



## wwPDB EM Validation Summary Report ⓘ

Sep 5, 2026 – 12:04 pm BST

PDB ID : 9TLH / pdb\_00009tlh  
EMDB ID : EMD-56055  
Title : Cryo-EM Structure of the oligomeric LPOR:Chlide:NADPH Complexes HF-23  
Authors : Gabruk, M.; Desfosses, A.; Estrozi, L.F.; Pintscher, S.; Rawski, M.  
Deposited on : 2025-12-10  
Resolution : 3.03 Å(reported)

This is a wwPDB EM Validation Summary 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>.

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

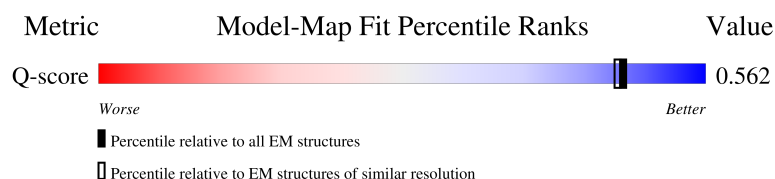
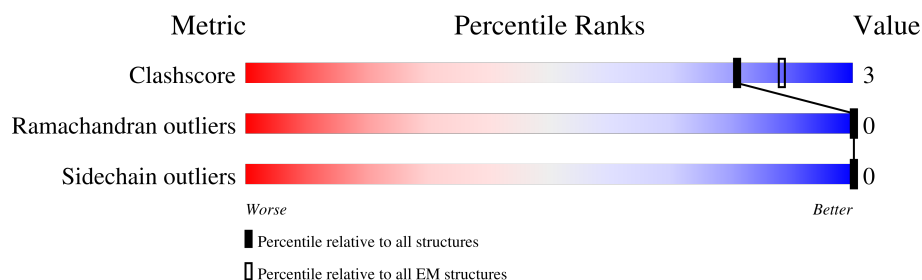
EMDB validation analysis : 0.0.1.dev133  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using 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

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

The reported resolution of this entry is 3.03 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.



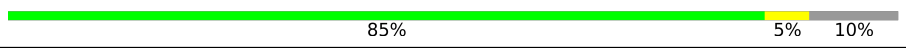
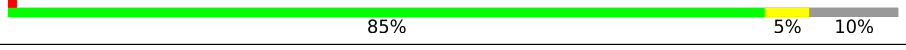
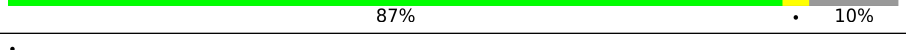
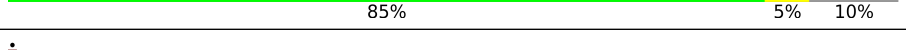
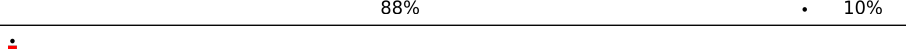
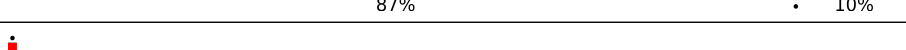
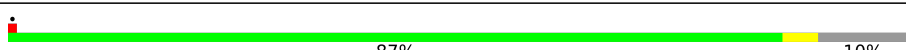
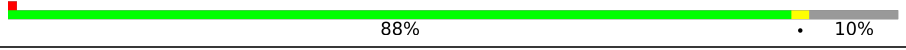
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 13929 ( 2.53 - 3.53 )                                    |

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   | AA    | 353    |                  |
| 1   | AB    | 353    |                  |
| 1   | AC    | 353    |                  |
| 1   | AD    | 353    |                  |

