409 | LHG  | O1-C1-C2-O2     |
| 17  | B     | 609  | CLA  | C16-C17-C18-C19 |
| 17  | b     | 5609 | CLA  | C16-C17-C18-C19 |
| 17  | A     | 403  | CLA  | C2B-C3B-CAB-CBB |
| 17  | B     | 605  | CLA  | C2B-C3B-CAB-CBB |
| 17  | C     | 501  | CLA  | C2B-C3B-CAB-CBB |
| 17  | C     | 502  | CLA  | C2B-C3B-CAB-CBB |
| 17  | D     | 405  | CLA  | C2B-C3B-CAB-CBB |
| 17  | a     | 5404 | CLA  | C2B-C3B-CAB-CBB |
| 17  | b     | 5605 | CLA  | C2B-C3B-CAB-CBB |
| 17  | c     | 5501 | CLA  | C2B-C3B-CAB-CBB |
| 17  | c     | 5502 | CLA  | C2B-C3B-CAB-CBB |
| 17  | d     | 5404 | CLA  | C2B-C3B-CAB-CBB |
| 25  | m     | 5103 | MGE  | C6B-C7B-C8B-C9B |
| 17  | C     | 512  | CLA  | O1A-CGA-O2A-C1  |
| 17  | c     | 5511 | CLA  | O1A-CGA-O2A-C1  |
| 23  | D     | 403  | SQD  | C13-C14-C15-C16 |
| 17  | B     | 615  | CLA  | C2-C1-O2A-CGA   |
| 17  | b     | 5615 | CLA  | C2-C1-O2A-CGA   |
| 26  | A     | 413  | DGD  | O6D-C5D-C6D-O5D |
| 26  | c     | 5515 | DGD  | O6D-C5D-C6D-O5D |
| 22  | T     | 101  | LMT  | C4'-C5'-C6'-O6' |
| 25  | B     | 619  | MGE  | C8A-C9A-CAA-CBA |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 25  | C     | 519  | MGE  | C6A-C7A-C8A-C9A |
| 25  | b     | 5620 | MGE  | C8A-C9A-CAA-CBA |
| 25  | c     | 5517 | MGE  | C6A-C7A-C8A-C9A |
| 22  | T     | 101  | LMT  | C1-C2-C3-C4     |
| 25  | d     | 5408 | MGE  | C5B-C6B-C7B-C8B |
| 20  | A     | 407  | BCR  | C5-C6-C7-C8     |
| 20  | C     | 514  | BCR  | C1-C6-C7-C8     |
| 20  | C     | 514  | BCR  | C5-C6-C7-C8     |
| 20  | C     | 515  | BCR  | C5-C6-C7-C8     |
| 20  | C     | 516  | BCR  | C1-C6-C7-C8     |
| 20  | C     | 516  | BCR  | C23-C24-C25-C30 |
| 20  | D     | 407  | BCR  | C1-C6-C7-C8     |
| 20  | D     | 407  | BCR  | C5-C6-C7-C8     |
| 20  | D     | 407  | BCR  | C23-C24-C25-C26 |
| 20  | a     | 5408 | BCR  | C5-C6-C7-C8     |
| 20  | b     | 5619 | BCR  | C5-C6-C7-C8     |
| 20  | b     | 5619 | BCR  | C23-C24-C25-C26 |
| 20  | b     | 5619 | BCR  | C23-C24-C25-C30 |
| 20  | c     | 5513 | BCR  | C1-C6-C7-C8     |
| 20  | c     | 5513 | BCR  | C5-C6-C7-C8     |
| 20  | c     | 5514 | BCR  | C1-C6-C7-C8     |
| 20  | c     | 5514 | BCR  | C23-C24-C25-C30 |
| 20  | d     | 5406 | BCR  | C1-C6-C7-C8     |
| 20  | d     | 5406 | BCR  | C5-C6-C7-C8     |
| 20  | d     | 5406 | BCR  | C23-C24-C25-C26 |
| 20  | t     | 5101 | BCR  | C5-C6-C7-C8     |
| 20  | t     | 5101 | BCR  | C23-C24-C25-C26 |
| 20  | t     | 5101 | BCR  | C23-C24-C25-C30 |
| 20  | t     | 5102 | BCR  | C5-C6-C7-C8     |
| 20  | z     | 5101 | BCR  | C5-C6-C7-C8     |
| 25  | D     | 410  | MGE  | O6D-C5D-C6D-O5D |
| 25  | d     | 5409 | MGE  | O6D-C5D-C6D-O5D |
| 26  | b     | 5621 | DGD  | C8A-C9A-CAA-CBA |
| 17  | C     | 505  | CLA  | CBA-CGA-O2A-C1  |
| 17  | c     | 5505 | CLA  | CBA-CGA-O2A-C1  |
| 17  | C     | 503  | CLA  | C8-C10-C11-C12  |
| 17  | C     | 511  | CLA  | C8-C10-C11-C12  |
| 17  | c     | 5503 | CLA  | C8-C10-C11-C12  |
| 17  | k     | 5501 | CLA  | C8-C10-C11-C12  |
| 18  | D     | 402  | PHO  | C10-C11-C12-C13 |
| 18  | d     | 5402 | PHO  | C10-C11-C12-C13 |
| 23  | A     | 410  | SQD  | C24-C23-O48-C46 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 25  | m     | 5103 | MGE  | C3A-C4A-C5A-C6A |
| 26  | D     | 411  | DGD  | C8A-C9A-CAA-CBA |
| 17  | B     | 613  | CLA  | O1A-CGA-O2A-C1  |
| 17  | b     | 5613 | CLA  | O1A-CGA-O2A-C1  |
| 17  | B     | 604  | CLA  | C4-C3-C5-C6     |
| 17  | b     | 5604 | CLA  | C4-C3-C5-C6     |
| 17  | A     | 402  | CLA  | C11-C12-C13-C15 |
| 17  | A     | 403  | CLA  | C2-C3-C5-C6     |
| 17  | B     | 602  | CLA  | C6-C7-C8-C10    |
| 17  | B     | 605  | CLA  | C12-C13-C15-C16 |
| 17  | B     | 609  | CLA  | C12-C13-C15-C16 |
| 17  | B     | 613  | CLA  | C12-C13-C15-C16 |
| 17  | C     | 503  | CLA  | C11-C12-C13-C15 |
| 17  | D     | 404  | CLA  | C6-C7-C8-C10    |
| 17  | a     | 5403 | CLA  | C11-C12-C13-C15 |
| 17  | a     | 5404 | CLA  | C2-C3-C5-C6     |
| 17  | b     | 5602 | CLA  | C6-C7-C8-C10    |
| 17  | b     | 5605 | CLA  | C12-C13-C15-C16 |
| 17  | b     | 5609 | CLA  | C12-C13-C15-C16 |
| 17  | b     | 5613 | CLA  | C12-C13-C15-C16 |
| 17  | c     | 5503 | CLA  | C11-C12-C13-C15 |
| 17  | d     | 5403 | CLA  | C6-C7-C8-C10    |
| 18  | A     | 404  | PHO  | C6-C7-C8-C10    |
| 18  | a     | 5405 | PHO  | C6-C7-C8-C10    |
| 17  | B     | 611  | CLA  | O1A-CGA-O2A-C1  |
| 17  | b     | 5611 | CLA  | O1A-CGA-O2A-C1  |
| 17  | B     | 613  | CLA  | C5-C6-C7-C8     |
| 17  | C     | 507  | CLA  | C10-C11-C12-C13 |
| 17  | b     | 5613 | CLA  | C5-C6-C7-C8     |
| 17  | c     | 5507 | CLA  | C10-C11-C12-C13 |
| 17  | k     | 5501 | CLA  | C5-C6-C7-C8     |
| 17  | B     | 609  | CLA  | CBA-CGA-O2A-C1  |
| 17  | B     | 615  | CLA  | CBA-CGA-O2A-C1  |
| 17  | b     | 5609 | CLA  | CBA-CGA-O2A-C1  |
| 17  | b     | 5615 | CLA  | CBA-CGA-O2A-C1  |
| 17  | C     | 504  | CLA  | C2A-CAA-CBA-CGA |
| 17  | c     | 5504 | CLA  | C2A-CAA-CBA-CGA |
| 17  | B     | 608  | CLA  | C8-C10-C11-C12  |
| 17  | C     | 511  | CLA  | C5-C6-C7-C8     |
| 17  | b     | 5608 | CLA  | C8-C10-C11-C12  |
| 17  | B     | 611  | CLA  | C10-C11-C12-C13 |
| 17  | b     | 5611 | CLA  | C10-C11-C12-C13 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 23  | l     | 5102 | SQD  | C11-C12-C13-C14 |
| 20  | B     | 617  | BCR  | C6-C7-C8-C9     |
| 20  | B     | 618  | BCR  | C6-C7-C8-C9     |
| 20  | b     | 5617 | BCR  | C6-C7-C8-C9     |
| 20  | b     | 5618 | BCR  | C6-C7-C8-C9     |
| 17  | B     | 612  | CLA  | C5-C6-C7-C8     |
| 17  | b     | 5612 | CLA  | C5-C6-C7-C8     |
| 23  | L     | 101  | SQD  | C27-C28-C29-C30 |
| 22  | T     | 101  | LMT  | C4-C5-C6-C7     |
| 23  | d     | 5407 | SQD  | C14-C15-C16-C17 |
| 23  | l     | 5102 | SQD  | C9-C10-C11-C12  |
| 26  | C     | 518  | DGD  | O1B-C1B-O2G-C2G |
| 26  | a     | 5411 | DGD  | O1B-C1B-O2G-C2G |
| 17  | B     | 604  | CLA  | C3-C5-C6-C7     |
| 17  | b     | 5604 | CLA  | C3-C5-C6-C7     |
| 25  | A     | 412  | MGE  | C2D-C1D-O3G-C3G |
| 25  | l     | 5101 | MGE  | C2D-C1D-O3G-C3G |
| 25  | D     | 410  | MGE  | O1G-C1G-C2G-O2G |
| 25  | d     | 5410 | MGE  | O1G-C1G-C2G-O2G |
| 25  | d     | 5410 | MGE  | O6D-C5D-C6D-O5D |
| 25  | m     | 5101 | MGE  | O6D-C5D-C6D-O5D |
| 23  | D     | 403  | SQD  | C14-C15-C16-C17 |
| 26  | b     | 5621 | DGD  | CBA-CCA-CDA-CEA |
| 17  | C     | 511  | CLA  | C16-C17-C18-C20 |
| 17  | k     | 5501 | CLA  | C16-C17-C18-C20 |
| 25  | D     | 410  | MGE  | C6B-C7B-C8B-C9B |
| 26  | A     | 413  | DGD  | C5B-C6B-C7B-C8B |
| 26  | D     | 411  | DGD  | CBA-CCA-CDA-CEA |
| 26  | c     | 5515 | DGD  | C5B-C6B-C7B-C8B |
| 17  | B     | 610  | CLA  | C8-C10-C11-C12  |
| 17  | B     | 612  | CLA  | C8-C10-C11-C12  |
| 17  | b     | 5610 | CLA  | C8-C10-C11-C12  |
| 17  | b     | 5612 | CLA  | C8-C10-C11-C12  |
| 17  | B     | 603  | CLA  | C2-C3-C5-C6     |
| 17  | b     | 5603 | CLA  | C2-C3-C5-C6     |
| 23  | L     | 101  | SQD  | C11-C10-C9-C8   |
| 17  | B     | 603  | CLA  | C14-C13-C15-C16 |
| 17  | B     | 609  | CLA  | C14-C13-C15-C16 |
| 17  | B     | 613  | CLA  | C14-C13-C15-C16 |
| 17  | C     | 501  | CLA  | C14-C13-C15-C16 |
| 17  | C     | 503  | CLA  | C11-C12-C13-C14 |
| 17  | C     | 503  | CLA  | C14-C13-C15-C16 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | b     | 5603 | CLA  | C14-C13-C15-C16 |
| 17  | b     | 5609 | CLA  | C14-C13-C15-C16 |
| 17  | b     | 5613 | CLA  | C14-C13-C15-C16 |
| 17  | c     | 5501 | CLA  | C14-C13-C15-C16 |
| 17  | c     | 5503 | CLA  | C11-C12-C13-C14 |
| 17  | c     | 5503 | CLA  | C14-C13-C15-C16 |
| 18  | A     | 404  | PHO  | C6-C7-C8-C9     |
| 18  | A     | 404  | PHO  | C14-C13-C15-C16 |
| 18  | a     | 5405 | PHO  | C6-C7-C8-C9     |
| 18  | a     | 5405 | PHO  | C14-C13-C15-C16 |
| 26  | D     | 411  | DGD  | C3B-C4B-C5B-C6B |
| 26  | b     | 5621 | DGD  | C3B-C4B-C5B-C6B |
| 17  | C     | 505  | CLA  | C2A-CAA-CBA-CGA |
| 17  | c     | 5505 | CLA  | C2A-CAA-CBA-CGA |
| 25  | D     | 408  | MGE  | O6D-C5D-C6D-O5D |
| 18  | A     | 404  | PHO  | C5-C6-C7-C8     |
| 18  | a     | 5405 | PHO  | C5-C6-C7-C8     |
| 22  | a     | 5410 | LMT  | C3-C4-C5-C6     |
| 23  | D     | 403  | SQD  | C32-C33-C34-C35 |
| 20  | B     | 618  | BCR  | C17-C18-C19-C20 |
| 20  | b     | 5618 | BCR  | C17-C18-C19-C20 |
| 17  | C     | 505  | CLA  | O1A-CGA-O2A-C1  |
| 17  | c     | 5505 | CLA  | O1A-CGA-O2A-C1  |
| 23  | D     | 403  | SQD  | O10-C23-O48-C46 |
| 17  | A     | 405  | CLA  | C1A-C2A-CAA-CBA |
| 17  | C     | 504  | CLA  | C1A-C2A-CAA-CBA |
| 17  | C     | 512  | CLA  | C1A-C2A-CAA-CBA |
| 17  | a     | 5406 | CLA  | C1A-C2A-CAA-CBA |
| 17  | c     | 5504 | CLA  | C1A-C2A-CAA-CBA |
| 17  | c     | 5511 | CLA  | C1A-C2A-CAA-CBA |
| 17  | C     | 511  | CLA  | C16-C17-C18-C19 |
| 17  | k     | 5501 | CLA  | C16-C17-C18-C19 |
| 23  | d     | 5407 | SQD  | O49-C7-O47-C45  |
| 25  | A     | 412  | MGE  | O1B-C1B-O2G-C2G |
| 25  | l     | 5101 | MGE  | O1B-C1B-O2G-C2G |
| 22  | a     | 5410 | LMT  | C2-C3-C4-C5     |
| 17  | B     | 613  | CLA  | C10-C11-C12-C13 |
| 17  | b     | 5613 | CLA  | C10-C11-C12-C13 |
| 21  | a     | 5409 | LHG  | C24-C25-C26-C27 |
| 22  | T     | 101  | LMT  | O1'-C1-C2-C3    |
| 22  | M     | 101  | LMT  | C4'-C5'-C6'-O6' |
| 21  | A     | 408  | LHG  | C24-C25-C26-C27 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 26  | b     | 5621 | DGD  | C5B-C6B-C7B-C8B |
| 17  | A     | 403  | CLA  | C4-C3-C5-C6     |
| 17  | a     | 5404 | CLA  | C4-C3-C5-C6     |
| 18  | A     | 404  | PHO  | C4-C3-C5-C6     |
| 18  | a     | 5405 | PHO  | C4-C3-C5-C6     |
| 26  | C     | 517  | DGD  | C5A-C6A-C7A-C8A |
| 26  | D     | 411  | DGD  | C5B-C6B-C7B-C8B |
| 26  | c     | 5516 | DGD  | C5A-C6A-C7A-C8A |
| 23  | d     | 5407 | SQD  | C12-C13-C14-C15 |
| 17  | B     | 609  | CLA  | O1A-CGA-O2A-C1  |
| 25  | d     | 5410 | MGE  | C3A-C4A-C5A-C6A |
| 23  | A     | 410  | SQD  | C44-C45-C46-O48 |
| 23  | D     | 403  | SQD  | O6-C44-C45-C46  |
| 23  | L     | 101  | SQD  | C44-C45-C46-O48 |
| 23  | l     | 5102 | SQD  | C44-C45-C46-O48 |
| 25  | d     | 5408 | MGE  | C1G-C2G-C3G-O3G |
| 25  | d     | 5409 | MGE  | O1G-C1G-C2G-C3G |
| 25  | m     | 5103 | MGE  | C1G-C2G-C3G-O3G |
| 26  | C     | 518  | DGD  | C1G-C2G-C3G-O3G |
| 26  | D     | 411  | DGD  | O1G-C1G-C2G-C3G |
| 26  | a     | 5411 | DGD  | C1G-C2G-C3G-O3G |
| 26  | b     | 5621 | DGD  | O1G-C1G-C2G-C3G |
| 23  | L     | 101  | SQD  | C11-C12-C13-C14 |
| 17  | b     | 5609 | CLA  | O1A-CGA-O2A-C1  |
| 25  | d     | 5408 | MGE  | C2G-C3G-O3G-C1D |
| 17  | A     | 403  | CLA  | O1D-CGD-O2D-CED |
| 17  | a     | 5404 | CLA  | O1D-CGD-O2D-CED |
| 23  | l     | 5102 | SQD  | C19-C20-C21-C22 |
| 22  | B     | 620  | LMT  | C2-C3-C4-C5     |
| 17  | C     | 505  | CLA  | C16-C17-C18-C20 |
| 17  | c     | 5505 | CLA  | C16-C17-C18-C20 |
| 26  | D     | 411  | DGD  | O6E-C5E-C6E-O5E |
| 26  | b     | 5621 | DGD  | O6E-C5E-C6E-O5E |
| 17  | B     | 615  | CLA  | O1A-CGA-O2A-C1  |
| 17  | b     | 5615 | CLA  | O1A-CGA-O2A-C1  |
| 17  | B     | 605  | CLA  | C13-C15-C16-C17 |
| 17  | b     | 5605 | CLA  | C13-C15-C16-C17 |
| 20  | B     | 618  | BCR  | C20-C21-C22-C37 |
| 20  | C     | 514  | BCR  | C11-C10-C9-C34  |
| 20  | C     | 515  | BCR  | C35-C13-C14-C15 |
| 20  | b     | 5618 | BCR  | C20-C21-C22-C37 |
| 20  | b     | 5619 | BCR  | C16-C17-C18-C36 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 20  | c     | 5513 | BCR  | C11-C10-C9-C34  |
| 20  | t     | 5101 | BCR  | C16-C17-C18-C36 |
| 20  | t     | 5102 | BCR  | C11-C10-C9-C34  |
| 20  | z     | 5101 | BCR  | C35-C13-C14-C15 |
| 25  | D     | 408  | MGE  | C1B-C2B-C3B-C4B |
| 17  | D     | 404  | CLA  | CBA-CGA-O2A-C1  |
| 17  | d     | 5403 | CLA  | CBA-CGA-O2A-C1  |
| 25  | d     | 5408 | MGE  | O6D-C5D-C6D-O5D |
| 17  | b     | 5607 | CLA  | C15-C16-C17-C18 |
| 23  | d     | 5407 | SQD  | C17-C18-C19-C20 |
| 17  | c     | 5507 | CLA  | C2A-CAA-CBA-CGA |
| 17  | B     | 604  | CLA  | C15-C16-C17-C18 |
| 17  | B     | 607  | CLA  | C5-C6-C7-C8     |
| 17  | B     | 607  | CLA  | C15-C16-C17-C18 |
| 17  | C     | 508  | CLA  | C8-C10-C11-C12  |
| 17  | b     | 5604 | CLA  | C15-C16-C17-C18 |
| 17  | b     | 5613 | CLA  | C13-C15-C16-C17 |
| 17  | c     | 5508 | CLA  | C8-C10-C11-C12  |
| 17  | A     | 403  | CLA  | C2-C1-O2A-CGA   |
| 17  | a     | 5404 | CLA  | C2-C1-O2A-CGA   |
| 17  | b     | 5607 | CLA  | C5-C6-C7-C8     |
| 17  | B     | 613  | CLA  | C13-C15-C16-C17 |
| 20  | B     | 617  | BCR  | C12-C13-C14-C15 |
| 20  | b     | 5617 | BCR  | C12-C13-C14-C15 |
| 25  | D     | 409  | MGE  | C2D-C1D-O3G-C3G |
| 25  | m     | 5103 | MGE  | C2D-C1D-O3G-C3G |
| 21  | A     | 408  | LHG  | O7-C5-C6-O8     |
| 21  | a     | 5409 | LHG  | O7-C5-C6-O8     |
| 25  | d     | 5408 | MGE  | O1G-C1G-C2G-O2G |
| 26  | C     | 517  | DGD  | O1G-C1G-C2G-O2G |
| 26  | c     | 5516 | DGD  | O1G-C1G-C2G-O2G |
| 25  | B     | 619  | MGE  | C7A-C8A-C9A-CAA |
| 25  | b     | 5620 | MGE  | C7A-C8A-C9A-CAA |
| 25  | d     | 5409 | MGE  | C2B-C3B-C4B-C5B |
| 17  | B     | 603  | CLA  | C6-C7-C8-C10    |
| 17  | B     | 603  | CLA  | C12-C13-C15-C16 |
| 17  | B     | 608  | CLA  | C12-C13-C15-C16 |
| 17  | B     | 609  | CLA  | C11-C10-C8-C7   |
| 17  | B     | 610  | CLA  | C6-C7-C8-C10    |
| 17  | B     | 612  | CLA  | C12-C13-C15-C16 |
| 17  | B     | 615  | CLA  | C6-C7-C8-C10    |
| 17  | B     | 615  | CLA  | C12-C13-C15-C16 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | C     | 501  | CLA  | C11-C12-C13-C15 |
| 17  | C     | 501  | CLA  | C12-C13-C15-C16 |
| 17  | C     | 505  | CLA  | C11-C10-C8-C7   |
| 17  | C     | 506  | CLA  | C6-C7-C8-C10    |
| 17  | D     | 404  | CLA  | C12-C13-C15-C16 |
| 17  | b     | 5603 | CLA  | C6-C7-C8-C10    |
| 17  | b     | 5603 | CLA  | C12-C13-C15-C16 |
| 17  | b     | 5608 | CLA  | C12-C13-C15-C16 |
| 17  | b     | 5609 | CLA  | C11-C10-C8-C7   |
| 17  | b     | 5610 | CLA  | C6-C7-C8-C10    |
| 17  | b     | 5612 | CLA  | C12-C13-C15-C16 |
| 17  | b     | 5615 | CLA  | C6-C7-C8-C10    |
| 17  | b     | 5615 | CLA  | C12-C13-C15-C16 |
| 17  | c     | 5501 | CLA  | C11-C12-C13-C15 |
| 17  | c     | 5501 | CLA  | C12-C13-C15-C16 |
| 17  | c     | 5505 | CLA  | C11-C10-C8-C7   |
| 17  | c     | 5506 | CLA  | C6-C7-C8-C10    |
| 17  | d     | 5403 | CLA  | C12-C13-C15-C16 |
| 17  | B     | 602  | CLA  | C11-C10-C8-C9   |
| 17  | B     | 602  | CLA  | C11-C12-C13-C14 |
| 17  | B     | 602  | CLA  | C14-C13-C15-C16 |
| 17  | B     | 603  | CLA  | C6-C7-C8-C9     |
| 17  | B     | 605  | CLA  | C11-C12-C13-C14 |
| 17  | B     | 610  | CLA  | C6-C7-C8-C9     |
| 17  | B     | 612  | CLA  | C11-C10-C8-C9   |
| 17  | B     | 612  | CLA  | C14-C13-C15-C16 |
| 17  | B     | 615  | CLA  | C11-C10-C8-C9   |
| 17  | B     | 615  | CLA  | C14-C13-C15-C16 |
| 17  | C     | 503  | CLA  | C6-C7-C8-C9     |
| 17  | C     | 505  | CLA  | C11-C10-C8-C9   |
| 17  | C     | 508  | CLA  | C14-C13-C15-C16 |
| 17  | D     | 404  | CLA  | C14-C13-C15-C16 |
| 17  | b     | 5602 | CLA  | C11-C10-C8-C9   |
| 17  | b     | 5602 | CLA  | C11-C12-C13-C14 |
| 17  | b     | 5602 | CLA  | C14-C13-C15-C16 |
| 17  | b     | 5603 | CLA  | C6-C7-C8-C9     |
| 17  | b     | 5605 | CLA  | C11-C12-C13-C14 |
| 17  | b     | 5610 | CLA  | C6-C7-C8-C9     |
| 17  | b     | 5612 | CLA  | C11-C10-C8-C9   |
| 17  | b     | 5612 | CLA  | C14-C13-C15-C16 |
| 17  | b     | 5615 | CLA  | C11-C10-C8-C9   |
| 17  | b     | 5615 | CLA  | C14-C13-C15-C16 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | c     | 5503 | CLA  | C6-C7-C8-C9     |
| 17  | c     | 5505 | CLA  | C11-C10-C8-C9   |
| 17  | c     | 5508 | CLA  | C14-C13-C15-C16 |
| 17  | d     | 5403 | CLA  | C14-C13-C15-C16 |
| 18  | D     | 402  | PHO  | C11-C12-C13-C14 |
| 18  | d     | 5402 | PHO  | C11-C12-C13-C14 |
| 25  | d     | 5409 | MGE  | C2A-C1A-O1G-C1G |
| 17  | C     | 507  | CLA  | C2A-CAA-CBA-CGA |
| 20  | D     | 407  | BCR  | C11-C12-C13-C14 |
| 20  | d     | 5406 | BCR  | C11-C12-C13-C14 |
| 22  | A     | 409  | LMT  | C3'-C4'-O1B-C1B |
| 18  | D     | 402  | PHO  | C3-C5-C6-C7     |
| 18  | d     | 5402 | PHO  | C3-C5-C6-C7     |
| 25  | C     | 519  | MGE  | C2B-C1B-O2G-C2G |
| 25  | c     | 5517 | MGE  | C2B-C1B-O2G-C2G |
| 25  | d     | 5410 | MGE  | C8B-C9B-CAB-CBB |
| 26  | A     | 413  | DGD  | C2A-C1A-O1G-C1G |
| 26  | c     | 5515 | DGD  | C2A-C1A-O1G-C1G |
| 25  | D     | 408  | MGE  | C5B-C6B-C7B-C8B |
| 21  | a     | 5409 | LHG  | C32-C33-C34-C35 |
| 21  | A     | 408  | LHG  | C32-C33-C34-C35 |
| 17  | A     | 401  | CLA  | C4B-C3B-CAB-CBB |
| 17  | B     | 603  | CLA  | C4B-C3B-CAB-CBB |
| 17  | B     | 604  | CLA  | C4B-C3B-CAB-CBB |
| 17  | D     | 405  | CLA  | C4B-C3B-CAB-CBB |
| 17  | a     | 5402 | CLA  | C4B-C3B-CAB-CBB |
| 17  | b     | 5603 | CLA  | C4B-C3B-CAB-CBB |
| 17  | b     | 5604 | CLA  | C4B-C3B-CAB-CBB |
| 17  | d     | 5404 | CLA  | C4B-C3B-CAB-CBB |
| 26  | C     | 517  | DGD  | C1B-C2B-C3B-C4B |
| 26  | c     | 5516 | DGD  | C1B-C2B-C3B-C4B |
| 21  | A     | 408  | LHG  | C33-C34-C35-C36 |
| 21  | a     | 5409 | LHG  | C33-C34-C35-C36 |
| 22  | a     | 5410 | LMT  | C7-C8-C9-C10    |
| 23  | l     | 5102 | SQD  | C11-C10-C9-C8   |
| 25  | D     | 408  | MGE  | C2A-C3A-C4A-C5A |
| 17  | A     | 405  | CLA  | C3A-C2A-CAA-CBA |
| 17  | B     | 607  | CLA  | C3A-C2A-CAA-CBA |
| 17  | a     | 5406 | CLA  | C3A-C2A-CAA-CBA |
| 17  | b     | 5607 | CLA  | C3A-C2A-CAA-CBA |
| 18  | A     | 404  | PHO  | C3A-C2A-CAA-CBA |
| 18  | a     | 5405 | PHO  | C3A-C2A-CAA-CBA |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 25  | A     | 412  | MGE  | C2A-C3A-C4A-C5A |
| 25  | l     | 5101 | MGE  | C2A-C3A-C4A-C5A |
| 25  | m     | 5103 | MGE  | C4A-C5A-C6A-C7A |
| 17  | B     | 615  | CLA  | C15-C16-C17-C18 |
| 18  | A     | 404  | PHO  | C15-C16-C17-C18 |
| 18  | a     | 5405 | PHO  | C15-C16-C17-C18 |
| 23  | D     | 403  | SQD  | C33-C34-C35-C36 |
| 17  | B     | 609  | CLA  | C5-C6-C7-C8     |
| 17  | b     | 5609 | CLA  | C5-C6-C7-C8     |
| 17  | b     | 5615 | CLA  | C15-C16-C17-C18 |
| 23  | d     | 5407 | SQD  | O6-C44-C45-C46  |
| 25  | C     | 519  | MGE  | C1G-C2G-C3G-O3G |
| 25  | D     | 410  | MGE  | O1G-C1G-C2G-C3G |
| 25  | c     | 5517 | MGE  | C1G-C2G-C3G-O3G |
| 25  | d     | 5408 | MGE  | O1G-C1G-C2G-C3G |
| 26  | C     | 518  | DGD  | O1G-C1G-C2G-C3G |
| 26  | a     | 5411 | DGD  | O1G-C1G-C2G-C3G |
| 22  | A     | 409  | LMT  | C5-C6-C7-C8     |
| 17  | C     | 510  | CLA  | C3-C5-C6-C7     |
| 17  | c     | 5510 | CLA  | C3-C5-C6-C7     |
| 17  | D     | 404  | CLA  | O1A-CGA-O2A-C1  |
| 17  | d     | 5403 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 620  | LMT  | C5-C6-C7-C8     |
| 25  | m     | 5103 | MGE  | O6D-C5D-C6D-O5D |
| 17  | B     | 607  | CLA  | C8-C10-C11-C12  |
| 17  | b     | 5607 | CLA  | C8-C10-C11-C12  |
| 25  | C     | 519  | MGE  | C1A-C2A-C3A-C4A |
| 25  | c     | 5517 | MGE  | C1A-C2A-C3A-C4A |
| 26  | C     | 517  | DGD  | O1A-C1A-O1G-C1G |
| 26  | c     | 5516 | DGD  | O1A-C1A-O1G-C1G |
| 25  | A     | 412  | MGE  | C7A-C8A-C9A-CAA |
| 17  | b     | 5613 | CLA  | C8-C10-C11-C12  |
| 17  | B     | 612  | CLA  | O1D-CGD-O2D-CED |
| 17  | C     | 505  | CLA  | C16-C17-C18-C19 |
| 17  | c     | 5505 | CLA  | C16-C17-C18-C19 |
| 17  | B     | 613  | CLA  | C8-C10-C11-C12  |
| 25  | l     | 5101 | MGE  | C7A-C8A-C9A-CAA |
| 17  | b     | 5612 | CLA  | O1D-CGD-O2D-CED |
| 17  | b     | 5610 | CLA  | CBD-CGD-O2D-CED |
| 17  | A     | 401  | CLA  | C2B-C3B-CAB-CBB |
| 17  | B     | 603  | CLA  | C2B-C3B-CAB-CBB |
| 17  | C     | 511  | CLA  | C2B-C3B-CAB-CBB |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | a     | 5402 | CLA  | C2B-C3B-CAB-CBB |
| 17  | b     | 5603 | CLA  | C2B-C3B-CAB-CBB |
| 17  | k     | 5501 | CLA  | C2B-C3B-CAB-CBB |
| 23  | A     | 410  | SQD  | O6-C44-C45-O47  |
| 23  | a     | 5401 | SQD  | O6-C44-C45-O47  |
| 25  | d     | 5409 | MGE  | O1G-C1G-C2G-O2G |
| 17  | B     | 610  | CLA  | CBD-CGD-O2D-CED |
| 22  | m     | 5102 | LMT  | C4'-C5'-C6'-O6' |
| 25  | D     | 410  | MGE  | C5A-C6A-C7A-C8A |
| 17  | C     | 501  | CLA  | C10-C11-C12-C13 |
| 17  | c     | 5501 | CLA  | C10-C11-C12-C13 |
| 26  | D     | 411  | DGD  | CCA-CDA-CEA-CFA |
| 26  | b     | 5621 | DGD  | CCA-CDA-CEA-CFA |
| 17  | B     | 608  | CLA  | C2-C1-O2A-CGA   |
| 17  | b     | 5608 | CLA  | C2-C1-O2A-CGA   |
| 17  | A     | 401  | CLA  | C11-C10-C8-C9   |
| 17  | A     | 402  | CLA  | C14-C13-C15-C16 |
| 17  | B     | 606  | CLA  | C14-C13-C15-C16 |
| 17  | B     | 611  | CLA  | C6-C7-C8-C9     |
| 17  | B     | 612  | CLA  | C6-C7-C8-C9     |
| 17  | C     | 501  | CLA  | C6-C7-C8-C9     |
| 17  | C     | 506  | CLA  | C6-C7-C8-C9     |
| 17  | a     | 5402 | CLA  | C11-C10-C8-C9   |
| 17  | a     | 5403 | CLA  | C14-C13-C15-C16 |
| 17  | b     | 5611 | CLA  | C6-C7-C8-C9     |
| 17  | b     | 5612 | CLA  | C6-C7-C8-C9     |
| 17  | c     | 5501 | CLA  | C6-C7-C8-C9     |
| 17  | c     | 5506 | CLA  | C6-C7-C8-C9     |
| 22  | A     | 409  | LMT  | C1-C2-C3-C4     |
| 22  | m     | 5102 | LMT  | C1-C2-C3-C4     |
| 25  | d     | 5409 | MGE  | O1A-C1A-O1G-C1G |
| 17  | B     | 615  | CLA  | C16-C17-C18-C19 |
| 17  | B     | 615  | CLA  | C16-C17-C18-C20 |
| 17  | b     | 5615 | CLA  | C16-C17-C18-C19 |
| 17  | b     | 5615 | CLA  | C16-C17-C18-C20 |
| 20  | B     | 617  | BCR  | C5-C6-C7-C8     |
| 20  | B     | 618  | BCR  | C23-C24-C25-C30 |
| 20  | C     | 514  | BCR  | C23-C24-C25-C26 |
| 20  | C     | 515  | BCR  | C23-C24-C25-C26 |
| 20  | C     | 515  | BCR  | C23-C24-C25-C30 |
| 20  | C     | 516  | BCR  | C5-C6-C7-C8     |
| 20  | H     | 101  | BCR  | C5-C6-C7-C8     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 20  | b     | 5617 | BCR  | C5-C6-C7-C8     |
| 20  | b     | 5618 | BCR  | C23-C24-C25-C30 |
| 20  | c     | 5513 | BCR  | C23-C24-C25-C26 |
| 20  | c     | 5514 | BCR  | C5-C6-C7-C8     |
| 20  | h     | 5101 | BCR  | C5-C6-C7-C8     |
| 20  | z     | 5101 | BCR  | C23-C24-C25-C26 |
| 20  | z     | 5101 | BCR  | C23-C24-C25-C30 |
| 17  | B     | 603  | CLA  | C15-C16-C17-C18 |
| 20  | k     | 5502 | BCR  | C11-C12-C13-C14 |
| 17  | b     | 5603 | CLA  | C15-C16-C17-C18 |
| 20  | H     | 101  | BCR  | C14-C15-C16-C17 |
| 20  | h     | 5101 | BCR  | C14-C15-C16-C17 |
| 25  | m     | 5103 | MGE  | CCB-CDB-CEB-CFB |
| 17  | D     | 404  | CLA  | C8-C10-C11-C12  |
| 17  | d     | 5403 | CLA  | C8-C10-C11-C12  |
| 17  | C     | 501  | CLA  | C13-C15-C16-C17 |
| 17  | c     | 5501 | CLA  | C13-C15-C16-C17 |
| 25  | B     | 619  | MGE  | C3A-C4A-C5A-C6A |
| 25  | b     | 5620 | MGE  | C3A-C4A-C5A-C6A |
| 17  | A     | 401  | CLA  | C6-C7-C8-C10    |
| 17  | A     | 402  | CLA  | C12-C13-C15-C16 |
| 17  | B     | 602  | CLA  | C11-C10-C8-C7   |
| 17  | B     | 602  | CLA  | C11-C12-C13-C15 |
| 17  | B     | 602  | CLA  | C12-C13-C15-C16 |
| 17  | B     | 606  | CLA  | C11-C12-C13-C15 |
| 17  | B     | 611  | CLA  | C6-C7-C8-C10    |
| 17  | B     | 615  | CLA  | C11-C10-C8-C7   |
| 17  | C     | 501  | CLA  | C6-C7-C8-C10    |
| 17  | C     | 503  | CLA  | C6-C7-C8-C10    |
| 17  | C     | 506  | CLA  | C11-C10-C8-C7   |
| 17  | C     | 506  | CLA  | C11-C12-C13-C15 |
| 17  | C     | 508  | CLA  | C12-C13-C15-C16 |
| 17  | a     | 5402 | CLA  | C6-C7-C8-C10    |
| 17  | a     | 5403 | CLA  | C12-C13-C15-C16 |
| 17  | b     | 5602 | CLA  | C11-C10-C8-C7   |
| 17  | b     | 5602 | CLA  | C11-C12-C13-C15 |
| 17  | b     | 5602 | CLA  | C12-C13-C15-C16 |
| 17  | b     | 5611 | CLA  | C6-C7-C8-C10    |
| 17  | b     | 5615 | CLA  | C11-C10-C8-C7   |
| 17  | c     | 5501 | CLA  | C6-C7-C8-C10    |
| 17  | c     | 5503 | CLA  | C6-C7-C8-C10    |
| 17  | c     | 5506 | CLA  | C11-C10-C8-C7   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | c     | 5506 | CLA  | C11-C12-C13-C15 |
| 17  | c     | 5508 | CLA  | C12-C13-C15-C16 |
| 25  | D     | 410  | MGE  | C6A-C7A-C8A-C9A |
| 20  | A     | 407  | BCR  | C19-C20-C21-C22 |
| 20  | a     | 5408 | BCR  | C19-C20-C21-C22 |
| 21  | A     | 408  | LHG  | C29-C30-C31-C32 |
| 21  | a     | 5409 | LHG  | C29-C30-C31-C32 |
| 20  | A     | 407  | BCR  | C35-C13-C14-C15 |
| 20  | B     | 618  | BCR  | C16-C17-C18-C36 |
| 20  | a     | 5408 | BCR  | C35-C13-C14-C15 |
| 20  | b     | 5618 | BCR  | C16-C17-C18-C36 |
| 17  | C     | 501  | CLA  | CBA-CGA-O2A-C1  |
| 17  | c     | 5501 | CLA  | CBA-CGA-O2A-C1  |
| 23  | l     | 5102 | SQD  | C24-C23-O48-C46 |
| 22  | M     | 101  | LMT  | C9-C10-C11-C12  |
| 25  | A     | 412  | MGE  | C3A-C4A-C5A-C6A |
| 25  | l     | 5101 | MGE  | C3A-C4A-C5A-C6A |
| 17  | C     | 502  | CLA  | C10-C11-C12-C13 |
| 17  | c     | 5502 | CLA  | C10-C11-C12-C13 |
| 17  | B     | 606  | CLA  | CAD-CBD-CGD-O2D |
| 17  | B     | 612  | CLA  | CAD-CBD-CGD-O2D |
| 17  | C     | 504  | CLA  | CAD-CBD-CGD-O2D |
| 17  | C     | 512  | CLA  | CAD-CBD-CGD-O2D |
| 17  | b     | 5606 | CLA  | CAD-CBD-CGD-O2D |
| 17  | b     | 5612 | CLA  | CAD-CBD-CGD-O2D |
| 17  | c     | 5504 | CLA  | CAD-CBD-CGD-O2D |
| 17  | c     | 5511 | CLA  | CAD-CBD-CGD-O2D |
| 22  | a     | 5410 | LMT  | C1-C2-C3-C4     |
| 20  | D     | 407  | BCR  | C6-C7-C8-C9     |
| 25  | A     | 412  | MGE  | O6D-C1D-O3G-C3G |
| 25  | l     | 5101 | MGE  | O6D-C1D-O3G-C3G |
| 23  | A     | 410  | SQD  | O6-C44-C45-C46  |
| 25  | D     | 409  | MGE  | C1G-C2G-C3G-O3G |
| 26  | A     | 413  | DGD  | C1G-C2G-C3G-O3G |
| 26  | c     | 5515 | DGD  | C1G-C2G-C3G-O3G |
| 21  | A     | 408  | LHG  | O6-C4-C5-O7     |
| 21  | a     | 5409 | LHG  | O6-C4-C5-O7     |
| 25  | d     | 5408 | MGE  | O2G-C1B-C2B-C3B |
| 29  | F     | 101  | HEM  | C4C-C3C-CAC-CBC |
| 29  | f     | 5101 | HEM  | C4C-C3C-CAC-CBC |
| 20  | D     | 407  | BCR  | C14-C15-C16-C17 |
| 20  | d     | 5406 | BCR  | C14-C15-C16-C17 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 25  | C     | 519  | MGE  | O1B-C1B-O2G-C2G |
| 25  | c     | 5517 | MGE  | O1B-C1B-O2G-C2G |
| 17  | A     | 402  | CLA  | CHA-CBD-CGD-O1D |
| 17  | A     | 402  | CLA  | CHA-CBD-CGD-O2D |
| 17  | A     | 405  | CLA  | CHA-CBD-CGD-O1D |
| 17  | B     | 602  | CLA  | CHA-CBD-CGD-O1D |
| 17  | B     | 608  | CLA  | CHA-CBD-CGD-O1D |
| 17  | B     | 608  | CLA  | CHA-CBD-CGD-O2D |
| 17  | B     | 610  | CLA  | CHA-CBD-CGD-O1D |
| 17  | B     | 610  | CLA  | CHA-CBD-CGD-O2D |
| 17  | B     | 614  | CLA  | CHA-CBD-CGD-O1D |
| 17  | C     | 502  | CLA  | CHA-CBD-CGD-O1D |
| 17  | C     | 502  | CLA  | CHA-CBD-CGD-O2D |
| 17  | C     | 503  | CLA  | CHA-CBD-CGD-O1D |
| 17  | C     | 503  | CLA  | CHA-CBD-CGD-O2D |
| 17  | C     | 506  | CLA  | CHA-CBD-CGD-O1D |
| 17  | C     | 506  | CLA  | CHA-CBD-CGD-O2D |
| 17  | C     | 508  | CLA  | CHA-CBD-CGD-O1D |
| 17  | C     | 508  | CLA  | CHA-CBD-CGD-O2D |
| 17  | C     | 510  | CLA  | CHA-CBD-CGD-O1D |
| 17  | C     | 510  | CLA  | CHA-CBD-CGD-O2D |
| 17  | D     | 405  | CLA  | CHA-CBD-CGD-O1D |
| 17  | D     | 405  | CLA  | CHA-CBD-CGD-O2D |
| 17  | a     | 5403 | CLA  | CHA-CBD-CGD-O1D |
| 17  | a     | 5403 | CLA  | CHA-CBD-CGD-O2D |
| 17  | a     | 5406 | CLA  | CHA-CBD-CGD-O1D |
| 17  | b     | 5602 | CLA  | CHA-CBD-CGD-O1D |
| 17  | b     | 5608 | CLA  | CHA-CBD-CGD-O1D |
| 17  | b     | 5608 | CLA  | CHA-CBD-CGD-O2D |
| 17  | b     | 5610 | CLA  | CHA-CBD-CGD-O1D |
| 17  | b     | 5610 | CLA  | CHA-CBD-CGD-O2D |
| 17  | b     | 5614 | CLA  | CHA-CBD-CGD-O1D |
| 17  | c     | 5502 | CLA  | CHA-CBD-CGD-O1D |
| 17  | c     | 5502 | CLA  | CHA-CBD-CGD-O2D |
| 17  | c     | 5503 | CLA  | CHA-CBD-CGD-O1D |
| 17  | c     | 5503 | CLA  | CHA-CBD-CGD-O2D |
| 17  | c     | 5506 | CLA  | CHA-CBD-CGD-O1D |
| 17  | c     | 5506 | CLA  | CHA-CBD-CGD-O2D |
| 17  | c     | 5508 | CLA  | CHA-CBD-CGD-O1D |
| 17  | c     | 5508 | CLA  | CHA-CBD-CGD-O2D |
| 17  | c     | 5510 | CLA  | CHA-CBD-CGD-O1D |
| 17  | c     | 5510 | CLA  | CHA-CBD-CGD-O2D |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | d     | 5404 | CLA  | CHA-CBD-CGD-O1D |
| 17  | d     | 5404 | CLA  | CHA-CBD-CGD-O2D |
| 23  | L     | 101  | SQD  | C28-C29-C30-C31 |
| 20  | t     | 5102 | BCR  | C16-C17-C18-C19 |
| 25  | D     | 410  | MGE  | CCB-CDB-CEB-CFB |
| 25  | d     | 5410 | MGE  | C3B-C4B-C5B-C6B |
| 23  | L     | 101  | SQD  | O6-C44-C45-O47  |
| 25  | B     | 619  | MGE  | O2G-C2G-C3G-O3G |
| 25  | D     | 409  | MGE  | O1G-C1G-C2G-O2G |
| 25  | b     | 5620 | MGE  | O2G-C2G-C3G-O3G |
| 25  | d     | 5408 | MGE  | O2G-C2G-C3G-O3G |
| 25  | m     | 5103 | MGE  | O2G-C2G-C3G-O3G |
| 26  | A     | 413  | DGD  | O2G-C2G-C3G-O3G |
| 26  | c     | 5515 | DGD  | O2G-C2G-C3G-O3G |
| 17  | B     | 608  | CLA  | O1D-CGD-O2D-CED |
| 17  | b     | 5608 | CLA  | O1D-CGD-O2D-CED |
| 23  | D     | 403  | SQD  | O49-C7-O47-C45  |
| 17  | A     | 402  | CLA  | C11-C10-C8-C9   |
| 17  | a     | 5403 | CLA  | C11-C10-C8-C9   |
| 26  | D     | 411  | DGD  | C5A-C6A-C7A-C8A |
| 26  | b     | 5621 | DGD  | C5A-C6A-C7A-C8A |
| 23  | A     | 410  | SQD  | C4-C5-C6-S      |
| 23  | D     | 403  | SQD  | C4-C5-C6-S      |
| 23  | d     | 5407 | SQD  | C4-C5-C6-S      |
| 23  | l     | 5102 | SQD  | C28-C29-C30-C31 |
| 17  | C     | 501  | CLA  | O1A-CGA-O2A-C1  |
| 17  | c     | 5501 | CLA  | O1A-CGA-O2A-C1  |
| 17  | B     | 607  | CLA  | C3-C5-C6-C7     |
| 25  | A     | 412  | MGE  | C7B-C8B-C9B-CAB |
| 25  | l     | 5101 | MGE  | C7B-C8B-C9B-CAB |
| 17  | B     | 604  | CLA  | C1A-C2A-CAA-CBA |
| 17  | C     | 513  | CLA  | C1A-C2A-CAA-CBA |
| 17  | b     | 5604 | CLA  | C1A-C2A-CAA-CBA |
| 17  | c     | 5512 | CLA  | C1A-C2A-CAA-CBA |
| 25  | m     | 5101 | MGE  | C4A-C5A-C6A-C7A |
| 17  | B     | 612  | CLA  | C2-C1-O2A-CGA   |
| 17  | C     | 502  | CLA  | C2-C1-O2A-CGA   |
| 17  | b     | 5612 | CLA  | C2-C1-O2A-CGA   |
| 17  | c     | 5502 | CLA  | C2-C1-O2A-CGA   |
| 17  | b     | 5607 | CLA  | C3-C5-C6-C7     |
| 17  | B     | 604  | CLA  | C2-C3-C5-C6     |
| 17  | b     | 5604 | CLA  | C2-C3-C5-C6     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 25  | d     | 5408 | MGE  | C4B-C5B-C6B-C7B |
| 17  | B     | 602  | CLA  | C4B-C3B-CAB-CBB |
| 17  | C     | 504  | CLA  | C4B-C3B-CAB-CBB |
| 17  | C     | 505  | CLA  | C4B-C3B-CAB-CBB |
| 17  | C     | 511  | CLA  | C4B-C3B-CAB-CBB |
| 17  | D     | 404  | CLA  | C4B-C3B-CAB-CBB |
| 17  | b     | 5602 | CLA  | C4B-C3B-CAB-CBB |
| 17  | c     | 5504 | CLA  | C4B-C3B-CAB-CBB |
| 17  | c     | 5505 | CLA  | C4B-C3B-CAB-CBB |
| 17  | d     | 5403 | CLA  | C4B-C3B-CAB-CBB |
| 17  | k     | 5501 | CLA  | C4B-C3B-CAB-CBB |
| 23  | D     | 403  | SQD  | C11-C10-C9-C8   |
| 23  | d     | 5407 | SQD  | C11-C10-C9-C8   |
| 25  | C     | 519  | MGE  | O6D-C1D-O3G-C3G |
| 25  | c     | 5517 | MGE  | O6D-C1D-O3G-C3G |
| 21  | A     | 408  | LHG  | O6-C4-C5-C6     |
| 21  | a     | 5409 | LHG  | O6-C4-C5-C6     |
| 17  | b     | 5616 | CLA  | C10-C11-C12-C13 |
| 23  | D     | 403  | SQD  | C26-C27-C28-C29 |
| 17  | B     | 603  | CLA  | CAD-CBD-CGD-O1D |
| 17  | B     | 605  | CLA  | CAD-CBD-CGD-O1D |
| 17  | B     | 607  | CLA  | CAD-CBD-CGD-O1D |
| 17  | B     | 613  | CLA  | CAD-CBD-CGD-O1D |
| 17  | C     | 501  | CLA  | CAD-CBD-CGD-O1D |
| 17  | C     | 502  | CLA  | CAD-CBD-CGD-O1D |
| 17  | C     | 506  | CLA  | CAD-CBD-CGD-O1D |
| 17  | C     | 510  | CLA  | CAD-CBD-CGD-O1D |
| 17  | b     | 5603 | CLA  | CAD-CBD-CGD-O1D |
| 17  | b     | 5605 | CLA  | CAD-CBD-CGD-O1D |
| 17  | b     | 5607 | CLA  | CAD-CBD-CGD-O1D |
| 17  | b     | 5613 | CLA  | CAD-CBD-CGD-O1D |
| 17  | c     | 5501 | CLA  | CAD-CBD-CGD-O1D |
| 17  | c     | 5502 | CLA  | CAD-CBD-CGD-O1D |
| 17  | c     | 5506 | CLA  | CAD-CBD-CGD-O1D |
| 17  | c     | 5510 | CLA  | CAD-CBD-CGD-O1D |
| 17  | B     | 616  | CLA  | C10-C11-C12-C13 |
| 26  | a     | 5411 | DGD  | C5B-C6B-C7B-C8B |
| 25  | C     | 519  | MGE  | C5A-C6A-C7A-C8A |
| 26  | C     | 518  | DGD  | C5B-C6B-C7B-C8B |
| 25  | B     | 619  | MGE  | CAA-CBA-CCA-CDA |
| 25  | c     | 5517 | MGE  | C5A-C6A-C7A-C8A |
| 26  | C     | 517  | DGD  | C4A-C5A-C6A-C7A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 26  | D     | 411  | DGD  | C3A-C4A-C5A-C6A |
| 26  | b     | 5621 | DGD  | C3A-C4A-C5A-C6A |
| 26  | c     | 5516 | DGD  | C4A-C5A-C6A-C7A |
| 17  | A     | 402  | CLA  | C11-C10-C8-C7   |
| 17  | B     | 604  | CLA  | C12-C13-C15-C16 |
| 17  | B     | 607  | CLA  | C11-C10-C8-C7   |
| 17  | C     | 505  | CLA  | C11-C12-C13-C15 |
| 17  | a     | 5403 | CLA  | C11-C10-C8-C7   |
| 17  | b     | 5604 | CLA  | C12-C13-C15-C16 |
| 17  | b     | 5607 | CLA  | C11-C10-C8-C7   |
| 17  | c     | 5505 | CLA  | C11-C12-C13-C15 |
| 18  | D     | 402  | PHO  | C12-C13-C15-C16 |
| 18  | d     | 5402 | PHO  | C12-C13-C15-C16 |
| 25  | b     | 5620 | MGE  | CAA-CBA-CCA-CDA |
| 17  | B     | 610  | CLA  | C5-C6-C7-C8     |
| 17  | b     | 5610 | CLA  | C5-C6-C7-C8     |
| 25  | B     | 619  | MGE  | C1B-C2B-C3B-C4B |
| 25  | b     | 5620 | MGE  | C1B-C2B-C3B-C4B |
| 17  | D     | 405  | CLA  | C2A-CAA-CBA-CGA |
| 17  | d     | 5404 | CLA  | C2A-CAA-CBA-CGA |
| 17  | B     | 604  | CLA  | C16-C17-C18-C20 |
| 17  | b     | 5604 | CLA  | C16-C17-C18-C20 |
| 23  | D     | 403  | SQD  | O6-C44-C45-O47  |
| 23  | d     | 5407 | SQD  | O6-C44-C45-O47  |
| 25  | d     | 5409 | MGE  | O2G-C2G-C3G-O3G |
| 26  | C     | 517  | DGD  | O2G-C2G-C3G-O3G |
| 26  | C     | 518  | DGD  | O1G-C1G-C2G-O2G |
| 26  | a     | 5411 | DGD  | O1G-C1G-C2G-O2G |
| 26  | c     | 5516 | DGD  | O2G-C2G-C3G-O3G |
| 22  | A     | 409  | LMT  | C3-C4-C5-C6     |
| 25  | D     | 408  | MGE  | C2G-C3G-O3G-C1D |
| 17  | A     | 402  | CLA  | C10-C11-C12-C13 |
| 17  | a     | 5403 | CLA  | C10-C11-C12-C13 |
| 21  | A     | 408  | LHG  | C2-C3-O3-P      |
| 21  | a     | 5409 | LHG  | C2-C3-O3-P      |
| 25  | m     | 5103 | MGE  | O1A-C1A-O1G-C1G |
| 25  | m     | 5103 | MGE  | C2A-C1A-O1G-C1G |
| 23  | L     | 101  | SQD  | C17-C18-C19-C20 |
| 17  | A     | 401  | CLA  | C6-C7-C8-C9     |
| 17  | B     | 607  | CLA  | C11-C10-C8-C9   |
| 17  | B     | 610  | CLA  | C14-C13-C15-C16 |
| 17  | B     | 615  | CLA  | C6-C7-C8-C9     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | C     | 507  | CLA  | C6-C7-C8-C9     |
| 17  | a     | 5402 | CLA  | C6-C7-C8-C9     |
| 17  | b     | 5607 | CLA  | C11-C10-C8-C9   |
| 17  | b     | 5608 | CLA  | C6-C7-C8-C9     |
| 17  | b     | 5615 | CLA  | C6-C7-C8-C9     |
| 17  | c     | 5507 | CLA  | C6-C7-C8-C9     |
| 20  | A     | 407  | BCR  | C22-C23-C24-C25 |
| 20  | a     | 5408 | BCR  | C22-C23-C24-C25 |
| 20  | d     | 5406 | BCR  | C6-C7-C8-C9     |
| 25  | D     | 410  | MGE  | CBB-CCB-CDB-CEB |
| 17  | B     | 604  | CLA  | C2B-C3B-CAB-CBB |
| 17  | C     | 504  | CLA  | C2B-C3B-CAB-CBB |
| 17  | b     | 5604 | CLA  | C2B-C3B-CAB-CBB |
| 17  | c     | 5504 | CLA  | C2B-C3B-CAB-CBB |
| 21  | a     | 5409 | LHG  | O10-C23-O8-C6   |
| 20  | k     | 5502 | BCR  | C16-C17-C18-C36 |
| 26  | C     | 517  | DGD  | C9A-CAA-CBA-CCA |
| 26  | c     | 5516 | DGD  | C9A-CAA-CBA-CCA |
| 21  | A     | 408  | LHG  | O10-C23-O8-C6   |
| 18  | a     | 5405 | PHO  | C2-C3-C5-C6     |
| 17  | C     | 510  | CLA  | C13-C15-C16-C17 |
| 17  | c     | 5510 | CLA  | C13-C15-C16-C17 |
| 23  | l     | 5102 | SQD  | C18-C19-C20-C21 |
| 25  | B     | 619  | MGE  | C1A-C2A-C3A-C4A |
| 25  | b     | 5620 | MGE  | C1A-C2A-C3A-C4A |
| 17  | C     | 503  | CLA  | CBA-CGA-O2A-C1  |
| 17  | c     | 5503 | CLA  | CBA-CGA-O2A-C1  |
| 23  | D     | 403  | SQD  | C25-C26-C27-C28 |
| 20  | A     | 407  | BCR  | C23-C24-C25-C30 |
| 20  | B     | 617  | BCR  | C1-C6-C7-C8     |
| 20  | B     | 618  | BCR  | C1-C6-C7-C8     |
| 20  | B     | 618  | BCR  | C23-C24-C25-C26 |
| 20  | C     | 514  | BCR  | C23-C24-C25-C30 |
| 20  | C     | 516  | BCR  | C23-C24-C25-C26 |
| 20  | H     | 101  | BCR  | C1-C6-C7-C8     |
| 20  | T     | 102  | BCR  | C1-C6-C7-C8     |
| 20  | T     | 102  | BCR  | C5-C6-C7-C8     |
| 20  | a     | 5408 | BCR  | C23-C24-C25-C30 |
| 20  | b     | 5617 | BCR  | C1-C6-C7-C8     |
| 20  | b     | 5618 | BCR  | C1-C6-C7-C8     |
| 20  | b     | 5618 | BCR  | C5-C6-C7-C8     |
| 20  | b     | 5618 | BCR  | C23-C24-C25-C26 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 20  | c     | 5513 | BCR  | C23-C24-C25-C30 |
| 20  | c     | 5514 | BCR  | C23-C24-C25-C26 |
| 20  | h     | 5101 | BCR  | C1-C6-C7-C8     |
| 18  | A     | 404  | PHO  | C2-C3-C5-C6     |
| 17  | D     | 404  | CLA  | C2A-CAA-CBA-CGA |
| 17  | d     | 5403 | CLA  | C2A-CAA-CBA-CGA |
| 19  | D     | 406  | PQ9  | C18-C20-C21-C22 |
| 19  | d     | 5405 | PQ9  | C18-C20-C21-C22 |
| 25  | D     | 410  | MGE  | C2D-C1D-O3G-C3G |
| 25  | B     | 619  | MGE  | O1G-C1G-C2G-O2G |
| 25  | D     | 408  | MGE  | O1G-C1G-C2G-O2G |
| 25  | b     | 5620 | MGE  | O1G-C1G-C2G-O2G |
| 17  | C     | 505  | CLA  | C15-C16-C17-C18 |
| 17  | c     | 5505 | CLA  | C15-C16-C17-C18 |
| 25  | d     | 5409 | MGE  | C6B-C7B-C8B-C9B |
| 18  | A     | 404  | PHO  | CHA-CBD-CGD-O1D |
| 18  | A     | 404  | PHO  | CHA-CBD-CGD-O2D |
| 18  | a     | 5405 | PHO  | CHA-CBD-CGD-O1D |
| 18  | a     | 5405 | PHO  | CHA-CBD-CGD-O2D |
| 17  | b     | 5615 | CLA  | C13-C15-C16-C17 |
| 25  | B     | 619  | MGE  | C1G-C2G-C3G-O3G |
| 26  | C     | 517  | DGD  | C1G-C2G-C3G-O3G |
| 26  | c     | 5516 | DGD  | C1G-C2G-C3G-O3G |
| 17  | C     | 507  | CLA  | C6-C7-C8-C10    |
| 17  | C     | 511  | CLA  | C12-C13-C15-C16 |
| 17  | D     | 404  | CLA  | C11-C10-C8-C7   |
| 17  | c     | 5507 | CLA  | C6-C7-C8-C10    |
| 17  | d     | 5403 | CLA  | C11-C10-C8-C7   |
| 17  | k     | 5501 | CLA  | C12-C13-C15-C16 |
| 17  | B     | 606  | CLA  | C11-C12-C13-C14 |
| 17  | B     | 608  | CLA  | C6-C7-C8-C9     |
| 17  | C     | 506  | CLA  | C11-C12-C13-C14 |
| 17  | C     | 511  | CLA  | C14-C13-C15-C16 |
| 17  | b     | 5610 | CLA  | C14-C13-C15-C16 |
| 17  | c     | 5506 | CLA  | C11-C12-C13-C14 |
| 17  | k     | 5501 | CLA  | C14-C13-C15-C16 |
| 20  | B     | 617  | BCR  | C15-C16-C17-C18 |
| 20  | C     | 514  | BCR  | C13-C14-C15-C16 |
| 20  | b     | 5617 | BCR  | C15-C16-C17-C18 |
| 20  | c     | 5513 | BCR  | C13-C14-C15-C16 |
| 17  | B     | 615  | CLA  | C13-C15-C16-C17 |
| 25  | c     | 5517 | MGE  | C5B-C6B-C7B-C8B |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 25  | C     | 519  | MGE  | C5B-C6B-C7B-C8B |
| 25  | m     | 5103 | MGE  | C5B-C6B-C7B-C8B |
| 17  | B     | 612  | CLA  | C4-C3-C5-C6     |
| 17  | b     | 5612 | CLA  | C4-C3-C5-C6     |
| 17  | C     | 503  | CLA  | O1A-CGA-O2A-C1  |
| 17  | B     | 604  | CLA  | C16-C17-C18-C19 |
| 17  | b     | 5604 | CLA  | C16-C17-C18-C19 |
| 17  | c     | 5503 | CLA  | O1A-CGA-O2A-C1  |
| 17  | C     | 511  | CLA  | C15-C16-C17-C18 |
| 17  | B     | 607  | CLA  | C2A-CAA-CBA-CGA |
| 17  | b     | 5607 | CLA  | C2A-CAA-CBA-CGA |
| 17  | k     | 5501 | CLA  | C15-C16-C17-C18 |
| 20  | H     | 101  | BCR  | C15-C16-C17-C18 |
| 20  | h     | 5101 | BCR  | C15-C16-C17-C18 |
| 18  | D     | 402  | PHO  | C13-C15-C16-C17 |
| 18  | d     | 5402 | PHO  | C13-C15-C16-C17 |
| 17  | B     | 613  | CLA  | C4-C3-C5-C6     |
| 17  | b     | 5613 | CLA  | C4-C3-C5-C6     |
| 17  | B     | 612  | CLA  | C2-C3-C5-C6     |
| 17  | b     | 5612 | CLA  | C2-C3-C5-C6     |
| 17  | D     | 404  | CLA  | C2-C1-O2A-CGA   |
| 17  | d     | 5403 | CLA  | C2-C1-O2A-CGA   |
| 17  | b     | 5610 | CLA  | O1D-CGD-O2D-CED |
| 25  | d     | 5410 | MGE  | C2D-C1D-O3G-C3G |
| 21  | A     | 408  | LHG  | C26-C27-C28-C29 |
| 17  | C     | 507  | CLA  | C8-C10-C11-C12  |
| 17  | c     | 5507 | CLA  | C8-C10-C11-C12  |
| 17  | B     | 603  | CLA  | C2A-CAA-CBA-CGA |
| 17  | C     | 501  | CLA  | C2A-CAA-CBA-CGA |
| 17  | b     | 5603 | CLA  | C2A-CAA-CBA-CGA |
| 17  | c     | 5501 | CLA  | C2A-CAA-CBA-CGA |
| 25  | m     | 5101 | MGE  | O1G-C1G-C2G-O2G |
| 21  | a     | 5409 | LHG  | C26-C27-C28-C29 |
| 25  | m     | 5101 | MGE  | C2B-C3B-C4B-C5B |
| 17  | B     | 608  | CLA  | C3A-C2A-CAA-CBA |
| 17  | C     | 505  | CLA  | C3A-C2A-CAA-CBA |
| 17  | C     | 506  | CLA  | C3A-C2A-CAA-CBA |
| 17  | b     | 5608 | CLA  | C3A-C2A-CAA-CBA |
| 17  | c     | 5505 | CLA  | C3A-C2A-CAA-CBA |
| 17  | c     | 5506 | CLA  | C3A-C2A-CAA-CBA |
| 17  | B     | 613  | CLA  | C16-C17-C18-C20 |
| 17  | b     | 5613 | CLA  | C16-C17-C18-C20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 26  | C     | 518  | DGD  | O2G-C1B-C2B-C3B |
| 26  | a     | 5411 | DGD  | O2G-C1B-C2B-C3B |
| 20  | H     | 101  | BCR  | C9-C10-C11-C12  |
| 20  | h     | 5101 | BCR  | C9-C10-C11-C12  |
| 17  | A     | 403  | CLA  | CBA-CGA-O2A-C1  |
| 17  | a     | 5404 | CLA  | CBA-CGA-O2A-C1  |
| 17  | B     | 607  | CLA  | C6-C7-C8-C9     |
| 17  | B     | 611  | CLA  | C14-C13-C15-C16 |
| 17  | b     | 5607 | CLA  | C6-C7-C8-C9     |
| 17  | b     | 5611 | CLA  | C14-C13-C15-C16 |
| 25  | D     | 410  | MGE  | C5B-C6B-C7B-C8B |
| 26  | D     | 411  | DGD  | C6B-C7B-C8B-C9B |
| 17  | B     | 610  | CLA  | O1D-CGD-O2D-CED |
| 26  | b     | 5621 | DGD  | C6B-C7B-C8B-C9B |
| 20  | b     | 5619 | BCR  | C20-C21-C22-C37 |
| 20  | t     | 5101 | BCR  | C20-C21-C22-C37 |
| 25  | B     | 619  | MGE  | O1G-C1G-C2G-C3G |
| 25  | b     | 5620 | MGE  | O1G-C1G-C2G-C3G |
| 25  | b     | 5620 | MGE  | C1G-C2G-C3G-O3G |
| 22  | a     | 5410 | LMT  | O5'-C1'-O1'-C1  |
| 25  | D     | 409  | MGE  | O6D-C1D-O3G-C3G |
| 26  | C     | 517  | DGD  | O6D-C1D-O3G-C3G |
| 26  | c     | 5516 | DGD  | O6D-C1D-O3G-C3G |
| 26  | A     | 413  | DGD  | CBA-CCA-CDA-CEA |
| 26  | c     | 5515 | DGD  | CBA-CCA-CDA-CEA |
| 25  | d     | 5408 | MGE  | C2A-C3A-C4A-C5A |
| 17  | B     | 607  | CLA  | C1A-C2A-CAA-CBA |
| 17  | C     | 501  | CLA  | C1A-C2A-CAA-CBA |
| 17  | b     | 5607 | CLA  | C1A-C2A-CAA-CBA |
| 17  | c     | 5501 | CLA  | C1A-C2A-CAA-CBA |
| 25  | l     | 5101 | MGE  | C5A-C6A-C7A-C8A |
| 17  | C     | 502  | CLA  | C6-C7-C8-C10    |
| 17  | C     | 507  | CLA  | C11-C10-C8-C7   |
| 17  | c     | 5502 | CLA  | C6-C7-C8-C10    |
| 17  | c     | 5507 | CLA  | C11-C10-C8-C7   |
| 17  | A     | 402  | CLA  | C2C-C3C-CAC-CBC |
| 25  | A     | 412  | MGE  | C5A-C6A-C7A-C8A |
| 17  | A     | 403  | CLA  | O1A-CGA-O2A-C1  |
| 17  | a     | 5404 | CLA  | O1A-CGA-O2A-C1  |
| 17  | C     | 506  | CLA  | C16-C17-C18-C20 |
| 17  | c     | 5506 | CLA  | C16-C17-C18-C20 |
| 22  | m     | 5102 | LMT  | O1'-C1-C2-C3    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | a     | 5403 | CLA  | C2C-C3C-CAC-CBC |
| 25  | d     | 5409 | MGE  | C2A-C3A-C4A-C5A |
| 17  | B     | 602  | CLA  | C2B-C3B-CAB-CBB |
| 17  | B     | 613  | CLA  | C2B-C3B-CAB-CBB |
| 17  | C     | 505  | CLA  | C2B-C3B-CAB-CBB |
| 17  | D     | 404  | CLA  | C2B-C3B-CAB-CBB |
| 17  | b     | 5602 | CLA  | C2B-C3B-CAB-CBB |
| 17  | b     | 5613 | CLA  | C2B-C3B-CAB-CBB |
| 17  | c     | 5505 | CLA  | C2B-C3B-CAB-CBB |
| 17  | d     | 5403 | CLA  | C2B-C3B-CAB-CBB |
| 20  | C     | 516  | BCR  | C16-C17-C18-C19 |
| 20  | c     | 5514 | BCR  | C16-C17-C18-C19 |
| 20  | C     | 515  | BCR  | C13-C14-C15-C16 |
| 20  | D     | 407  | BCR  | C19-C20-C21-C22 |
| 20  | d     | 5406 | BCR  | C19-C20-C21-C22 |
| 20  | z     | 5101 | BCR  | C13-C14-C15-C16 |
| 20  | Y     | 101  | BCR  | C9-C10-C11-C12  |
| 17  | B     | 610  | CLA  | O1A-CGA-O2A-C1  |
| 17  | A     | 401  | CLA  | C15-C16-C17-C18 |
| 17  | C     | 502  | CLA  | C4-C3-C5-C6     |
| 17  | c     | 5502 | CLA  | C4-C3-C5-C6     |
| 17  | B     | 613  | CLA  | C2-C1-O2A-CGA   |
| 17  | b     | 5613 | CLA  | C2-C1-O2A-CGA   |
| 25  | D     | 409  | MGE  | C6B-C7B-C8B-C9B |
| 17  | b     | 5610 | CLA  | O1A-CGA-O2A-C1  |
| 17  | a     | 5402 | CLA  | C15-C16-C17-C18 |
| 22  | M     | 101  | LMT  | C1-C2-C3-C4     |
| 23  | d     | 5407 | SQD  | C10-C11-C12-C13 |
| 20  | A     | 407  | BCR  | C23-C24-C25-C26 |
| 20  | B     | 618  | BCR  | C5-C6-C7-C8     |
| 20  | a     | 5408 | BCR  | C23-C24-C25-C26 |
| 20  | k     | 5502 | BCR  | C1-C6-C7-C8     |
| 20  | Y     | 101  | BCR  | C1-C6-C7-C8     |
| 25  | D     | 408  | MGE  | O1G-C1G-C2G-C3G |
| 26  | C     | 517  | DGD  | O1G-C1G-C2G-C3G |
| 26  | c     | 5516 | DGD  | O1G-C1G-C2G-C3G |
| 20  | C     | 514  | BCR  | C15-C16-C17-C18 |
| 20  | C     | 515  | BCR  | C15-C16-C17-C18 |
| 20  | c     | 5513 | BCR  | C15-C16-C17-C18 |
| 20  | z     | 5101 | BCR  | C15-C16-C17-C18 |
| 20  | D     | 407  | BCR  | C17-C18-C19-C20 |
| 20  | d     | 5406 | BCR  | C17-C18-C19-C20 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | B     | 602  | CLA  | CAA-CBA-CGA-O2A |
| 17  | b     | 5602 | CLA  | CAA-CBA-CGA-O2A |
| 17  | B     | 610  | CLA  | CBA-CGA-O2A-C1  |
| 17  | b     | 5610 | CLA  | CBA-CGA-O2A-C1  |
| 17  | B     | 613  | CLA  | C4B-C3B-CAB-CBB |
| 17  | C     | 506  | CLA  | C4B-C3B-CAB-CBB |
| 17  | b     | 5613 | CLA  | C4B-C3B-CAB-CBB |
| 17  | c     | 5506 | CLA  | C4B-C3B-CAB-CBB |
| 17  | A     | 402  | CLA  | C4C-C3C-CAC-CBC |
| 17  | B     | 612  | CLA  | C6-C7-C8-C10    |
| 17  | b     | 5612 | CLA  | C6-C7-C8-C10    |
| 18  | D     | 402  | PHO  | C11-C12-C13-C15 |
| 18  | d     | 5402 | PHO  | C11-C12-C13-C15 |
| 17  | a     | 5403 | CLA  | C4C-C3C-CAC-CBC |
| 23  | l     | 5102 | SQD  | O48-C23-C24-C25 |
| 17  | B     | 605  | CLA  | C16-C17-C18-C20 |
| 17  | b     | 5605 | CLA  | C16-C17-C18-C20 |
| 17  | B     | 614  | CLA  | CBA-CGA-O2A-C1  |
| 17  | b     | 5614 | CLA  | CBA-CGA-O2A-C1  |
| 17  | C     | 507  | CLA  | CAA-CBA-CGA-O2A |
| 17  | c     | 5507 | CLA  | CAA-CBA-CGA-O2A |
| 17  | C     | 502  | CLA  | C2-C3-C5-C6     |
| 17  | c     | 5502 | CLA  | C2-C3-C5-C6     |
| 25  | m     | 5103 | MGE  | O2G-C1B-C2B-C3B |
| 17  | B     | 605  | CLA  | C11-C10-C8-C9   |
| 17  | C     | 505  | CLA  | C6-C7-C8-C9     |
| 17  | C     | 505  | CLA  | C11-C12-C13-C14 |
| 17  | D     | 404  | CLA  | C11-C10-C8-C9   |
| 17  | b     | 5605 | CLA  | C11-C10-C8-C9   |
| 17  | c     | 5505 | CLA  | C6-C7-C8-C9     |
| 17  | c     | 5505 | CLA  | C11-C12-C13-C14 |
| 17  | d     | 5403 | CLA  | C11-C10-C8-C9   |
| 25  | d     | 5410 | MGE  | C6B-C7B-C8B-C9B |
| 25  | D     | 409  | MGE  | C2A-C3A-C4A-C5A |
| 26  | D     | 411  | DGD  | C4B-C5B-C6B-C7B |
| 17  | B     | 602  | CLA  | CAD-CBD-CGD-O2D |
| 17  | B     | 614  | CLA  | CAD-CBD-CGD-O2D |
| 17  | B     | 616  | CLA  | CAD-CBD-CGD-O2D |
| 17  | C     | 505  | CLA  | CAD-CBD-CGD-O2D |
| 17  | C     | 511  | CLA  | CAD-CBD-CGD-O2D |
| 17  | b     | 5602 | CLA  | CAD-CBD-CGD-O2D |
| 17  | b     | 5614 | CLA  | CAD-CBD-CGD-O2D |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | b     | 5616 | CLA  | CAD-CBD-CGD-O2D |
| 17  | c     | 5505 | CLA  | CAD-CBD-CGD-O2D |
| 17  | k     | 5501 | CLA  | CAD-CBD-CGD-O2D |
| 25  | m     | 5103 | MGE  | C1G-C2G-O2G-C1B |
| 25  | m     | 5103 | MGE  | C3G-C2G-O2G-C1B |
| 26  | b     | 5621 | DGD  | C4B-C5B-C6B-C7B |
| 25  | m     | 5101 | MGE  | O1B-C1B-O2G-C2G |
| 17  | B     | 614  | CLA  | C4C-C3C-CAC-CBC |
| 17  | b     | 5614 | CLA  | C4C-C3C-CAC-CBC |
| 25  | m     | 5101 | MGE  | C4B-C5B-C6B-C7B |
| 23  | L     | 101  | SQD  | O48-C23-C24-C25 |
| 25  | d     | 5408 | MGE  | C9A-CAA-CBA-CCA |
| 23  | a     | 5401 | SQD  | O6-C44-C45-C46  |
| 17  | B     | 614  | CLA  | O1A-CGA-O2A-C1  |
| 23  | D     | 403  | SQD  | C12-C13-C14-C15 |
| 17  | A     | 401  | CLA  | O2A-C1-C2-C3    |
| 17  | C     | 512  | CLA  | O2A-C1-C2-C3    |
| 17  | a     | 5402 | CLA  | O2A-C1-C2-C3    |
| 17  | c     | 5511 | CLA  | O2A-C1-C2-C3    |
| 25  | D     | 409  | MGE  | C3B-C4B-C5B-C6B |
| 17  | b     | 5614 | CLA  | O1A-CGA-O2A-C1  |
| 17  | A     | 405  | CLA  | CHA-CBD-CGD-O2D |
| 17  | B     | 602  | CLA  | CHA-CBD-CGD-O2D |
| 17  | B     | 614  | CLA  | CHA-CBD-CGD-O2D |
| 17  | B     | 616  | CLA  | CHA-CBD-CGD-O1D |
| 17  | C     | 509  | CLA  | CHA-CBD-CGD-O1D |
| 17  | C     | 511  | CLA  | CHA-CBD-CGD-O1D |
| 17  | a     | 5406 | CLA  | CHA-CBD-CGD-O2D |
| 17  | b     | 5602 | CLA  | CHA-CBD-CGD-O2D |
| 17  | b     | 5614 | CLA  | CHA-CBD-CGD-O2D |
| 17  | b     | 5616 | CLA  | CHA-CBD-CGD-O1D |
| 17  | c     | 5509 | CLA  | CHA-CBD-CGD-O1D |
| 17  | k     | 5501 | CLA  | CHA-CBD-CGD-O1D |
| 17  | C     | 512  | CLA  | CAA-CBA-CGA-O2A |
| 17  | c     | 5511 | CLA  | CAA-CBA-CGA-O2A |
| 17  | C     | 506  | CLA  | C10-C11-C12-C13 |
| 17  | B     | 613  | CLA  | CAA-CBA-CGA-O2A |
| 17  | b     | 5613 | CLA  | CAA-CBA-CGA-O2A |
| 25  | m     | 5103 | MGE  | O1G-C1G-C2G-O2G |
| 17  | c     | 5506 | CLA  | C10-C11-C12-C13 |
| 26  | D     | 411  | DGD  | O2G-C1B-C2B-C3B |
| 26  | b     | 5621 | DGD  | O2G-C1B-C2B-C3B |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 25  | D     | 408  | MGE  | C2B-C1B-O2G-C2G |
| 17  | B     | 614  | CLA  | CAA-CBA-CGA-O2A |
| 17  | b     | 5614 | CLA  | CAA-CBA-CGA-O2A |
| 17  | B     | 609  | CLA  | C2-C3-C5-C6     |
| 17  | C     | 508  | CLA  | C11-C10-C8-C7   |
| 17  | b     | 5609 | CLA  | C2-C3-C5-C6     |
| 17  | c     | 5508 | CLA  | C11-C10-C8-C7   |
| 17  | B     | 610  | CLA  | C16-C17-C18-C19 |
| 17  | b     | 5610 | CLA  | C16-C17-C18-C19 |
| 20  | B     | 617  | BCR  | C19-C20-C21-C22 |
| 20  | b     | 5617 | BCR  | C19-C20-C21-C22 |
| 20  | k     | 5502 | BCR  | C15-C16-C17-C18 |
| 17  | C     | 504  | CLA  | CAA-CBA-CGA-O2A |
| 17  | c     | 5504 | CLA  | CAA-CBA-CGA-O2A |
| 23  | L     | 101  | SQD  | C4-C5-C6-S      |
| 17  | B     | 610  | CLA  | C16-C17-C18-C20 |
| 17  | b     | 5610 | CLA  | C16-C17-C18-C20 |
| 25  | m     | 5101 | MGE  | C2B-C1B-O2G-C2G |
| 17  | A     | 401  | CLA  | C2A-CAA-CBA-CGA |
| 17  | a     | 5402 | CLA  | C2A-CAA-CBA-CGA |
| 20  | C     | 516  | BCR  | C37-C22-C23-C24 |
| 20  | c     | 5514 | BCR  | C37-C22-C23-C24 |
| 25  | d     | 5410 | MGE  | C9B-CAB-CBB-CCB |
| 17  | C     | 503  | CLA  | CAA-CBA-CGA-O2A |
| 17  | C     | 507  | CLA  | CAA-CBA-CGA-O1A |
| 17  | c     | 5507 | CLA  | CAA-CBA-CGA-O1A |
| 17  | C     | 509  | CLA  | C1A-C2A-CAA-CBA |
| 17  | c     | 5509 | CLA  | C1A-C2A-CAA-CBA |
| 25  | m     | 5103 | MGE  | O1B-C1B-C2B-C3B |
| 17  | c     | 5503 | CLA  | CAA-CBA-CGA-O2A |
| 25  | m     | 5101 | MGE  | O1G-C1G-C2G-C3G |
| 22  | A     | 409  | LMT  | C9-C10-C11-C12  |
| 21  | A     | 408  | LHG  | C30-C31-C32-C33 |
| 17  | B     | 611  | CLA  | C4-C3-C5-C6     |
| 17  | b     | 5611 | CLA  | C4-C3-C5-C6     |
| 25  | B     | 619  | MGE  | C7B-C8B-C9B-CAB |
| 17  | B     | 613  | CLA  | C2-C3-C5-C6     |
| 21  | a     | 5409 | LHG  | C30-C31-C32-C33 |
| 25  | b     | 5620 | MGE  | C7B-C8B-C9B-CAB |
| 17  | C     | 504  | CLA  | CAA-CBA-CGA-O1A |
| 17  | C     | 512  | CLA  | CAA-CBA-CGA-O1A |
| 17  | c     | 5504 | CLA  | CAA-CBA-CGA-O1A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | c     | 5511 | CLA  | CAA-CBA-CGA-O1A |
| 20  | c     | 5513 | BCR  | C16-C17-C18-C36 |
| 20  | k     | 5502 | BCR  | C5-C6-C7-C8     |
| 20  | Y     | 101  | BCR  | C5-C6-C7-C8     |
| 25  | l     | 5101 | MGE  | CDB-CEB-CFB-CGB |
| 25  | C     | 519  | MGE  | C8A-C9A-CAA-CBA |
| 25  | c     | 5517 | MGE  | C8A-C9A-CAA-CBA |
| 25  | D     | 408  | MGE  | O1B-C1B-O2G-C2G |
| 17  | B     | 604  | CLA  | C2C-C3C-CAC-CBC |
| 17  | b     | 5604 | CLA  | C2C-C3C-CAC-CBC |
| 17  | b     | 5613 | CLA  | CAA-CBA-CGA-O1A |
| 25  | A     | 412  | MGE  | CDB-CEB-CFB-CGB |
| 17  | B     | 613  | CLA  | CAA-CBA-CGA-O1A |
| 17  | B     | 614  | CLA  | CAA-CBA-CGA-O1A |
| 17  | b     | 5613 | CLA  | C2-C3-C5-C6     |
| 17  | B     | 606  | CLA  | CAD-CBD-CGD-O1D |
| 17  | B     | 612  | CLA  | CAD-CBD-CGD-O1D |
| 17  | C     | 507  | CLA  | CAD-CBD-CGD-O1D |
| 17  | C     | 509  | CLA  | CAD-CBD-CGD-O1D |
| 17  | b     | 5606 | CLA  | CAD-CBD-CGD-O1D |
| 17  | b     | 5612 | CLA  | CAD-CBD-CGD-O1D |
| 17  | c     | 5507 | CLA  | CAD-CBD-CGD-O1D |
| 17  | c     | 5509 | CLA  | CAD-CBD-CGD-O1D |
| 17  | b     | 5614 | CLA  | CAA-CBA-CGA-O1A |
| 25  | d     | 5408 | MGE  | O1B-C1B-C2B-C3B |
| 25  | b     | 5620 | MGE  | C2B-C3B-C4B-C5B |
| 17  | A     | 402  | CLA  | C11-C12-C13-C14 |
| 17  | a     | 5403 | CLA  | C11-C12-C13-C14 |
| 22  | m     | 5102 | LMT  | C11-C10-C9-C8   |
| 25  | B     | 619  | MGE  | C2B-C3B-C4B-C5B |
| 25  | d     | 5410 | MGE  | CBB-CCB-CDB-CEB |
| 17  | B     | 609  | CLA  | C4-C3-C5-C6     |
| 17  | b     | 5609 | CLA  | C4-C3-C5-C6     |
| 19  | D     | 406  | PQ9  | C39-C38-C40-C41 |
| 19  | d     | 5405 | PQ9  | C39-C38-C40-C41 |
| 17  | B     | 605  | CLA  | C11-C10-C8-C7   |
| 17  | C     | 505  | CLA  | C6-C7-C8-C10    |
| 17  | C     | 505  | CLA  | C12-C13-C15-C16 |
| 17  | C     | 511  | CLA  | C6-C7-C8-C10    |
| 17  | b     | 5605 | CLA  | C11-C10-C8-C7   |
| 17  | c     | 5505 | CLA  | C6-C7-C8-C10    |
| 17  | c     | 5505 | CLA  | C12-C13-C15-C16 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | k     | 5501 | CLA  | C6-C7-C8-C10    |
| 25  | D     | 410  | MGE  | C9A-CAA-CBA-CCA |
| 25  | D     | 410  | MGE  | O2G-C1B-C2B-C3B |
| 17  | B     | 602  | CLA  | C10-C11-C12-C13 |
| 17  | b     | 5602 | CLA  | C10-C11-C12-C13 |
| 20  | b     | 5619 | BCR  | C7-C8-C9-C10    |
| 20  | t     | 5101 | BCR  | C7-C8-C9-C10    |
| 22  | a     | 5410 | LMT  | C2-C1-O1'-C1'   |
| 17  | D     | 404  | CLA  | CAA-CBA-CGA-O2A |
| 17  | d     | 5403 | CLA  | CAA-CBA-CGA-O2A |
| 29  | F     | 101  | HEM  | CAA-CBA-CGA-O1A |
| 29  | f     | 5101 | HEM  | CAA-CBA-CGA-O1A |
| 17  | B     | 606  | CLA  | C8-C10-C11-C12  |
| 26  | c     | 5515 | DGD  | C9A-CAA-CBA-CCA |
| 26  | A     | 413  | DGD  | C9A-CAA-CBA-CCA |
| 17  | b     | 5613 | CLA  | C3-C5-C6-C7     |