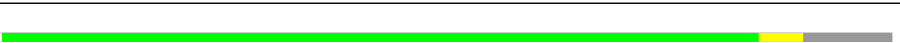
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | AE    | 353    |    |
| 1   | AF    | 353    |    |
| 1   | AG    | 353    |    |
| 1   | AH    | 353    |    |
| 1   | AI    | 353    |    |
| 1   | AJ    | 353    |    |
| 1   | AK    | 353    |    |
| 1   | AL    | 353    |    |
| 1   | BA    | 353    |    |
| 1   | BB    | 353    |    |
| 1   | BC    | 353    |    |
| 1   | BD    | 353    |  |
| 1   | BE    | 353    |  |
| 1   | BF    | 353    |  |
| 1   | BG    | 353    |  |
| 1   | BH    | 353    |  |
| 1   | BI    | 353    |  |
| 1   | BJ    | 353    |  |
| 1   | BK    | 353    |  |
| 1   | BL    | 353    |  |
| 1   | CA    | 353    |  |
| 1   | CB    | 353    |  |
| 1   | CC    | 353    |  |
| 1   | CD    | 353    |  |
| 1   | CE    | 353    |  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | CF    | 353    |    |
| 1   | CG    | 353    |    |
| 1   | CH    | 353    |    |
| 1   | CI    | 353    |    |
| 1   | CJ    | 353    |    |
| 1   | CK    | 353    |    |
| 1   | CL    | 353    |    |
| 1   | DA    | 353    |    |
| 1   | DB    | 353    |    |
| 1   | DC    | 353    |    |
| 1   | DD    | 353    |    |
| 1   | DE    | 353    |    |
| 1   | DF    | 353    |  |
| 1   | DG    | 353    |  |
| 1   | DH    | 353    |  |

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 |
|-----|-------|-------|-----|-----------|----------|---------|------------------|
| 4   | A1JWG | AA    | 503 | X         | -        | -       | -                |
| 4   | A1JWG | AB    | 502 | X         | -        | -       | -                |
| 4   | A1JWG | AC    | 502 | X         | -        | -       | -                |
| 4   | A1JWG | AD    | 503 | X         | -        | -       | -                |
| 4   | A1JWG | AE    | 701 | X         | -        | -       | -                |
| 4   | A1JWG | AF    | 503 | X         | -        | -       | -                |
| 4   | A1JWG | AG    | 701 | X         | -        | -       | -                |
| 4   | A1JWG | AH    | 701 | X         | -        | -       | -                |
| 4   | A1JWG | AI    | 503 | X         | -        | -       | -                |
| 4   | A1JWG | AJ    | 502 | X         | -        | -       | -                |
| 4   | A1JWG | AK    | 503 | X         | -        | -       | -                |
| 4   | A1JWG | AL    | 502 | X         | -        | -       | -                |

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| Mol | Type  | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|-------|-------|-----|-----------|----------|---------|------------------|
| 4   | A1JWG | BA    | 503 | X         | -        | -       | -                |
| 4   | A1JWG | BB    | 503 | X         | -        | -       | -                |
| 4   | A1JWG | BC    | 502 | X         | -        | -       | -                |
| 4   | A1JWG | BD    | 503 | X         | -        | -       | -                |
| 4   | A1JWG | BE    | 503 | X         | -        | -       | -                |
| 4   | A1JWG | BF    | 503 | X         | -        | -       | -                |
| 4   | A1JWG | BG    | 502 | X         | -        | -       | -                |
| 4   | A1JWG | BH    | 701 | X         | -        | -       | -                |
| 4   | A1JWG | BI    | 701 | X         | -        | -       | -                |
| 4   | A1JWG | BJ    | 502 | X         | -        | -       | -                |
| 4   | A1JWG | BK    | 503 | X         | -        | -       | -                |
| 4   | A1JWG | BL    | 701 | X         | -        | -       | -                |
| 4   | A1JWG | CA    | 701 | X         | -        | -       | -                |
| 4   | A1JWG | CB    | 502 | X         | -        | -       | -                |
| 4   | A1JWG | CC    | 503 | X         | -        | -       | -                |
| 4   | A1JWG | CD    | 503 | X         | -        | -       | -                |
| 4   | A1JWG | CE    | 502 | X         | -        | -       | -                |
| 4   | A1JWG | CF    | 503 | X         | -        | -       | -                |
| 4   | A1JWG | CG    | 503 | X         | -        | -       | -                |
| 4   | A1JWG | CH    | 503 | X         | -        | -       | -                |
| 4   | A1JWG | CI    | 502 | X         | -        | -       | -                |
| 4   | A1JWG | CJ    | 503 | X         | -        | -       | -                |
| 4   | A1JWG | CK    | 502 | X         | -        | -       | -                |
| 4   | A1JWG | CL    | 503 | X         | -        | -       | -                |
| 4   | A1JWG | DA    | 502 | X         | -        | -       | -                |
| 4   | A1JWG | DB    | 701 | X         | -        | -       | -                |
| 4   | A1JWG | DC    | 701 | X         | -        | -       | -                |
| 4   | A1JWG | DD    | 701 | X         | -        | -       | -                |
| 4   | A1JWG | DE    | 701 | X         | -        | -       | -                |
| 4   | A1JWG | DF    | 502 | X         | -        | -       | -                |
| 4   | A1JWG | DG    | 502 | X         | -        | -       | -                |
| 4   | A1JWG | DH    | 503 | X         | -        | -       | -                |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 219249 atoms, of which 106890 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 Protochlorophyllide reductase B, chloroplastic.