There are no ring outliers.

133 monomers are involved in 701 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 20  | A     | 407  | BCR  | 3       | 0            |
| 17  | D     | 404  | CLA  | 10      | 0            |
| 17  | C     | 507  | CLA  | 6       | 0            |
| 25  | d     | 5408 | MGE  | 4       | 0            |
| 17  | c     | 5502 | CLA  | 3       | 0            |
| 17  | c     | 5512 | CLA  | 6       | 0            |
| 17  | B     | 615  | CLA  | 4       | 0            |
| 25  | D     | 410  | MGE  | 13      | 0            |
| 20  | k     | 5502 | BCR  | 9       | 0            |
| 17  | C     | 511  | CLA  | 9       | 0            |
| 26  | a     | 5411 | DGD  | 2       | 0            |
| 20  | t     | 5101 | BCR  | 3       | 0            |
| 17  | b     | 5605 | CLA  | 5       | 0            |
| 26  | C     | 518  | DGD  | 3       | 0            |
| 17  | C     | 503  | CLA  | 8       | 0            |
| 26  | D     | 411  | DGD  | 7       | 0            |
| 17  | a     | 5402 | CLA  | 13      | 0            |
| 25  | D     | 408  | MGE  | 6       | 0            |
| 17  | b     | 5604 | CLA  | 7       | 0            |
| 20  | Y     | 101  | BCR  | 9       | 0            |
| 17  | B     | 607  | CLA  | 10      | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 24  | A     | 411  | BCT  | 8       | 0            |
| 25  | l     | 5101 | MGE  | 9       | 0            |
| 20  | C     | 516  | BCR  | 5       | 0            |
| 17  | a     | 5406 | CLA  | 1       | 0            |
| 17  | c     | 5506 | CLA  | 5       | 0            |
| 17  | B     | 601  | CLA  | 5       | 0            |
| 17  | B     | 614  | CLA  | 6       | 0            |
| 22  | B     | 620  | LMT  | 1       | 0            |
| 23  | L     | 101  | SQD  | 16      | 0            |
| 18  | d     | 5402 | PHO  | 14      | 0            |
| 17  | b     | 5610 | CLA  | 4       | 0            |
| 17  | B     | 608  | CLA  | 7       | 0            |
| 17  | C     | 502  | CLA  | 3       | 0            |
| 17  | d     | 5403 | CLA  | 8       | 0            |
| 17  | c     | 5508 | CLA  | 6       | 0            |
| 17  | C     | 504  | CLA  | 1       | 0            |
| 17  | b     | 5603 | CLA  | 11      | 0            |
| 25  | B     | 619  | MGE  | 6       | 0            |
| 20  | t     | 5102 | BCR  | 6       | 0            |
| 20  | b     | 5619 | BCR  | 3       | 0            |
| 17  | a     | 5403 | CLA  | 12      | 0            |
| 17  | B     | 612  | CLA  | 12      | 0            |
| 20  | B     | 617  | BCR  | 6       | 0            |
| 20  | d     | 5406 | BCR  | 4       | 0            |
| 17  | A     | 402  | CLA  | 9       | 0            |
| 26  | c     | 5515 | DGD  | 7       | 0            |
| 17  | A     | 401  | CLA  | 15      | 0            |
| 25  | d     | 5409 | MGE  | 8       | 0            |
| 17  | B     | 604  | CLA  | 7       | 0            |
| 17  | d     | 5404 | CLA  | 1       | 0            |
| 17  | A     | 403  | CLA  | 1       | 0            |
| 26  | b     | 5621 | DGD  | 7       | 0            |
| 19  | a     | 5407 | PQ9  | 2       | 0            |
| 17  | b     | 5612 | CLA  | 11      | 0            |
| 20  | b     | 5617 | BCR  | 8       | 0            |
| 17  | B     | 603  | CLA  | 12      | 0            |
| 25  | d     | 5410 | MGE  | 13      | 0            |
| 20  | D     | 407  | BCR  | 5       | 0            |
| 17  | C     | 508  | CLA  | 7       | 0            |
| 29  | f     | 5101 | HEM  | 4       | 0            |
| 17  | C     | 509  | CLA  | 1       | 0            |
| 17  | c     | 5503 | CLA  | 8       | 0            |

*Continued on next page...*

*Continued from previous page...*

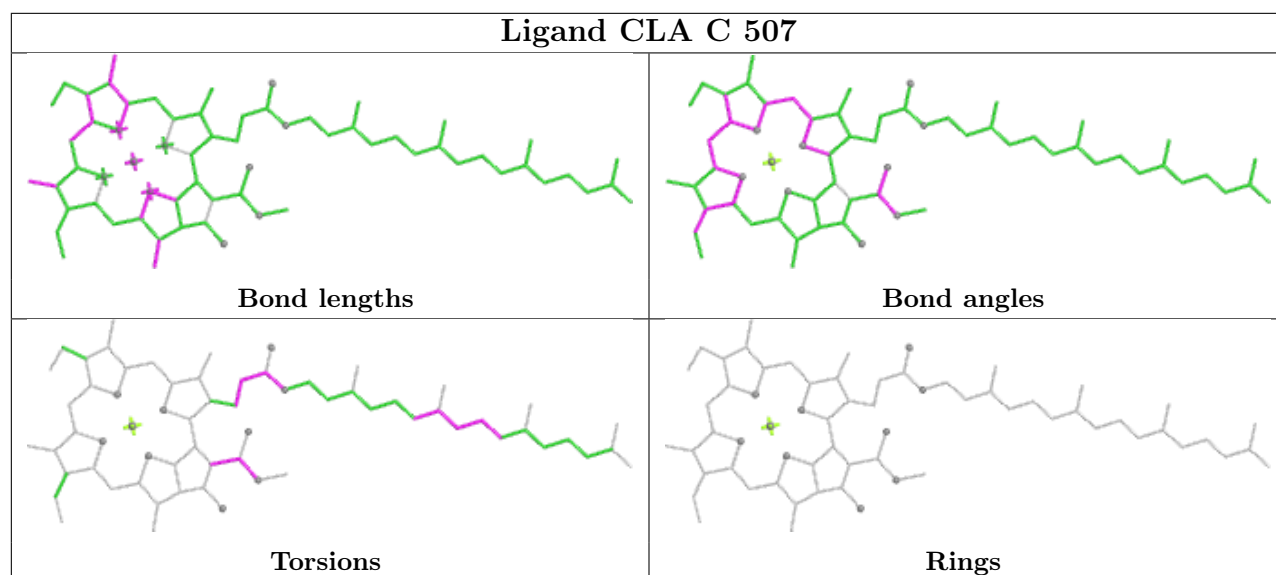
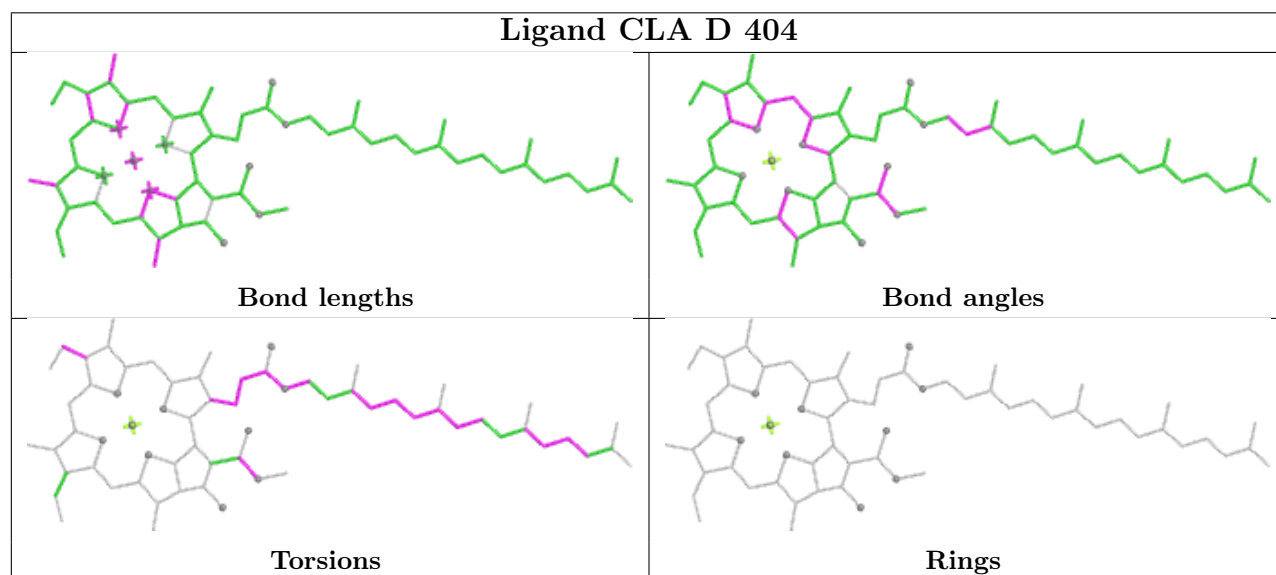
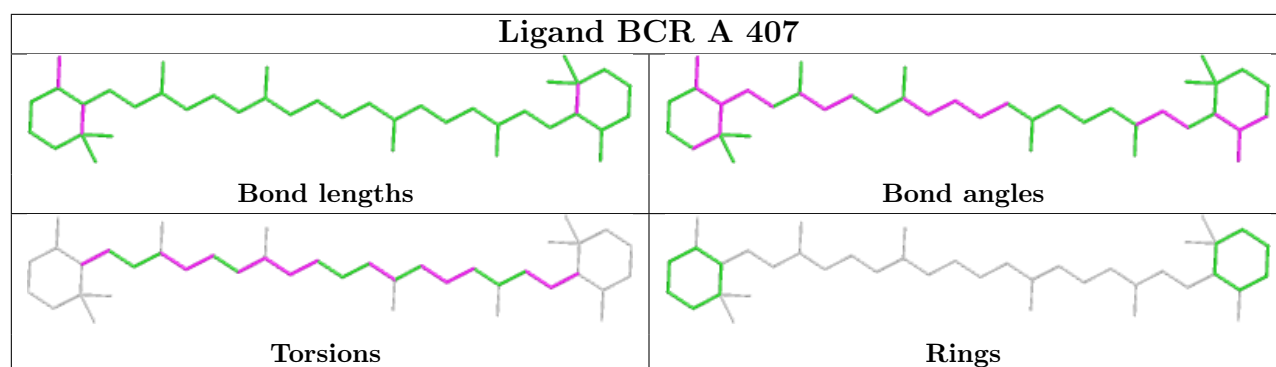
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 20  | a     | 5408 | BCR  | 5       | 0            |
| 17  | B     | 602  | CLA  | 5       | 0            |
| 17  | A     | 405  | CLA  | 5       | 0            |
| 17  | B     | 609  | CLA  | 9       | 0            |
| 17  | b     | 5601 | CLA  | 6       | 0            |
| 23  | l     | 5102 | SQD  | 13      | 0            |
| 23  | d     | 5407 | SQD  | 2       | 0            |
| 17  | c     | 5510 | CLA  | 3       | 0            |
| 20  | c     | 5513 | BCR  | 4       | 0            |
| 17  | D     | 405  | CLA  | 2       | 0            |
| 22  | A     | 409  | LMT  | 3       | 0            |
| 25  | b     | 5620 | MGE  | 6       | 0            |
| 17  | b     | 5614 | CLA  | 6       | 0            |
| 20  | B     | 618  | BCR  | 1       | 0            |
| 17  | b     | 5606 | CLA  | 3       | 0            |
| 17  | b     | 5611 | CLA  | 8       | 0            |
| 19  | d     | 5405 | PQ9  | 8       | 0            |
| 17  | C     | 512  | CLA  | 3       | 0            |
| 17  | b     | 5615 | CLA  | 3       | 0            |
| 20  | b     | 5618 | BCR  | 1       | 0            |
| 20  | C     | 515  | BCR  | 3       | 0            |
| 25  | m     | 5101 | MGE  | 10      | 0            |
| 17  | B     | 606  | CLA  | 9       | 0            |
| 18  | D     | 402  | PHO  | 7       | 0            |
| 22  | M     | 101  | LMT  | 2       | 0            |
| 23  | D     | 403  | SQD  | 6       | 0            |
| 17  | a     | 5404 | CLA  | 4       | 0            |
| 25  | c     | 5517 | MGE  | 5       | 0            |
| 19  | A     | 406  | PQ9  | 7       | 0            |
| 25  | m     | 5103 | MGE  | 9       | 0            |
| 24  | a     | 5412 | BCT  | 6       | 0            |
| 21  | a     | 5409 | LHG  | 3       | 0            |
| 19  | D     | 406  | PQ9  | 7       | 0            |
| 17  | k     | 5501 | CLA  | 7       | 0            |
| 20  | H     | 101  | BCR  | 6       | 0            |
| 17  | B     | 605  | CLA  | 6       | 0            |
| 17  | C     | 513  | CLA  | 7       | 0            |
| 17  | B     | 611  | CLA  | 8       | 0            |
| 17  | b     | 5608 | CLA  | 8       | 0            |
| 17  | C     | 510  | CLA  | 3       | 0            |
| 17  | C     | 501  | CLA  | 8       | 0            |
| 20  | c     | 5514 | BCR  | 5       | 0            |

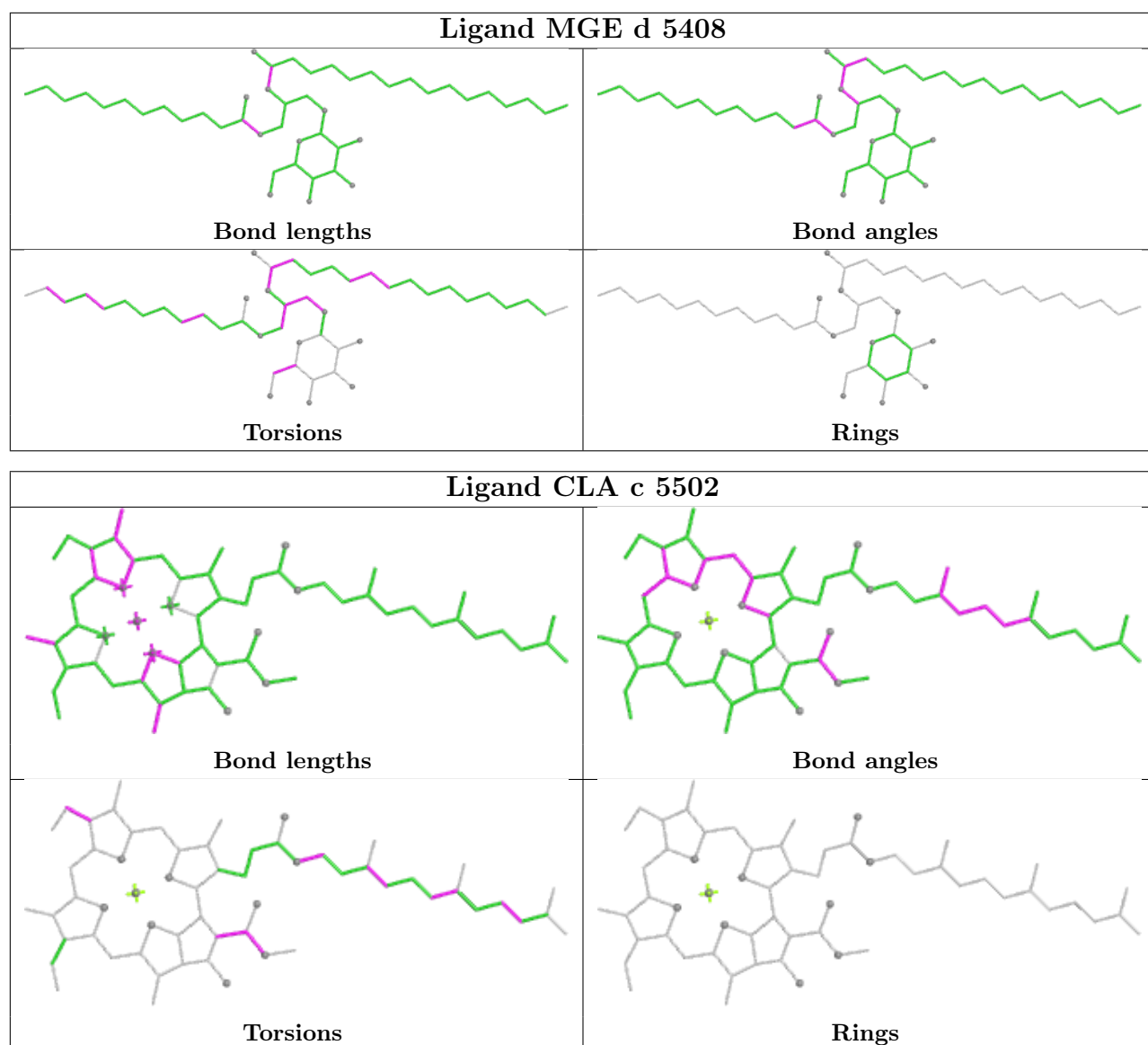
*Continued on next page...*

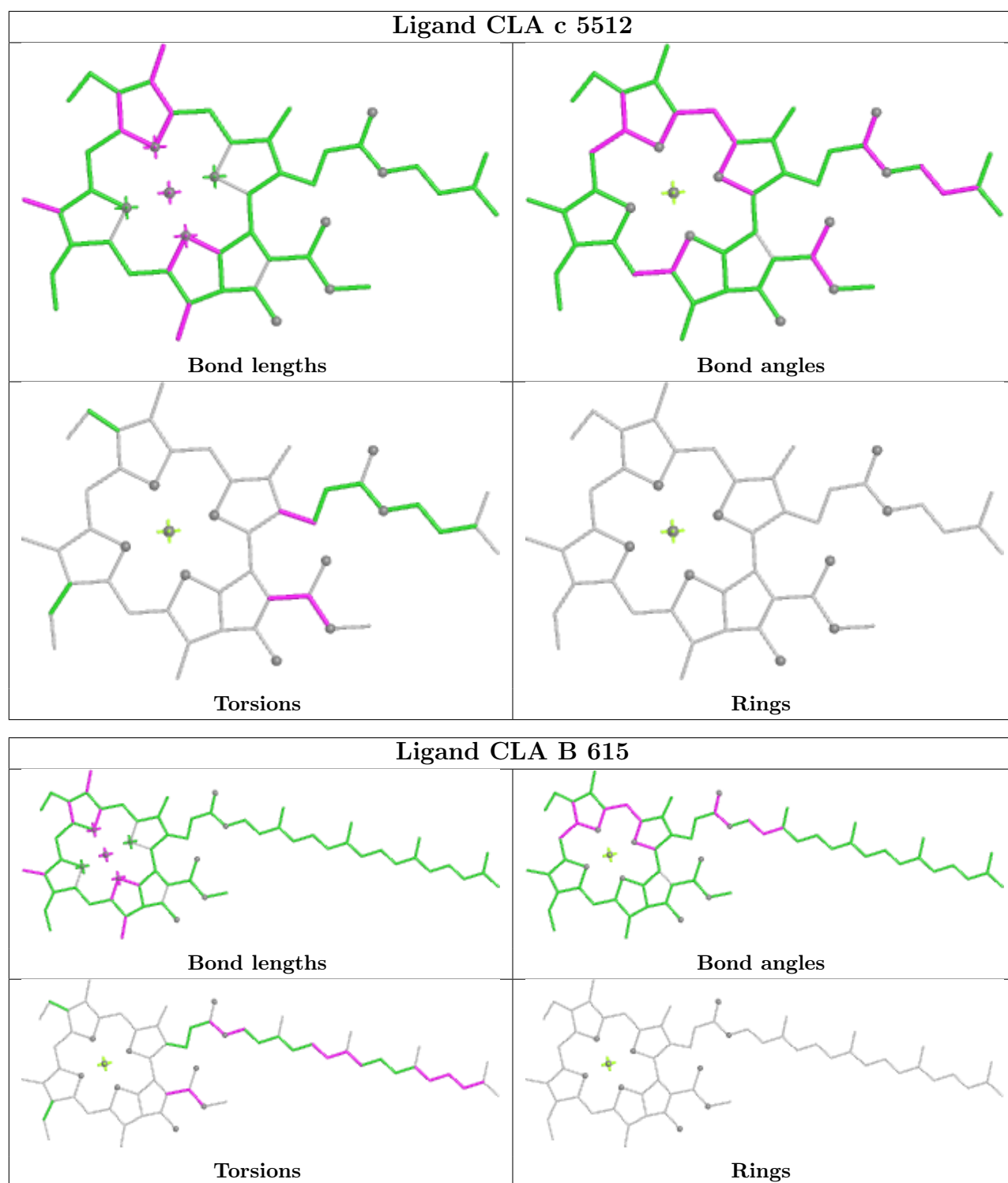
*Continued from previous page...*

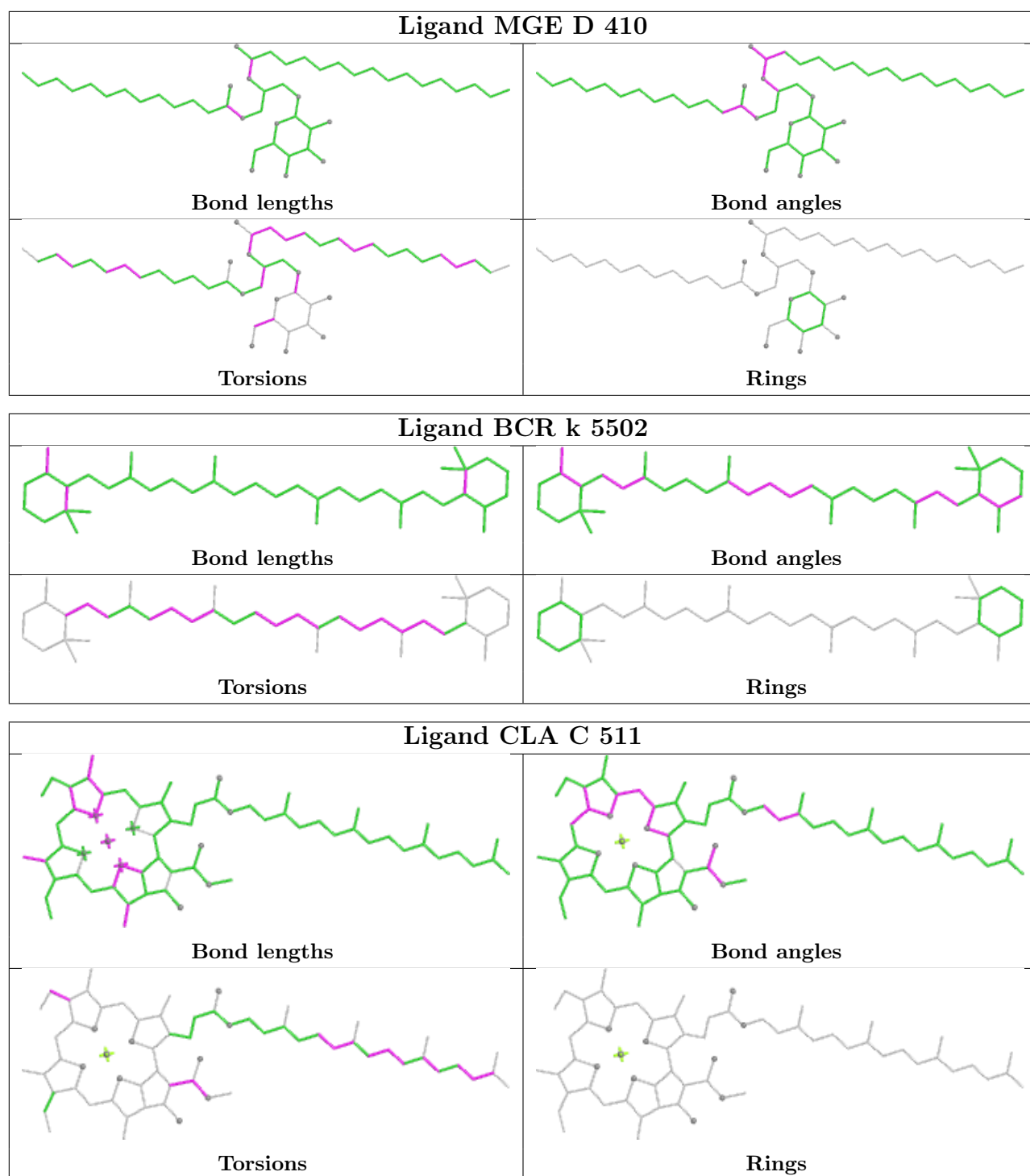
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 20  | h     | 5101 | BCR  | 7       | 0            |
| 25  | D     | 409  | MGE  | 5       | 0            |
| 17  | c     | 5505 | CLA  | 11      | 0            |
| 18  | a     | 5405 | PHO  | 9       | 0            |
| 17  | c     | 5501 | CLA  | 8       | 0            |
| 22  | m     | 5102 | LMT  | 1       | 0            |
| 17  | b     | 5607 | CLA  | 10      | 0            |
| 17  | C     | 505  | CLA  | 10      | 0            |
| 17  | C     | 506  | CLA  | 4       | 0            |
| 21  | A     | 408  | LHG  | 2       | 0            |
| 17  | c     | 5507 | CLA  | 5       | 0            |
| 25  | C     | 519  | MGE  | 5       | 0            |
| 17  | B     | 610  | CLA  | 6       | 0            |
| 20  | z     | 5101 | BCR  | 4       | 0            |
| 29  | F     | 101  | HEM  | 8       | 0            |
| 25  | A     | 412  | MGE  | 12      | 0            |
| 18  | A     | 404  | PHO  | 7       | 0            |
| 17  | B     | 616  | CLA  | 4       | 0            |
| 20  | C     | 514  | BCR  | 4       | 0            |
| 17  | c     | 5511 | CLA  | 3       | 0            |
| 17  | b     | 5613 | CLA  | 10      | 0            |
| 17  | b     | 5609 | CLA  | 8       | 0            |
| 17  | b     | 5602 | CLA  | 10      | 0            |
| 26  | A     | 413  | DGD  | 7       | 0            |
| 17  | B     | 613  | CLA  | 12      | 0            |
| 20  | T     | 102  | BCR  | 6       | 0            |
| 17  | b     | 5616 | CLA  | 5       | 0            |
| 17  | c     | 5509 | CLA  | 1       | 0            |