| Mol | Chain | Residues | Atoms         |           |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|-----------|----------|----------|---------|---------|-------|
| 1   | AA    | 319      | Total<br>4843 | C<br>1550 | H<br>2397 | N<br>423 | O<br>463 | S<br>10 | 0       | 0     |
| 1   | AB    | 319      | Total<br>4843 | C<br>1550 | H<br>2397 | N<br>423 | O<br>463 | S<br>10 | 0       | 0     |
| 1   | AC    | 319      | Total<br>4843 | C<br>1550 | H<br>2397 | N<br>423 | O<br>463 | S<br>10 | 0       | 0     |
| 1   | AD    | 315      | Total<br>4800 | C<br>1528 | H<br>2387 | N<br>417 | O<br>458 | S<br>10 | 0       | 0     |
| 1   | AE    | 319      | Total<br>4843 | C<br>1550 | H<br>2397 | N<br>423 | O<br>463 | S<br>10 | 0       | 0     |
| 1   | AF    | 317      | Total<br>4825 | C<br>1538 | H<br>2397 | N<br>419 | O<br>461 | S<br>10 | 0       | 0     |
| 1   | AG    | 317      | Total<br>4825 | C<br>1538 | H<br>2397 | N<br>419 | O<br>461 | S<br>10 | 0       | 0     |
| 1   | AH    | 319      | Total<br>4843 | C<br>1550 | H<br>2397 | N<br>423 | O<br>463 | S<br>10 | 0       | 0     |
| 1   | AI    | 317      | Total<br>4825 | C<br>1538 | H<br>2397 | N<br>419 | O<br>461 | S<br>10 | 0       | 0     |
| 1   | AJ    | 319      | Total<br>4843 | C<br>1550 | H<br>2397 | N<br>423 | O<br>463 | S<br>10 | 0       | 0     |
| 1   | AK    | 317      | Total<br>4825 | C<br>1538 | H<br>2397 | N<br>419 | O<br>461 | S<br>10 | 0       | 0     |
| 1   | AL    | 319      | Total<br>4843 | C<br>1550 | H<br>2397 | N<br>423 | O<br>463 | S<br>10 | 0       | 0     |
| 1   | BA    | 319      | Total<br>4843 | C<br>1550 | H<br>2397 | N<br>423 | O<br>463 | S<br>10 | 0       | 0     |
| 1   | BB    | 319      | Total<br>4843 | C<br>1550 | H<br>2397 | N<br>423 | O<br>463 | S<br>10 | 0       | 0     |
| 1   | BC    | 319      | Total<br>4843 | C<br>1550 | H<br>2397 | N<br>423 | O<br>463 | S<br>10 | 0       | 0     |
| 1   | BD    | 315      | Total<br>4800 | C<br>1528 | H<br>2387 | N<br>417 | O<br>458 | S<br>10 | 0       | 0     |
| 1   | BE    | 319      | Total<br>4843 | C<br>1550 | H<br>2397 | N<br>423 | O<br>463 | S<br>10 | 0       | 0     |

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| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 1   | BF    | 317      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4825  | 1538 | 2397 | 419 | 461 | 10 |         |       |
| 1   | BG    | 317      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4825  | 1538 | 2397 | 419 | 461 | 10 |         |       |
| 1   | BH    | 319      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4843  | 1550 | 2397 | 423 | 463 | 10 |         |       |
| 1   | BI    | 317      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4825  | 1538 | 2397 | 419 | 461 | 10 |         |       |
| 1   | BJ    | 319      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4843  | 1550 | 2397 | 423 | 463 | 10 |         |       |
| 1   | BK    | 317      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4825  | 1538 | 2397 | 419 | 461 | 10 |         |       |
| 1   | BL    | 319      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4843  | 1550 | 2397 | 423 | 463 | 10 |         |       |
| 1   | CA    | 319      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4843  | 1550 | 2397 | 423 | 463 | 10 |         |       |
| 1   | CB    | 319      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4843  | 1550 | 2397 | 423 | 463 | 10 |         |       |
| 1   | CC    | 319      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4843  | 1550 | 2397 | 423 | 463 | 10 |         |       |
| 1   | CD    | 315      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4800  | 1528 | 2387 | 417 | 458 | 10 |         |       |
| 1   | CE    | 319      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4843  | 1550 | 2397 | 423 | 463 | 10 |         |       |
| 1   | CF    | 317      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4825  | 1538 | 2397 | 419 | 461 | 10 |         |       |
| 1   | CG    | 317      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4825  | 1538 | 2397 | 419 | 461 | 10 |         |       |
| 1   | CH    | 319      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4843  | 1550 | 2397 | 423 | 463 | 10 |         |       |
| 1   | CI    | 317      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4825  | 1538 | 2397 | 419 | 461 | 10 |         |       |
| 1   | CJ    | 319      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4843  | 1550 | 2397 | 423 | 463 | 10 |         |       |
| 1   | CK    | 317      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4825  | 1538 | 2397 | 419 | 461 | 10 |         |       |
| 1   | CL    | 319      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4843  | 1550 | 2397 | 423 | 463 | 10 |         |       |
| 1   | DA    | 319      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4843  | 1550 | 2397 | 423 | 463 | 10 |         |       |
| 1   | DB    | 319      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4843  | 1550 | 2397 | 423 | 463 | 10 |         |       |

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| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 1   | DC    | 319      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4843  | 1550 | 2397 | 423 | 463 | 10 |         |       |
| 1   | DD    | 317      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4825  | 1538 | 2397 | 419 | 461 | 10 |         |       |
| 1   | DE    | 317      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4825  | 1538 | 2397 | 419 | 461 | 10 |         |       |
| 1   | DF    | 319      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4843  | 1550 | 2397 | 423 | 463 | 10 |         |       |
| 1   | DG    | 317      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4825  | 1538 | 2397 | 419 | 461 | 10 |         |       |
| 1   | DH    | 319      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4843  | 1550 | 2397 | 423 | 463 | 10 |         |       |