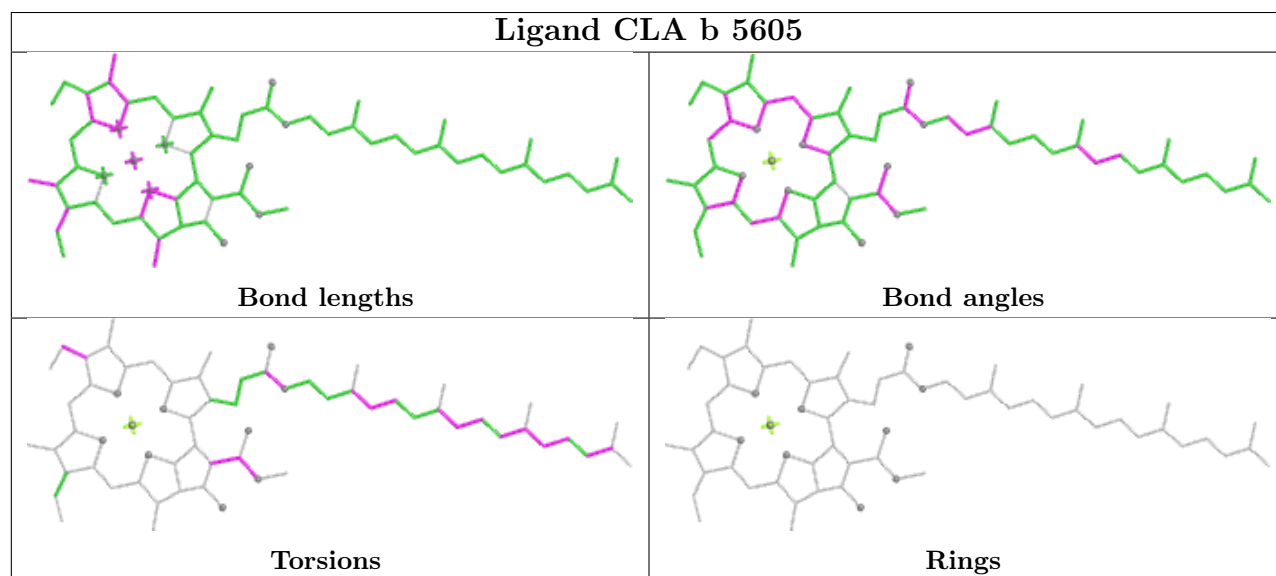
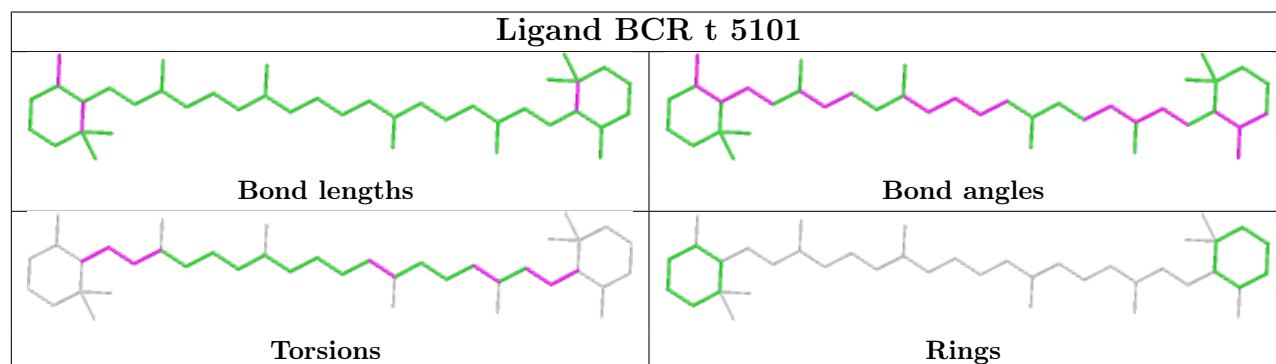
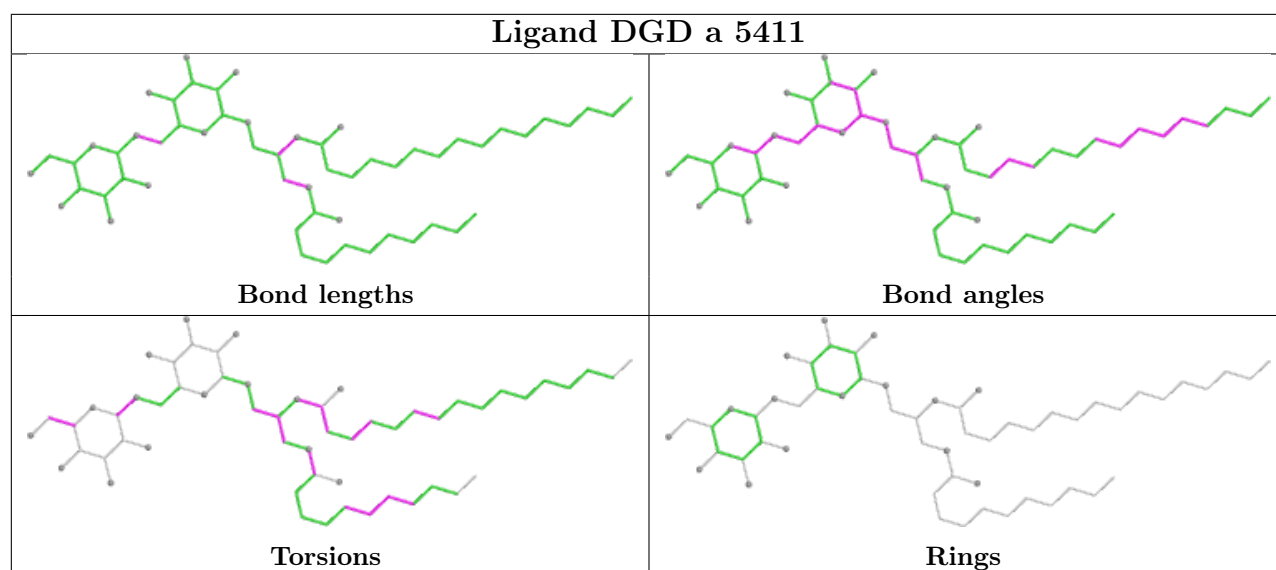
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

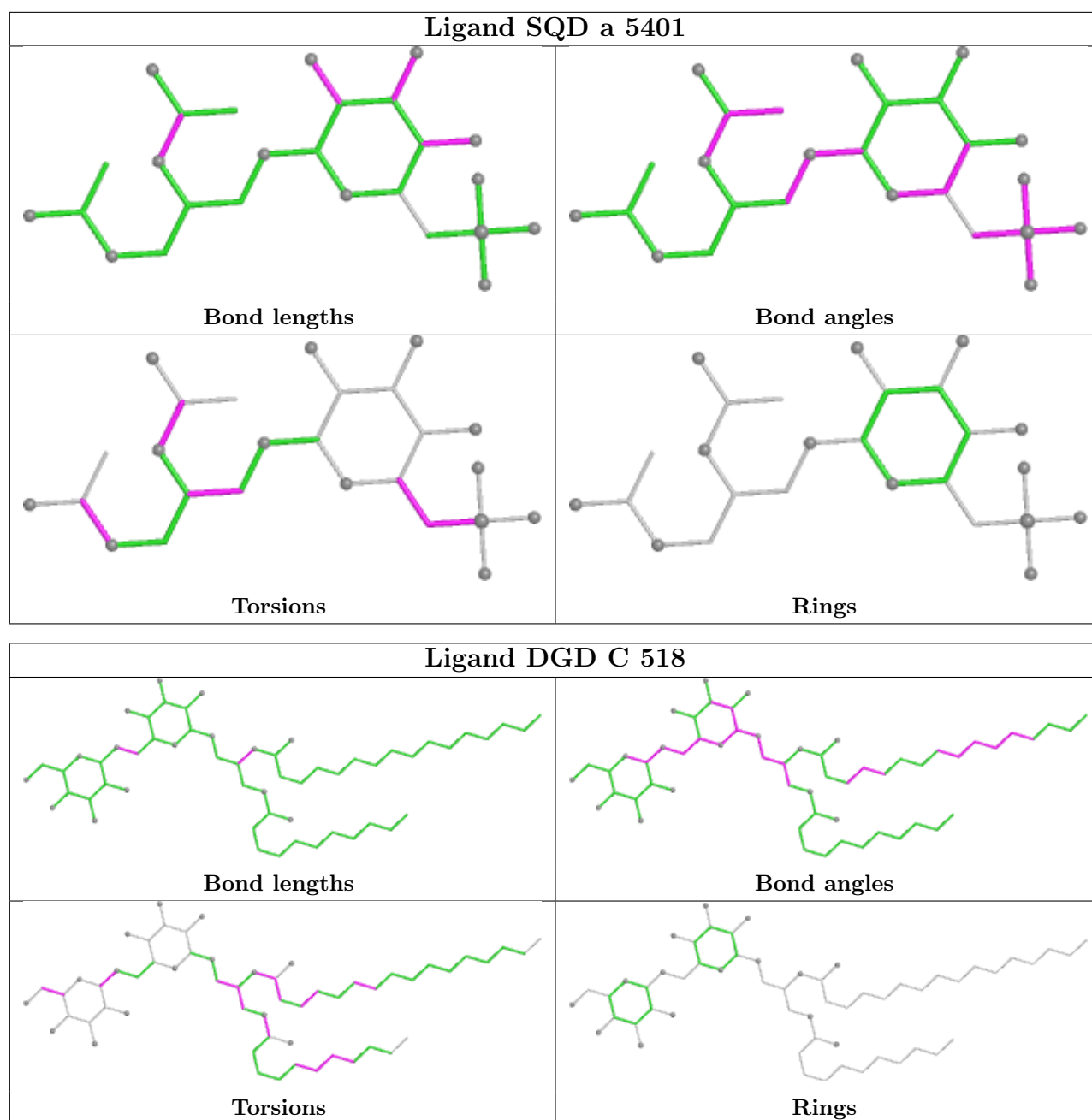


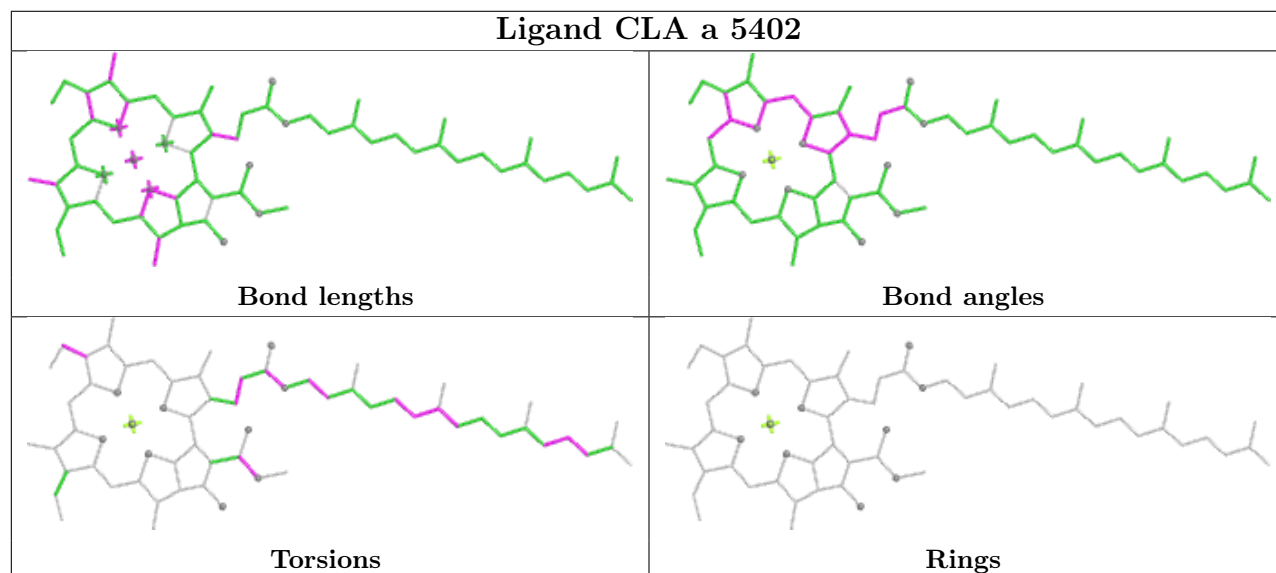
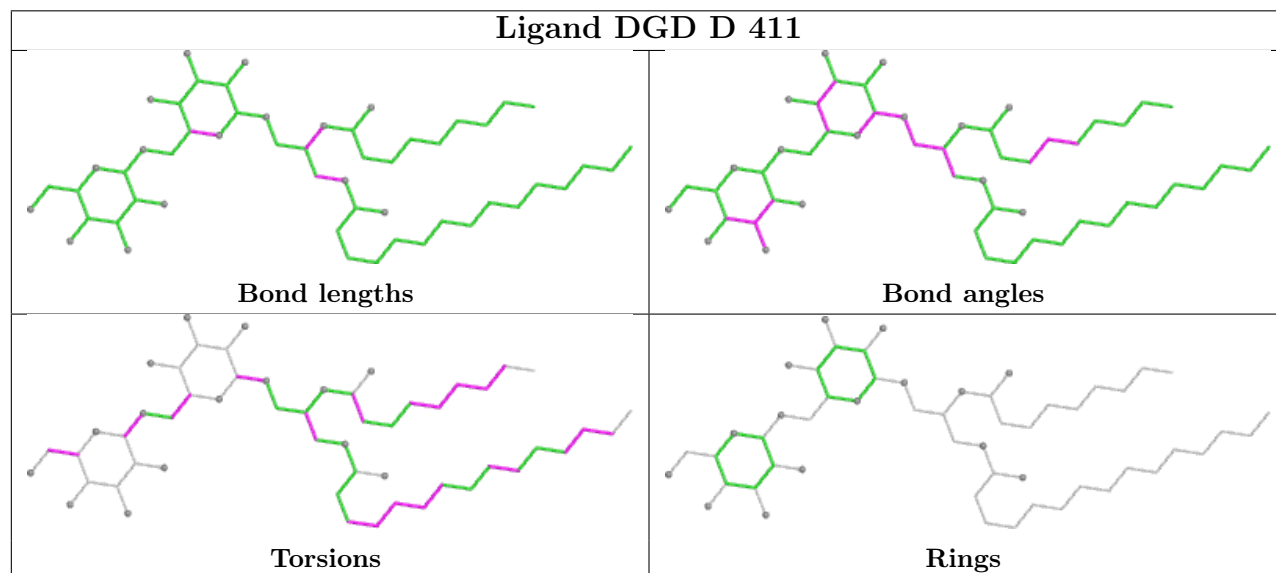
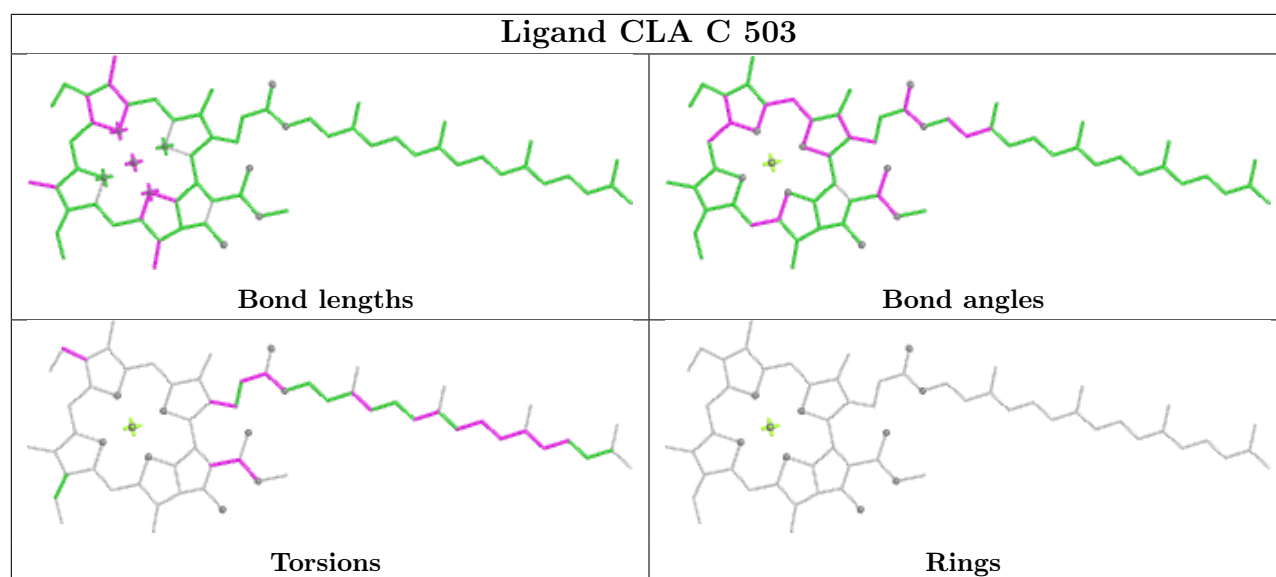


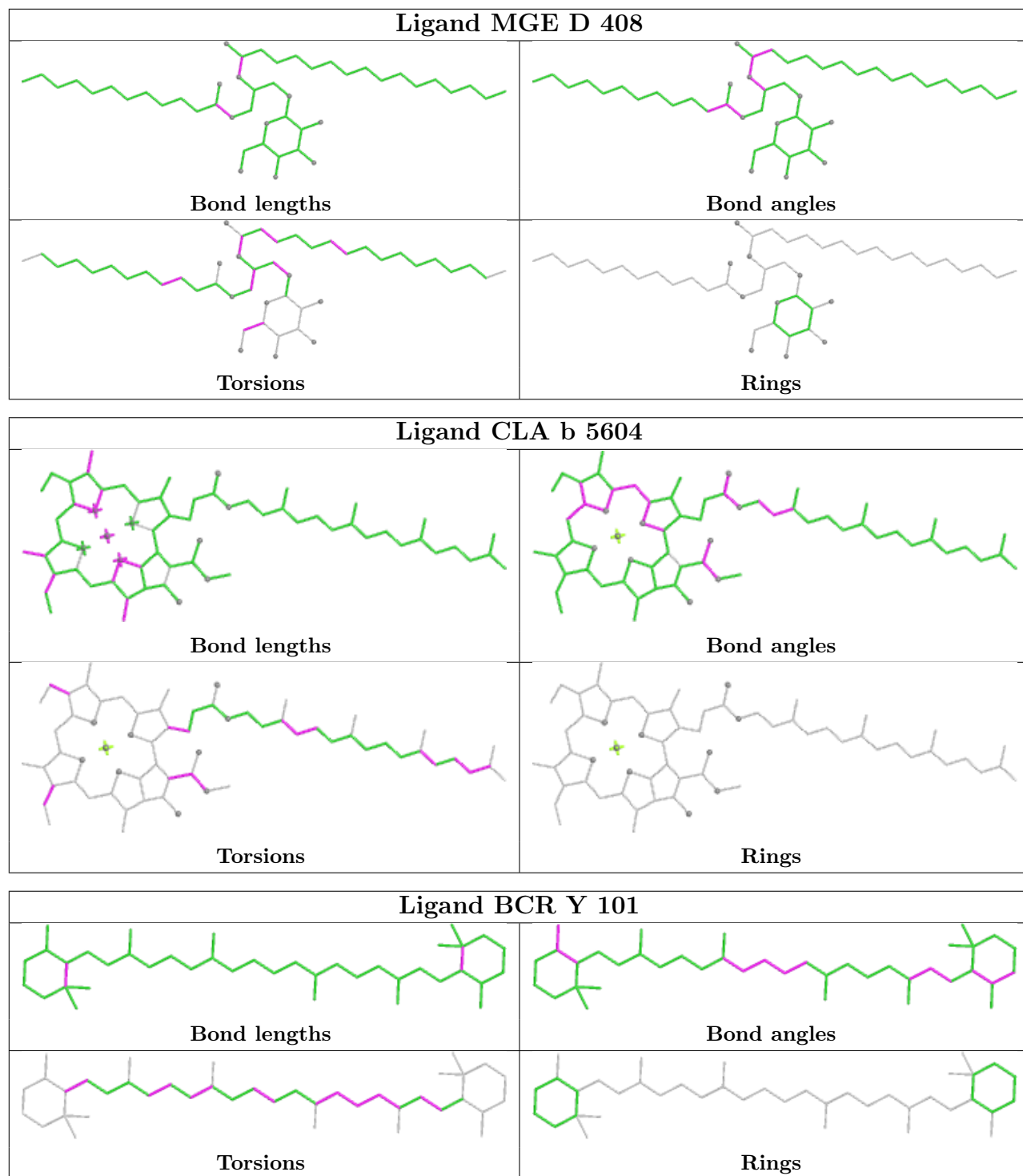


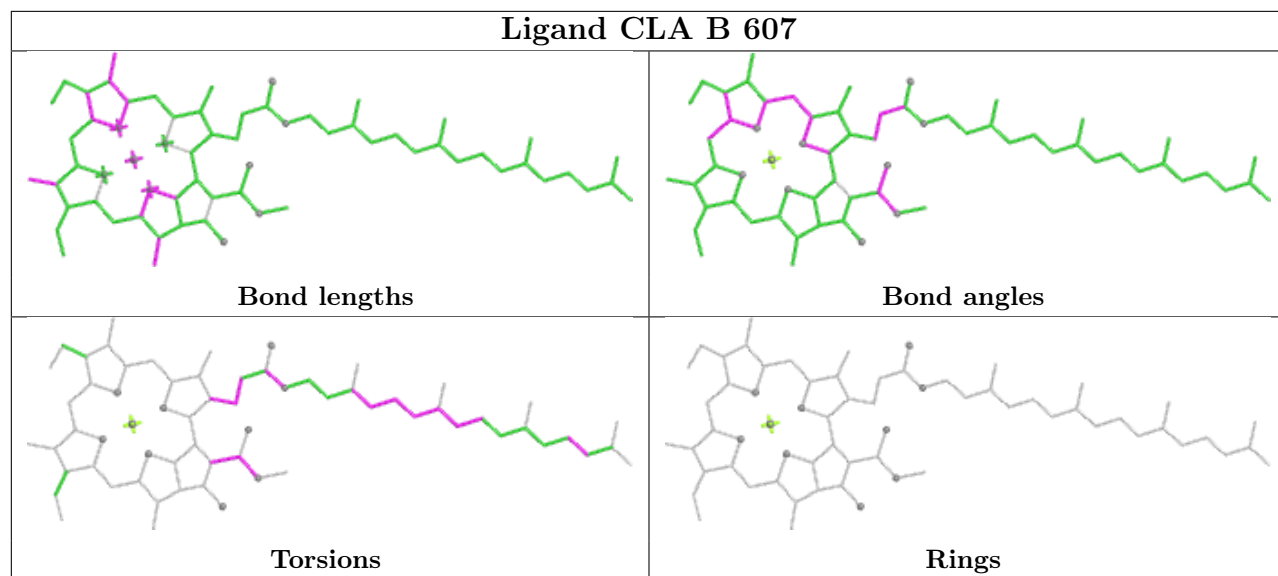


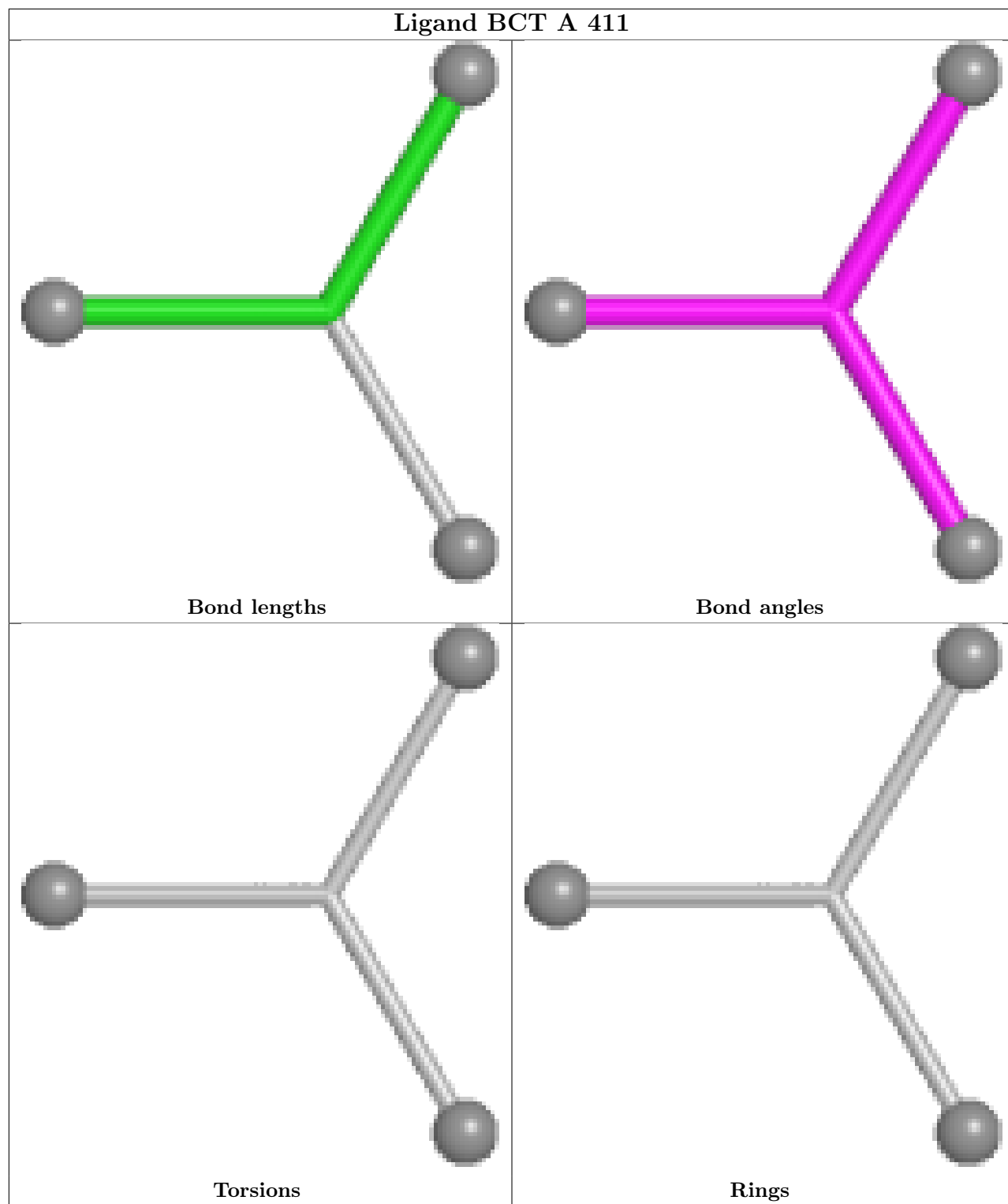


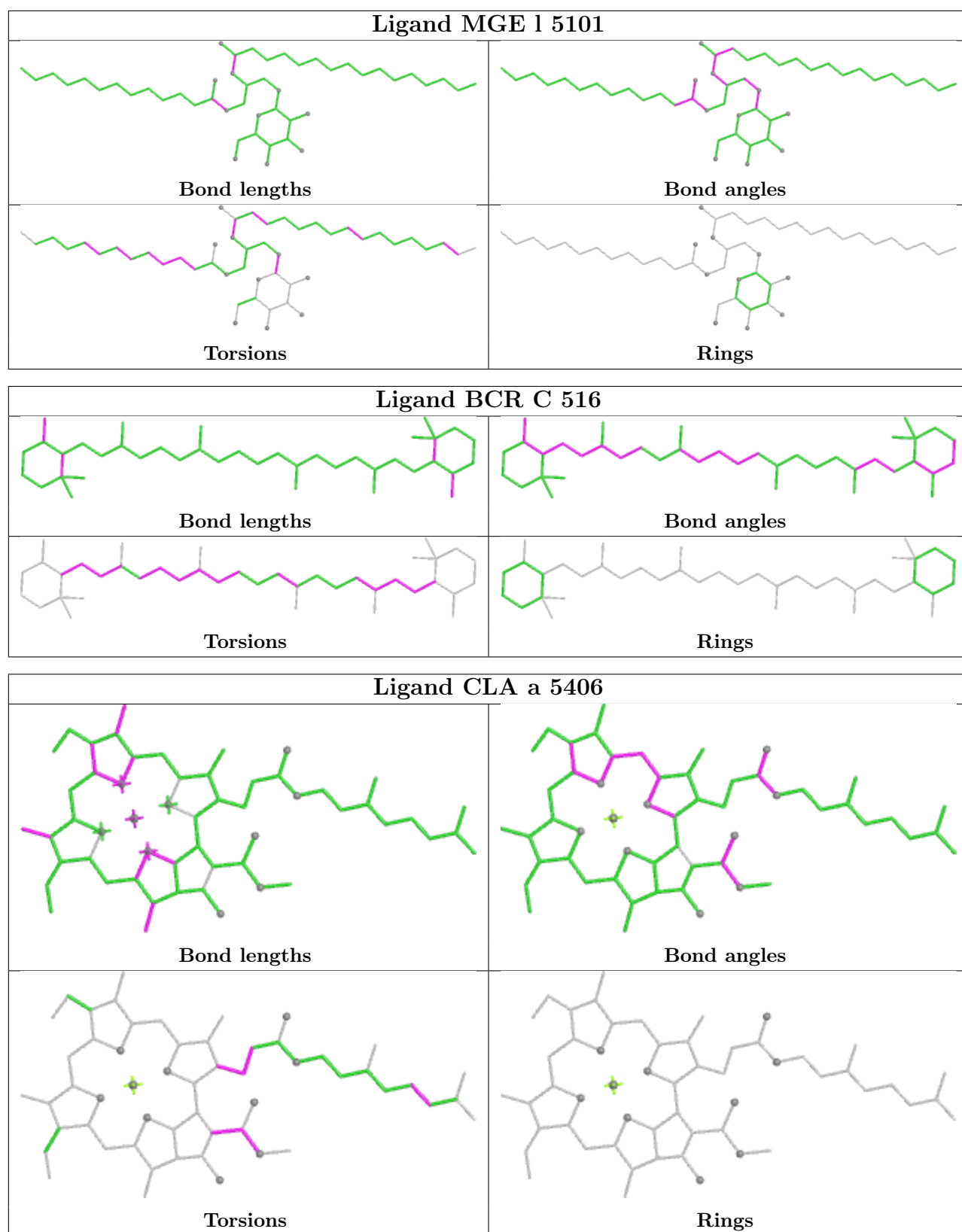


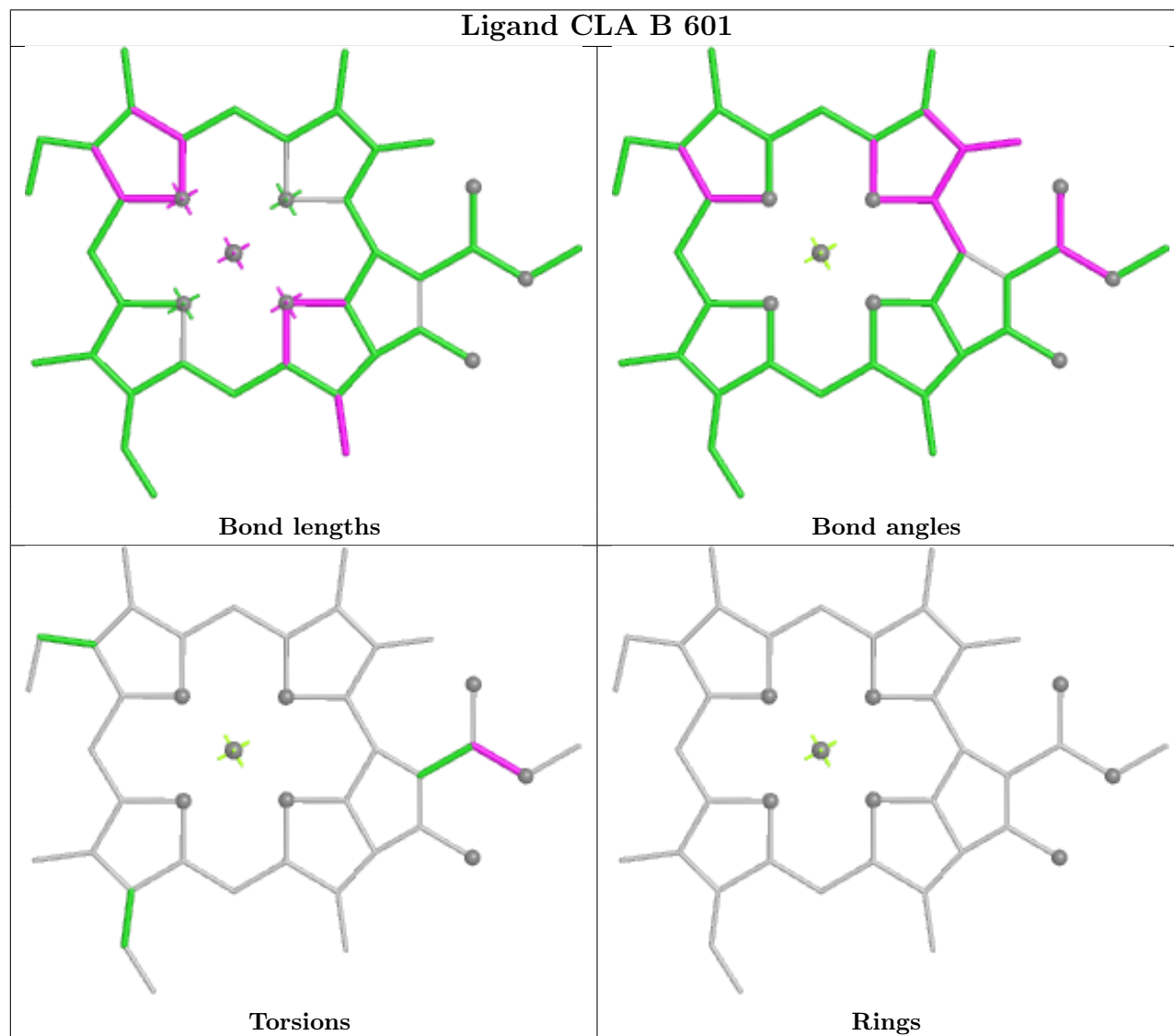
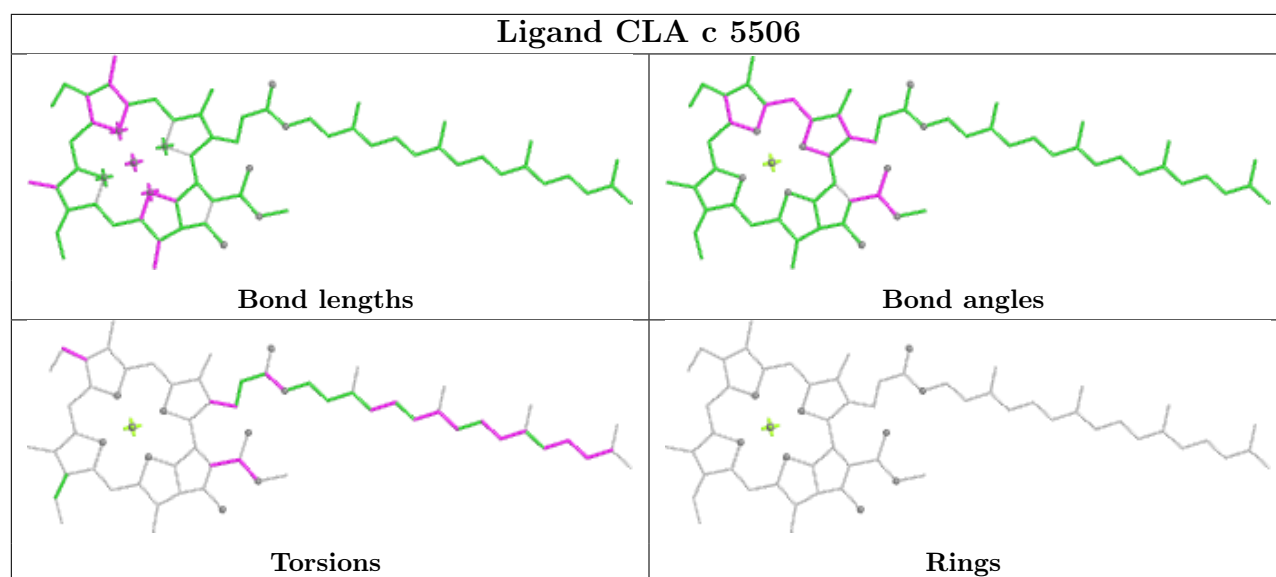




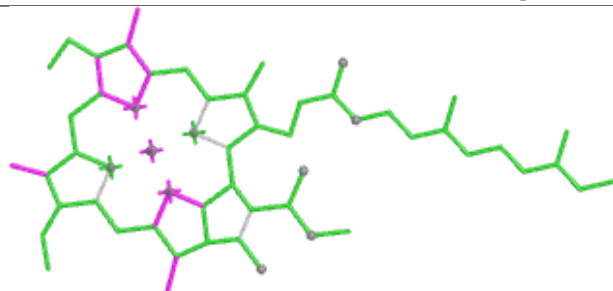




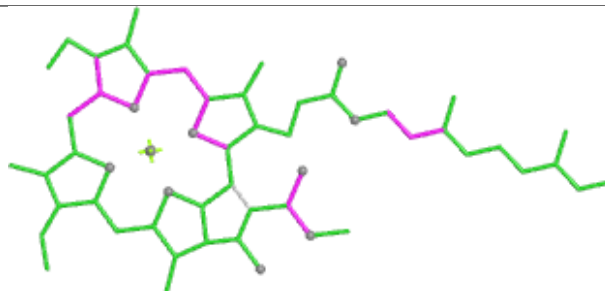




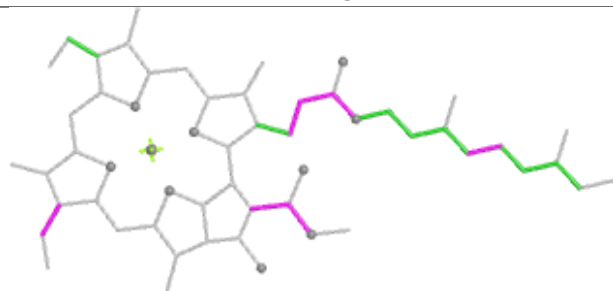
## Ligand CLA B 614



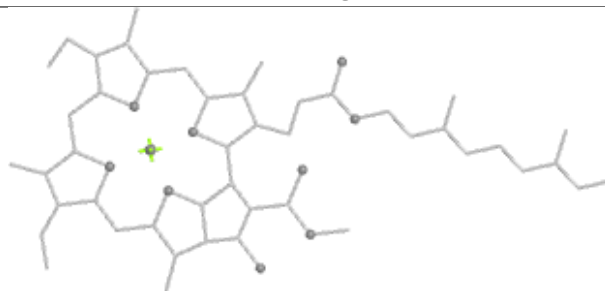
Bond lengths



Bond angles

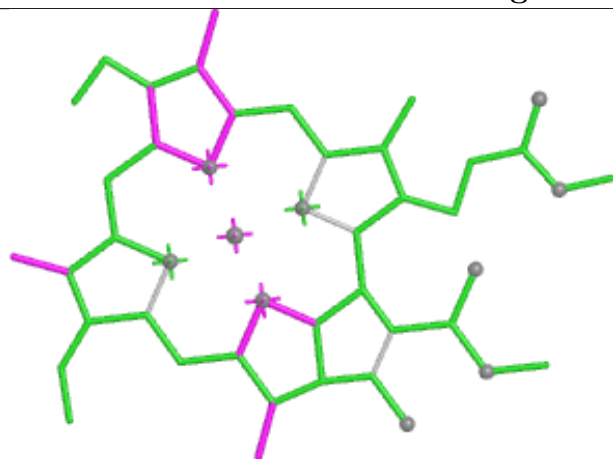


Torsions

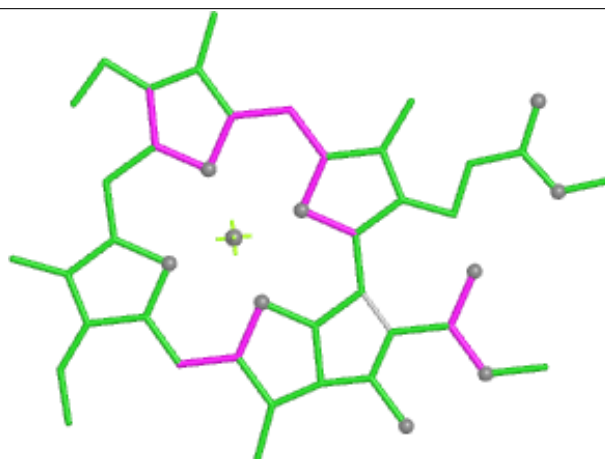


Rings

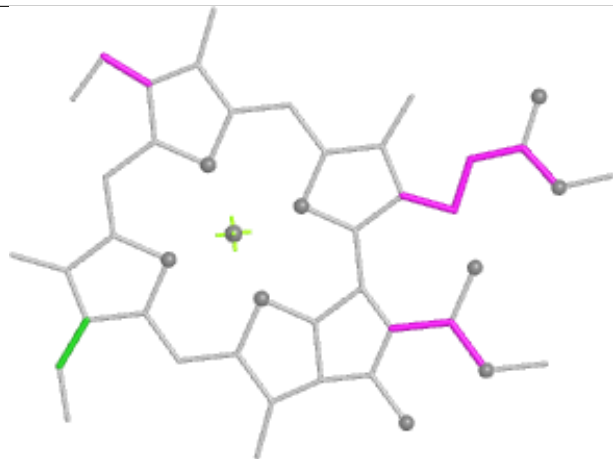
## Ligand CLA c 5504



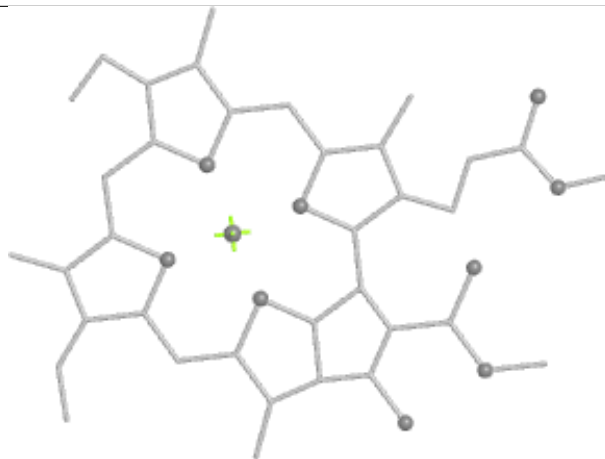
Bond lengths



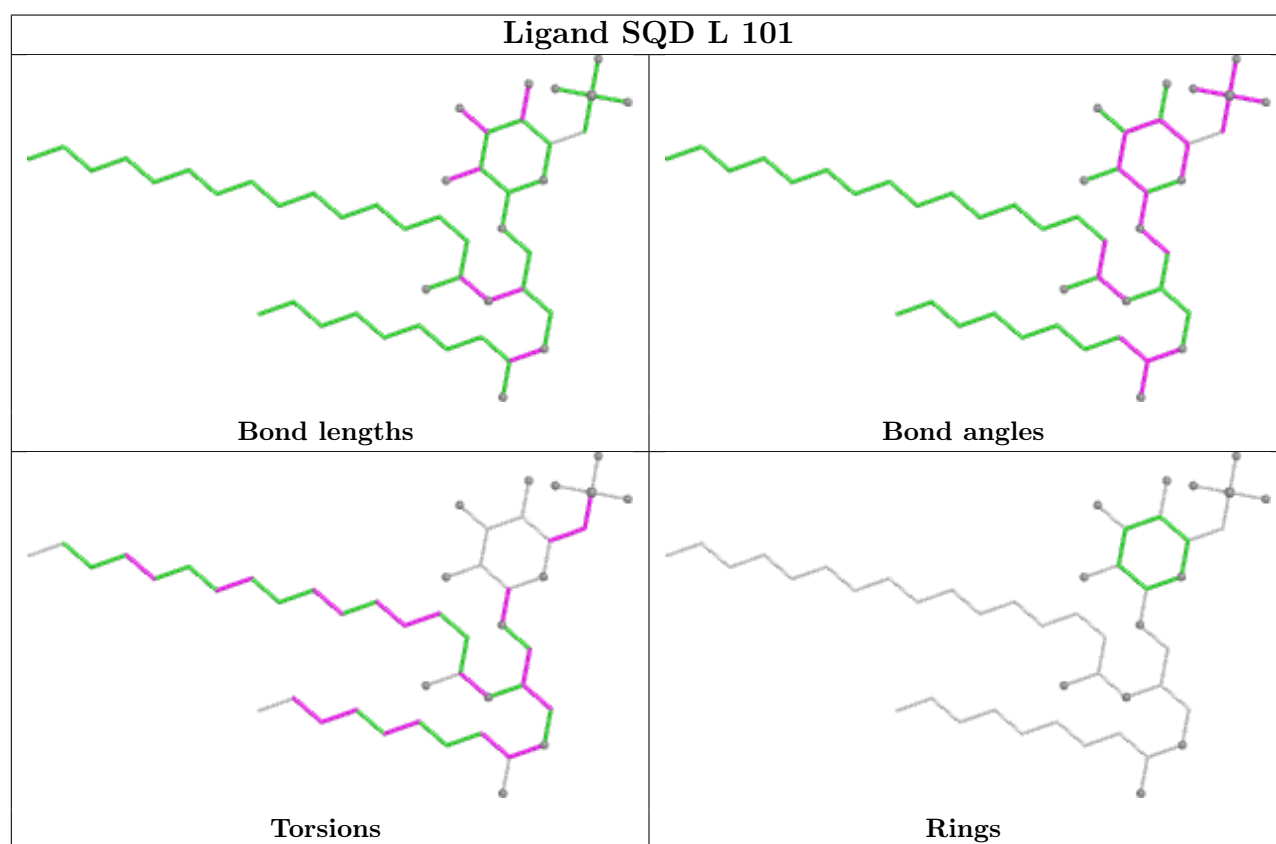
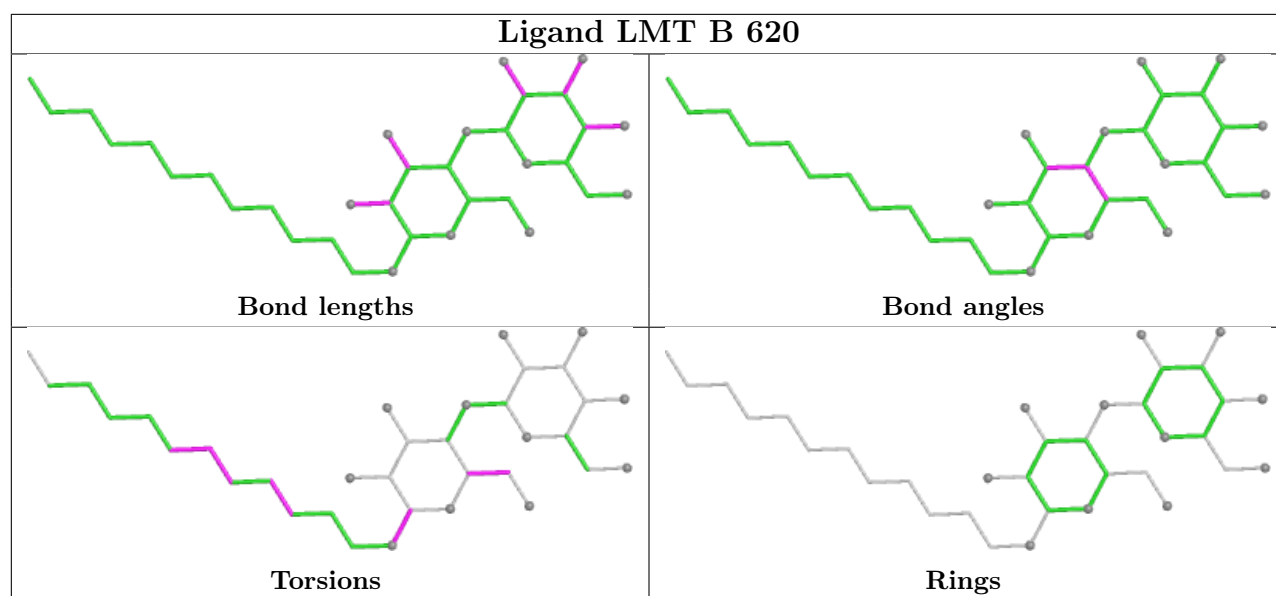
Bond angles