There are 836 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| AA    | 49      | MET      | -      | initiating methionine | UNP P21218 |
| AA    | 50      | GLY      | -      | expression tag        | UNP P21218 |
| AA    | 51      | SER      | -      | expression tag        | UNP P21218 |
| AA    | 52      | SER      | -      | expression tag        | UNP P21218 |
| AA    | 53      | HIS      | -      | expression tag        | UNP P21218 |
| AA    | 54      | HIS      | -      | expression tag        | UNP P21218 |
| AA    | 55      | HIS      | -      | expression tag        | UNP P21218 |
| AA    | 56      | HIS      | -      | expression tag        | UNP P21218 |
| AA    | 57      | HIS      | -      | expression tag        | UNP P21218 |
| AA    | 58      | HIS      | -      | expression tag        | UNP P21218 |
| AA    | 59      | SER      | -      | expression tag        | UNP P21218 |
| AA    | 60      | SER      | -      | expression tag        | UNP P21218 |
| AA    | 61      | GLY      | -      | expression tag        | UNP P21218 |
| AA    | 62      | LEU      | -      | expression tag        | UNP P21218 |
| AA    | 63      | VAL      | -      | expression tag        | UNP P21218 |
| AA    | 64      | PRO      | -      | expression tag        | UNP P21218 |
| AA    | 65      | ARG      | -      | expression tag        | UNP P21218 |
| AA    | 66      | GLY      | -      | expression tag        | UNP P21218 |
| AA    | 67      | SER      | -      | expression tag        | UNP P21218 |
| AB    | 49      | MET      | -      | initiating methionine | UNP P21218 |
| AB    | 50      | GLY      | -      | expression tag        | UNP P21218 |
| AB    | 51      | SER      | -      | expression tag        | UNP P21218 |
| AB    | 52      | SER      | -      | expression tag        | UNP P21218 |
| AB    | 53      | HIS      | -      | expression tag        | UNP P21218 |
| AB    | 54      | HIS      | -      | expression tag        | UNP P21218 |
| AB    | 55      | HIS      | -      | expression tag        | UNP P21218 |
| AB    | 56      | HIS      | -      | expression tag        | UNP P21218 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| AB    | 57      | HIS      | -      | expression tag        | UNP P21218 |
| AB    | 58      | HIS      | -      | expression tag        | UNP P21218 |
| AB    | 59      | SER      | -      | expression tag        | UNP P21218 |
| AB    | 60      | SER      | -      | expression tag        | UNP P21218 |
| AB    | 61      | GLY      | -      | expression tag        | UNP P21218 |
| AB    | 62      | LEU      | -      | expression tag        | UNP P21218 |
| AB    | 63      | VAL      | -      | expression tag        | UNP P21218 |
| AB    | 64      | PRO      | -      | expression tag        | UNP P21218 |
| AB    | 65      | ARG      | -      | expression tag        | UNP P21218 |
| AB    | 66      | GLY      | -      | expression tag        | UNP P21218 |
| AB    | 67      | SER      | -      | expression tag        | UNP P21218 |
| AC    | 49      | MET      | -      | initiating methionine | UNP P21218 |
| AC    | 50      | GLY      | -      | expression tag        | UNP P21218 |
| AC    | 51      | SER      | -      | expression tag        | UNP P21218 |
| AC    | 52      | SER      | -      | expression tag        | UNP P21218 |
| AC    | 53      | HIS      | -      | expression tag        | UNP P21218 |
| AC    | 54      | HIS      | -      | expression tag        | UNP P21218 |
| AC    | 55      | HIS      | -      | expression tag        | UNP P21218 |
| AC    | 56      | HIS      | -      | expression tag        | UNP P21218 |
| AC    | 57      | HIS      | -      | expression tag        | UNP P21218 |
| AC    | 58      | HIS      | -      | expression tag        | UNP P21218 |
| AC    | 59      | SER      | -      | expression tag        | UNP P21218 |
| AC    | 60      | SER      | -      | expression tag        | UNP P21218 |
| AC    | 61      | GLY      | -      | expression tag        | UNP P21218 |
| AC    | 62      | LEU      | -      | expression tag        | UNP P21218 |
| AC    | 63      | VAL      | -      | expression tag        | UNP P21218 |
| AC    | 64      | PRO      | -      | expression tag        | UNP P21218 |
| AC    | 65      | ARG      | -      | expression tag        | UNP P21218 |
| AC    | 66      | GLY      | -      | expression tag        | UNP P21218 |