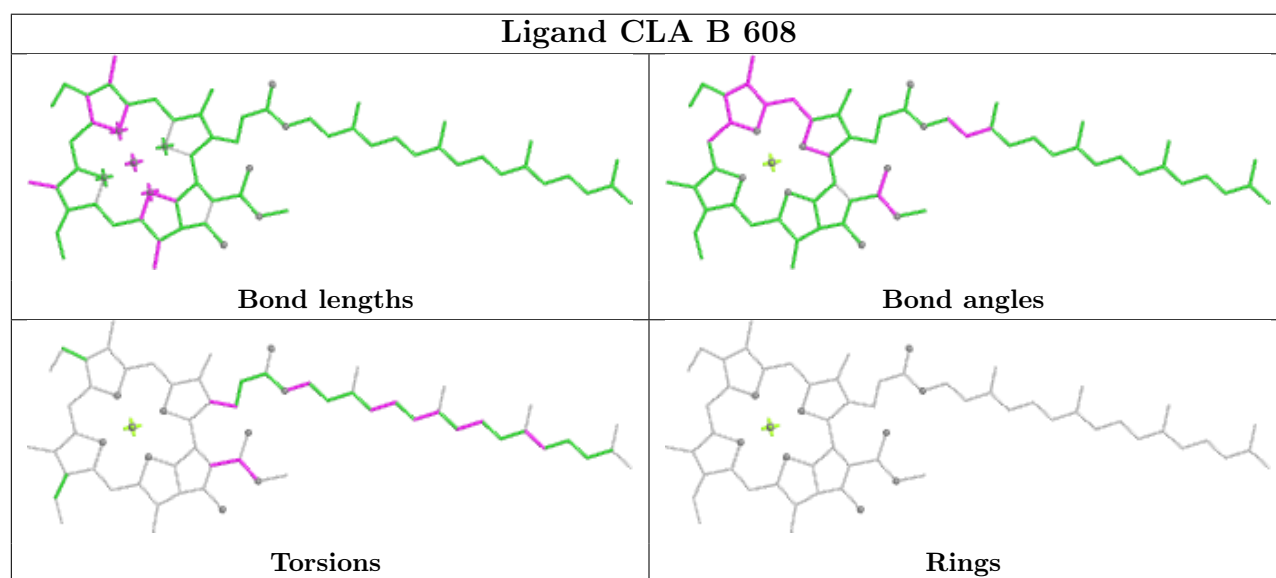
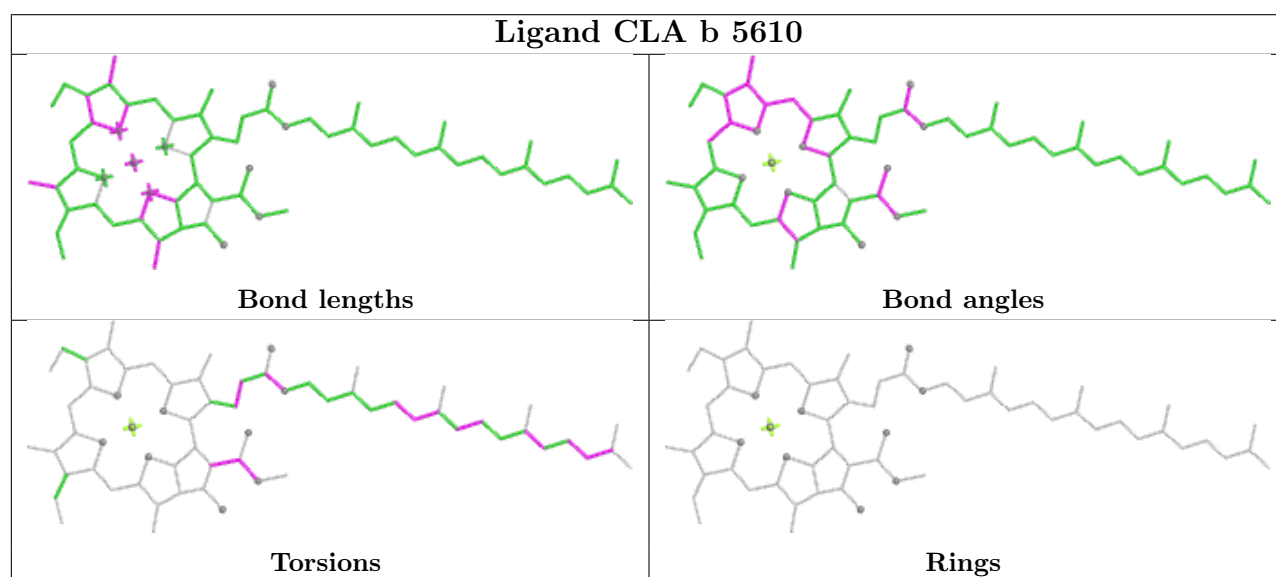
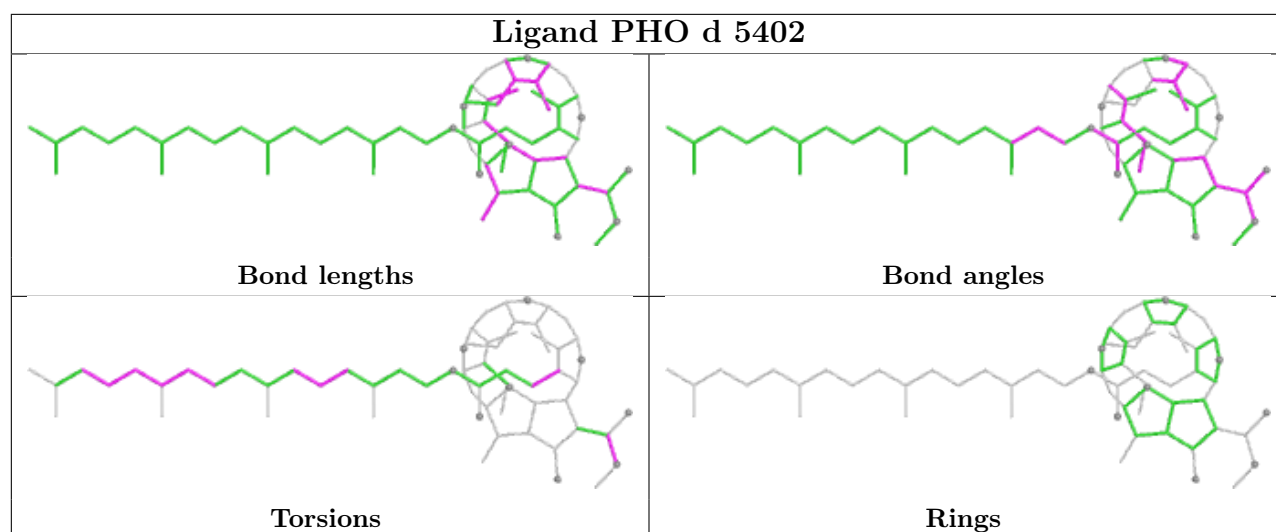


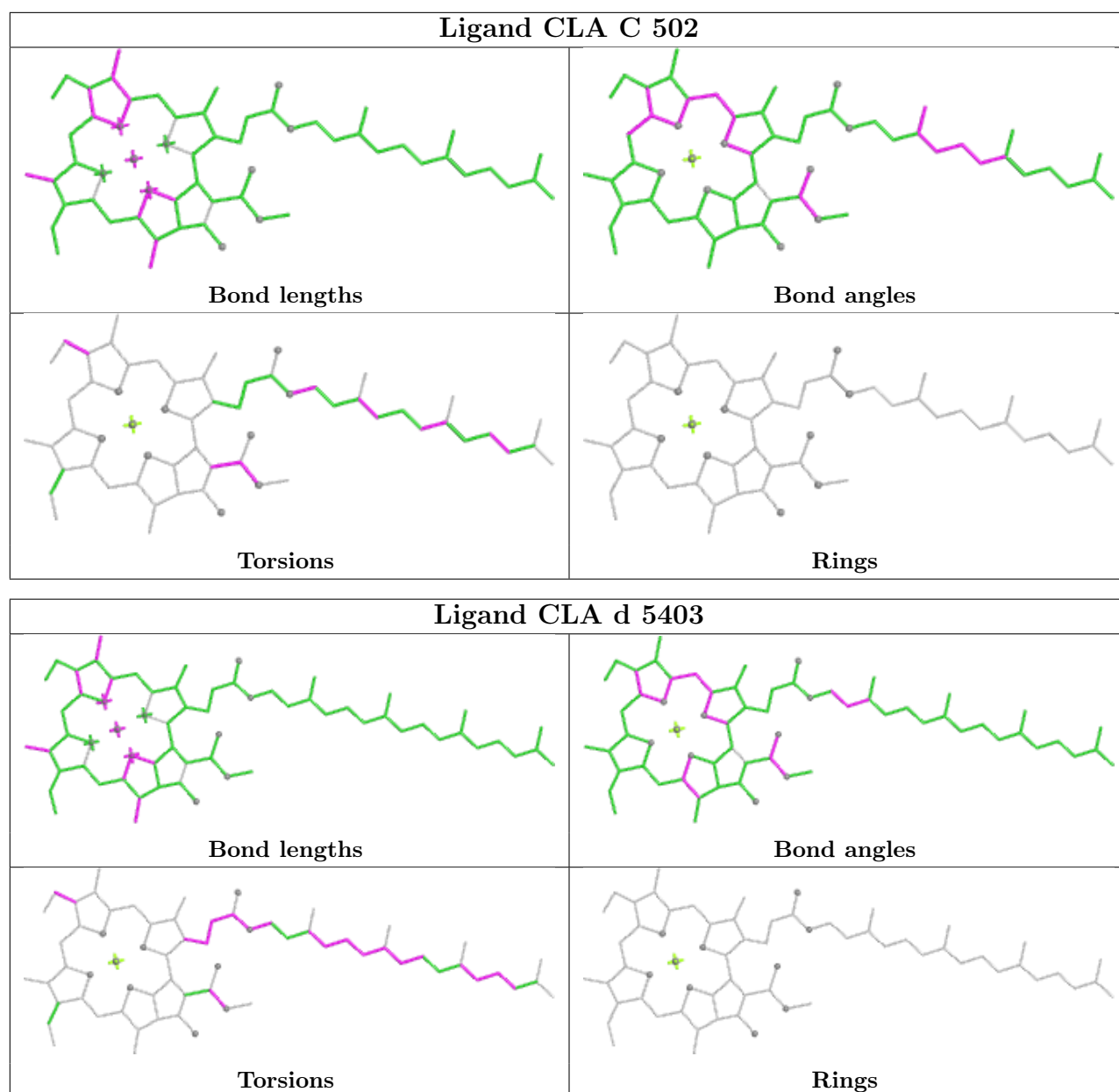
Torsions

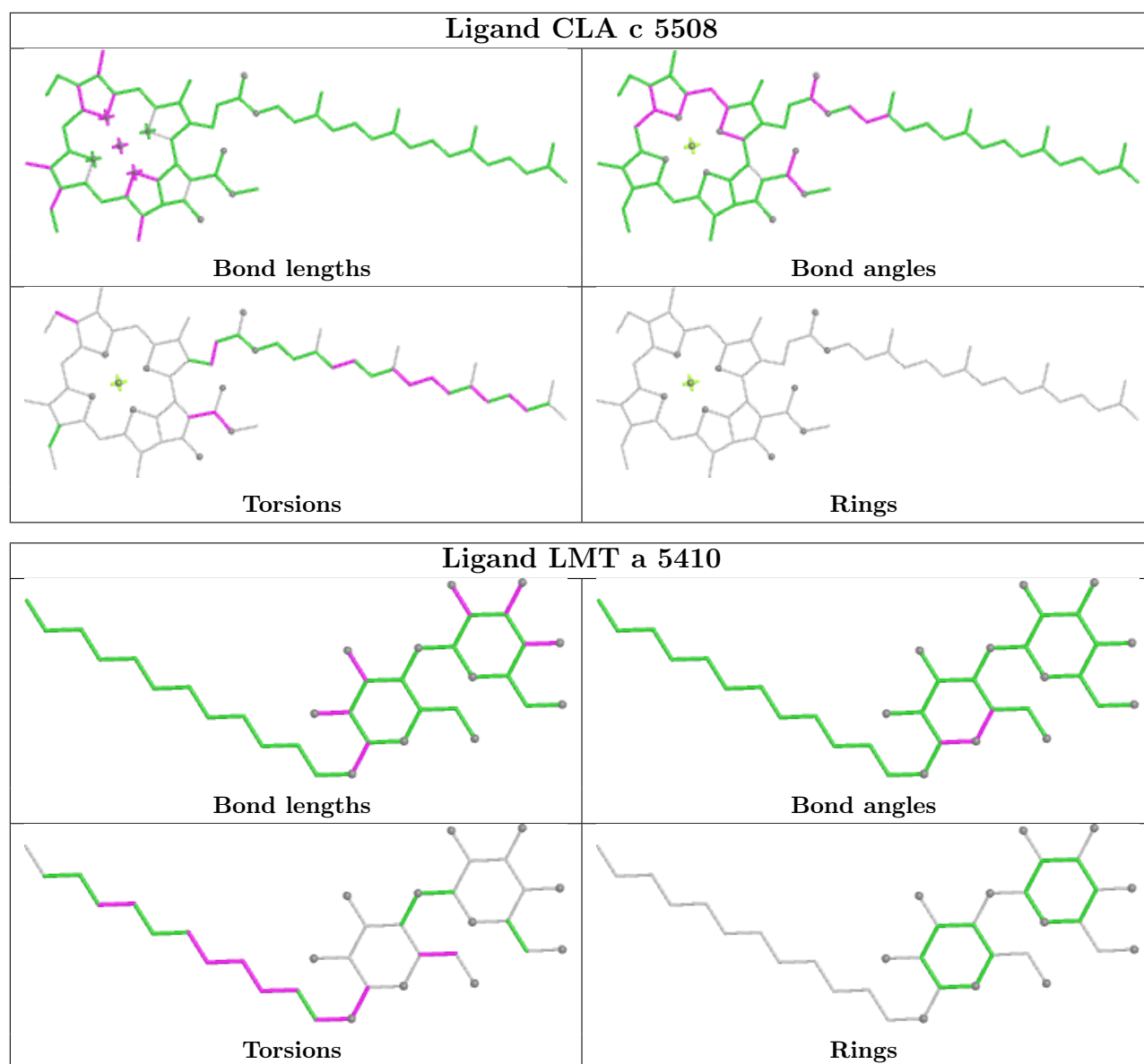


Rings

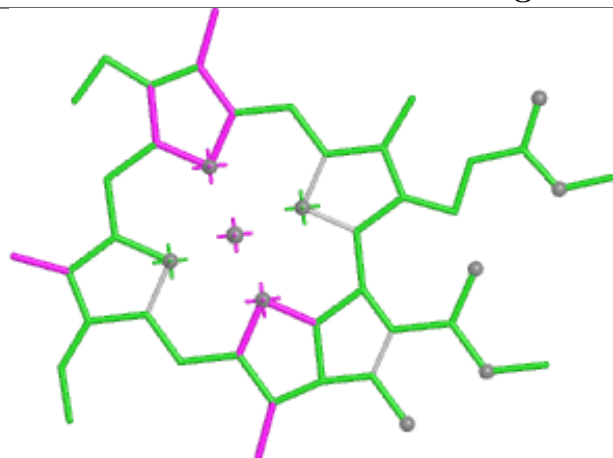




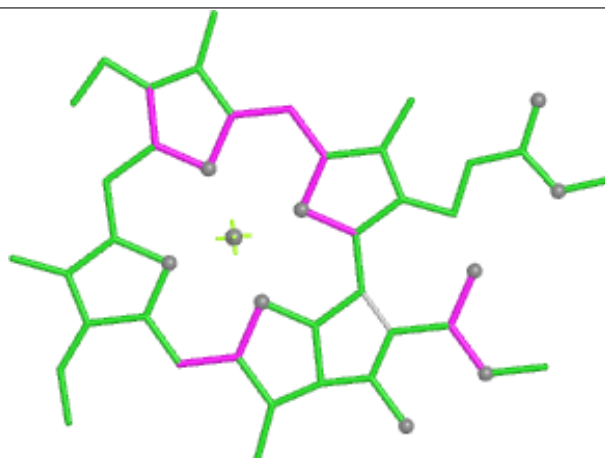




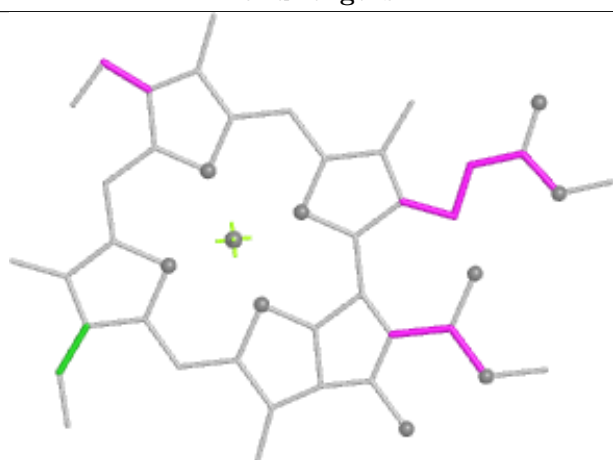
## Ligand CLA C 504



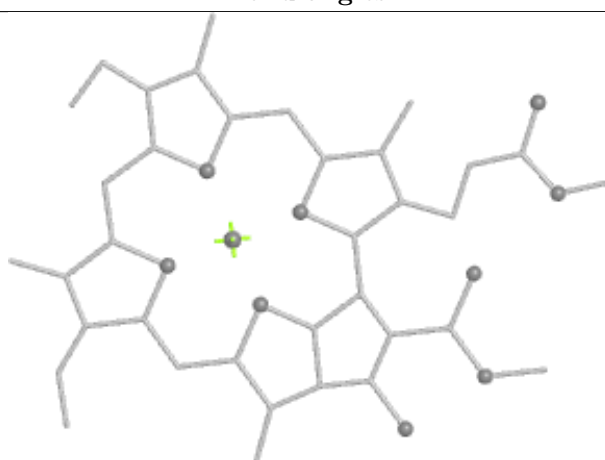
Bond lengths



Bond angles

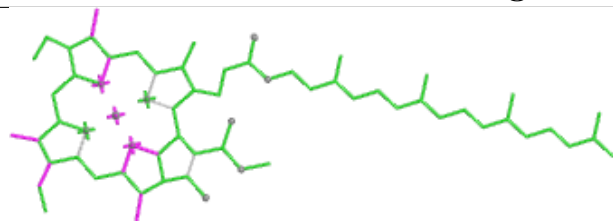


Torsions

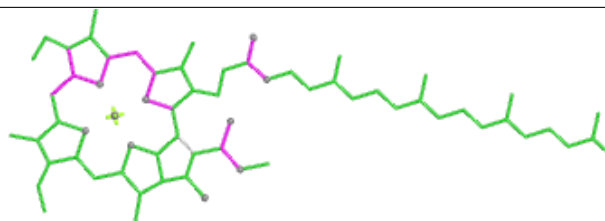


Rings

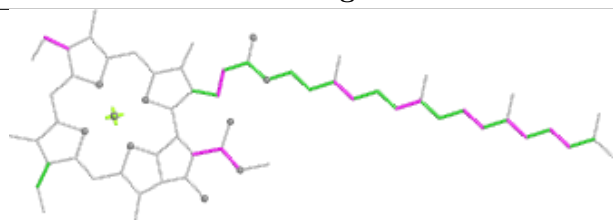
## Ligand CLA b 5603



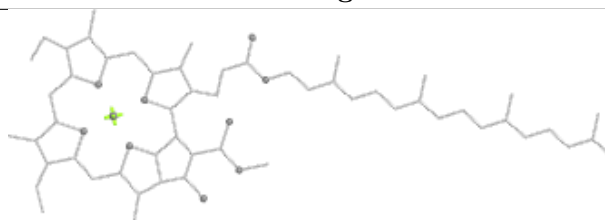
Bond lengths



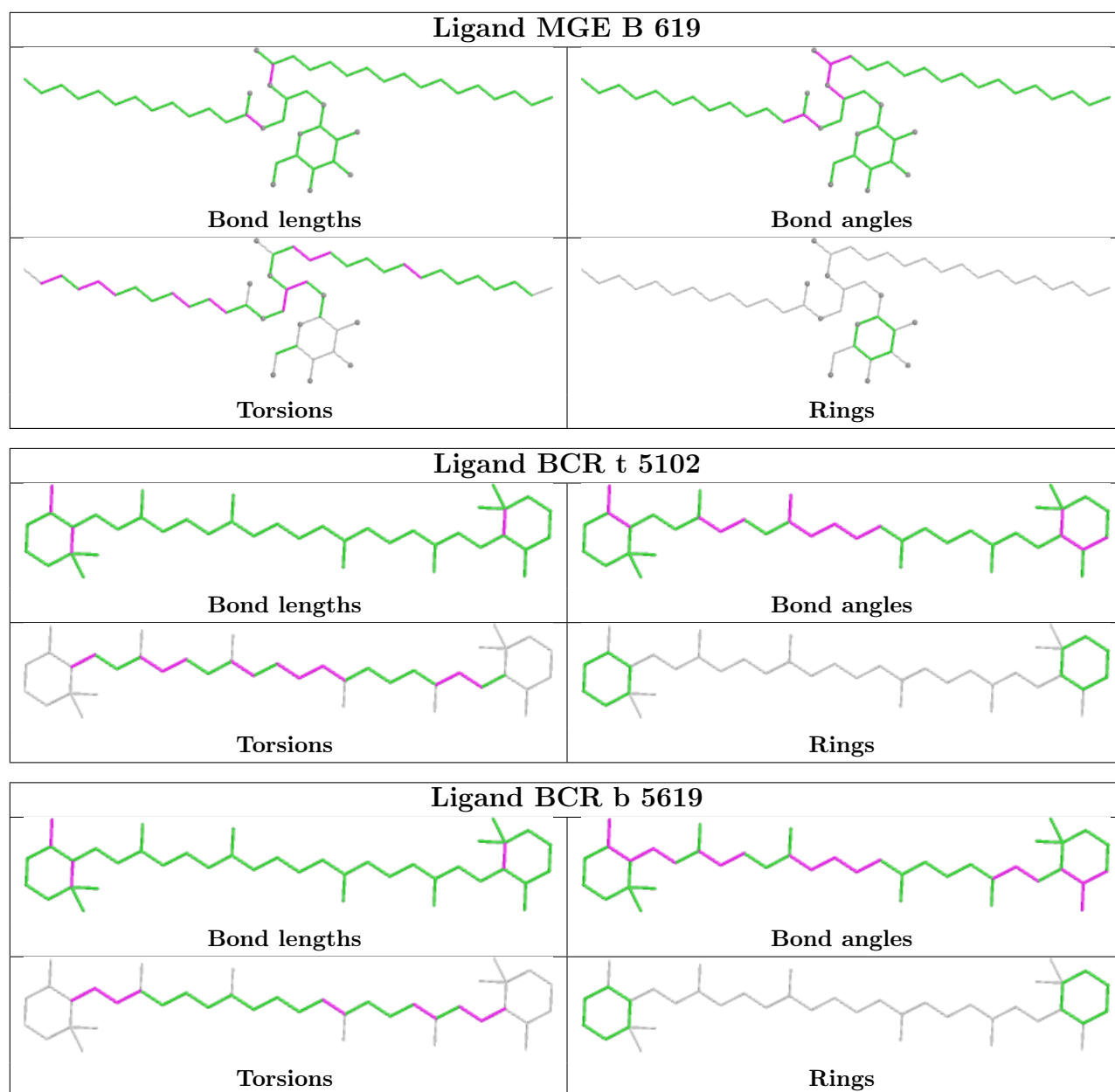
Bond angles

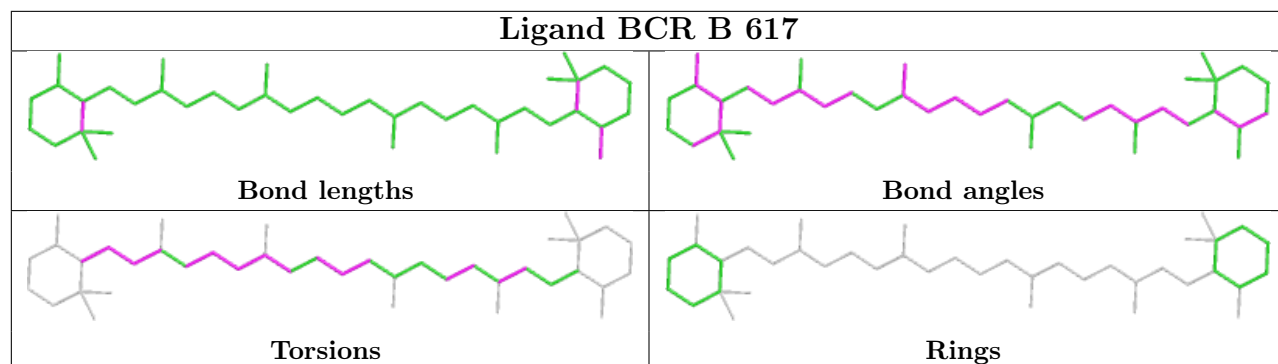
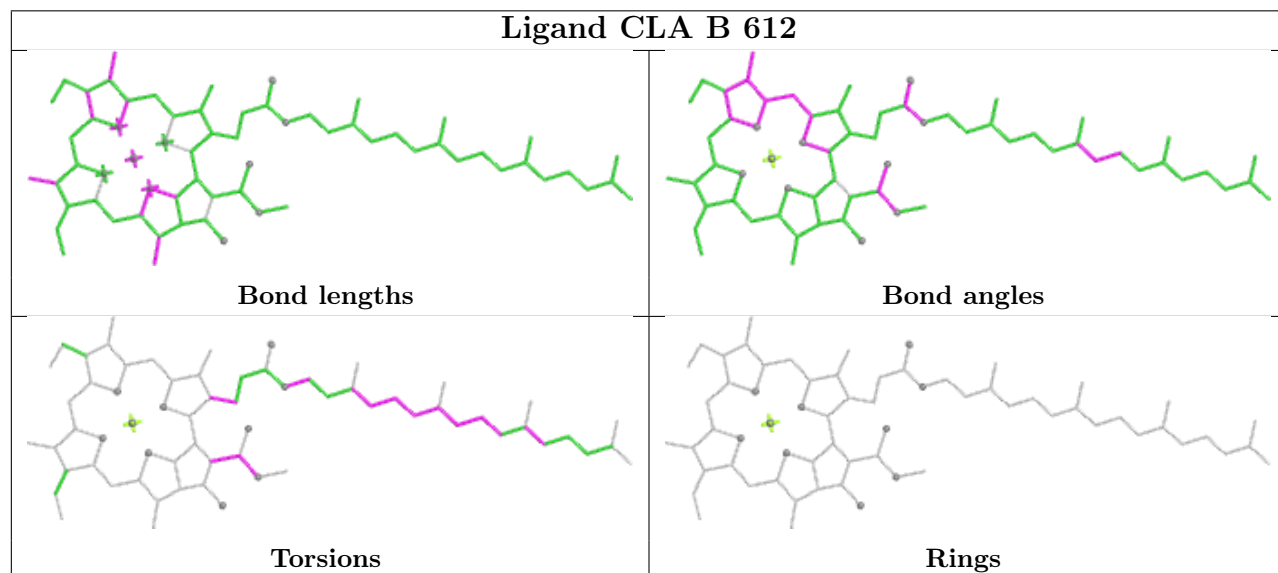
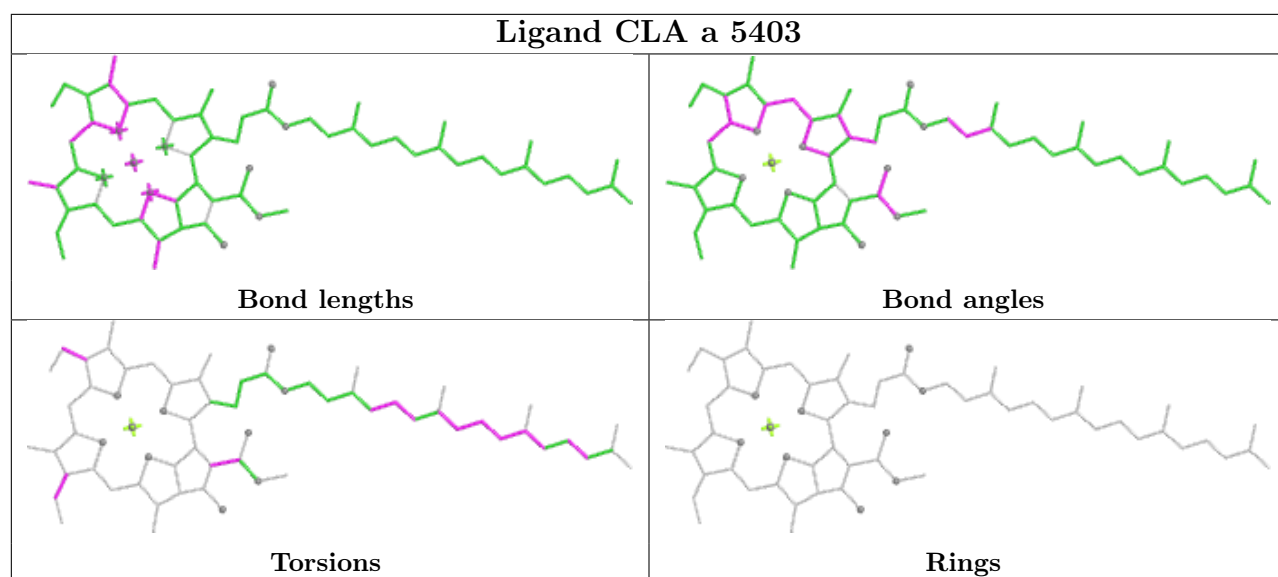


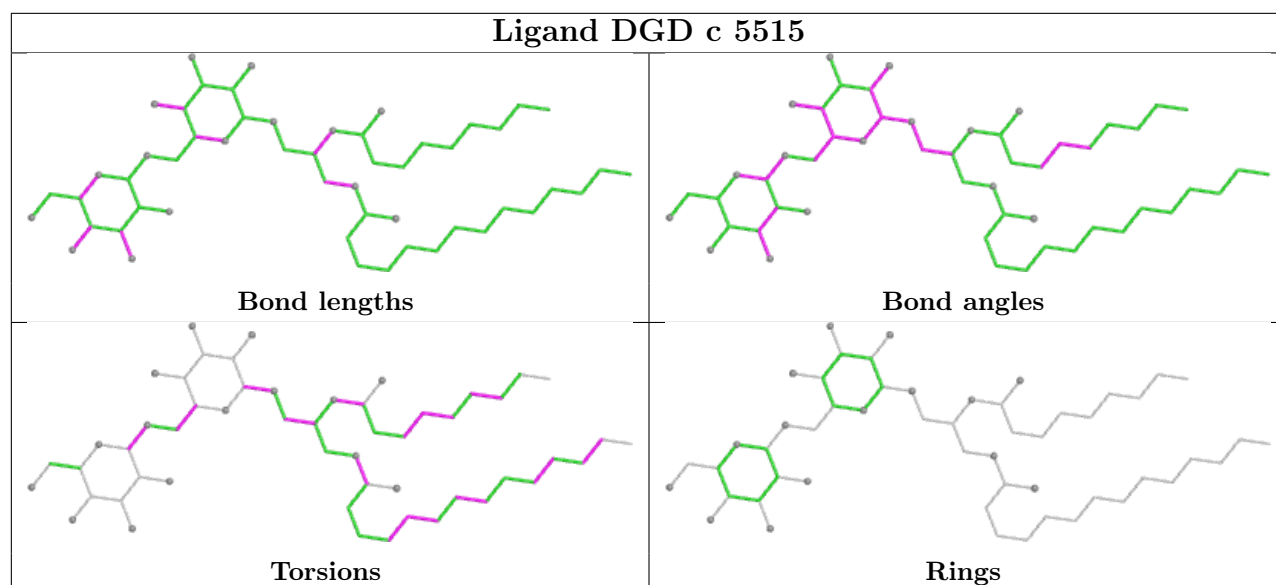
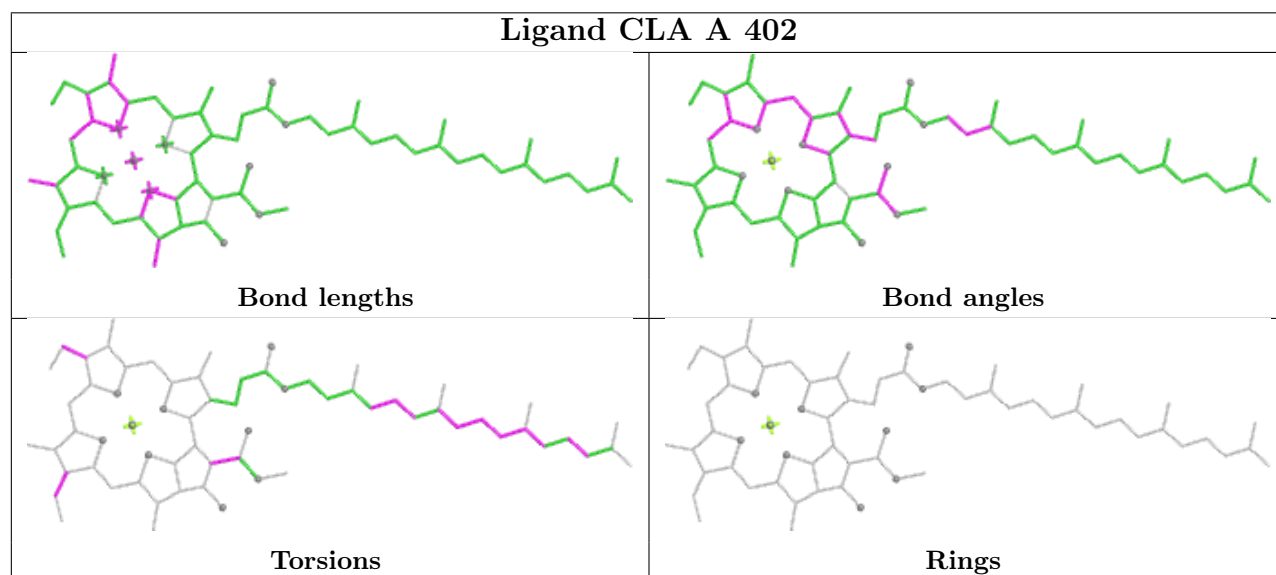
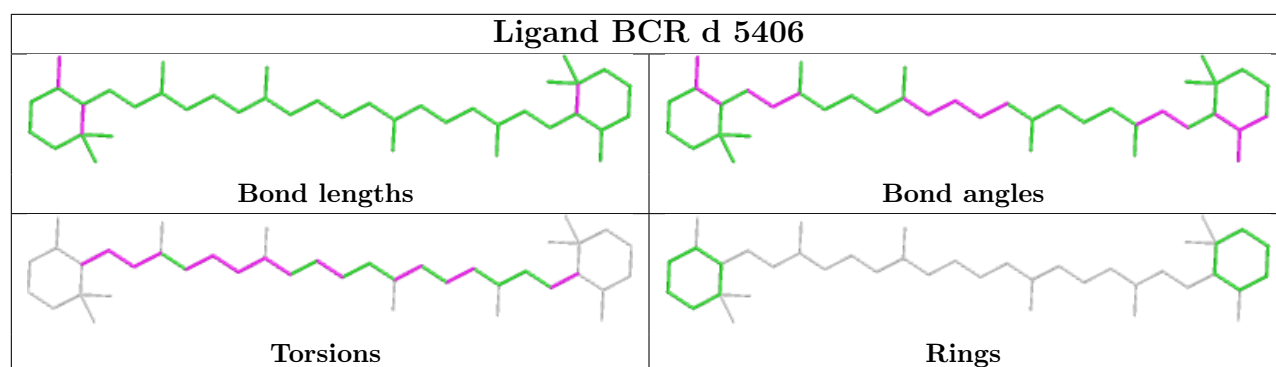
Torsions

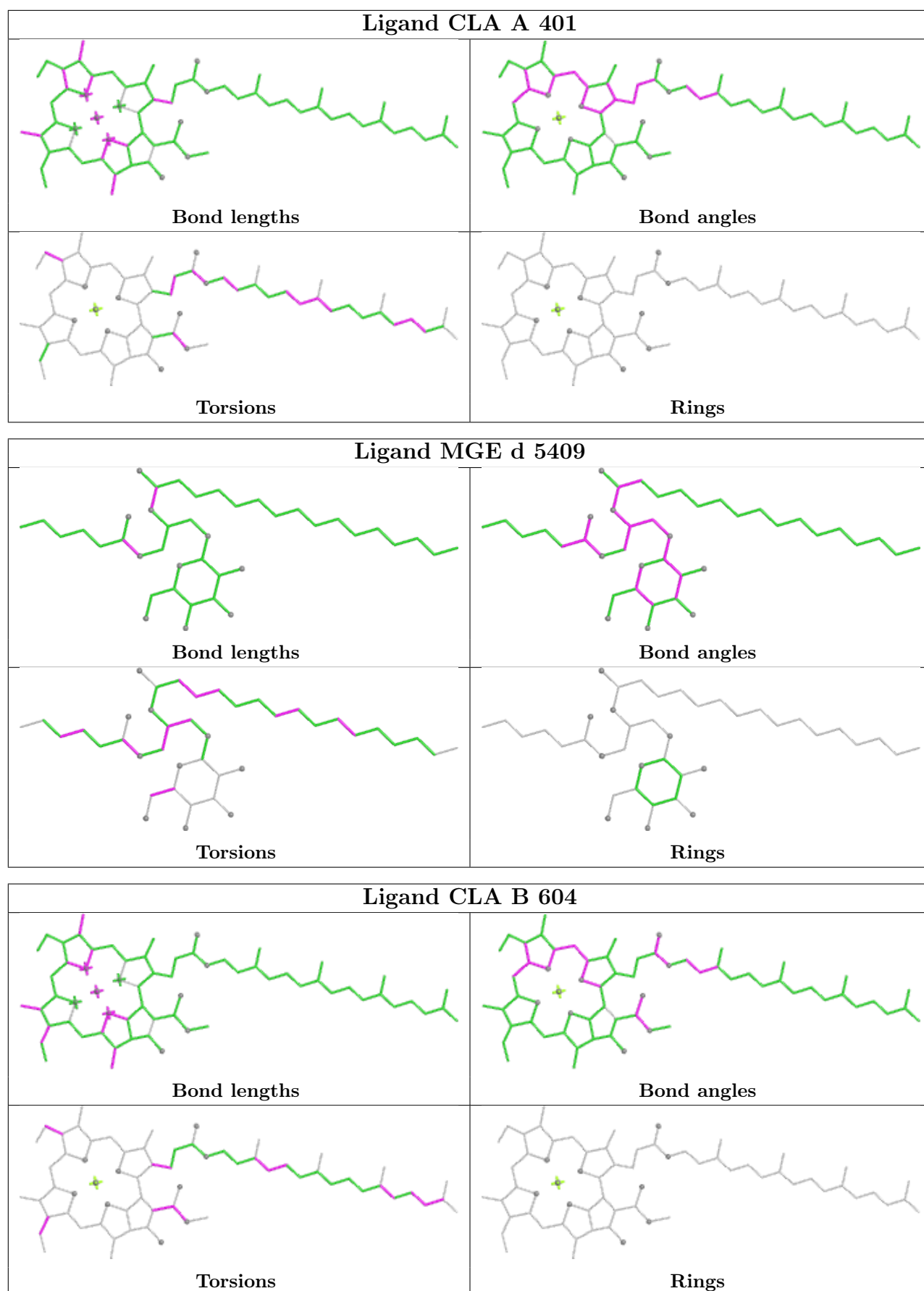


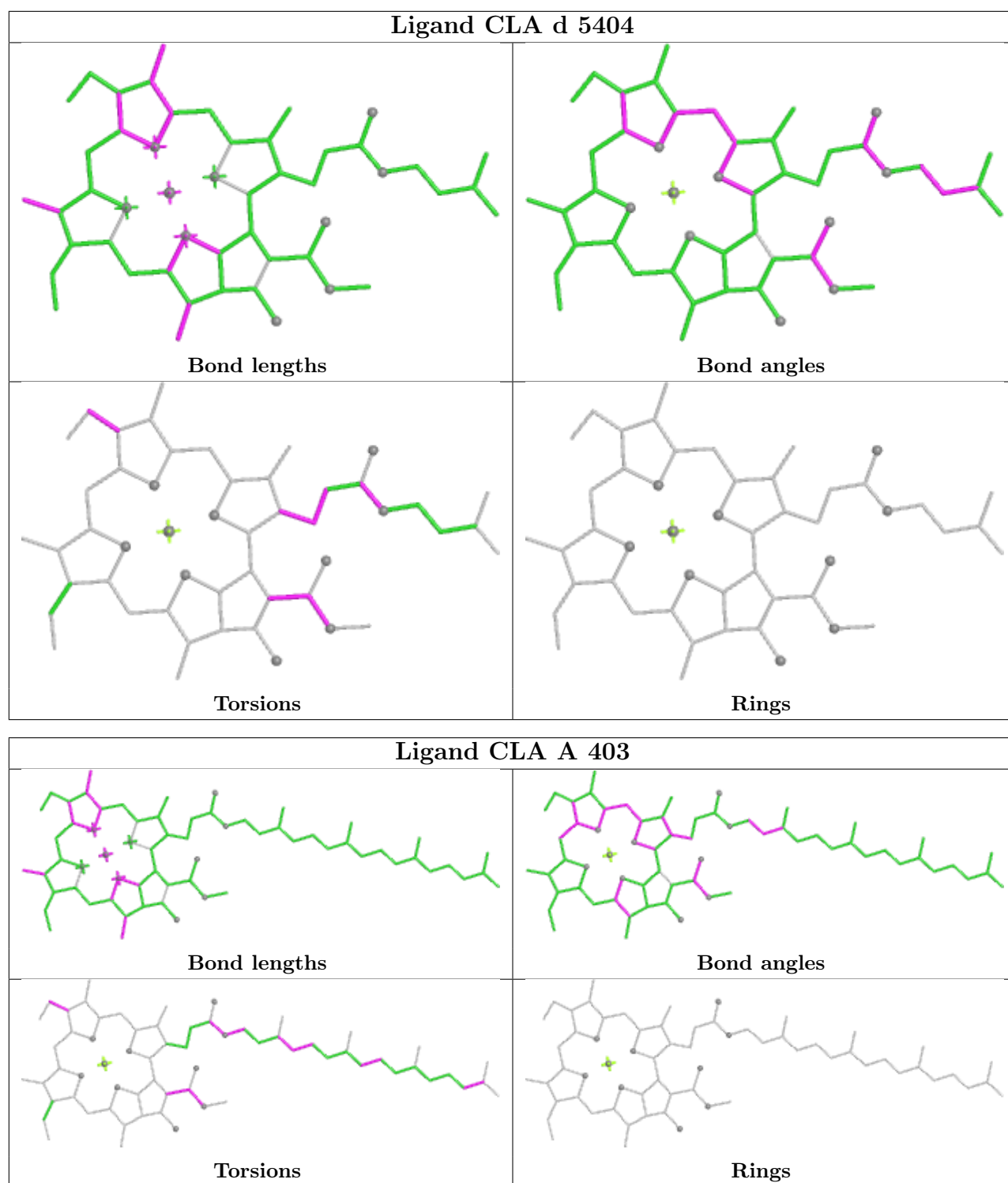
Rings

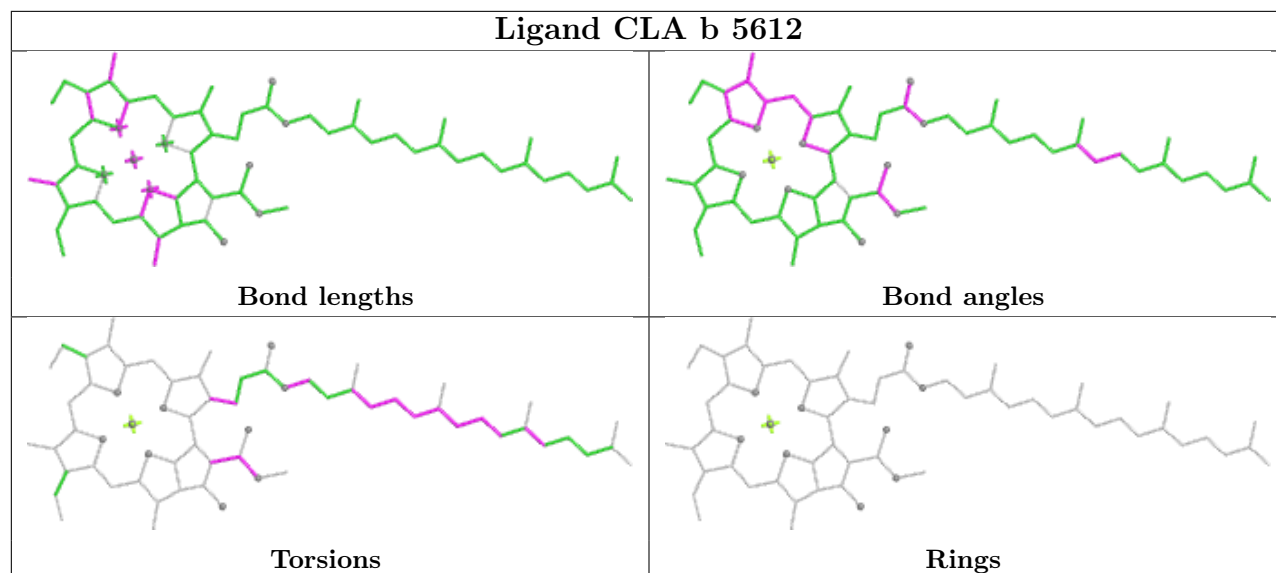
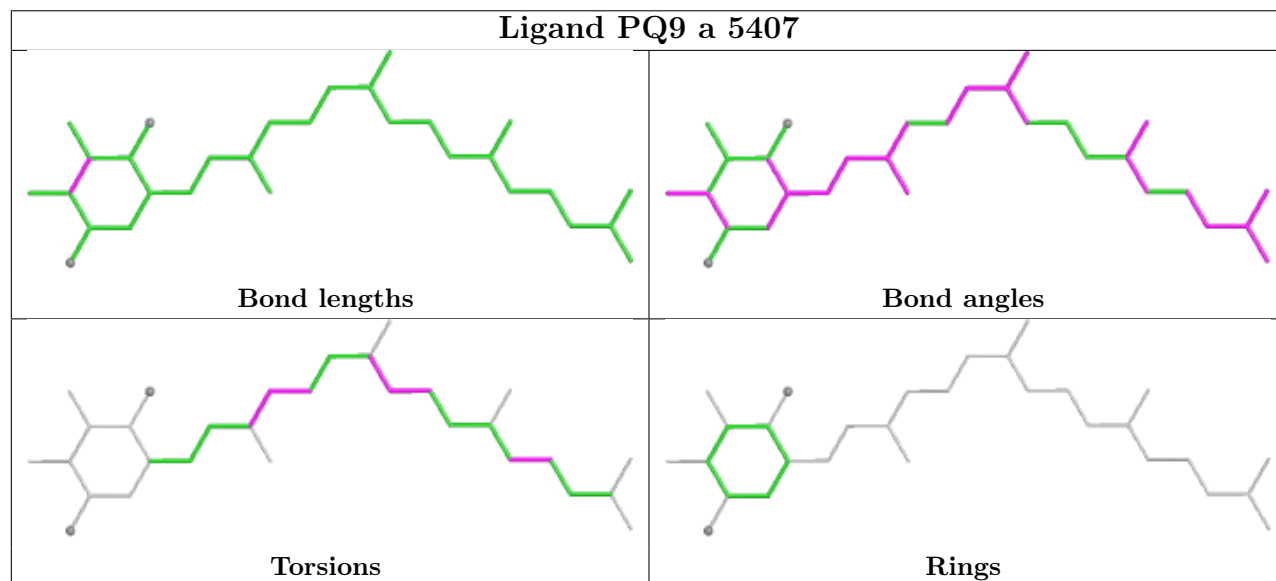
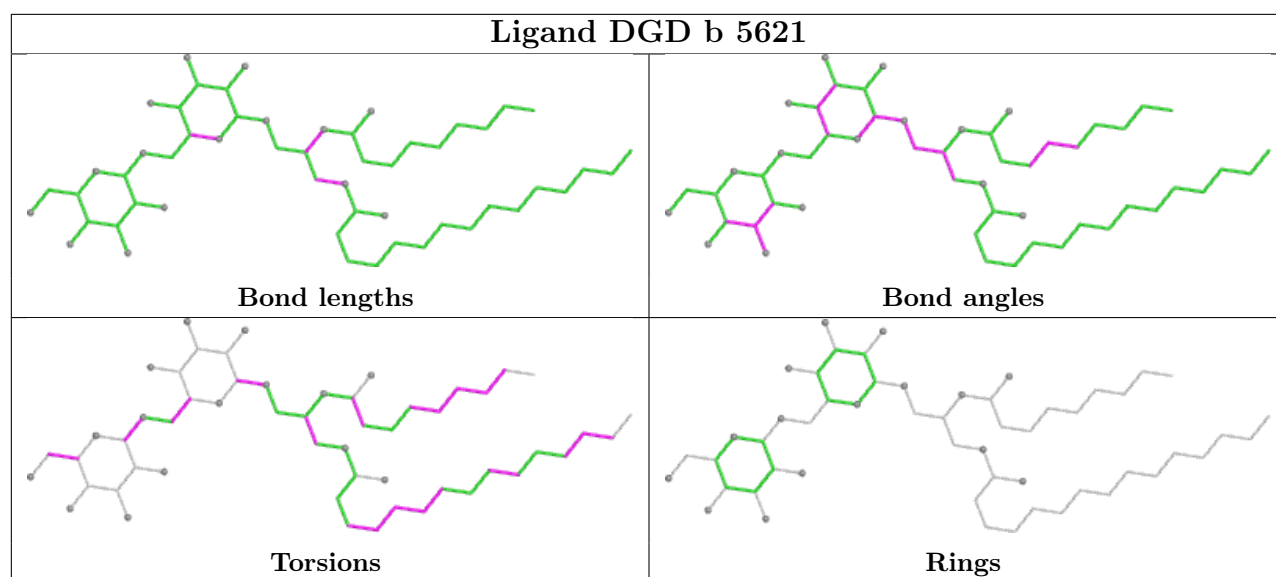


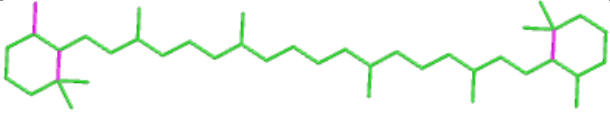
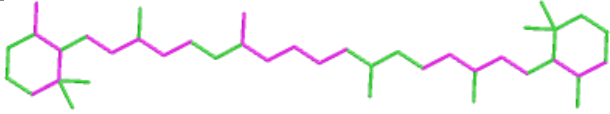
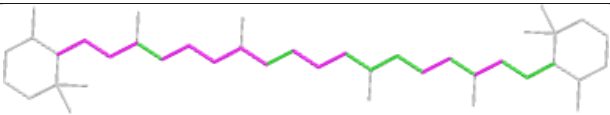
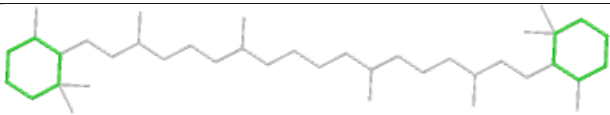
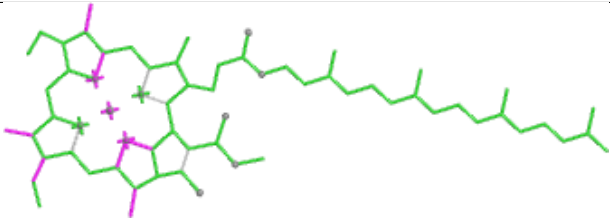
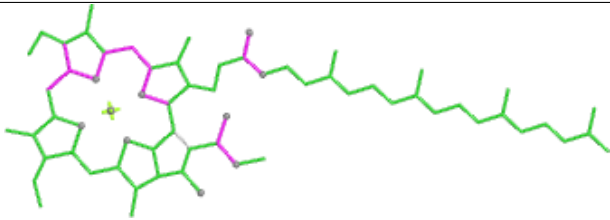
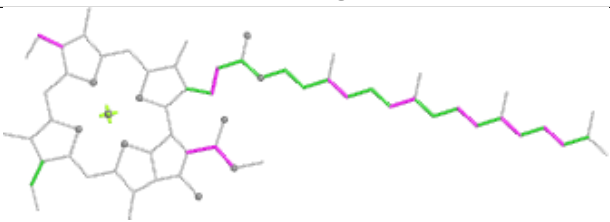
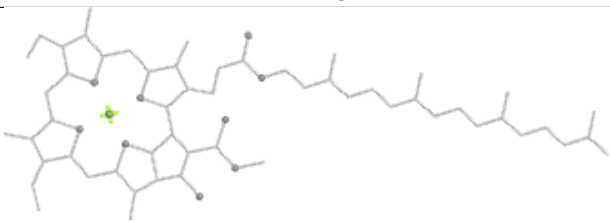
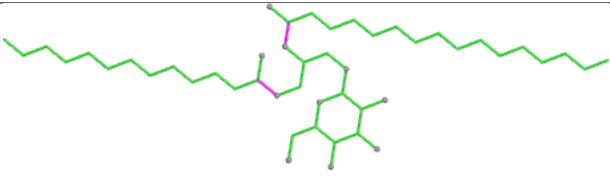
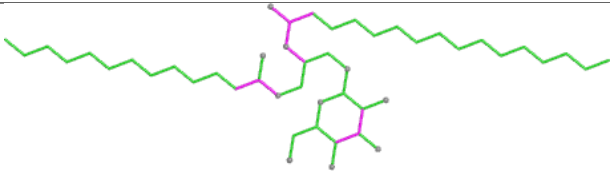
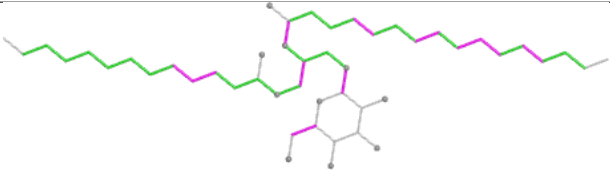
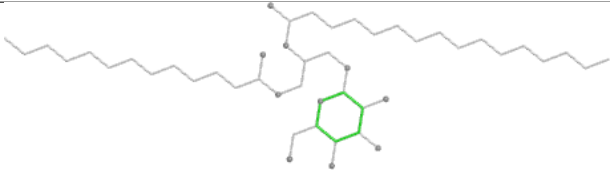


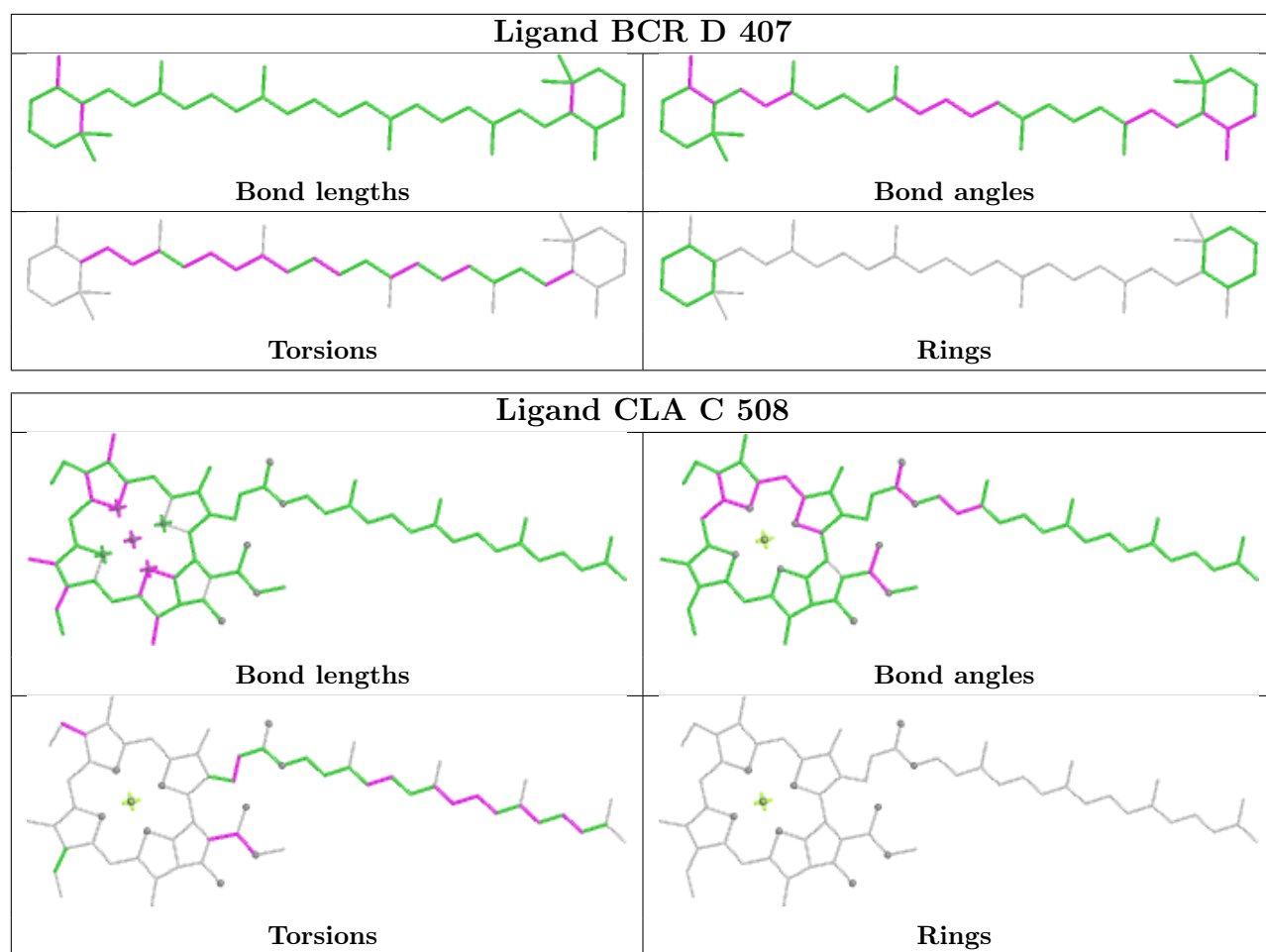


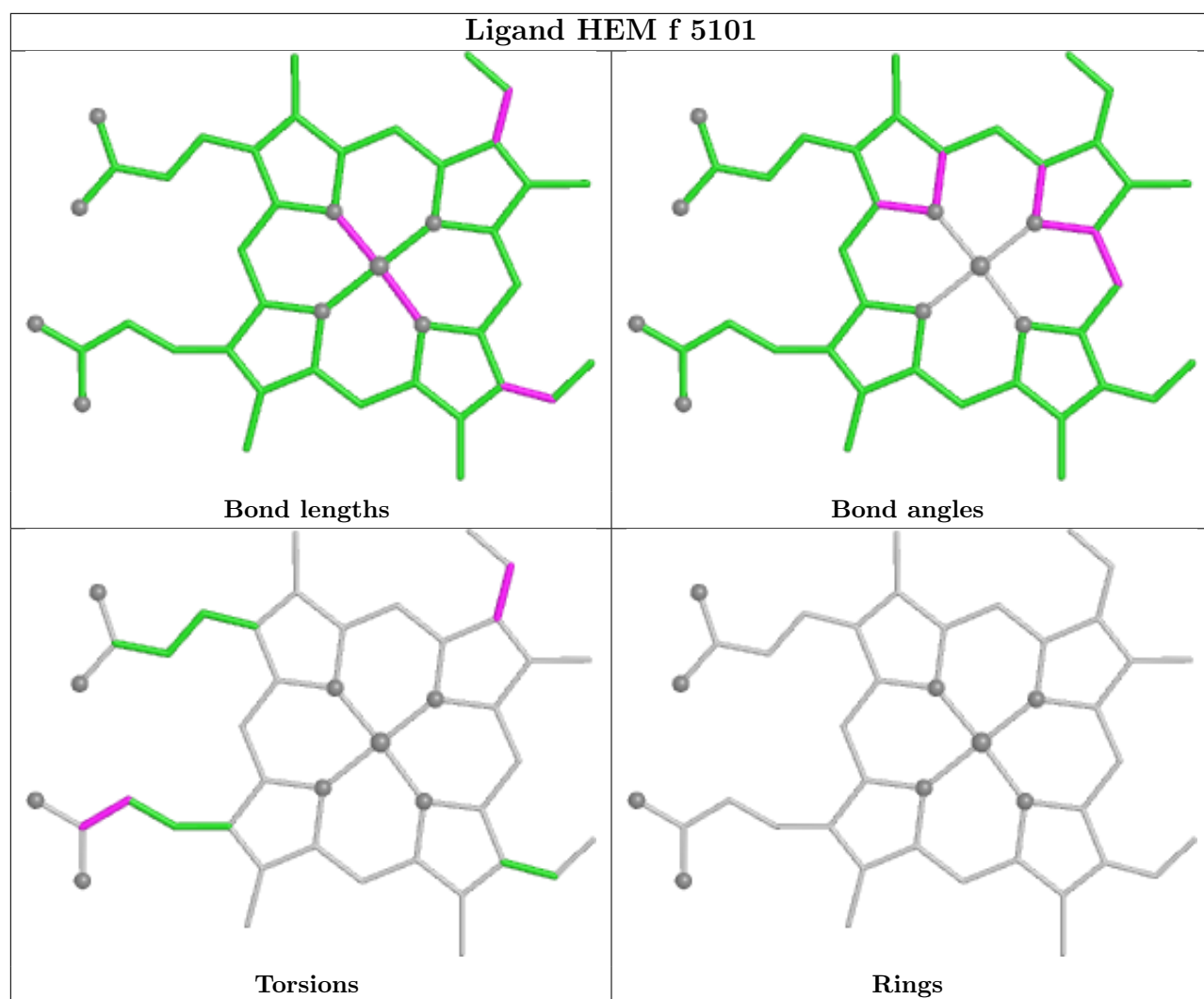




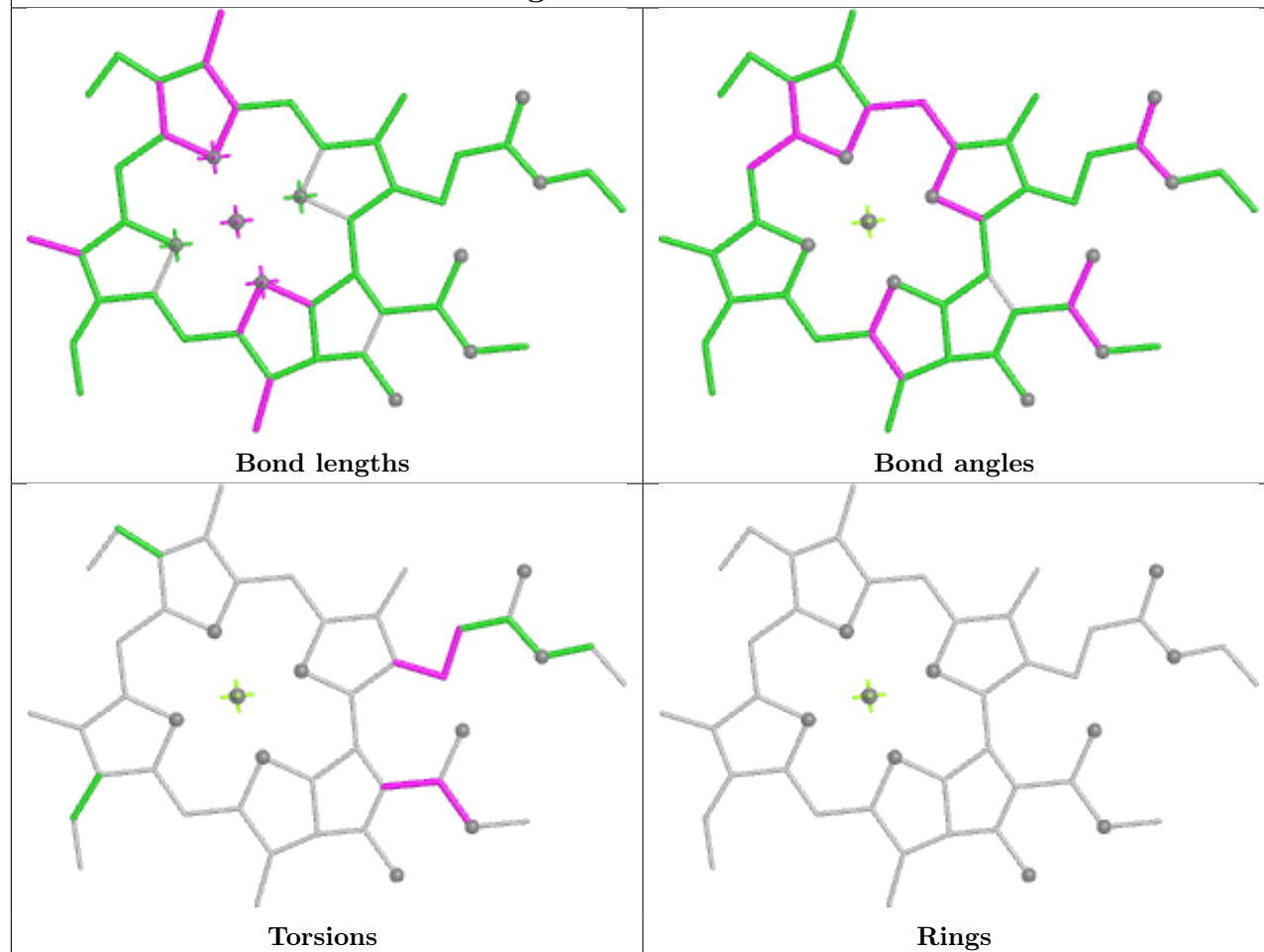


| Ligand BCR b 5617                                                                                       |                                                                                                         |
|---------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------|
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>       |  <p>Rings</p>         |
| Ligand CLA B 603                                                                                        |                                                                                                         |
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>      |  <p>Rings</p>        |
| Ligand MGE d 5410                                                                                       |                                                                                                         |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>     |  <p>Rings</p>       |

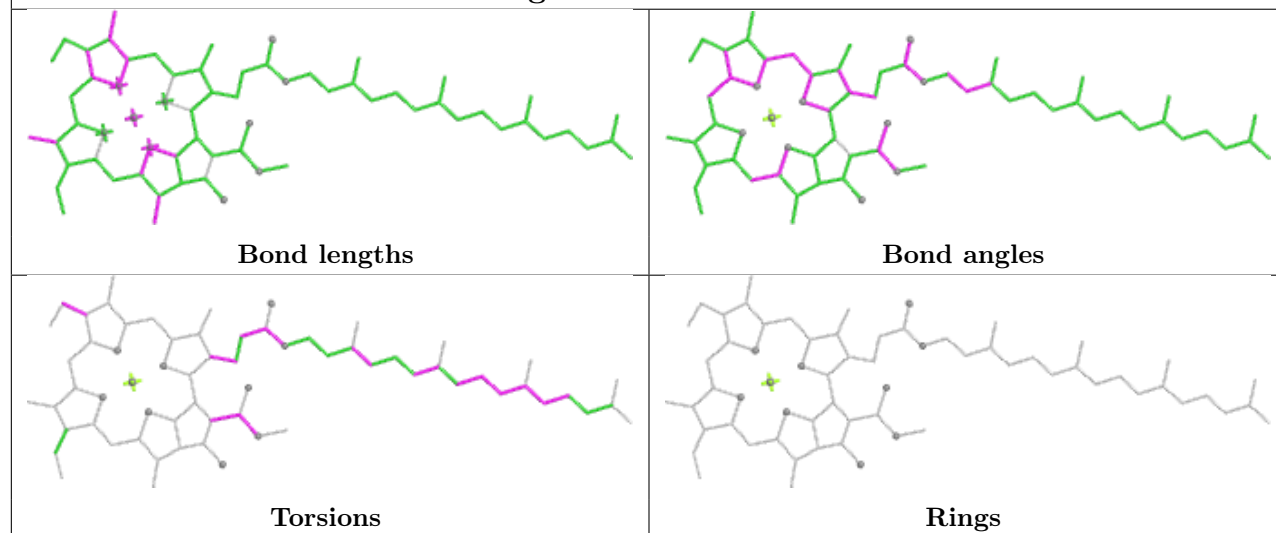


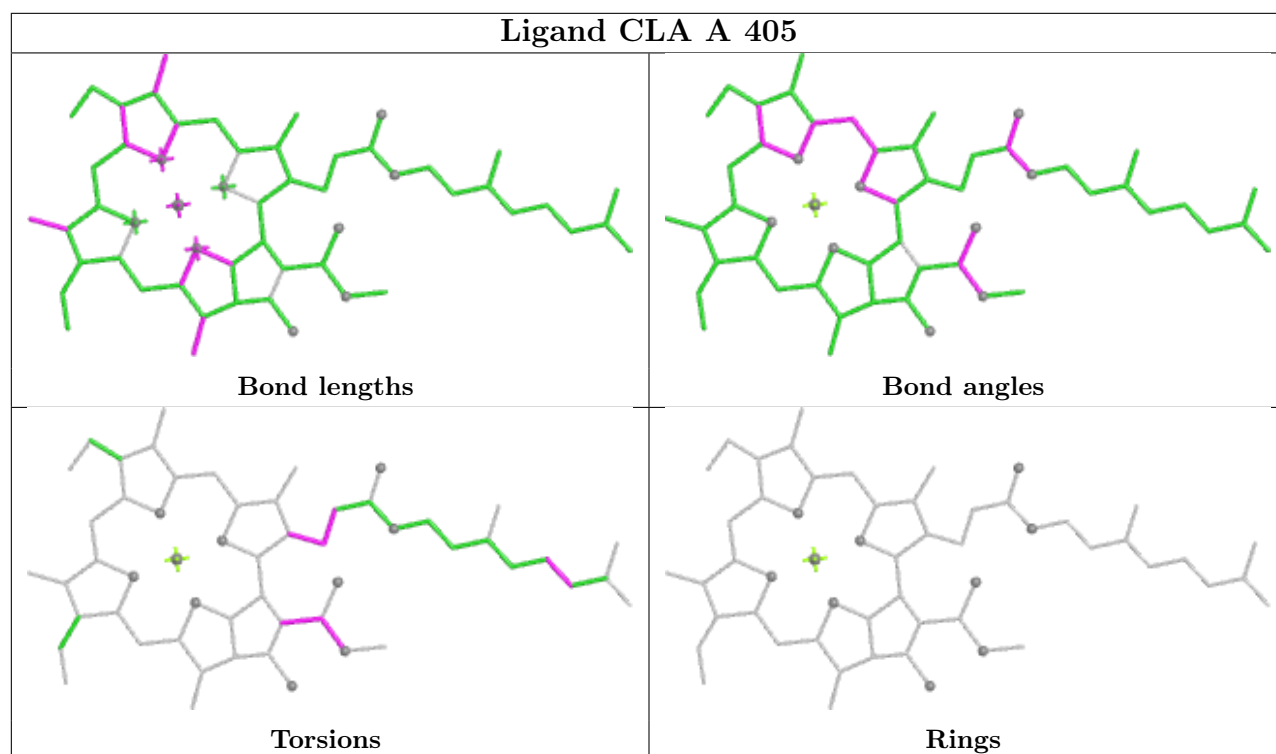
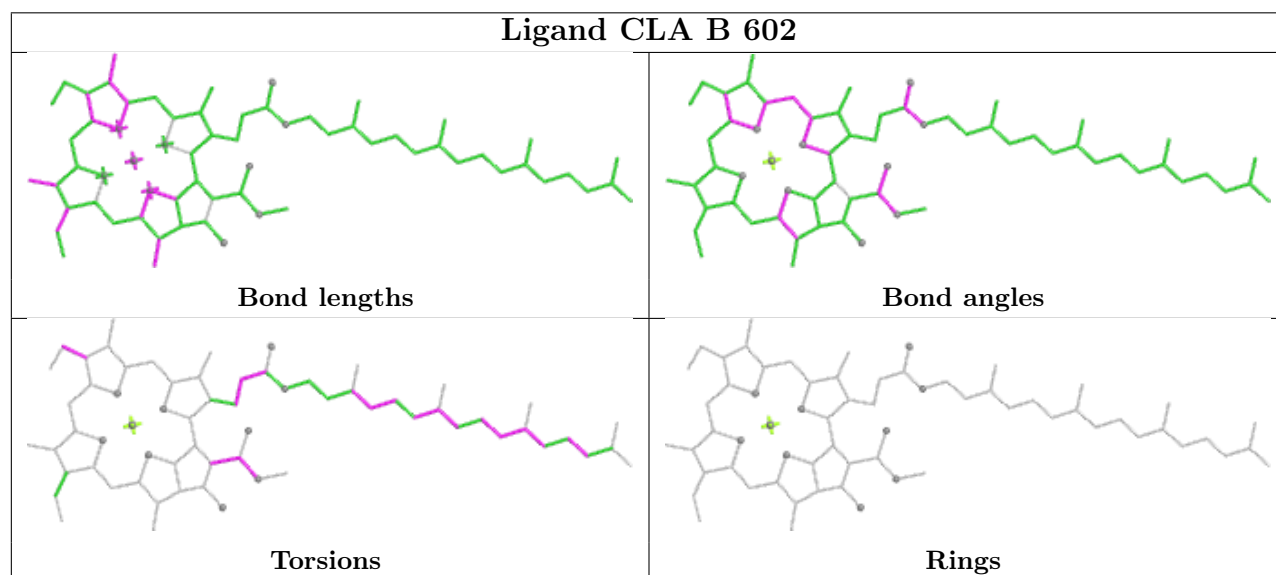
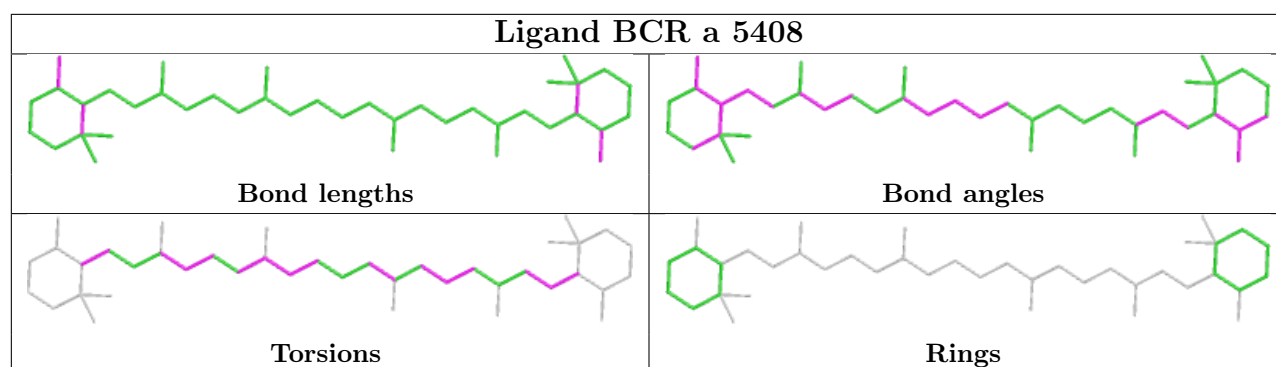


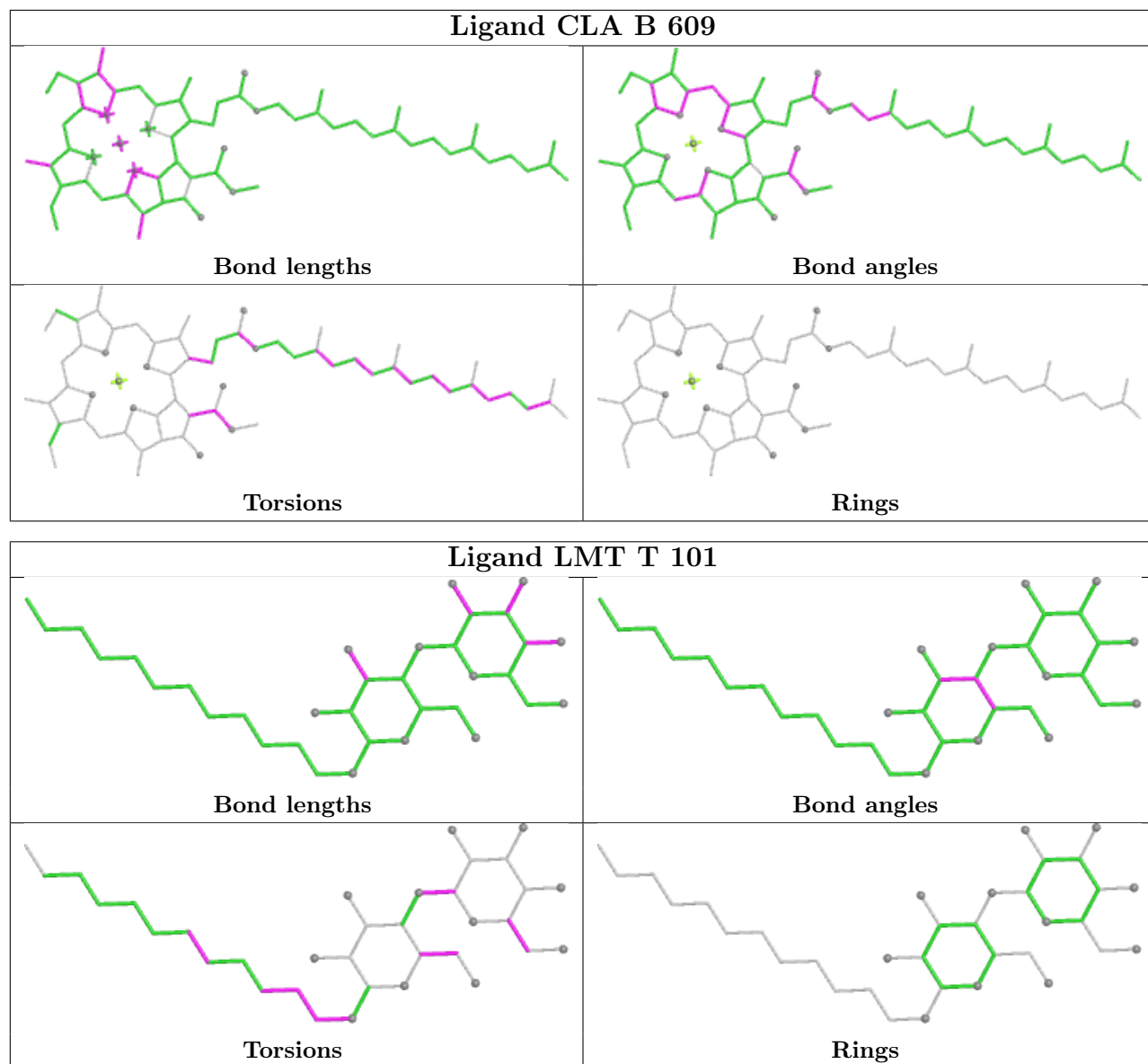
## Ligand CLA C 509

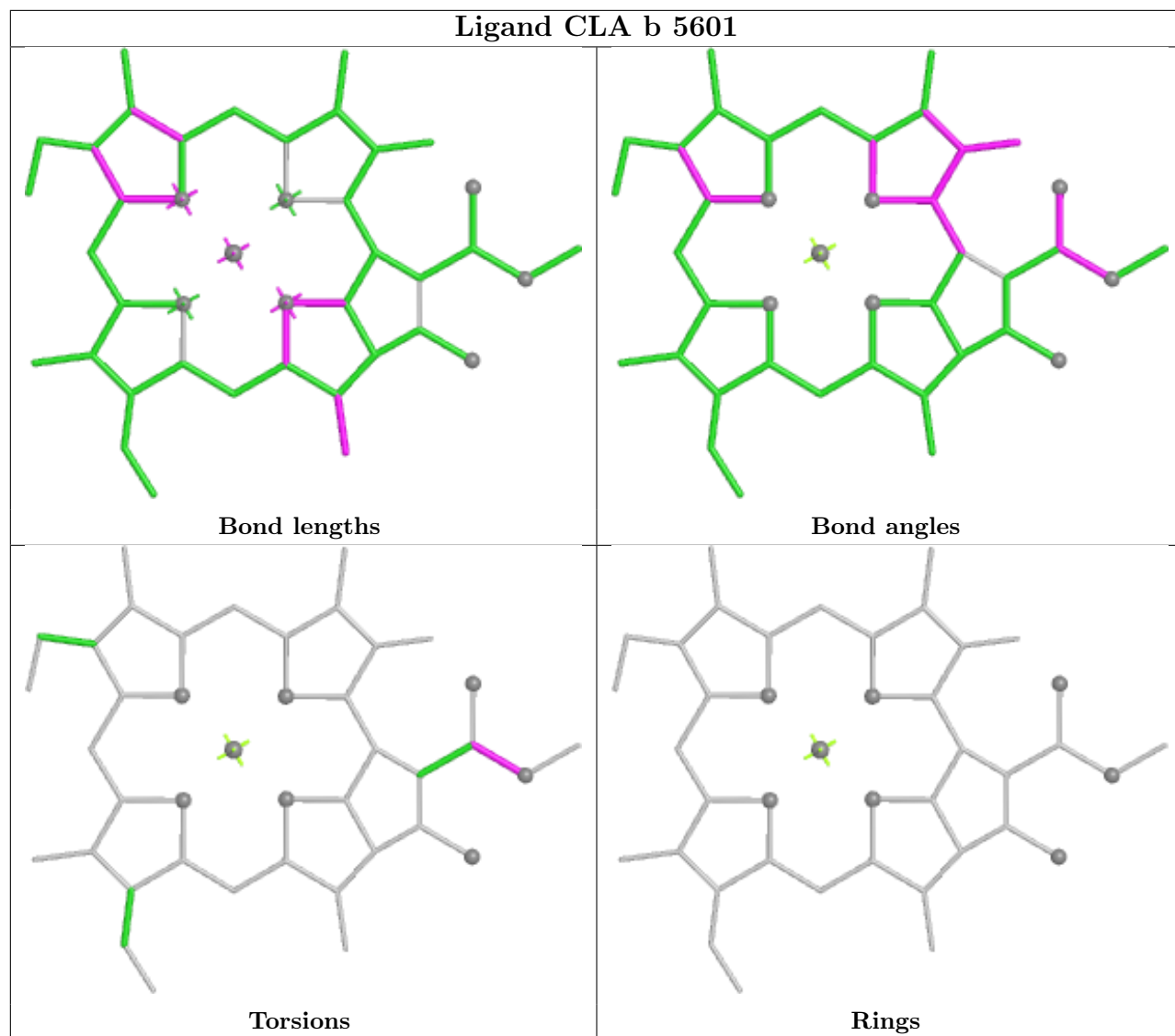


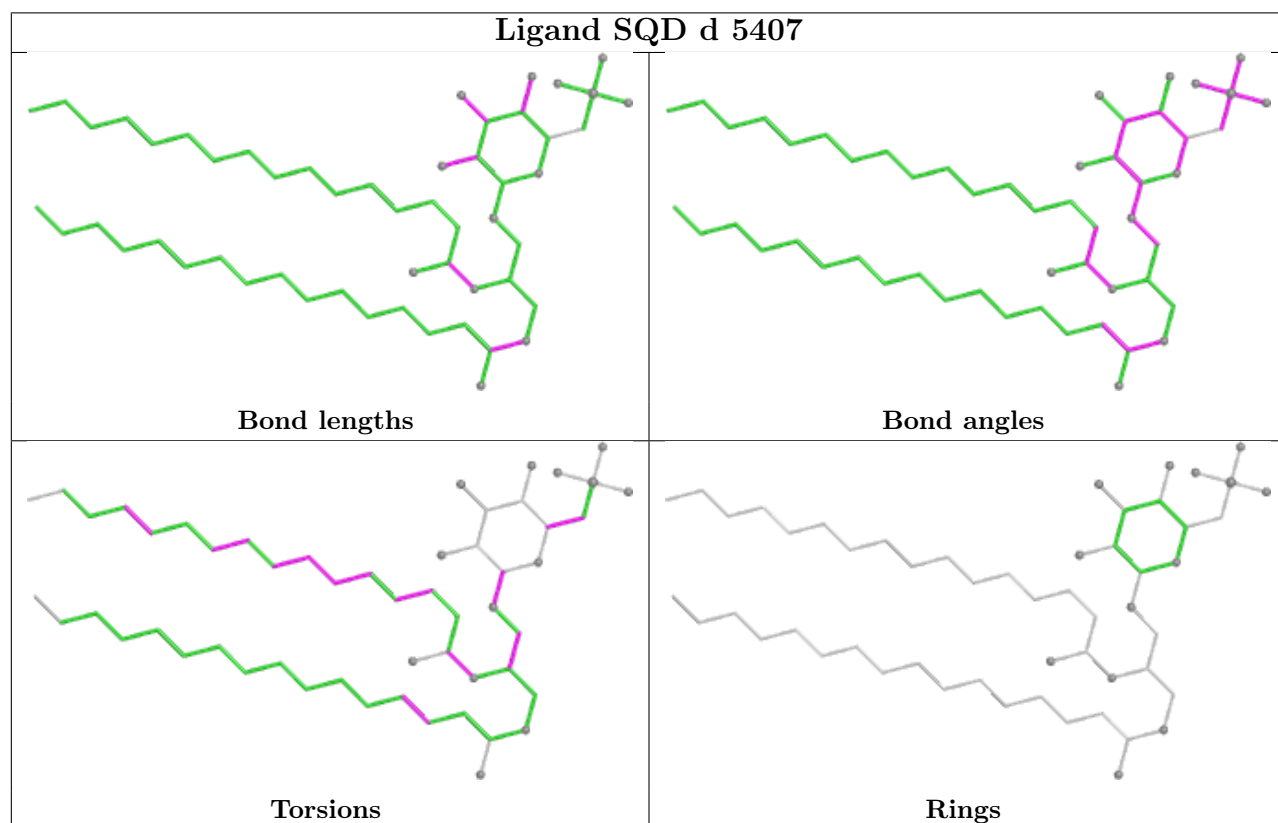
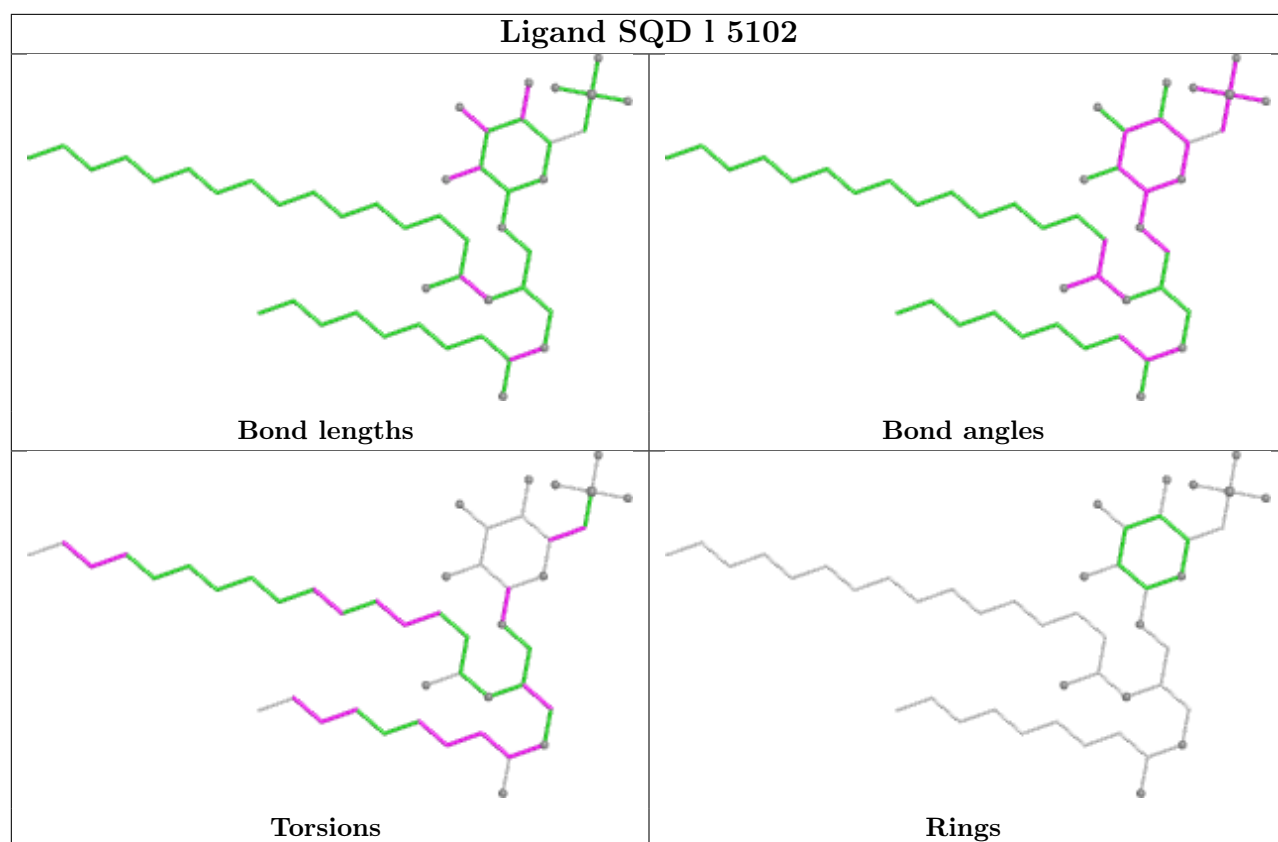
## Ligand CLA c 5503

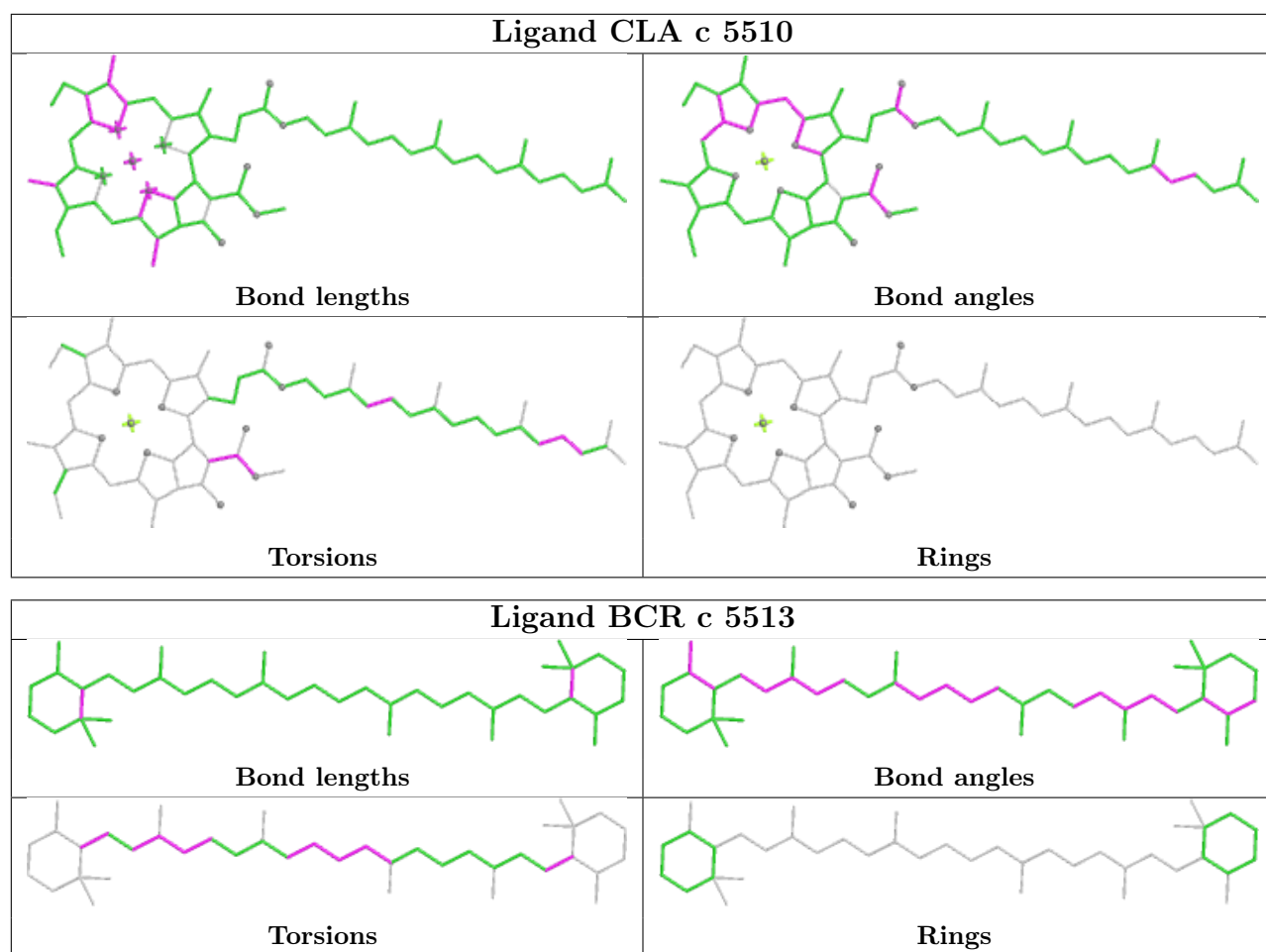




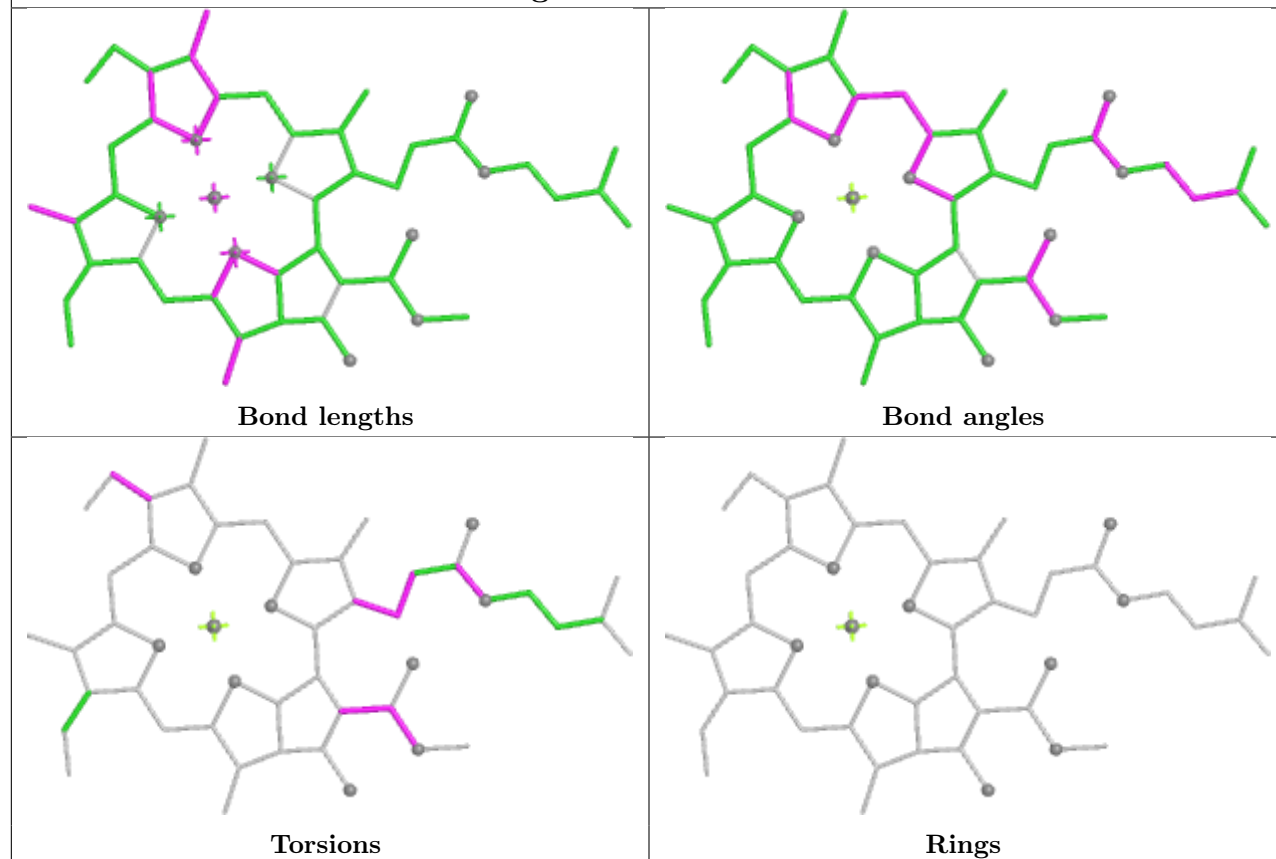




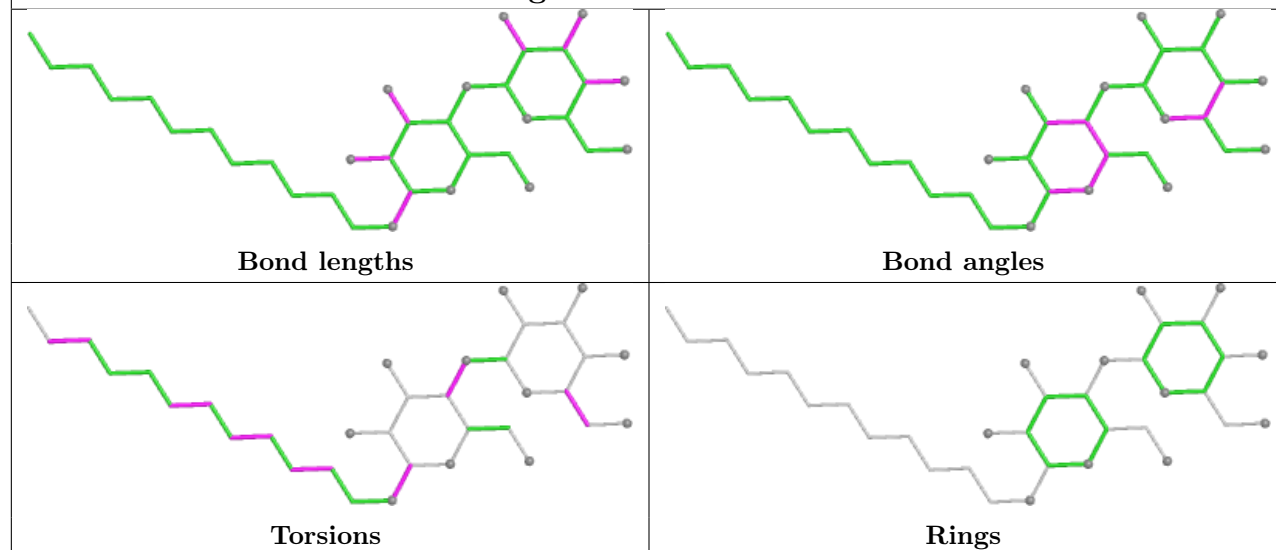


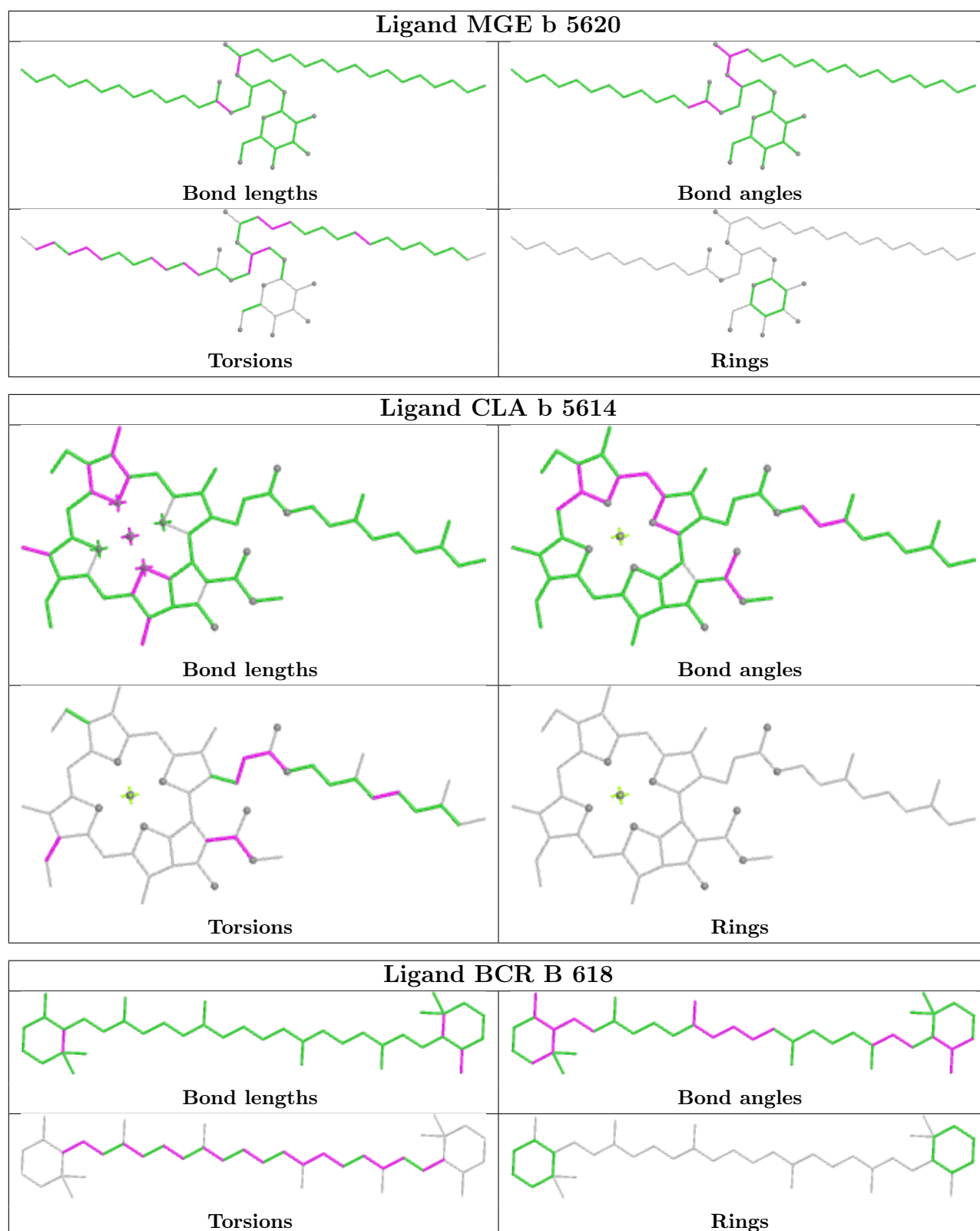


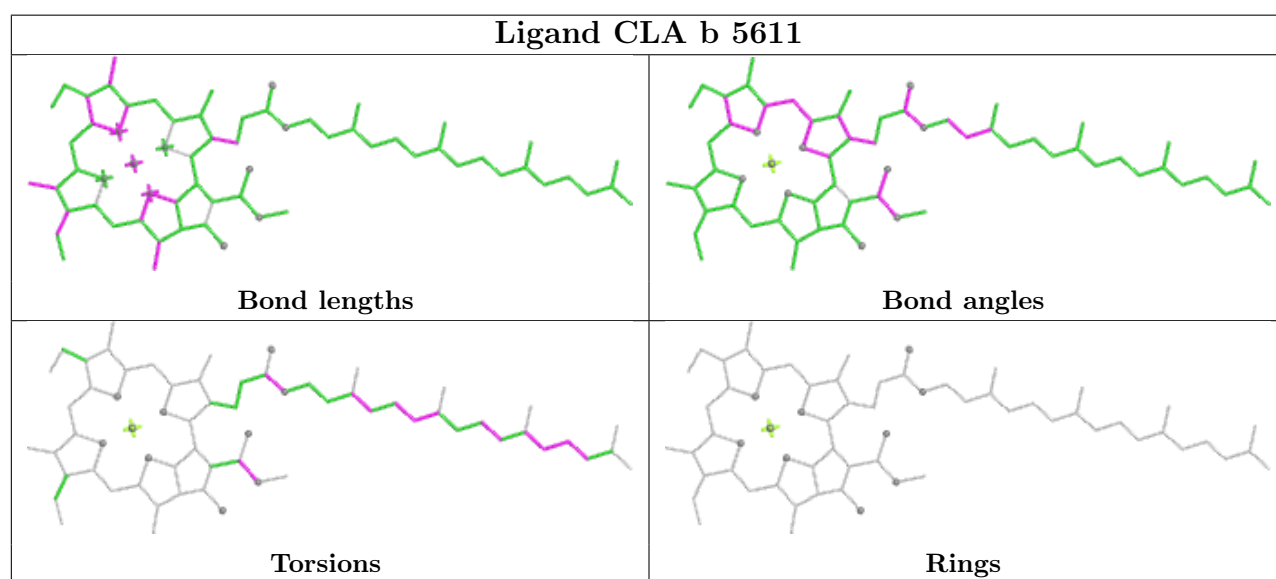
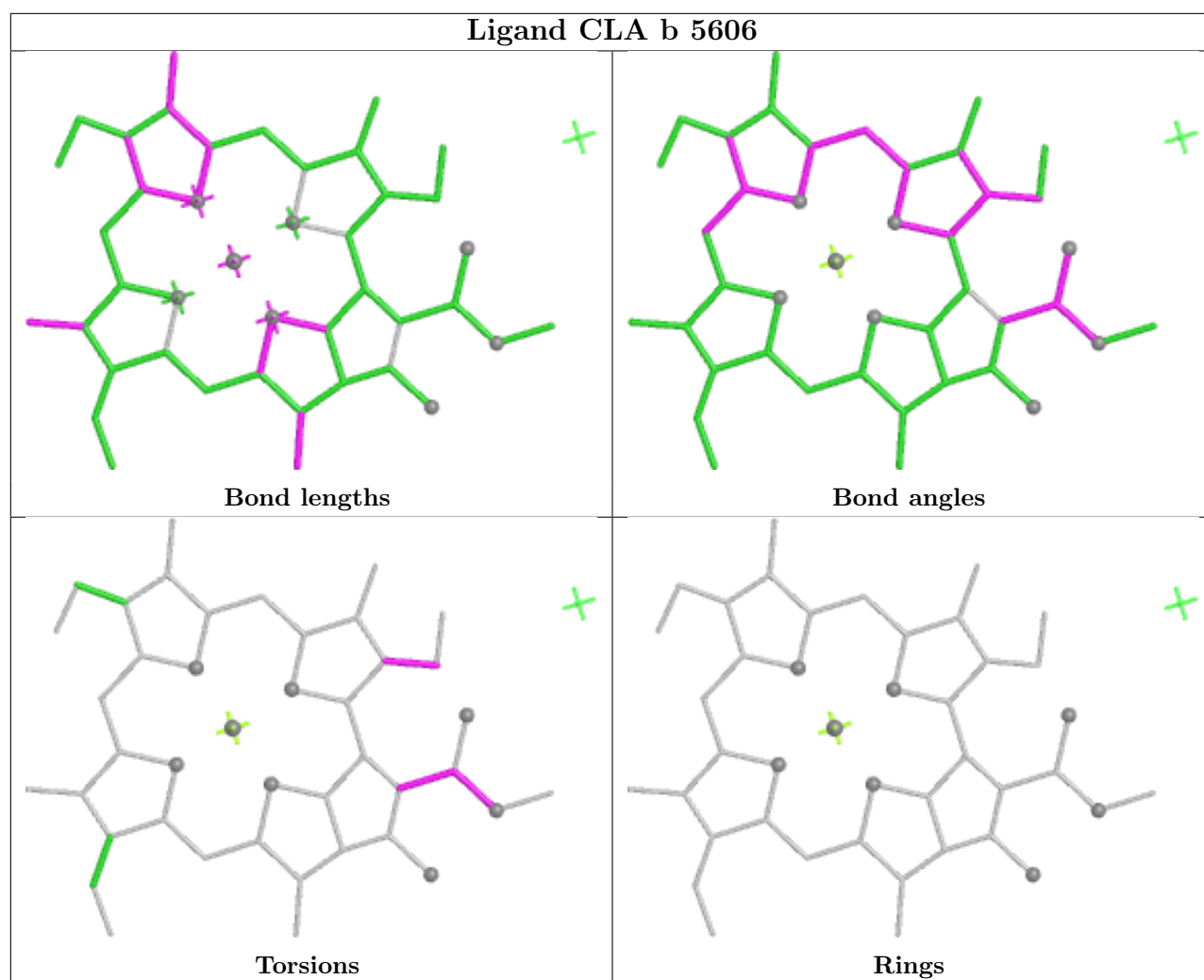
## Ligand CLA D 405