| AC    | 67      | SER      | -      | expression tag        | UNP P21218 |
| AD    | 49      | MET      | -      | initiating methionine | UNP P21218 |
| AD    | 50      | GLY      | -      | expression tag        | UNP P21218 |
| AD    | 51      | SER      | -      | expression tag        | UNP P21218 |
| AD    | 52      | SER      | -      | expression tag        | UNP P21218 |
| AD    | 53      | HIS      | -      | expression tag        | UNP P21218 |
| AD    | 54      | HIS      | -      | expression tag        | UNP P21218 |
| AD    | 55      | HIS      | -      | expression tag        | UNP P21218 |
| AD    | 56      | HIS      | -      | expression tag        | UNP P21218 |
| AD    | 57      | HIS      | -      | expression tag        | UNP P21218 |
| AD    | 58      | HIS      | -      | expression tag        | UNP P21218 |
| AD    | 59      | SER      | -      | expression tag        | UNP P21218 |
| AD    | 60      | SER      | -      | expression tag        | UNP P21218 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| AD    | 61      | GLY      | -      | expression tag        | UNP P21218 |
| AD    | 62      | LEU      | -      | expression tag        | UNP P21218 |
| AD    | 63      | VAL      | -      | expression tag        | UNP P21218 |
| AD    | 64      | PRO      | -      | expression tag        | UNP P21218 |
| AD    | 65      | ARG      | -      | expression tag        | UNP P21218 |
| AD    | 66      | GLY      | -      | expression tag        | UNP P21218 |
| AD    | 67      | SER      | -      | expression tag        | UNP P21218 |
| AE    | 49      | MET      | -      | initiating methionine | UNP P21218 |
| AE    | 50      | GLY      | -      | expression tag        | UNP P21218 |
| AE    | 51      | SER      | -      | expression tag        | UNP P21218 |
| AE    | 52      | SER      | -      | expression tag        | UNP P21218 |
| AE    | 53      | HIS      | -      | expression tag        | UNP P21218 |
| AE    | 54      | HIS      | -      | expression tag        | UNP P21218 |
| AE    | 55      | HIS      | -      | expression tag        | UNP P21218 |
| AE    | 56      | HIS      | -      | expression tag        | UNP P21218 |
| AE    | 57      | HIS      | -      | expression tag        | UNP P21218 |
| AE    | 58      | HIS      | -      | expression tag        | UNP P21218 |
| AE    | 59      | SER      | -      | expression tag        | UNP P21218 |
| AE    | 60      | SER      | -      | expression tag        | UNP P21218 |
| AE    | 61      | GLY      | -      | expression tag        | UNP P21218 |
| AE    | 62      | LEU      | -      | expression tag        | UNP P21218 |
| AE    | 63      | VAL      | -      | expression tag        | UNP P21218 |
| AE    | 64      | PRO      | -      | expression tag        | UNP P21218 |
| AE    | 65      | ARG      | -      | expression tag        | UNP P21218 |
| AE    | 66      | GLY      | -      | expression tag        | UNP P21218 |
| AE    | 67      | SER      | -      | expression tag        | UNP P21218 |
| AF    | 49      | MET      | -      | initiating methionine | UNP P21218 |
| AF    | 50      | GLY      | -      | expression tag        | UNP P21218 |
| AF    | 51      | SER      | -      | expression tag        | UNP P21218 |
| AF    | 52      | SER      | -      | expression tag        | UNP P21218 |
| AF    | 53      | HIS      | -      | expression tag        | UNP P21218 |
| AF    | 54      | HIS      | -      | expression tag        | UNP P21218 |
| AF    | 55      | HIS      | -      | expression tag        | UNP P21218 |
| AF    | 56      | HIS      | -      | expression tag        | UNP P21218 |
| AF    | 57      | HIS      | -      | expression tag        | UNP P21218 |
| AF    | 58      | HIS      | -      | expression tag        | UNP P21218 |
| AF    | 59      | SER      | -      | expression tag        | UNP P21218 |
| AF    | 60      | SER      | -      | expression tag        | UNP P21218 |
| AF    | 61      | GLY      | -      | expression tag        | UNP P21218 |
| AF    | 62      | LEU      | -      | expression tag        | UNP P21218 |
| AF    | 63      | VAL      | -      | expression tag        | UNP P21218 |
| AF    | 64      | PRO      | -      | expression tag        | UNP P21218 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| AF    | 65      | ARG      | -      | expression tag        | UNP P21218 |
| AF    | 66      | GLY      | -      | expression tag        | UNP P21218 |