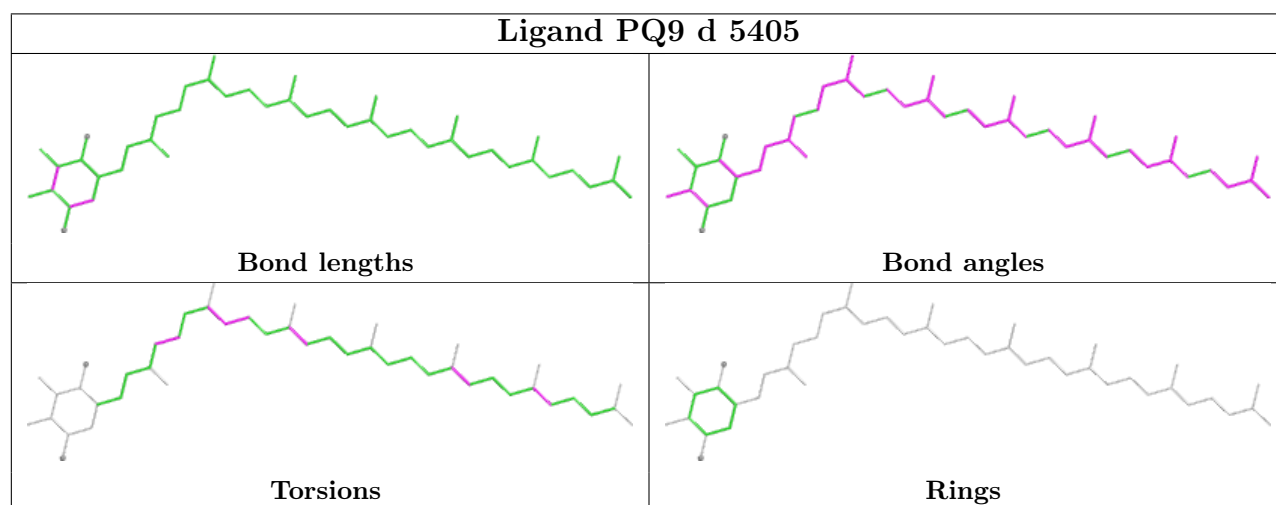
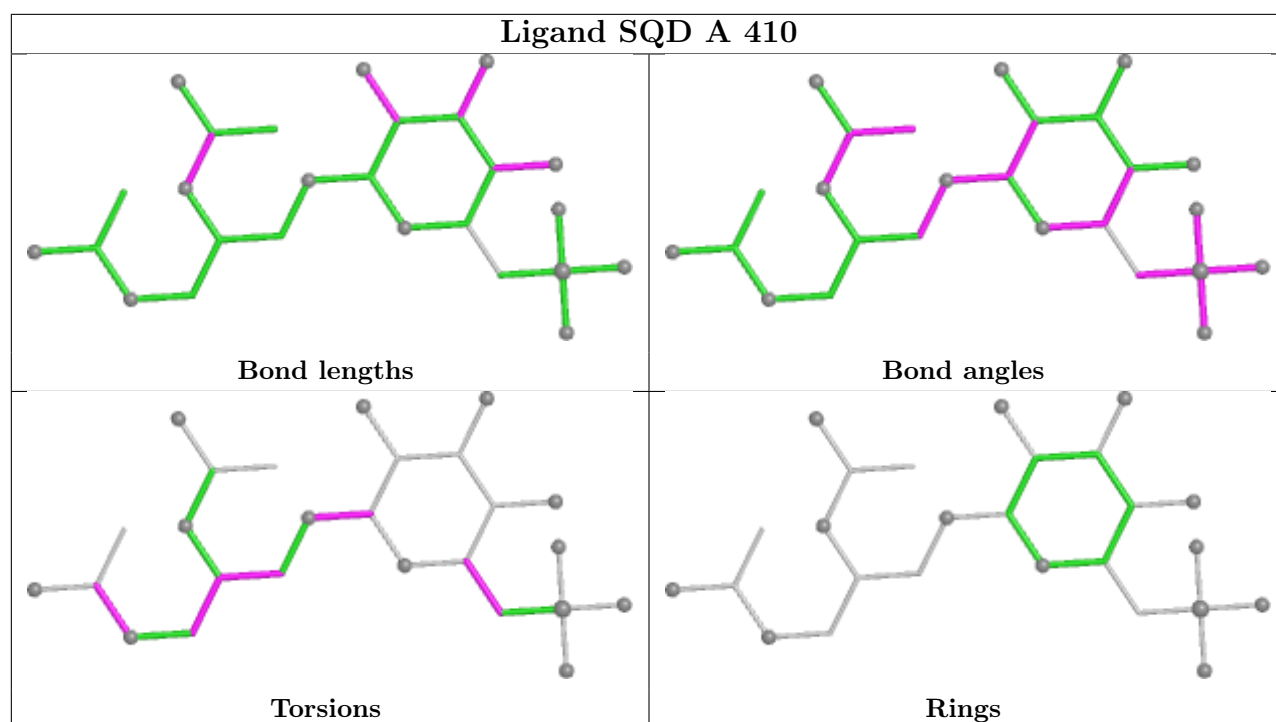


## Ligand LMT A 409

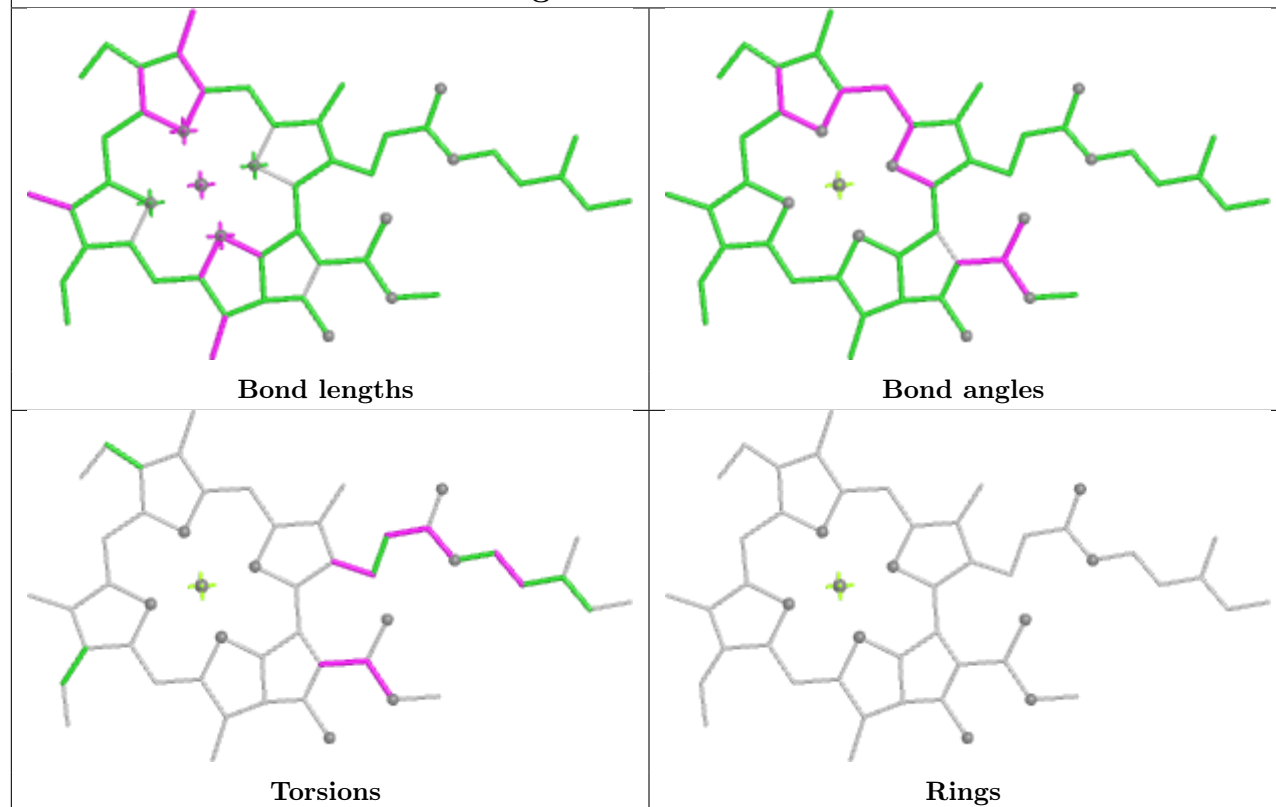




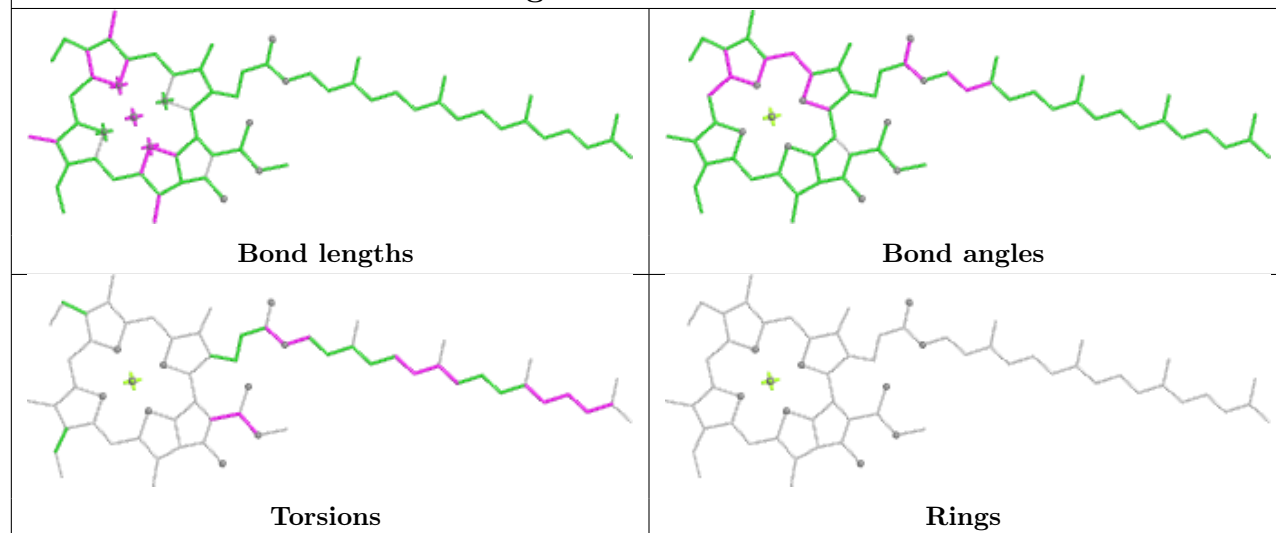


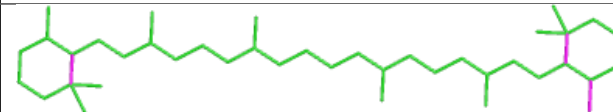
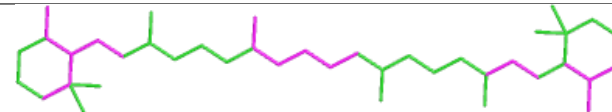
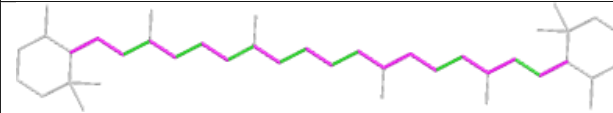
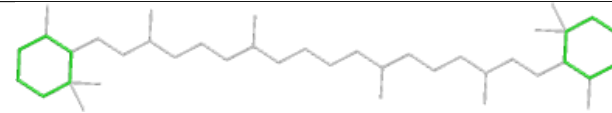


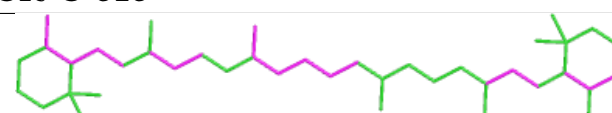
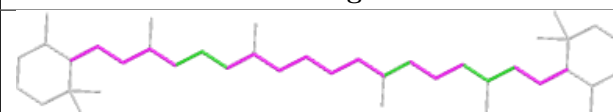
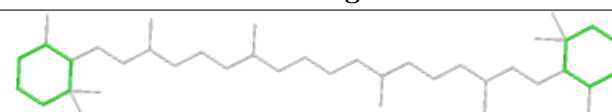
## Ligand CLA C 512

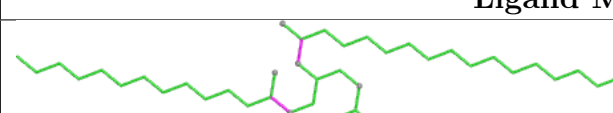
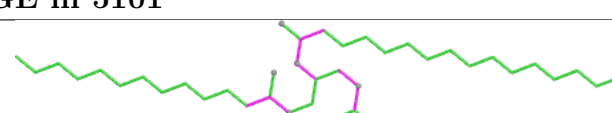
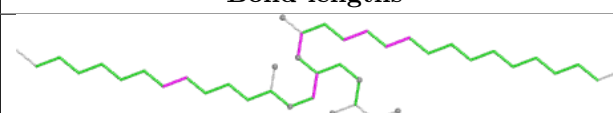
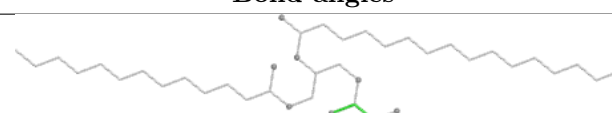


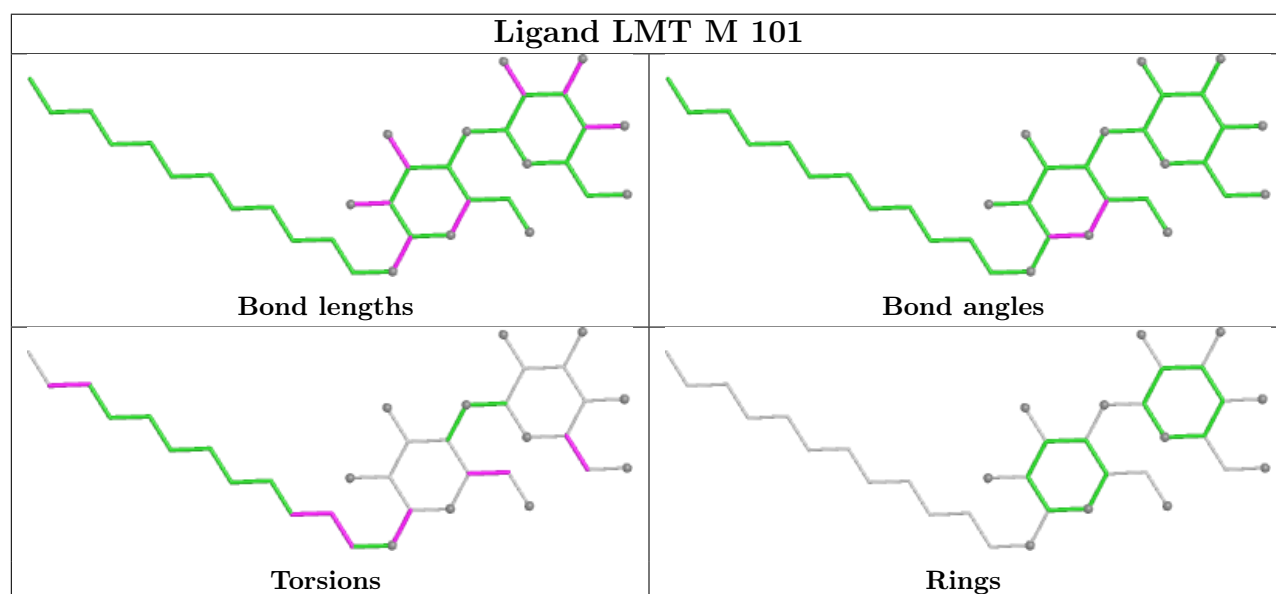
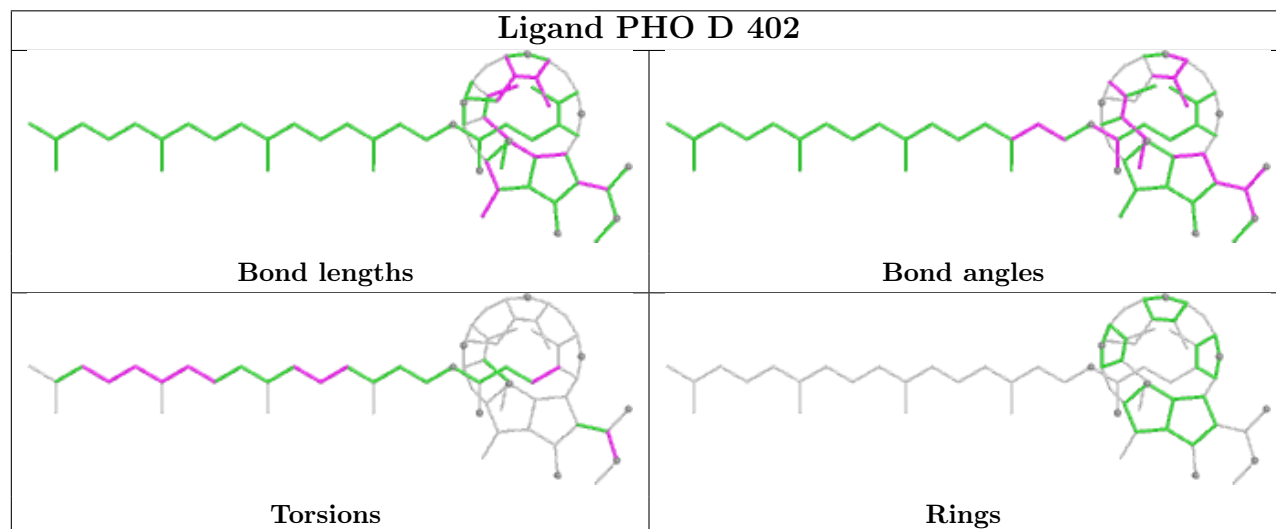
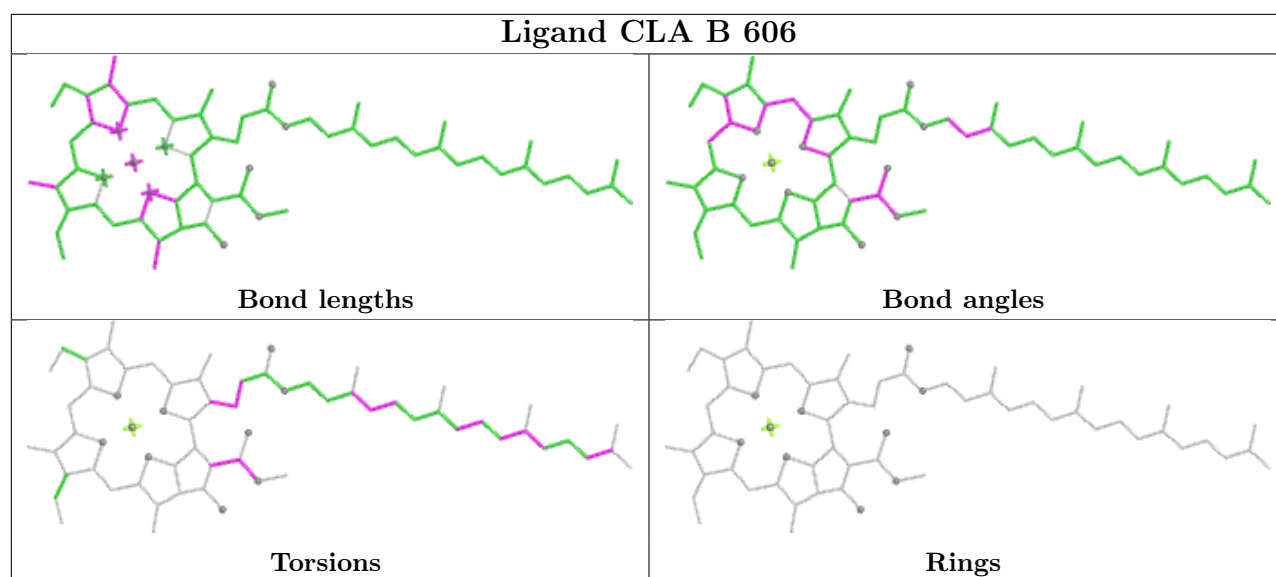
## Ligand CLA b 5615

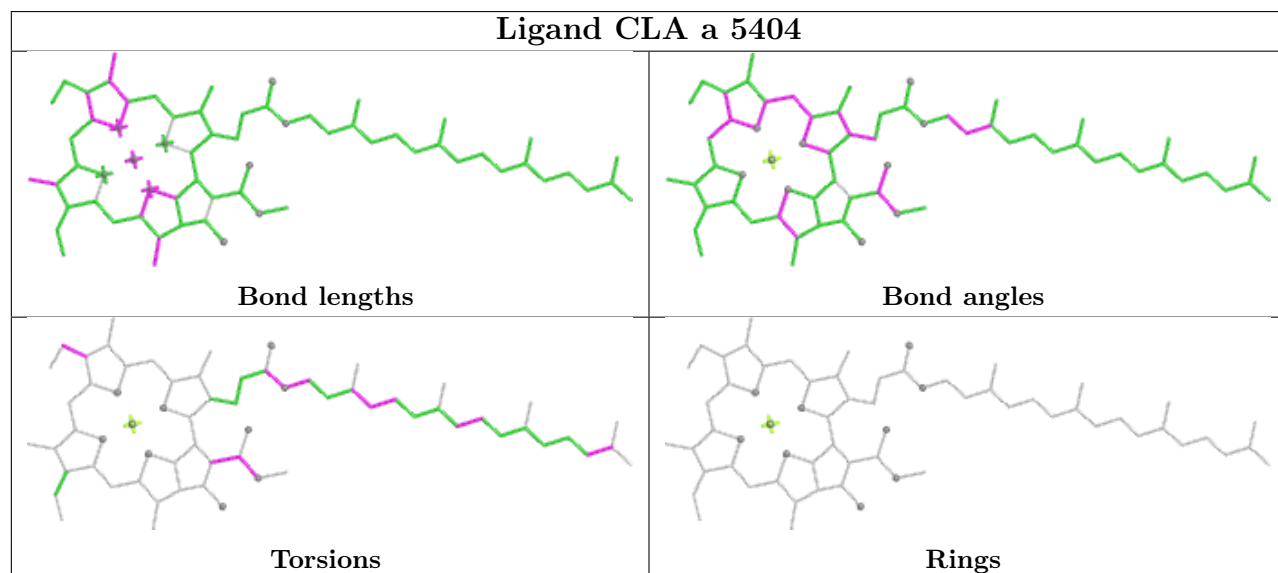
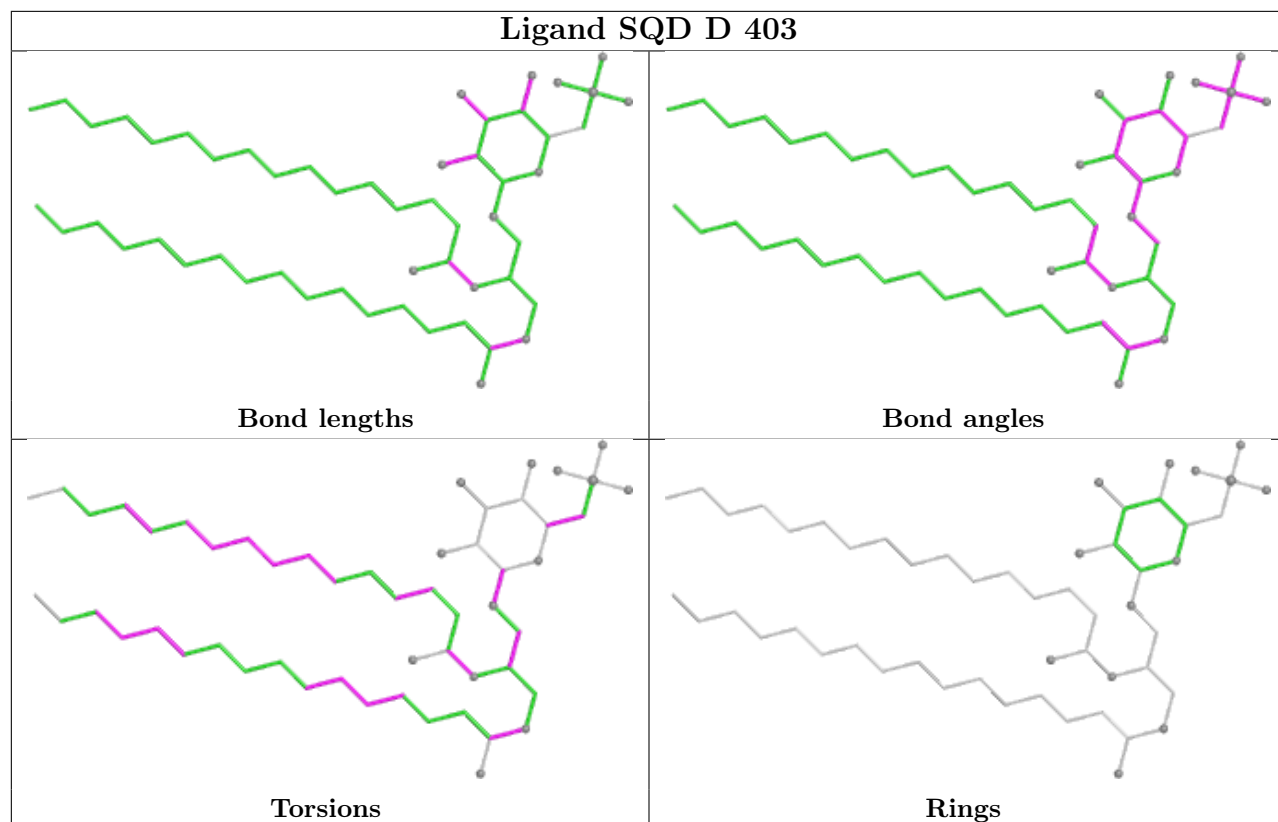


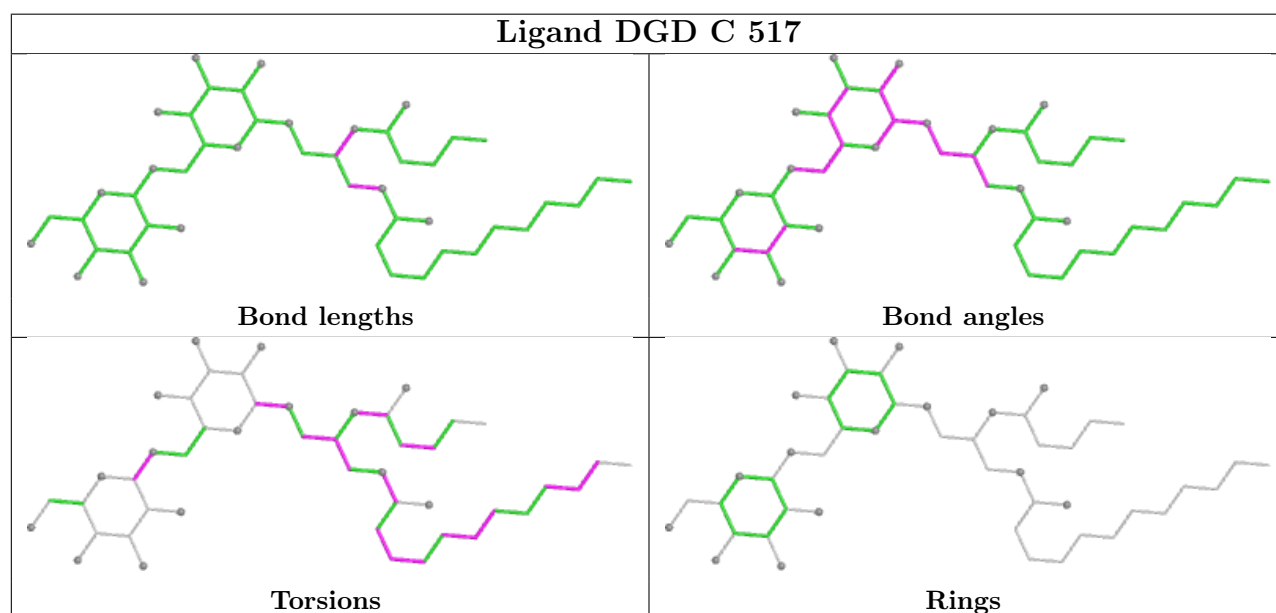
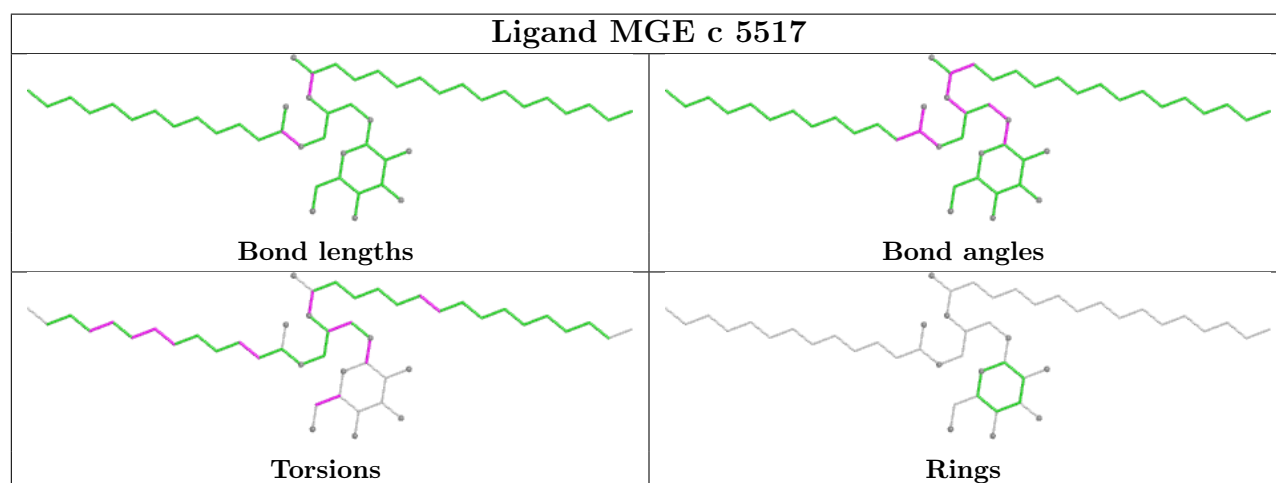
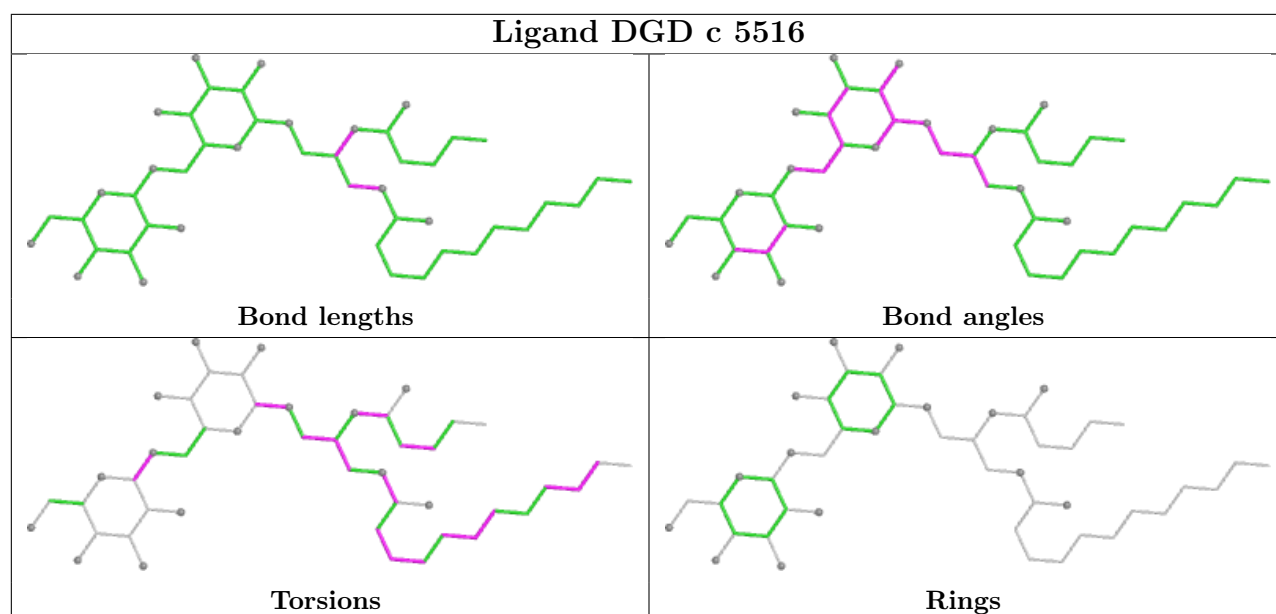
| Ligand BCR b 5618                                                                 |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

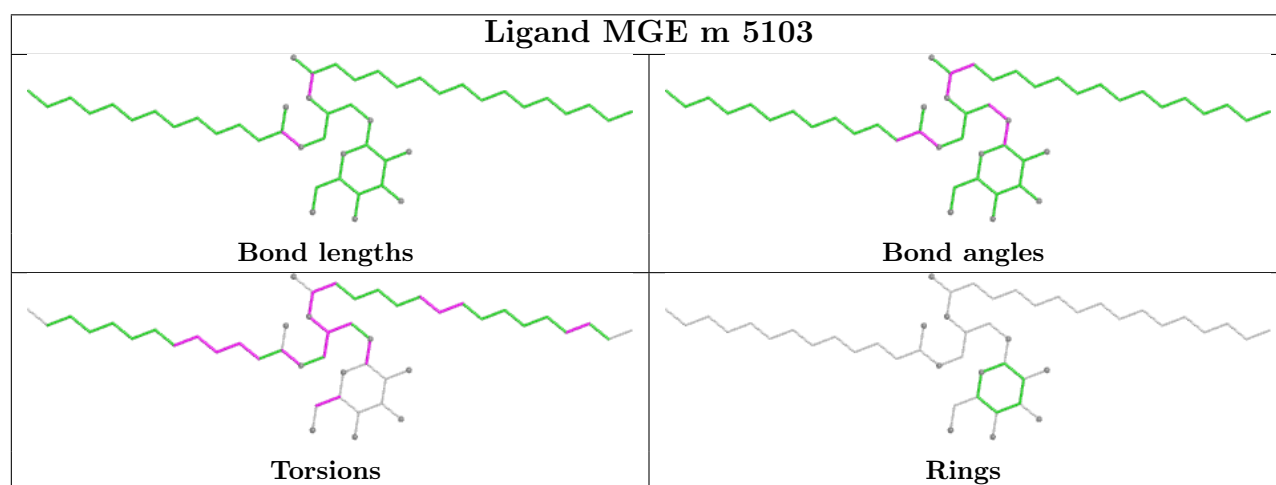
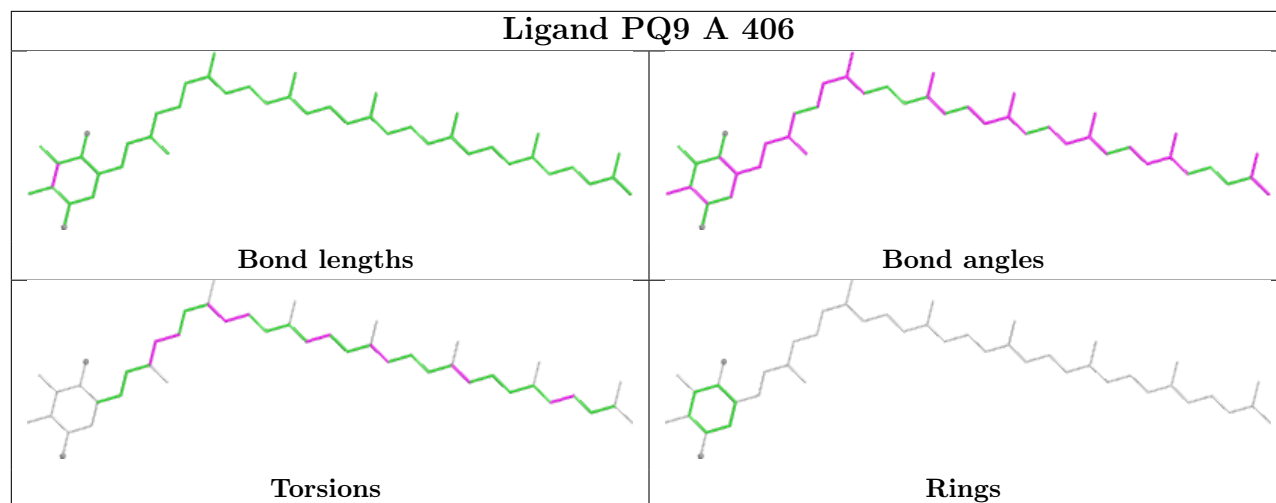
| Ligand BCR C 515                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

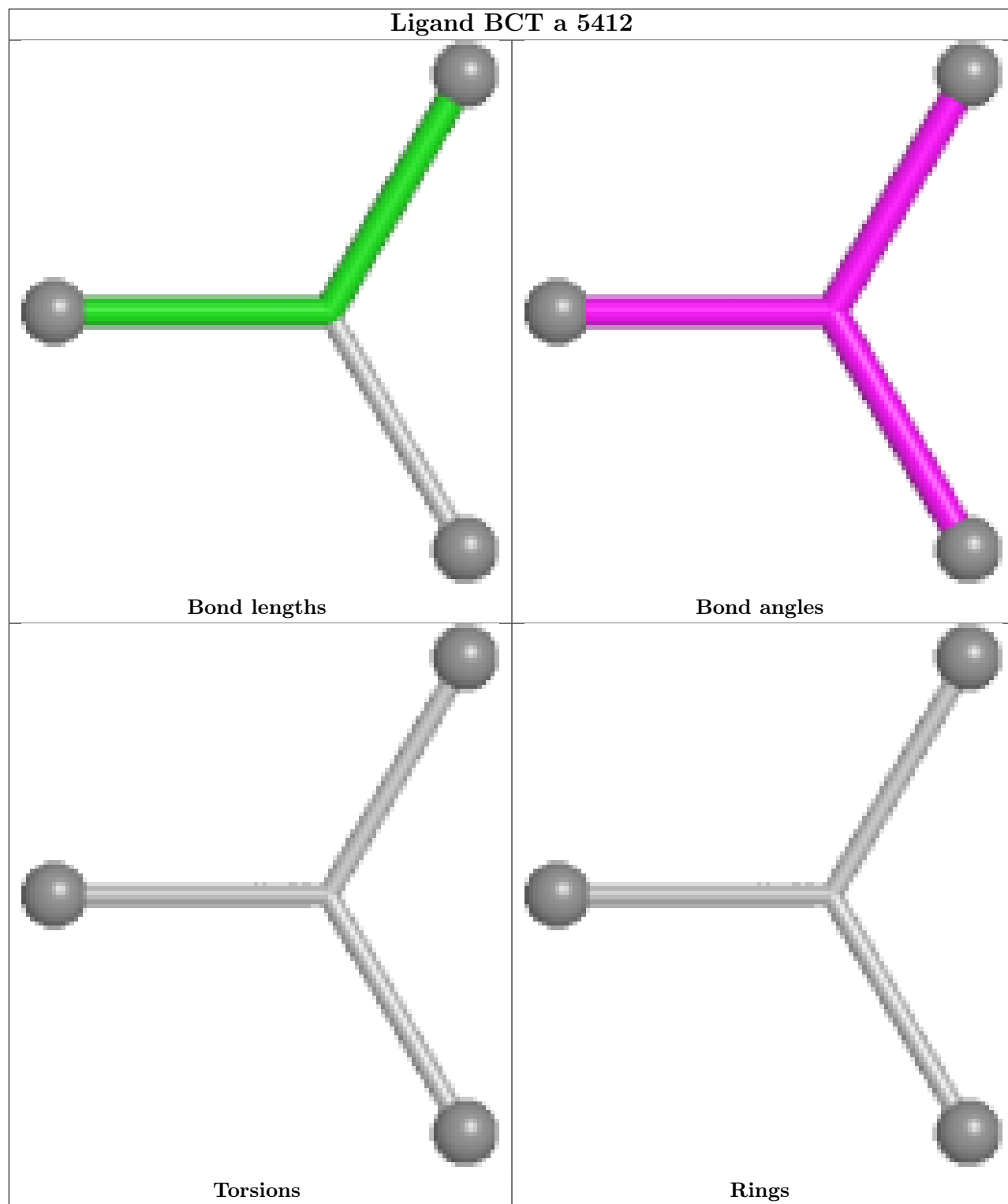
| Ligand MGE m 5101                                                                   |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

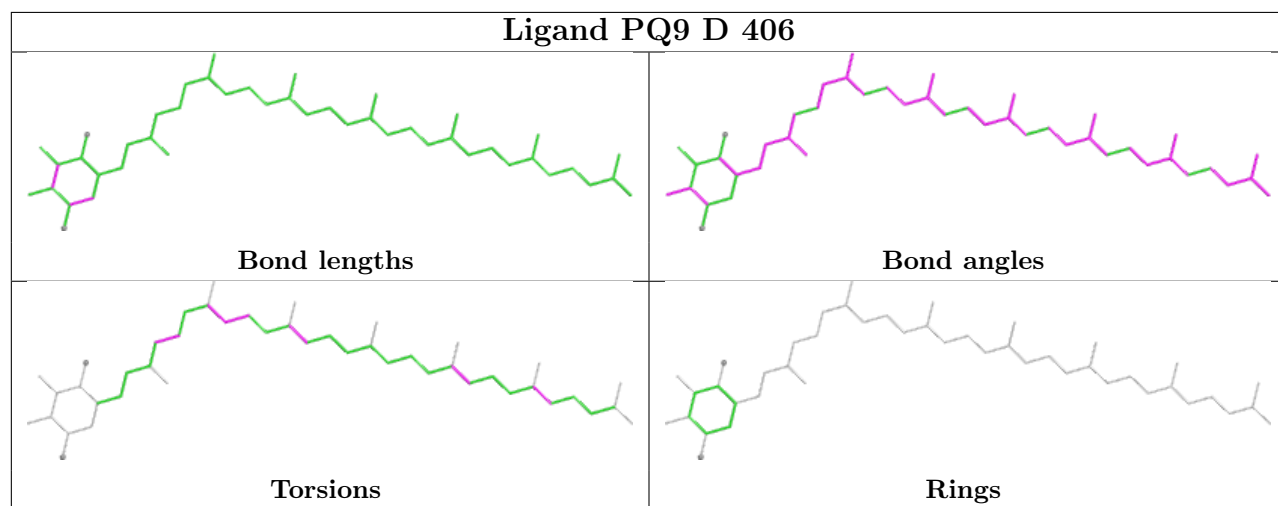
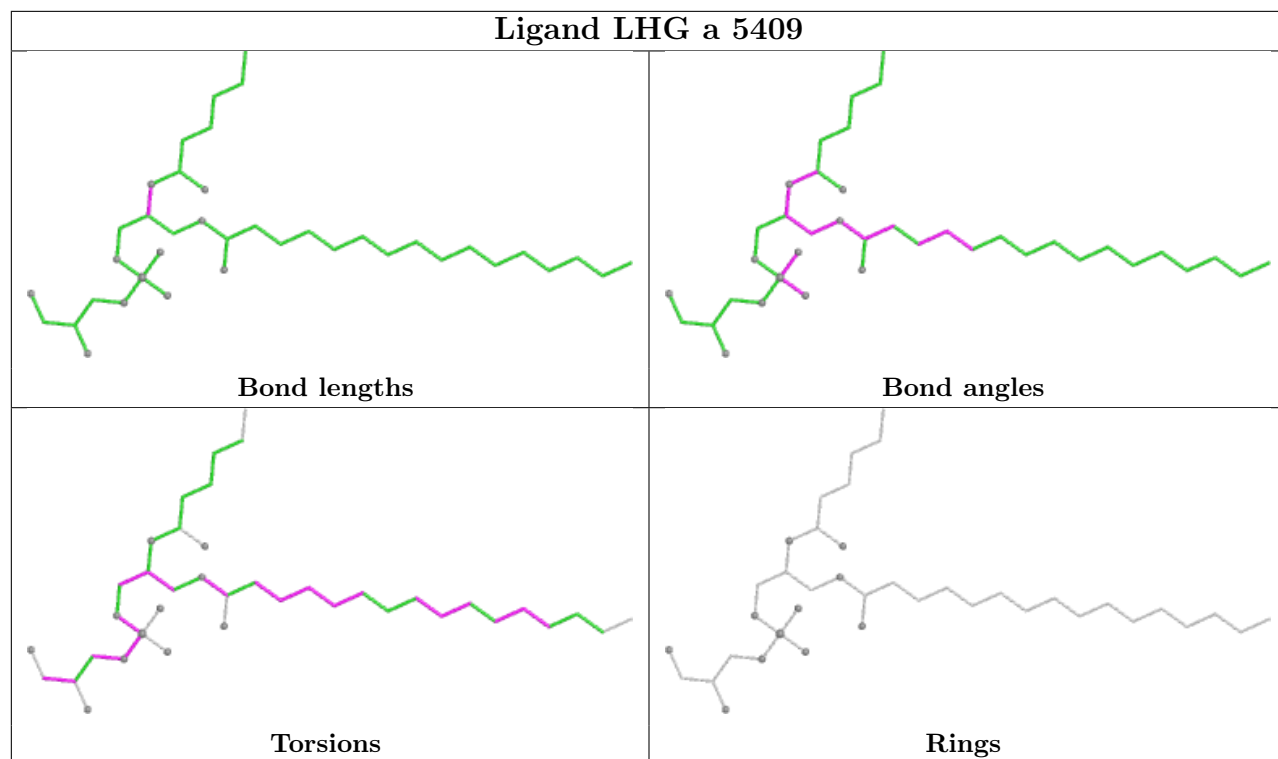


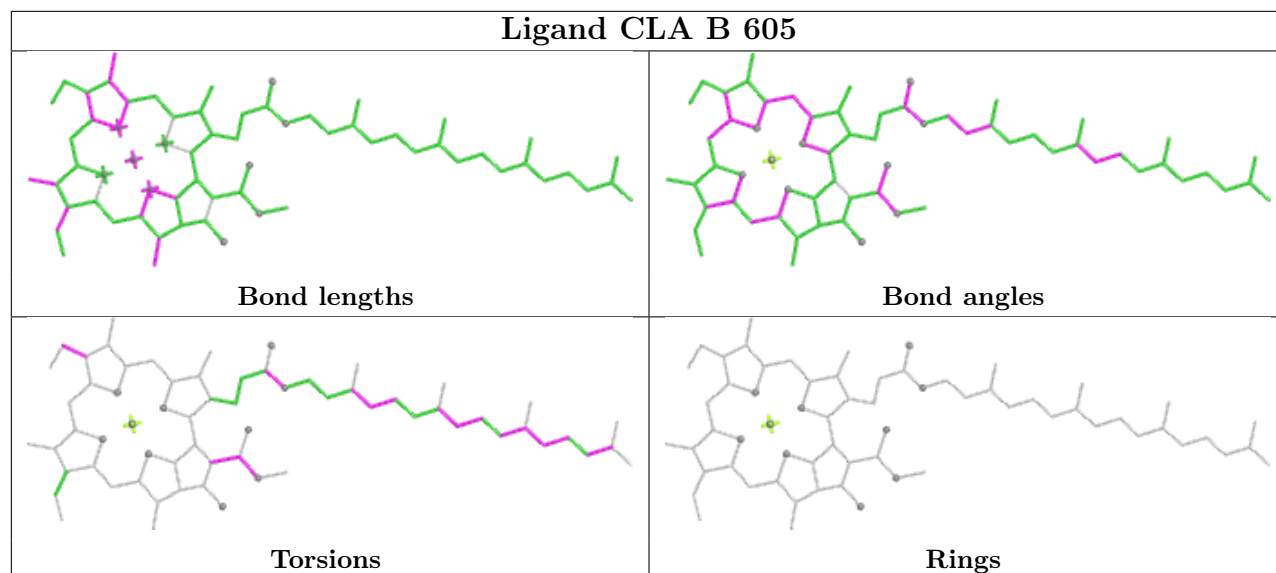
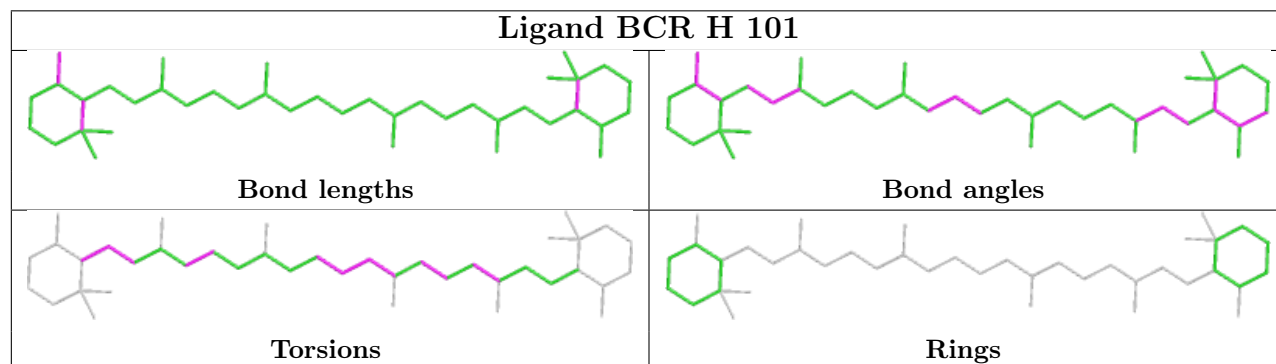
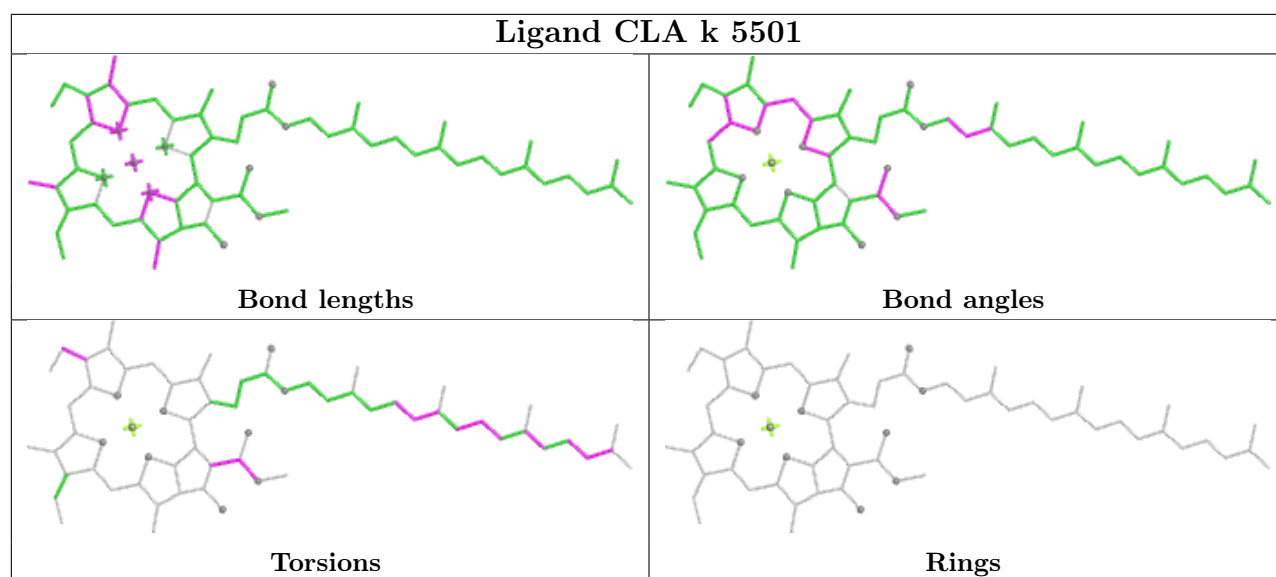




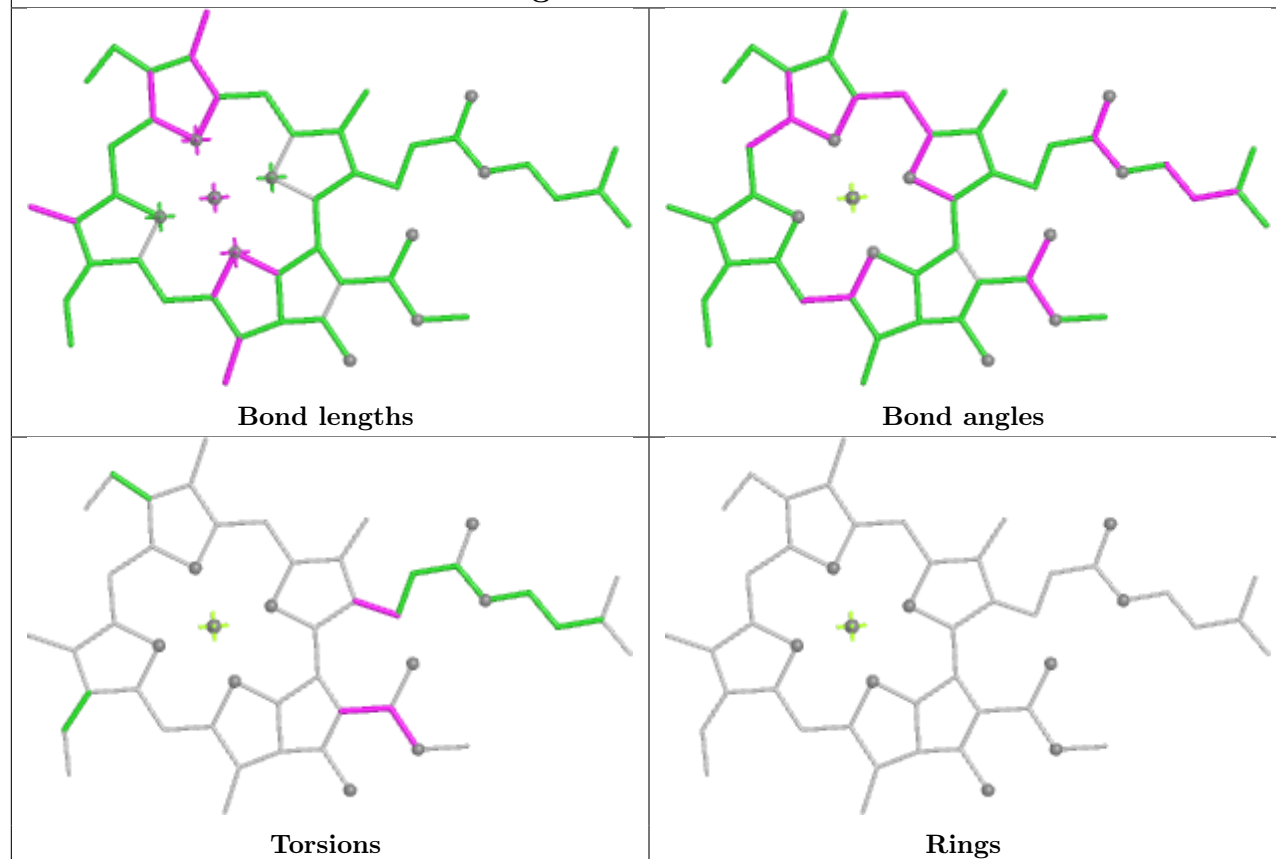




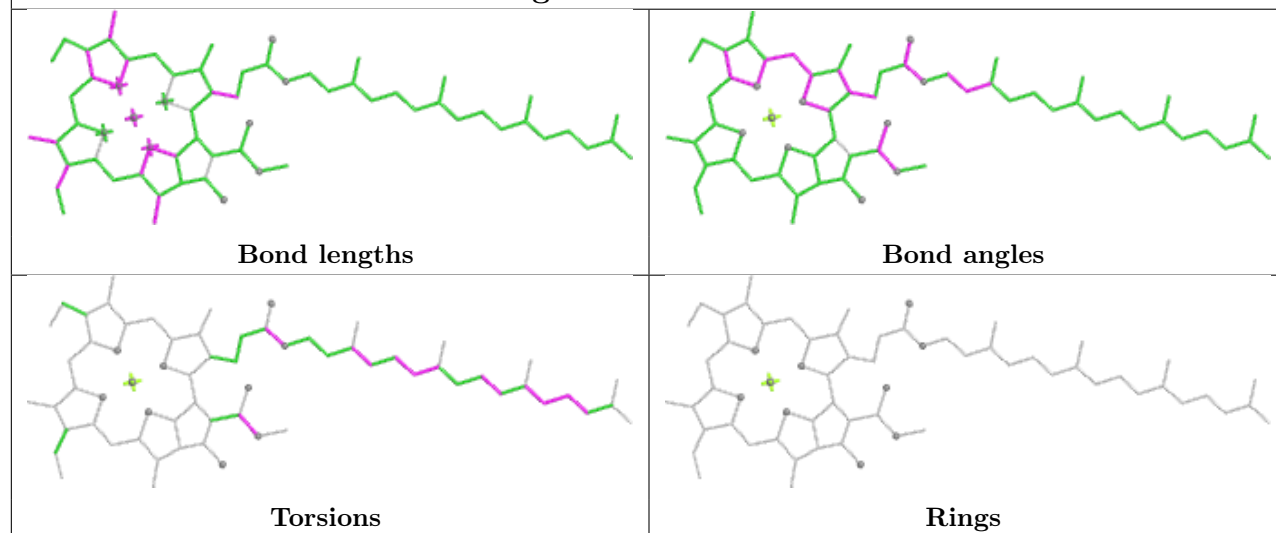


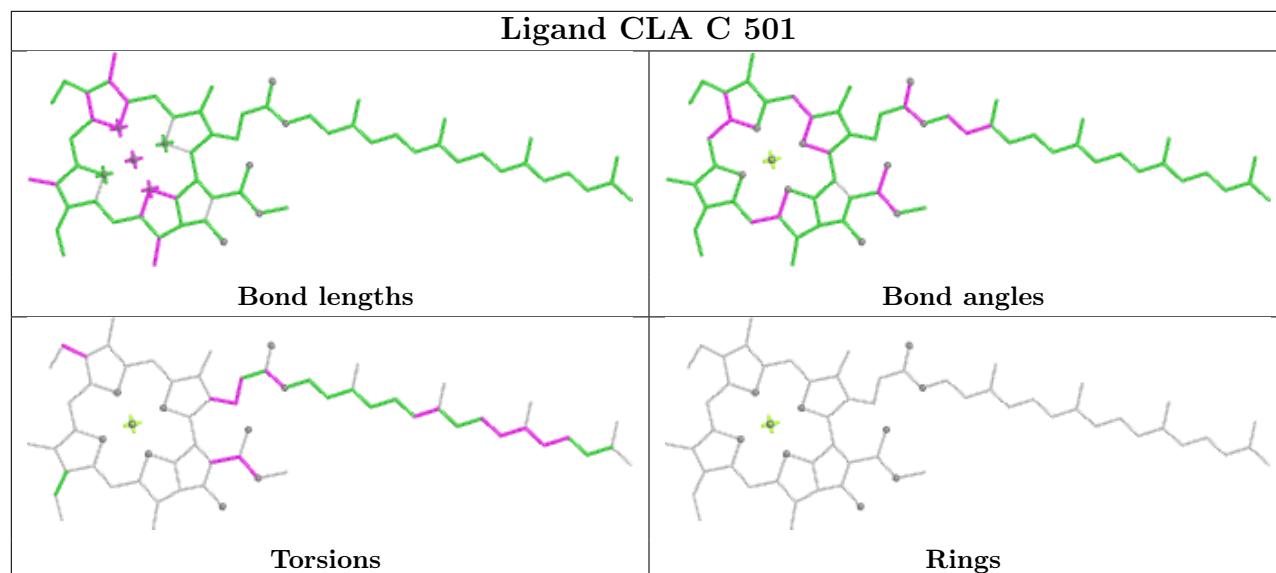
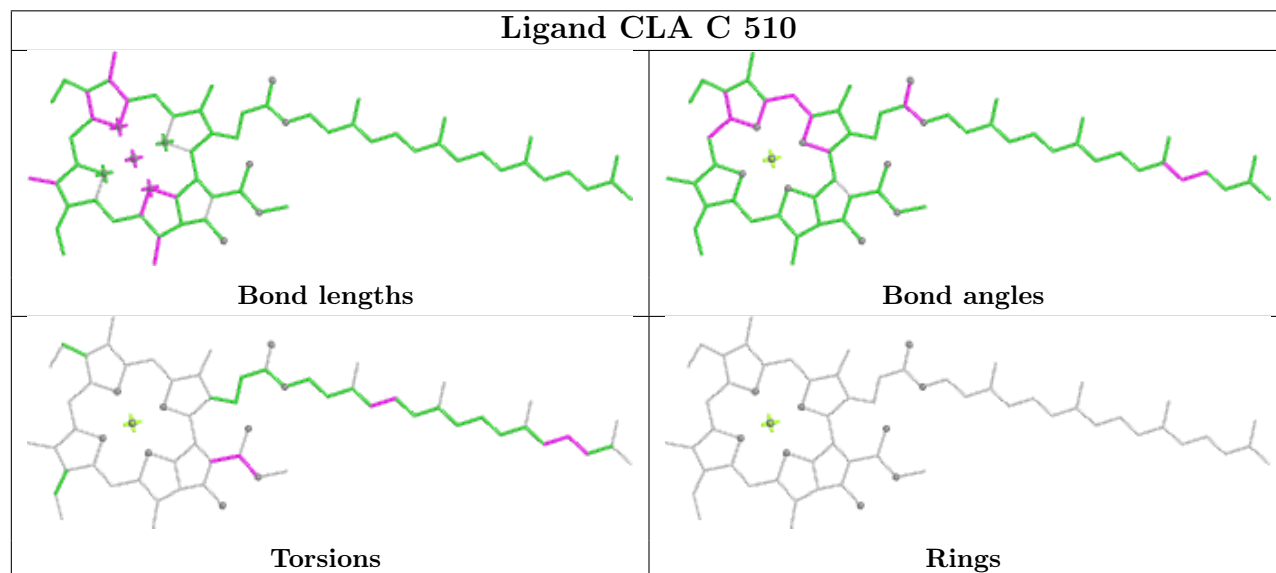
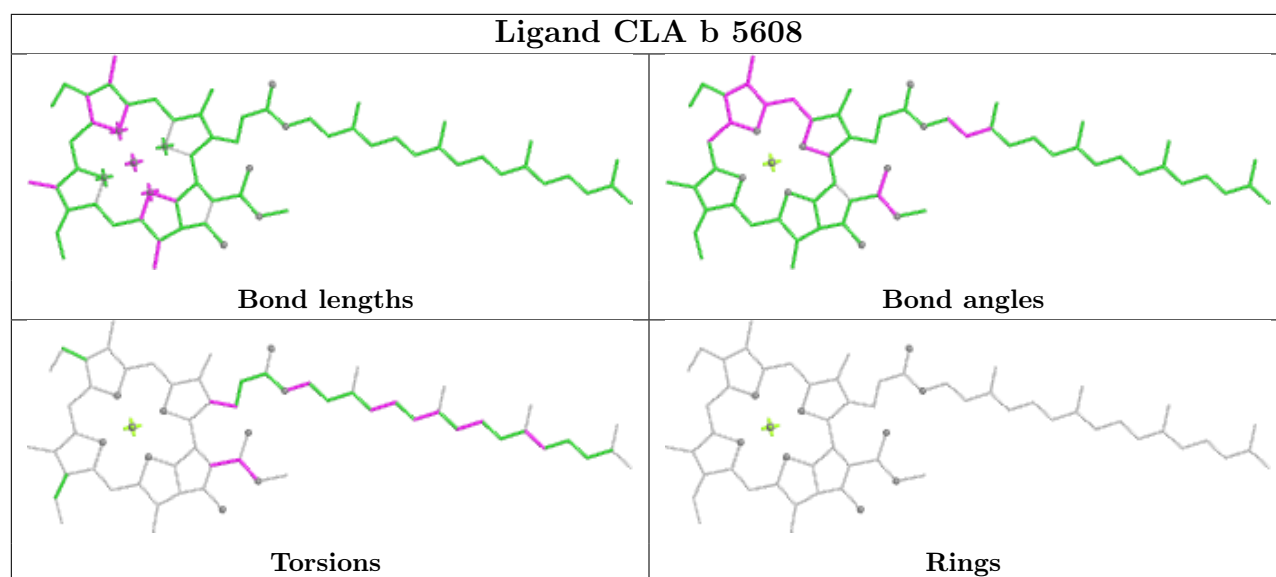


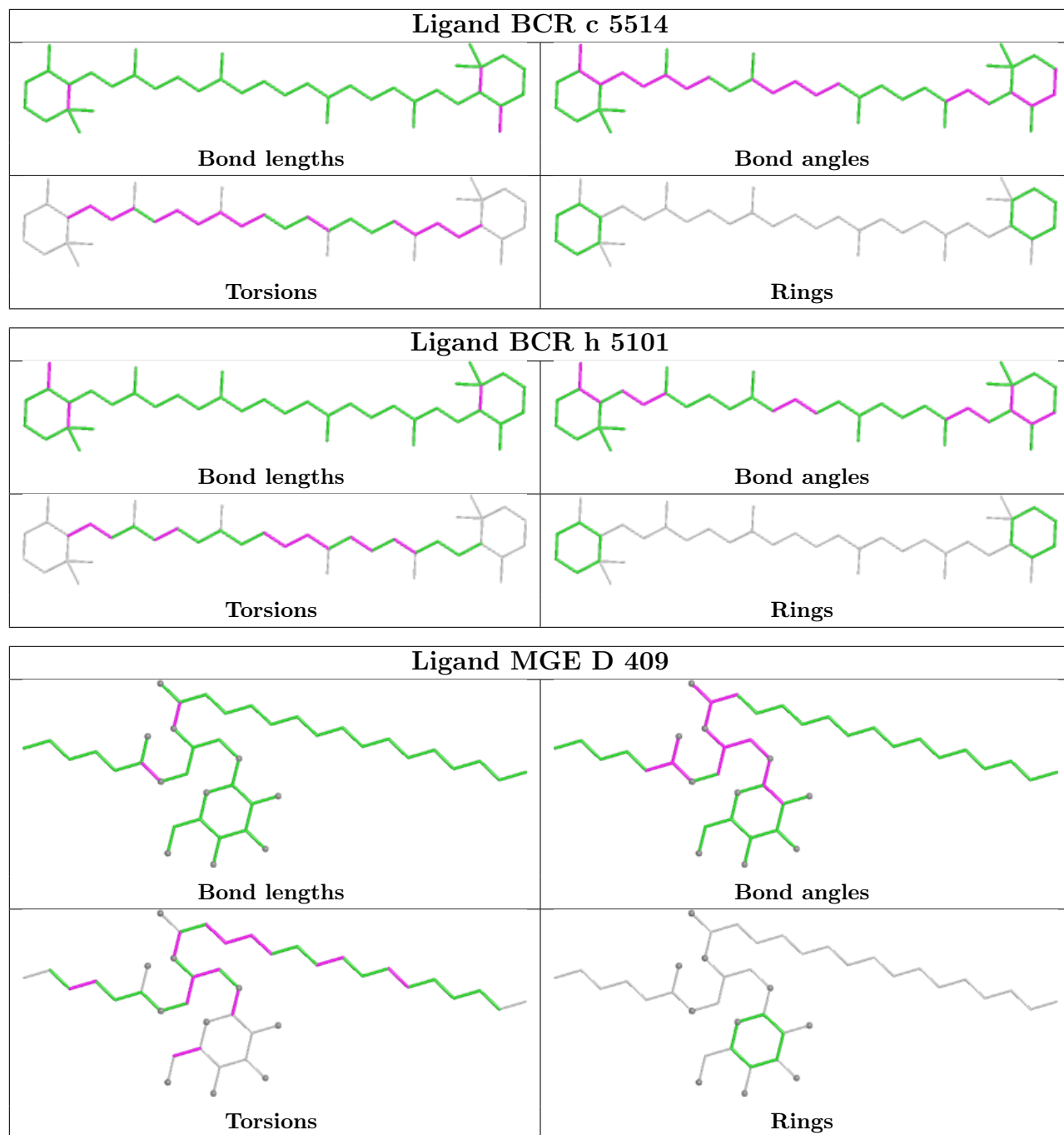
## Ligand CLA C 513

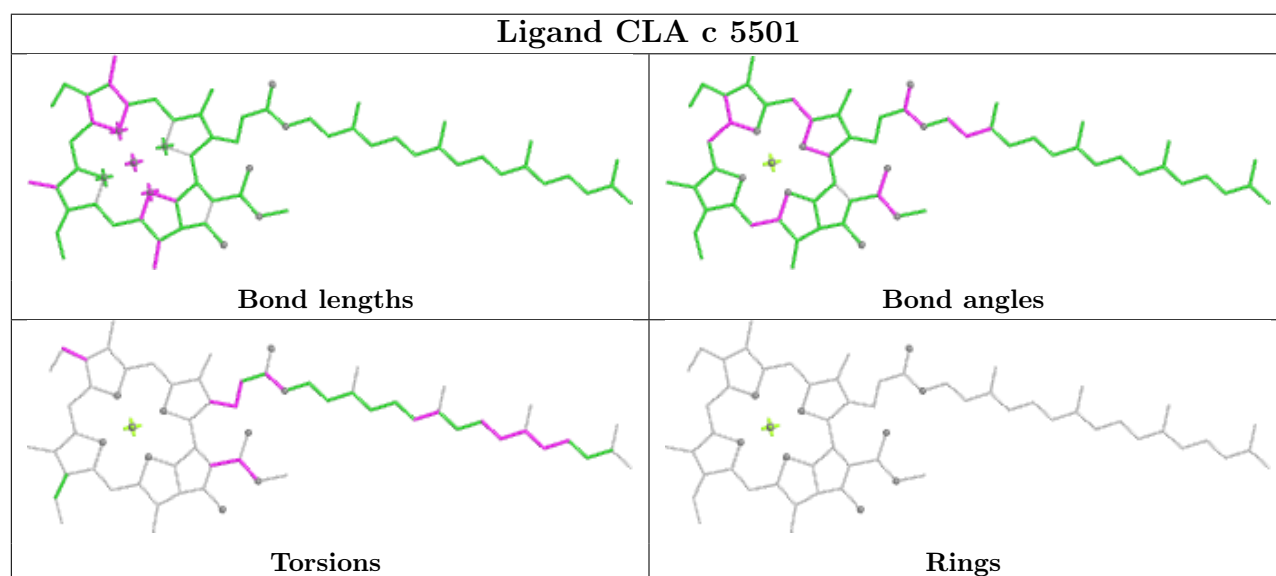
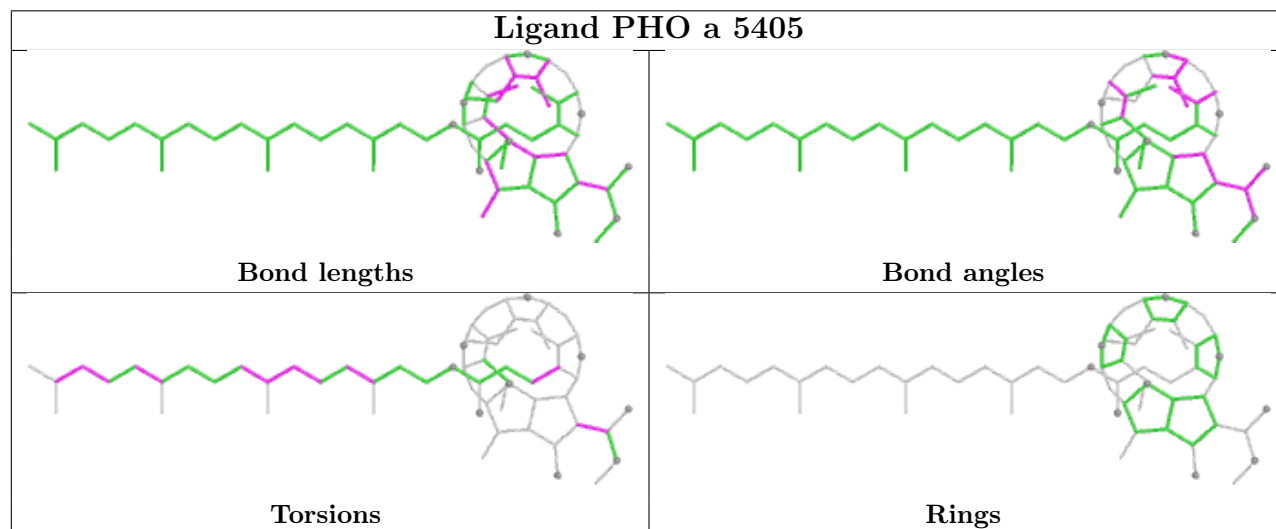
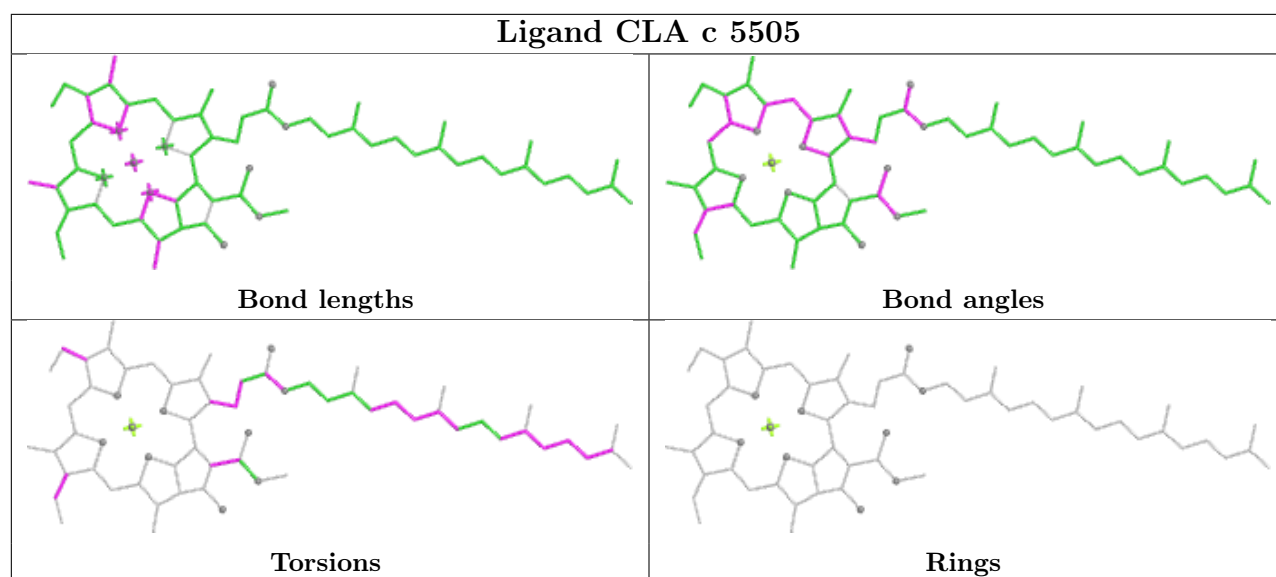


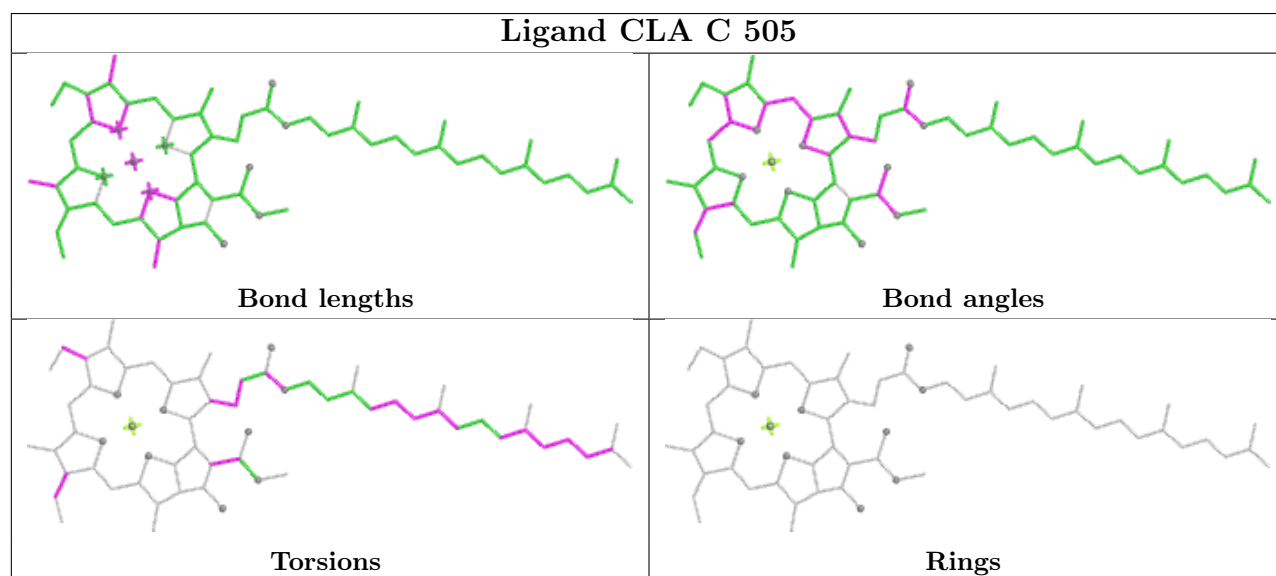
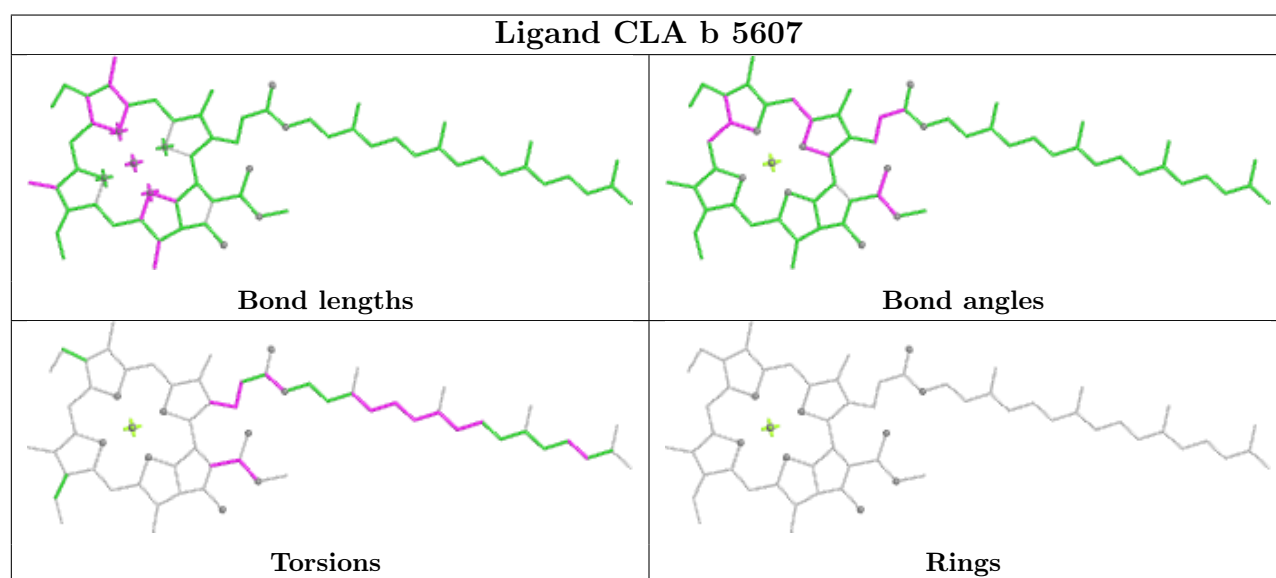
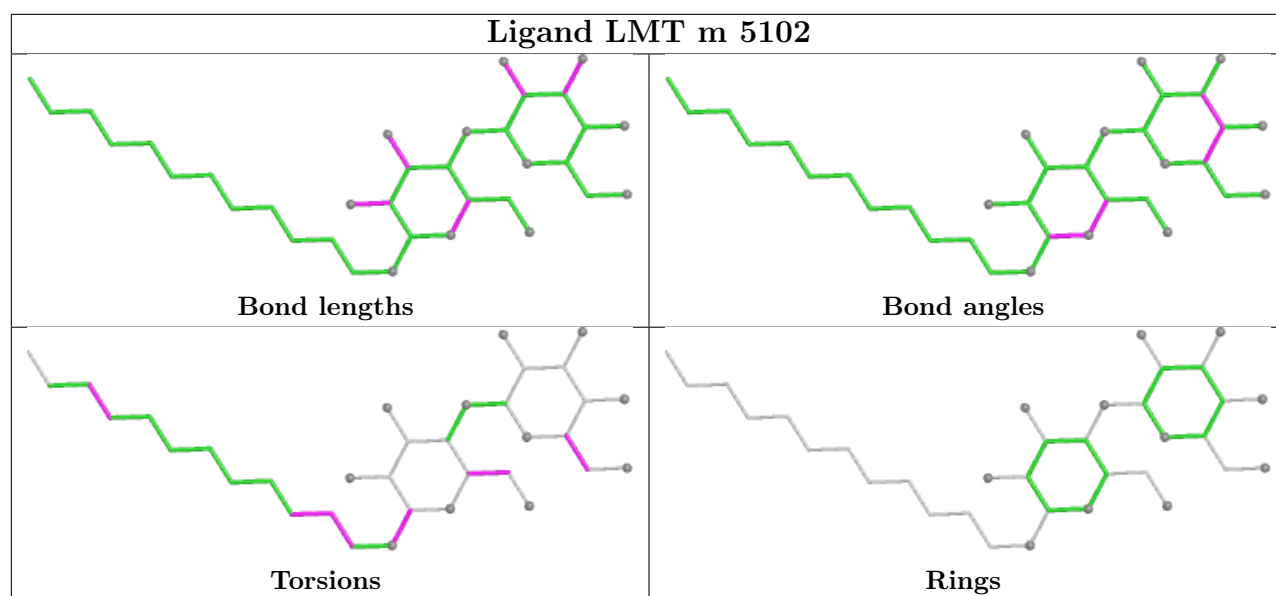
## Ligand CLA B 611

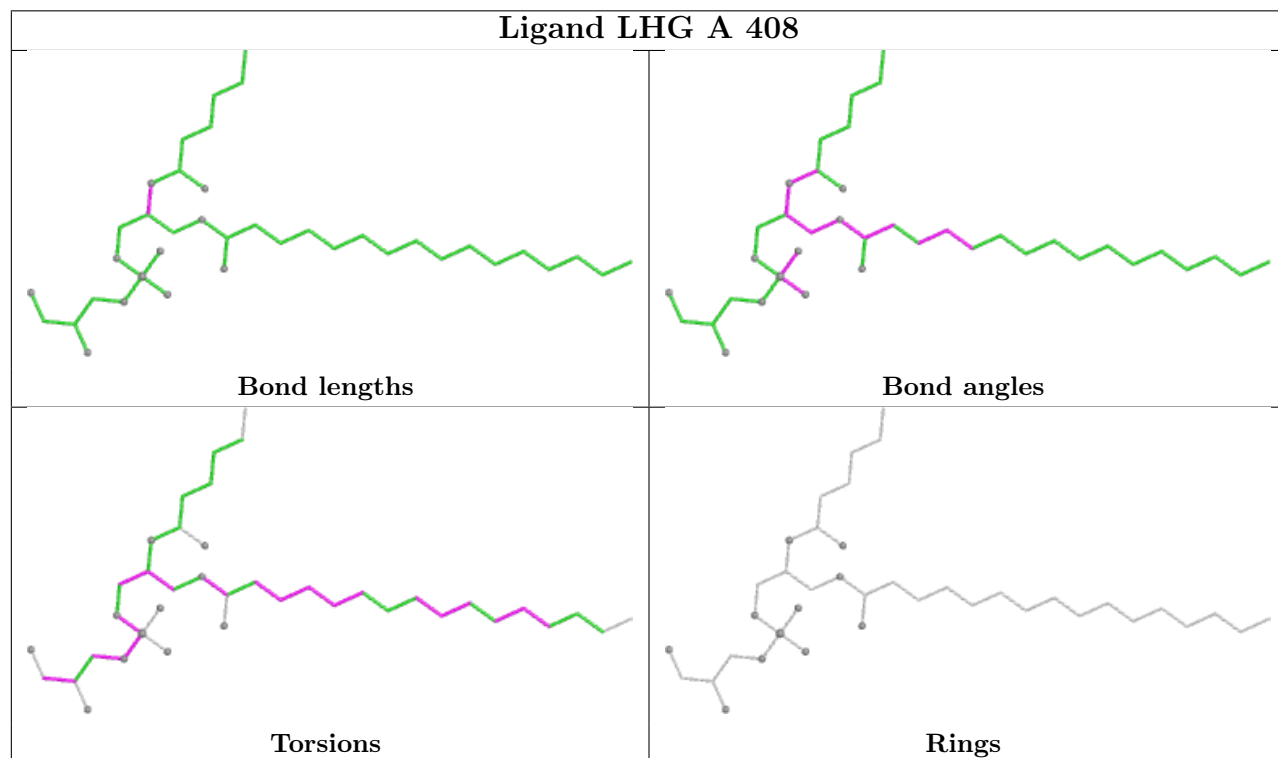
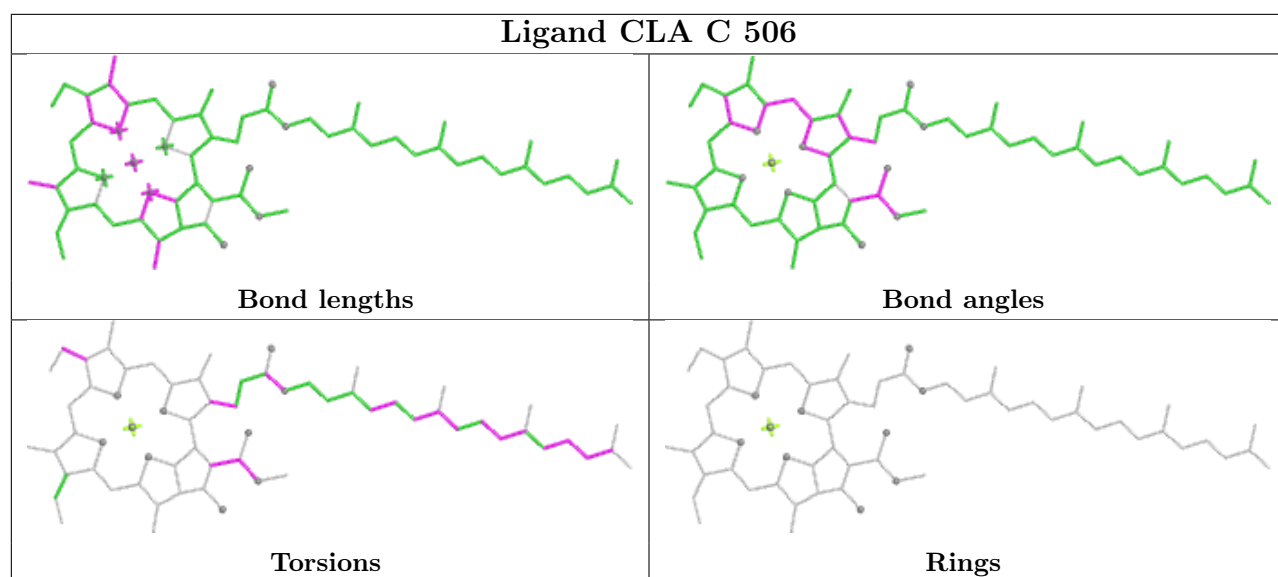


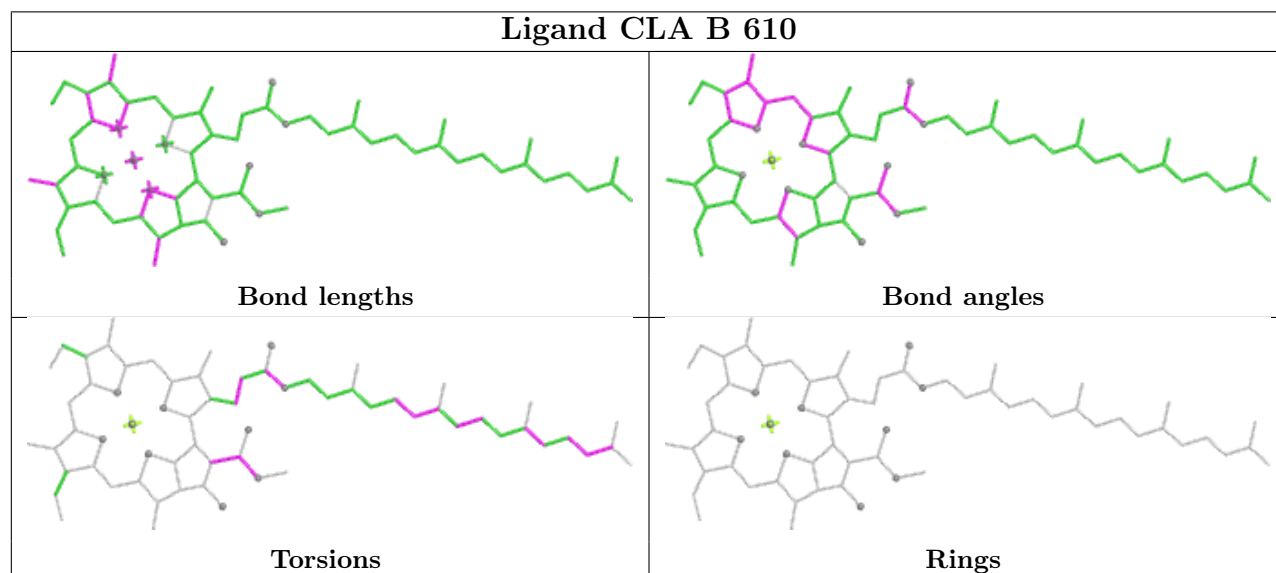
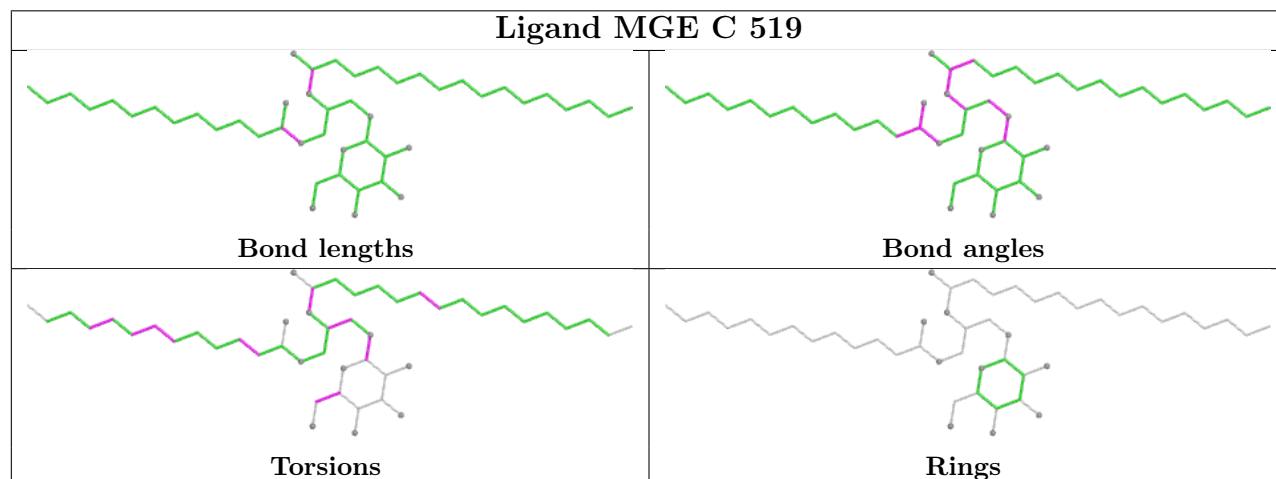
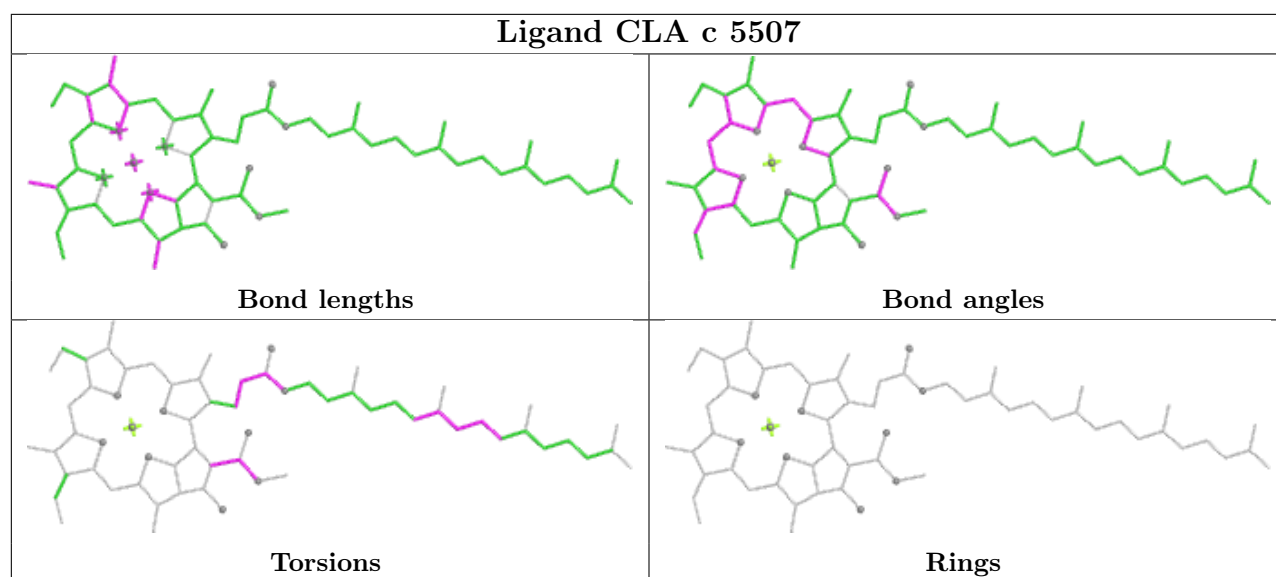


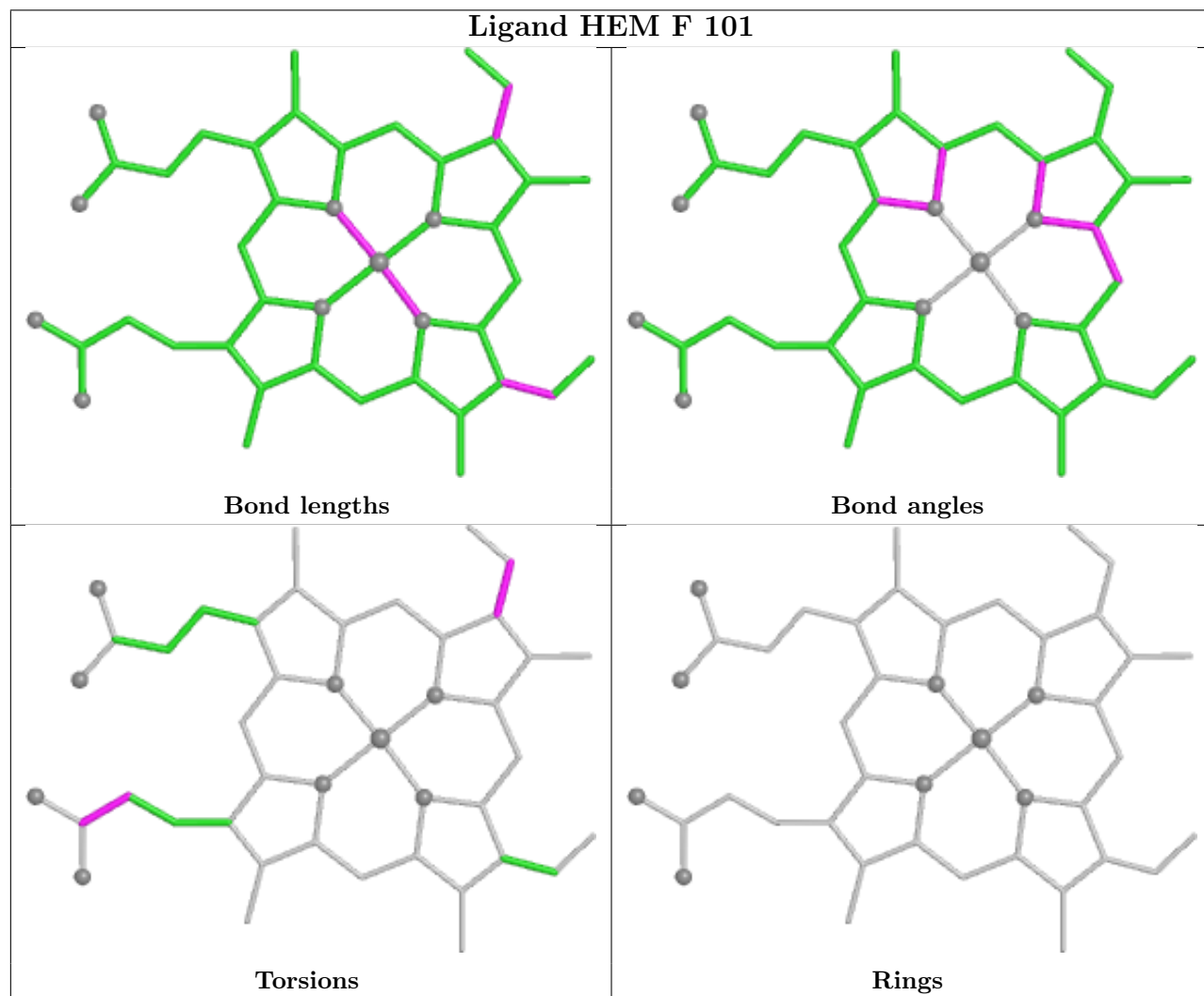
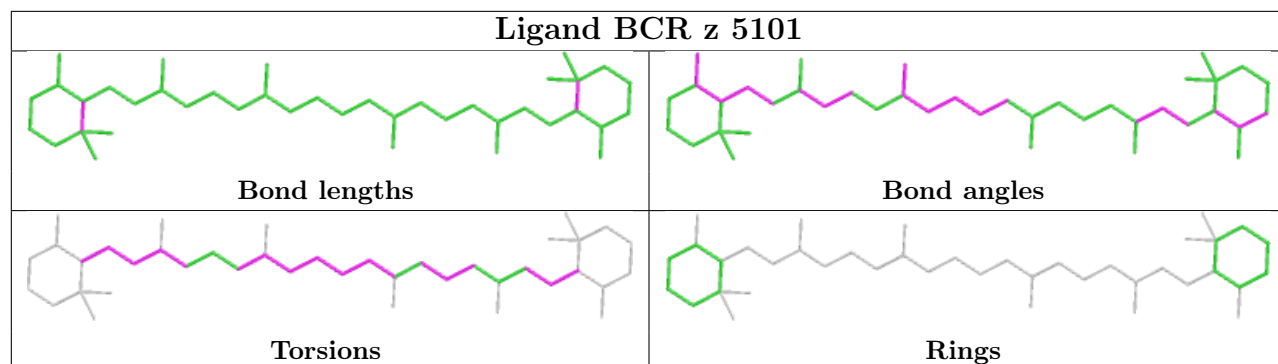


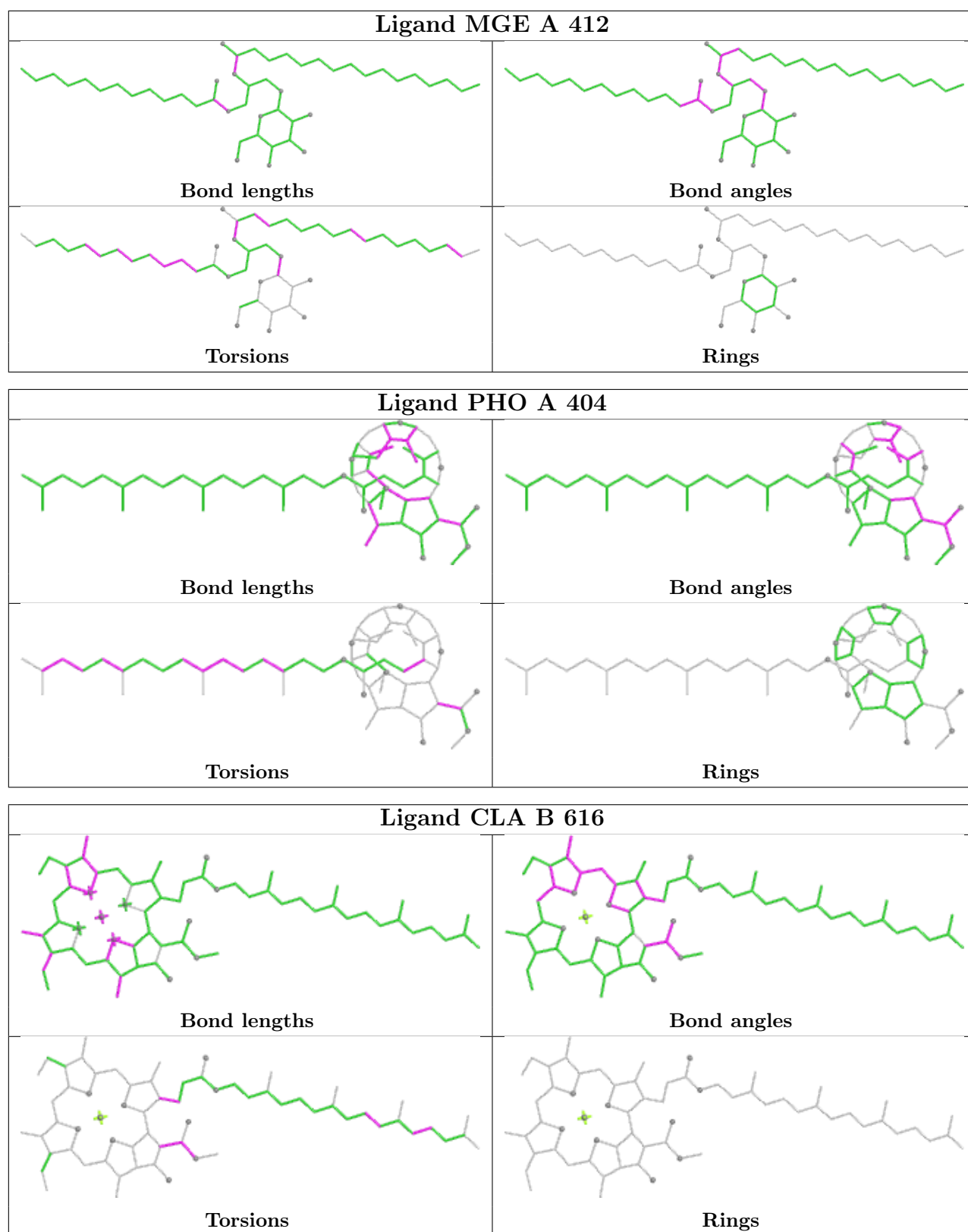


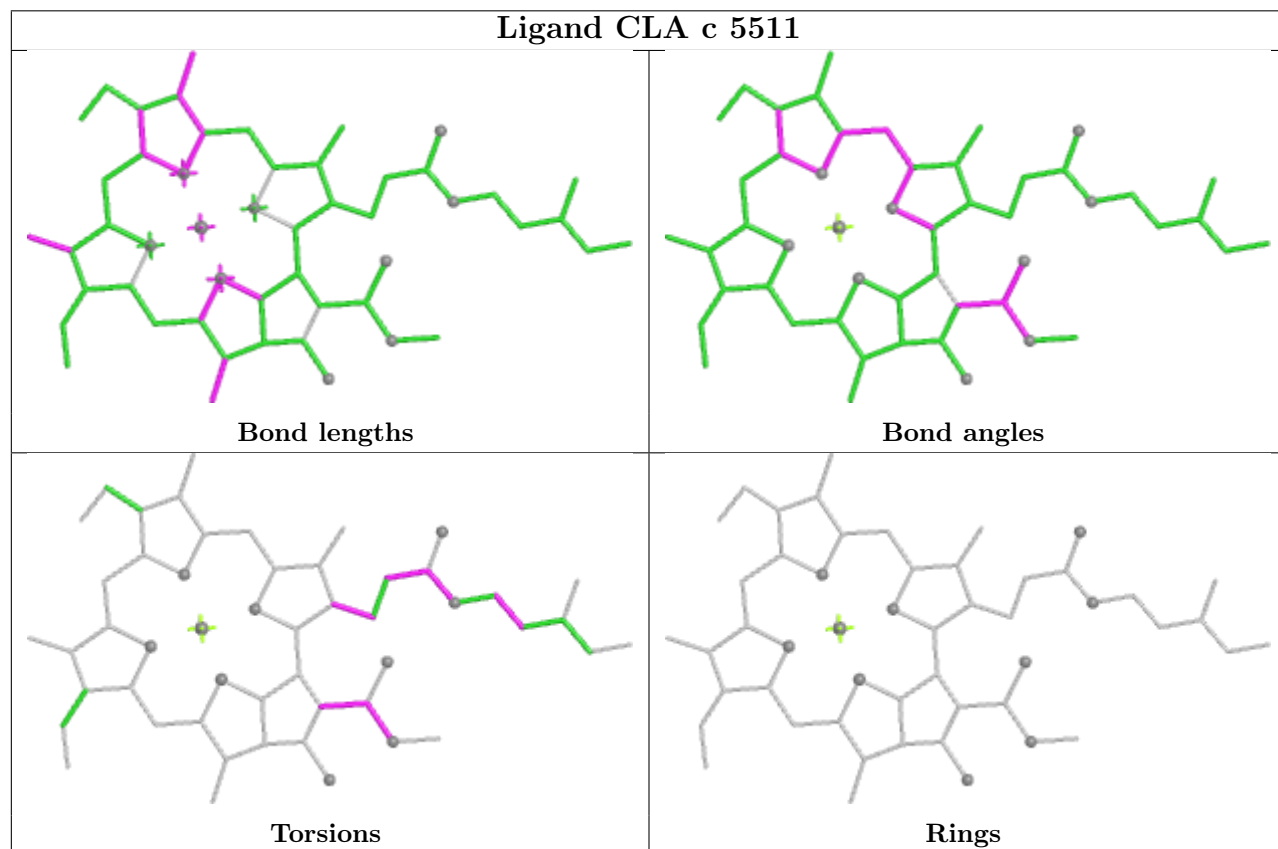
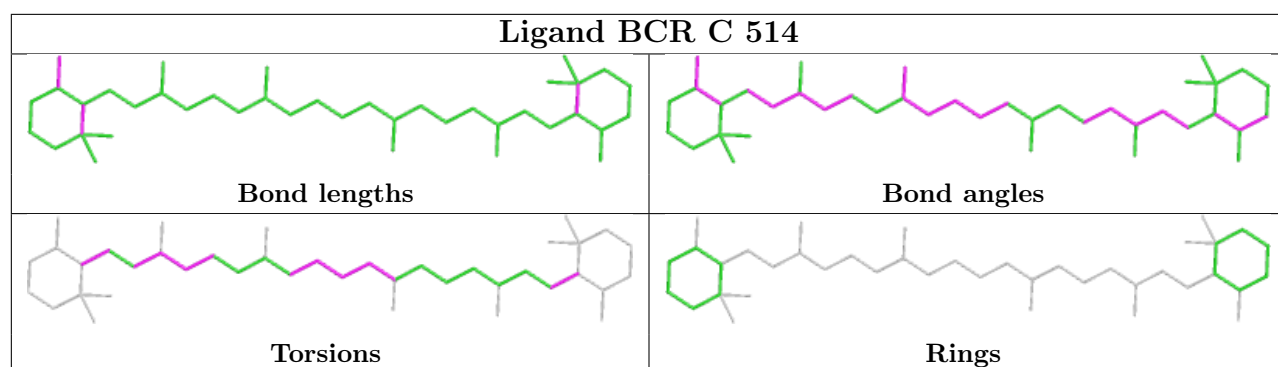


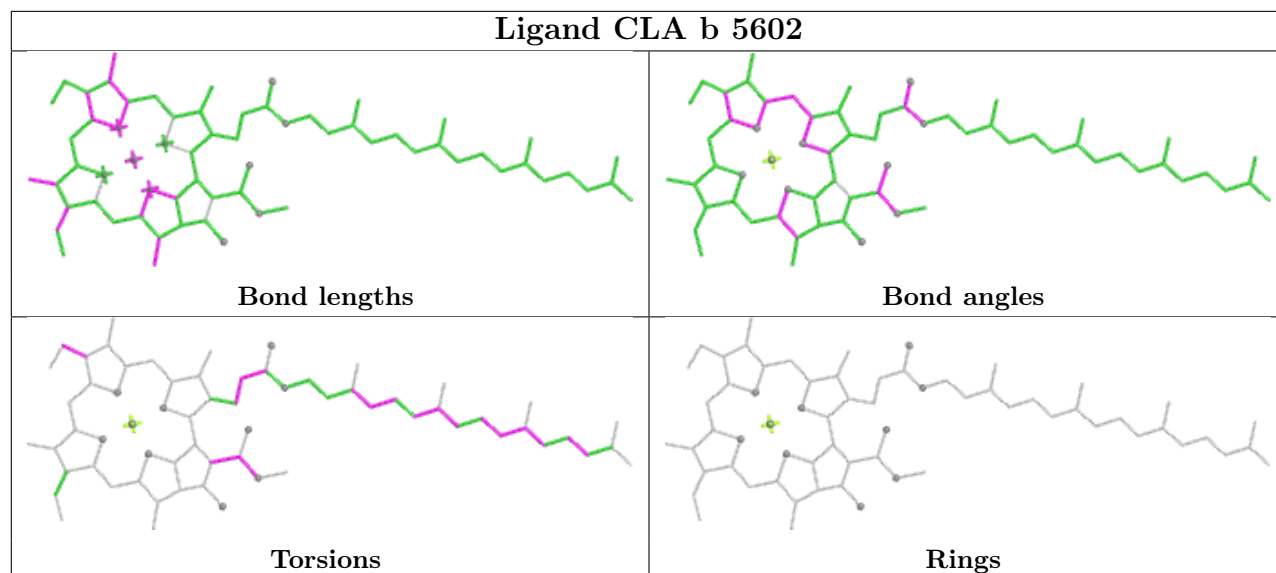
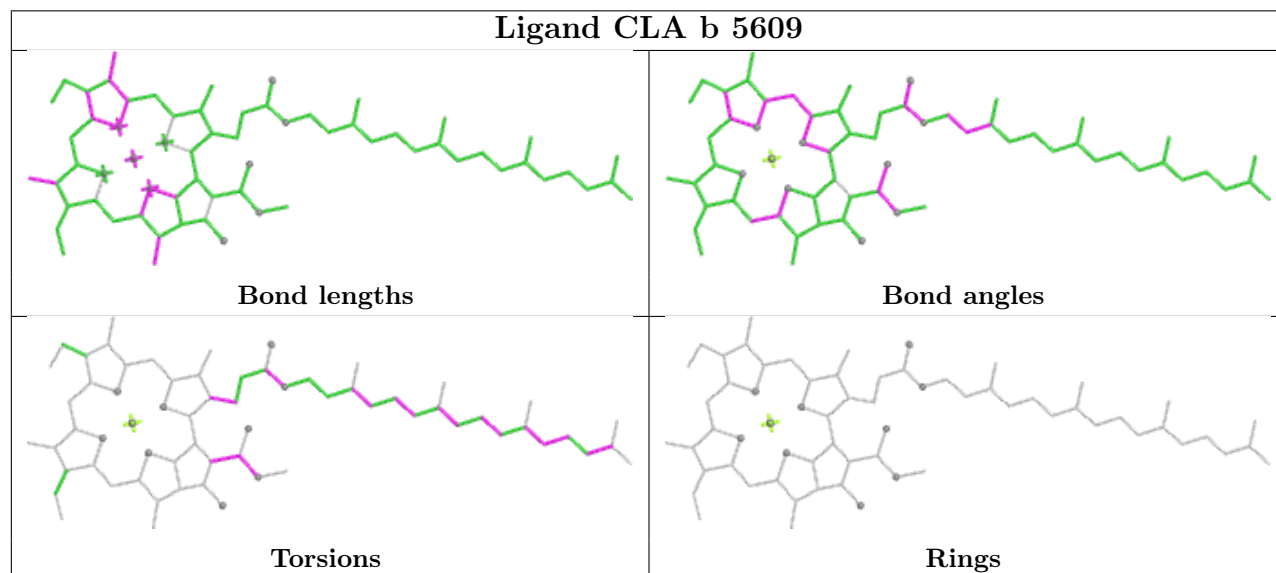
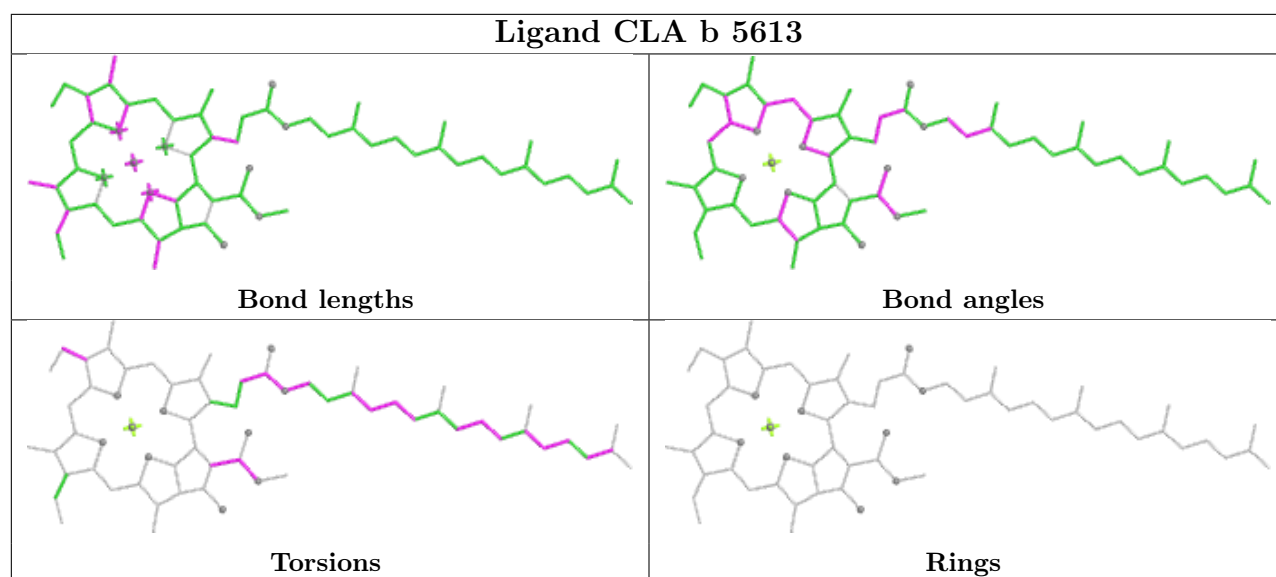


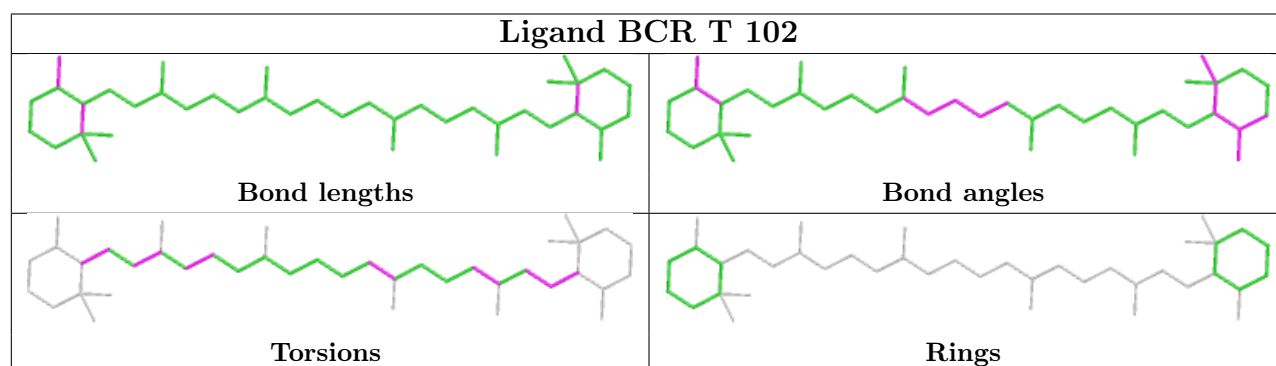
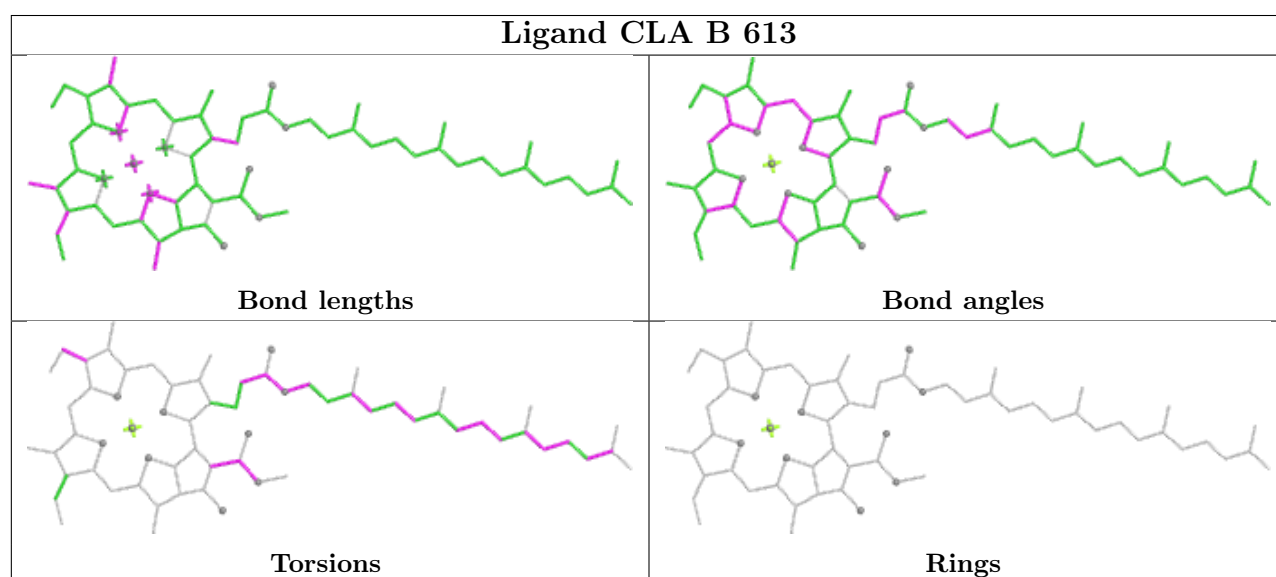
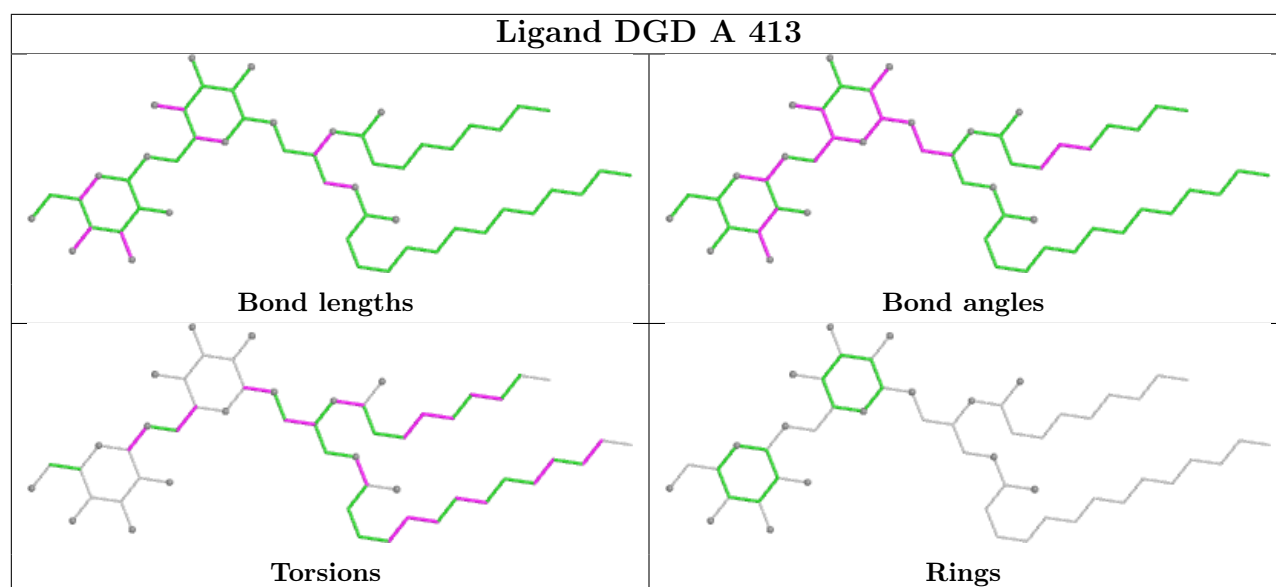


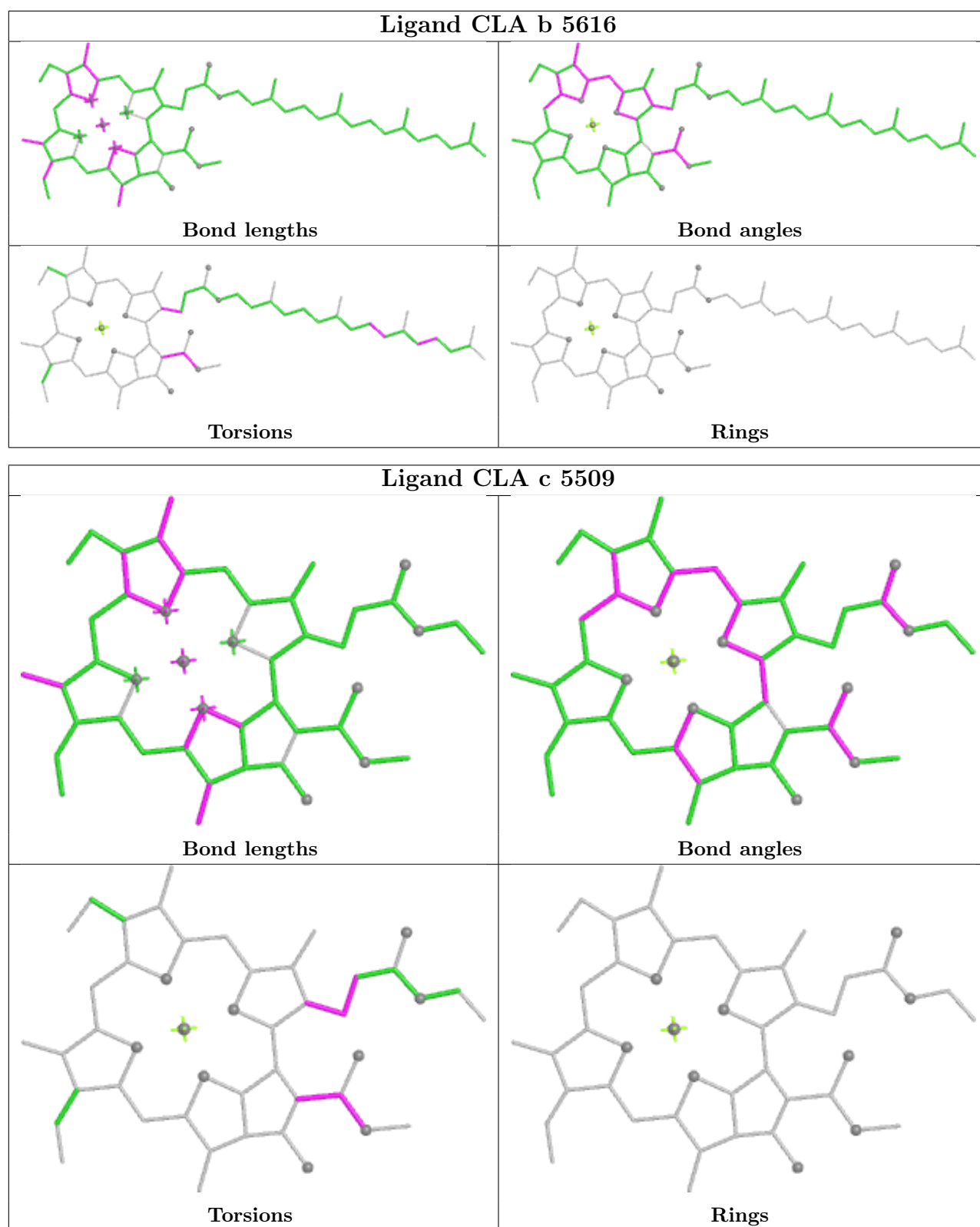












## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

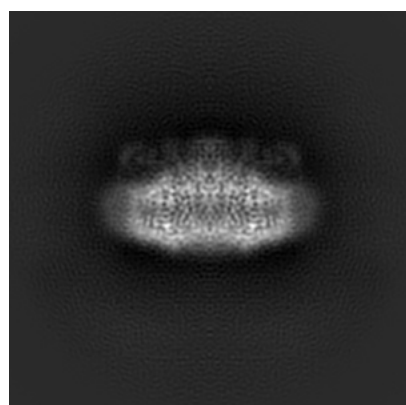
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30511. These allow visual inspection of the internal detail of the map and identification of artifacts.

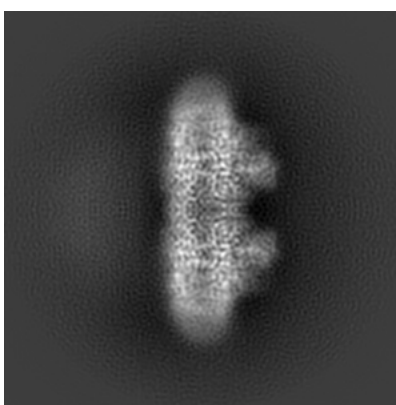
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

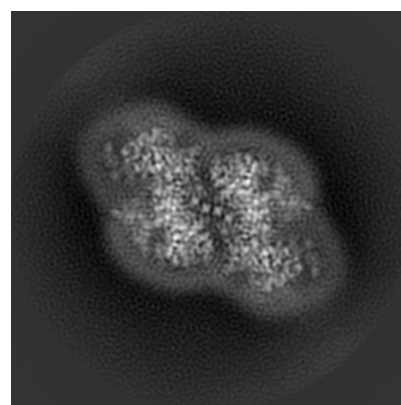
#### 6.1.1 Primary map



X



Y

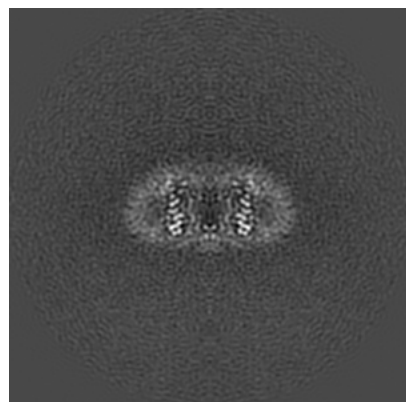


Z

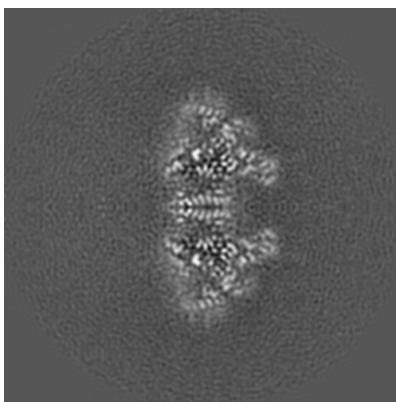
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

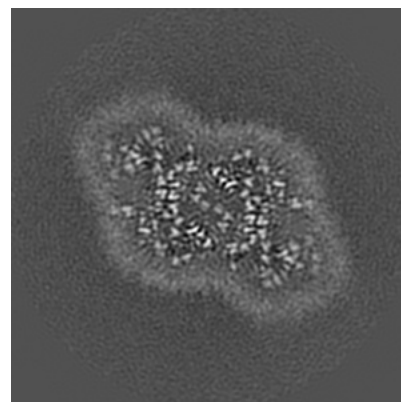
#### 6.2.1 Primary map



X Index: 120



Y Index: 120

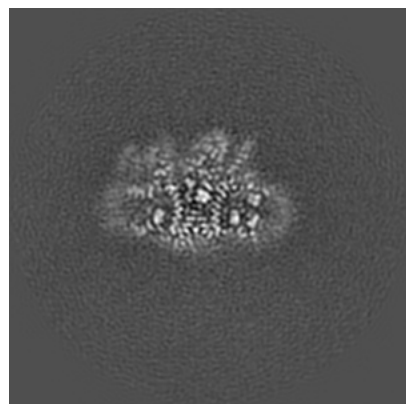


Z Index: 120

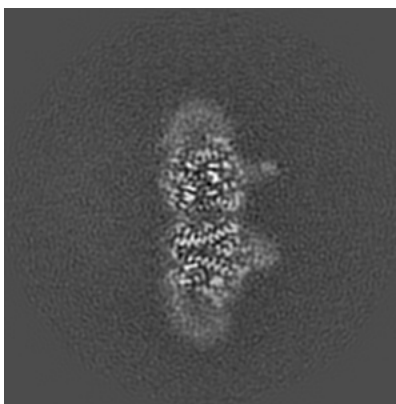
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

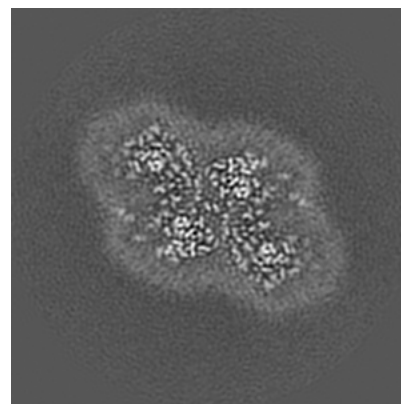
### 6.3.1 Primary map



X Index: 146



Y Index: 144

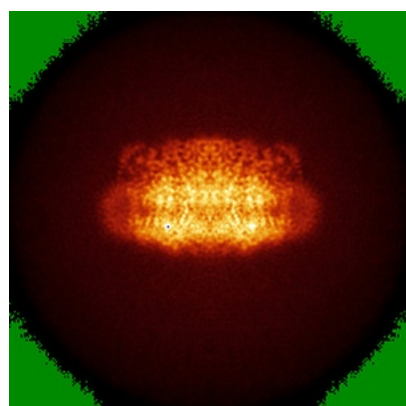


Z Index: 111

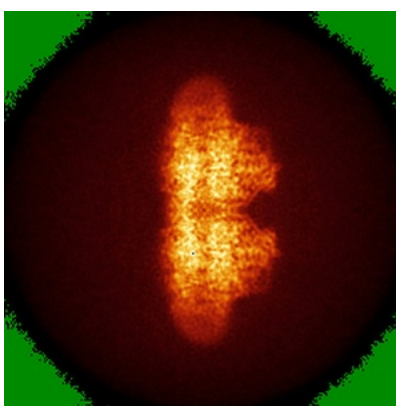
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

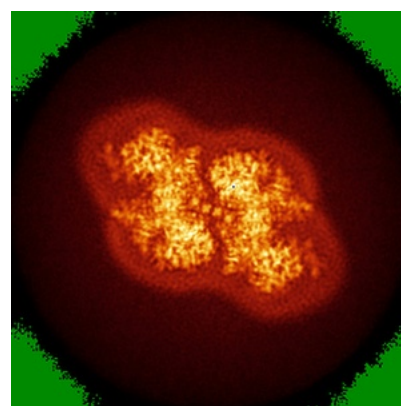
### 6.4.1 Primary map



X



Y

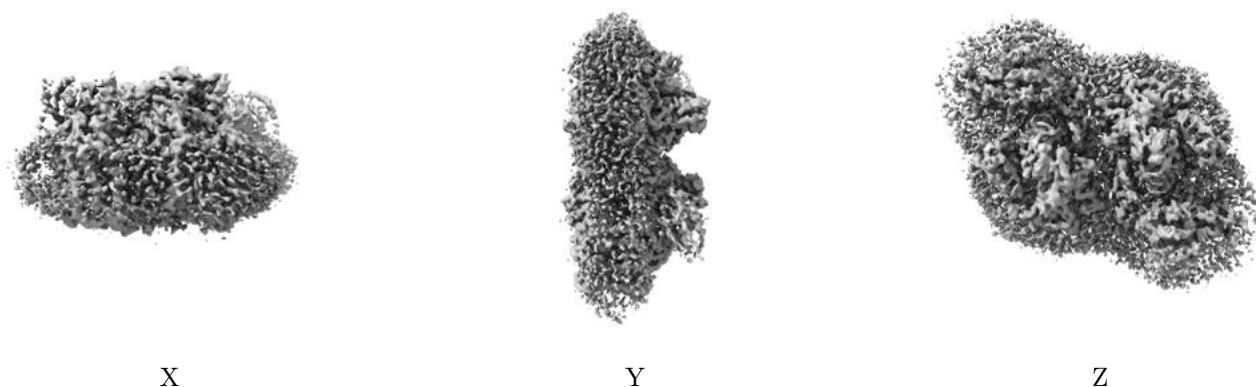


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.038. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

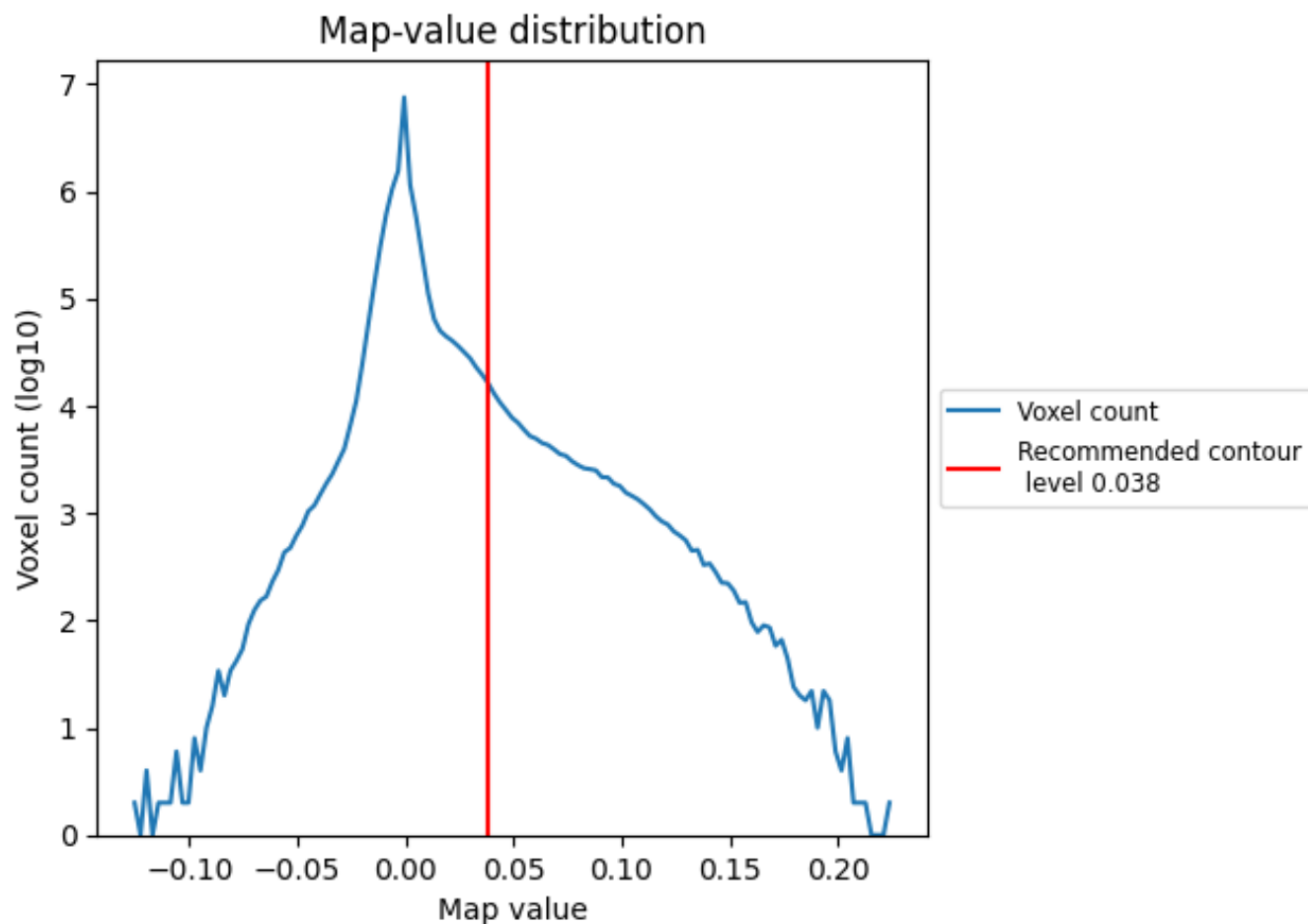
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

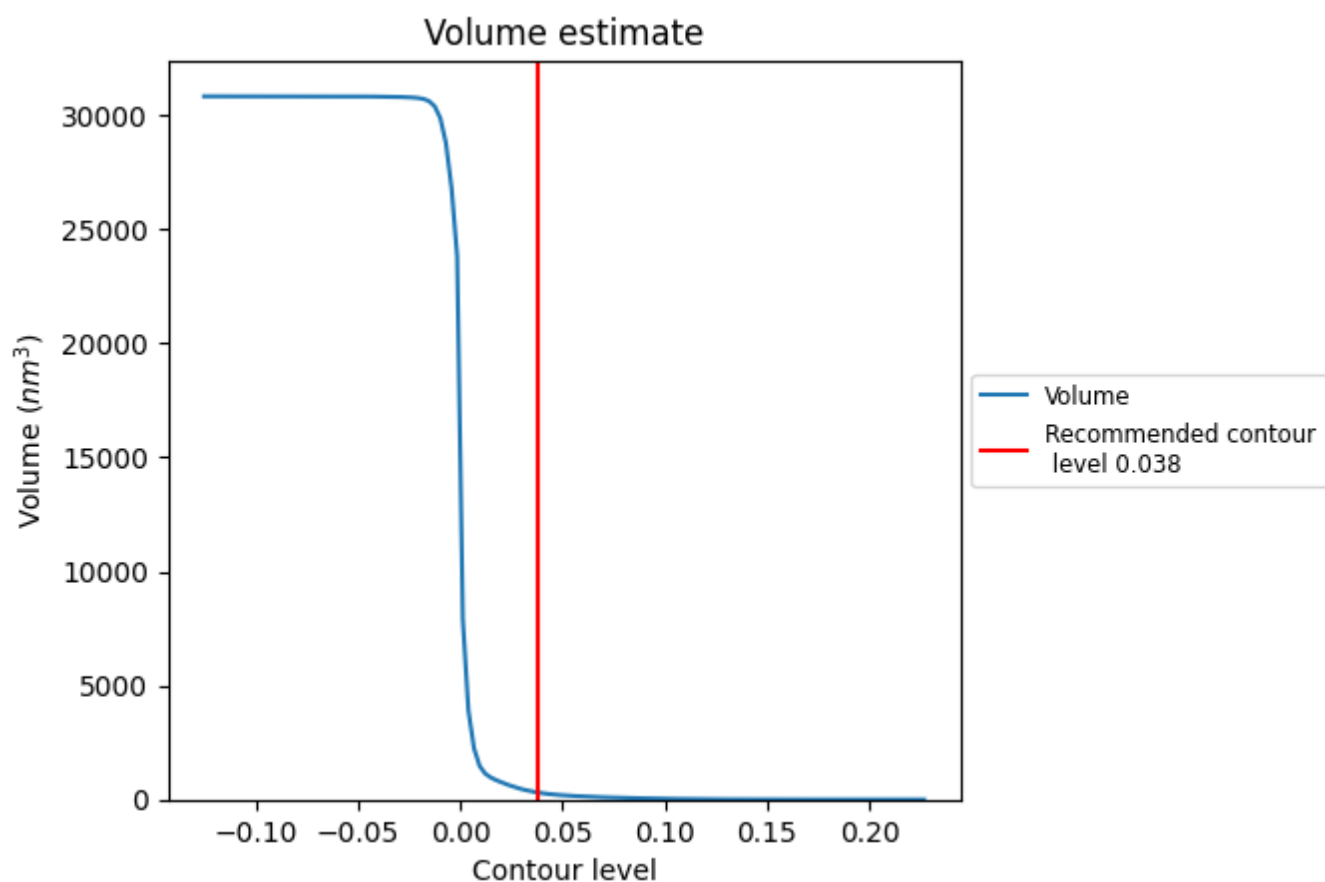
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

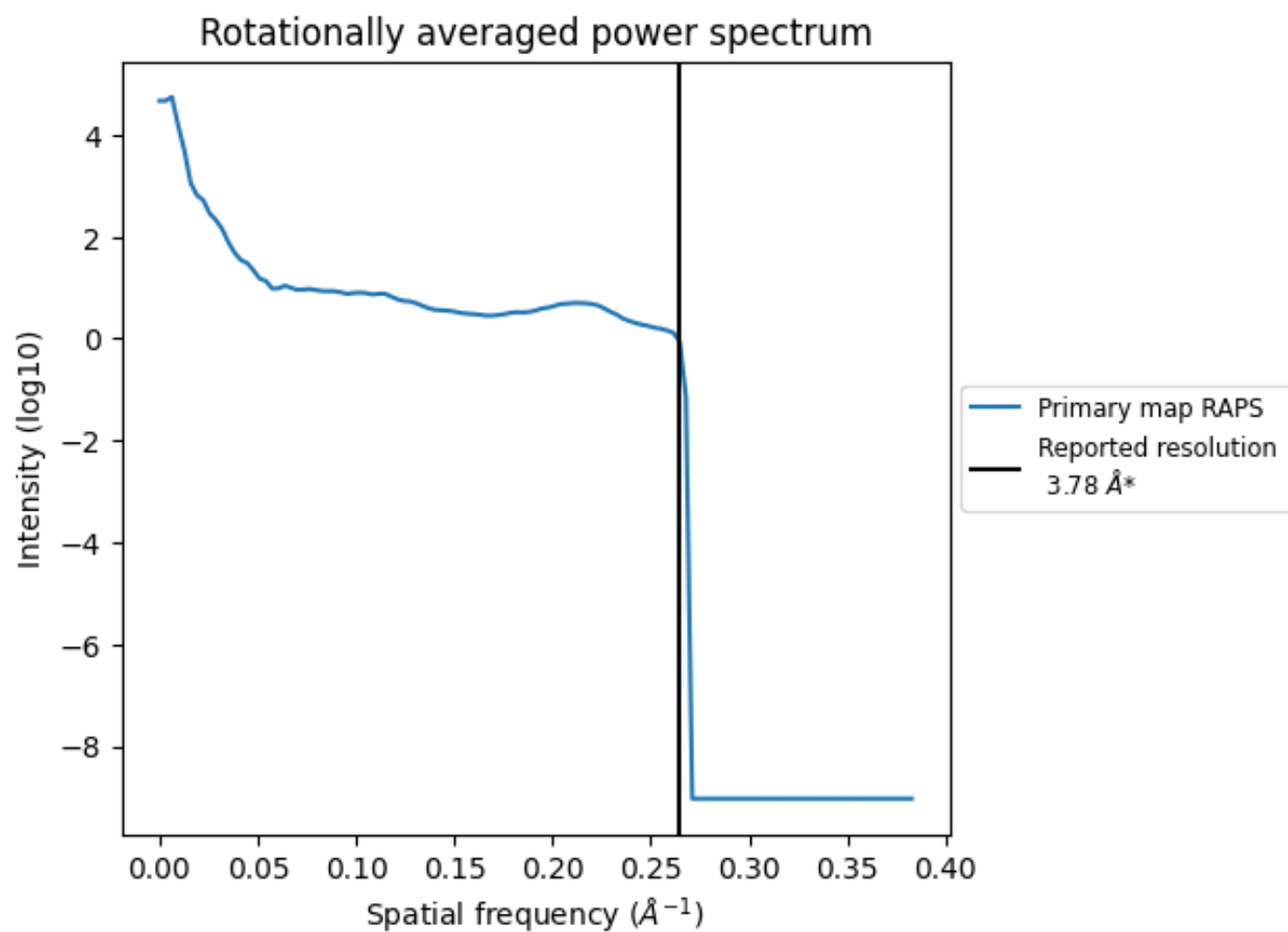
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 307 nm<sup>3</sup>; this corresponds to an approximate mass of 277 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.265 Å<sup>-1</sup>

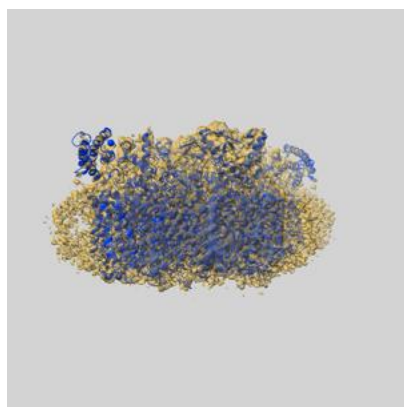
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

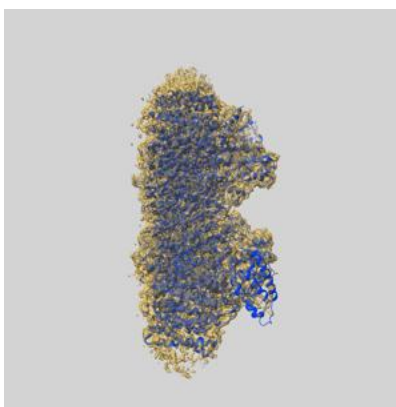
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30511 and PDB model 7CZL. Per-residue inclusion information can be found in [section 3](#) on [page 22](#).

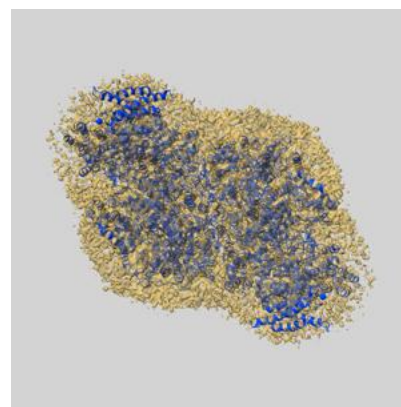
### 9.1 Map-model overlay [i](#)



X



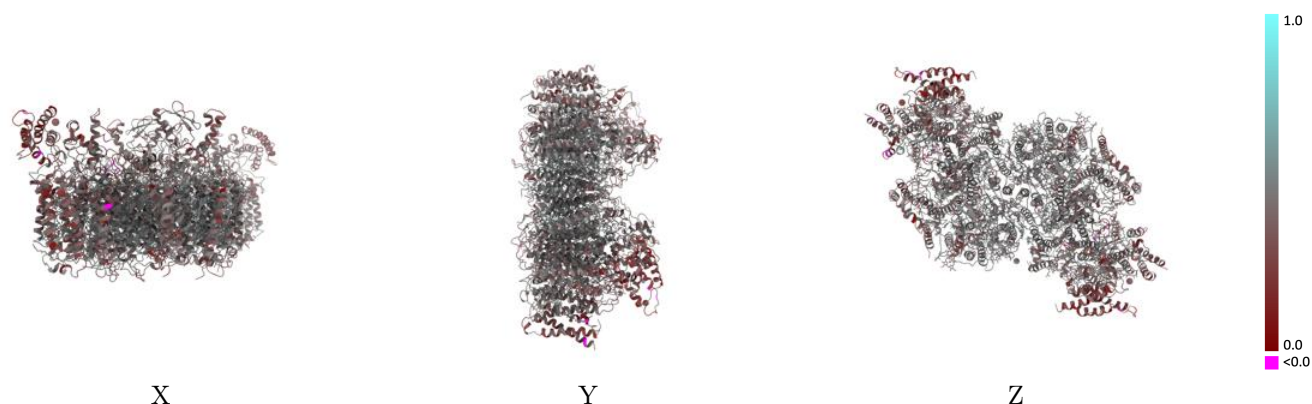
Y



Z

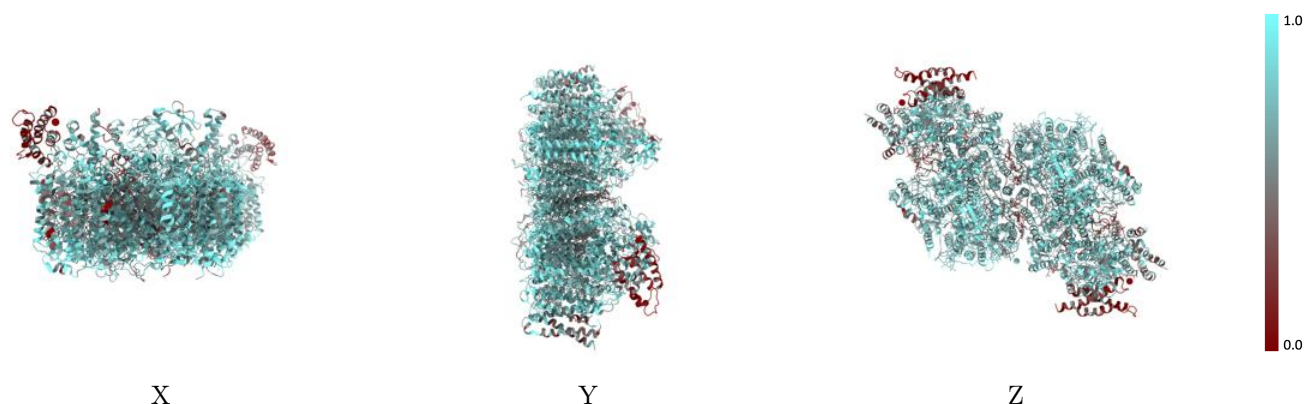
The images above show the 3D surface view of the map at the recommended contour level 0.038 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



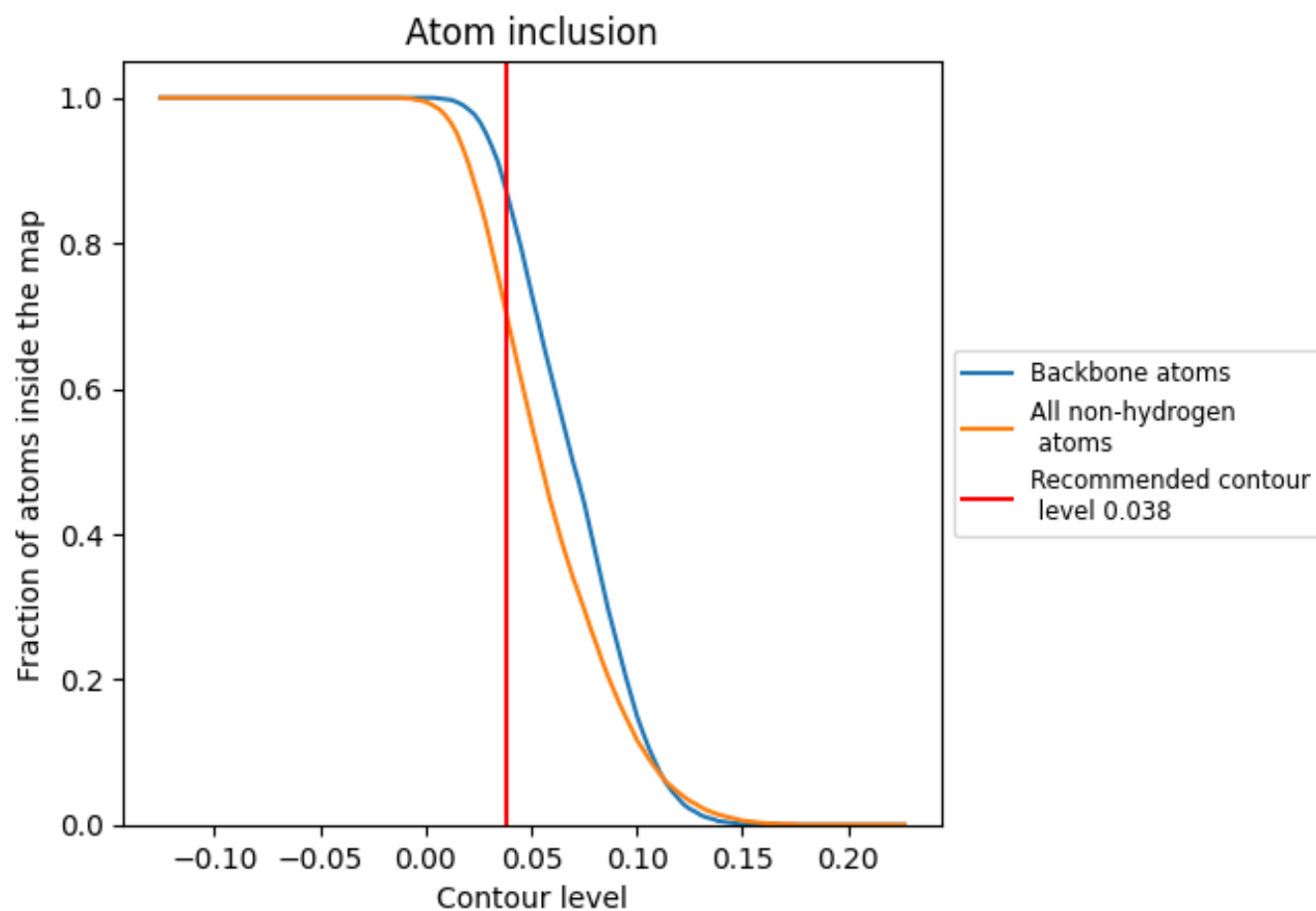
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.038).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.038) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.7080   |  0.4220   |
| A     |  0.7320   |  0.4420   |
| B     |  0.7710   |  0.4490   |
| C     |  0.6990   |  0.4070   |
| D     |  0.7690   |  0.4500   |
| E     |  0.6800   |  0.3720   |
| F     |  0.7410   |  0.3800   |
| H     |  0.8110   |  0.4300   |
| I     |  0.7650   |  0.4150   |
| K     |  0.6700   |  0.3670   |
| L     |  0.6960   |  0.4470   |
| M     |  0.6060   |  0.4270   |
| N     |  0.2210   |  0.2790   |
| T     |  0.6080   |  0.4550   |
| X     |  0.7360  |  0.3700  |
| Y     |  0.4900 |  0.3980 |
| Z     |  0.5290 |  0.3190 |
| a     |  0.7330 |  0.4390 |
| b     |  0.7750 |  0.4510 |
| c     |  0.7080 |  0.4070 |
| d     |  0.7670 |  0.4470 |
| e     |  0.6860 |  0.3680 |
| f     |  0.7410 |  0.3550 |
| h     |  0.7890 |  0.4260 |
| i     |  0.7680 |  0.4200 |
| k     |  0.6530 |  0.4010 |
| l     |  0.6610 |  0.4700 |
| m     |  0.5950 |  0.4350 |
| n     |  0.2060 |  0.2740 |
| t     |  0.6630 |  0.4710 |
| x     |  0.7640 |  0.3980 |
| y     |  0.5020 |  0.3350 |
| z     |  0.5150 |  0.3210 |