| AF    | 67      | SER      | -      | expression tag        | UNP P21218 |
| AG    | 49      | MET      | -      | initiating methionine | UNP P21218 |
| AG    | 50      | GLY      | -      | expression tag        | UNP P21218 |
| AG    | 51      | SER      | -      | expression tag        | UNP P21218 |
| AG    | 52      | SER      | -      | expression tag        | UNP P21218 |
| AG    | 53      | HIS      | -      | expression tag        | UNP P21218 |
| AG    | 54      | HIS      | -      | expression tag        | UNP P21218 |
| AG    | 55      | HIS      | -      | expression tag        | UNP P21218 |
| AG    | 56      | HIS      | -      | expression tag        | UNP P21218 |
| AG    | 57      | HIS      | -      | expression tag        | UNP P21218 |
| AG    | 58      | HIS      | -      | expression tag        | UNP P21218 |
| AG    | 59      | SER      | -      | expression tag        | UNP P21218 |
| AG    | 60      | SER      | -      | expression tag        | UNP P21218 |
| AG    | 61      | GLY      | -      | expression tag        | UNP P21218 |
| AG    | 62      | LEU      | -      | expression tag        | UNP P21218 |
| AG    | 63      | VAL      | -      | expression tag        | UNP P21218 |
| AG    | 64      | PRO      | -      | expression tag        | UNP P21218 |
| AG    | 65      | ARG      | -      | expression tag        | UNP P21218 |
| AG    | 66      | GLY      | -      | expression tag        | UNP P21218 |
| AG    | 67      | SER      | -      | expression tag        | UNP P21218 |
| AH    | 49      | MET      | -      | initiating methionine | UNP P21218 |
| AH    | 50      | GLY      | -      | expression tag        | UNP P21218 |
| AH    | 51      | SER      | -      | expression tag        | UNP P21218 |
| AH    | 52      | SER      | -      | expression tag        | UNP P21218 |
| AH    | 53      | HIS      | -      | expression tag        | UNP P21218 |
| AH    | 54      | HIS      | -      | expression tag        | UNP P21218 |
| AH    | 55      | HIS      | -      | expression tag        | UNP P21218 |
| AH    | 56      | HIS      | -      | expression tag        | UNP P21218 |
| AH    | 57      | HIS      | -      | expression tag        | UNP P21218 |
| AH    | 58      | HIS      | -      | expression tag        | UNP P21218 |
| AH    | 59      | SER      | -      | expression tag        | UNP P21218 |
| AH    | 60      | SER      | -      | expression tag        | UNP P21218 |
| AH    | 61      | GLY      | -      | expression tag        | UNP P21218 |
| AH    | 62      | LEU      | -      | expression tag        | UNP P21218 |
| AH    | 63      | VAL      | -      | expression tag        | UNP P21218 |
| AH    | 64      | PRO      | -      | expression tag        | UNP P21218 |
| AH    | 65      | ARG      | -      | expression tag        | UNP P21218 |
| AH    | 66      | GLY      | -      | expression tag        | UNP P21218 |
| AH    | 67      | SER      | -      | expression tag        | UNP P21218 |
| AI    | 49      | MET      | -      | initiating methionine | UNP P21218 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| AI    | 50      | GLY      | -      | expression tag        | UNP P21218 |
| AI    | 51      | SER      | -      | expression tag        | UNP P21218 |
| AI    | 52      | SER      | -      | expression tag        | UNP P21218 |
| AI    | 53      | HIS      | -      | expression tag        | UNP P21218 |
| AI    | 54      | HIS      | -      | expression tag        | UNP P21218 |
| AI    | 55      | HIS      | -      | expression tag        | UNP P21218 |
| AI    | 56      | HIS      | -      | expression tag        | UNP P21218 |
| AI    | 57      | HIS      | -      | expression tag        | UNP P21218 |
| AI    | 58      | HIS      | -      | expression tag        | UNP P21218 |
| AI    | 59      | SER      | -      | expression tag        | UNP P21218 |
| AI    | 60      | SER      | -      | expression tag        | UNP P21218 |
| AI    | 61      | GLY      | -      | expression tag        | UNP P21218 |
| AI    | 62      | LEU      | -      | expression tag        | UNP P21218 |
| AI    | 63      | VAL      | -      | expression tag        | UNP P21218 |
| AI    | 64      | PRO      | -      | expression tag        | UNP P21218 |
| AI    | 65      | ARG      | -      | expression tag        | UNP P21218 |
| AI    | 66      | GLY      | -      | expression tag        | UNP P21218 |
| AI    | 67      | SER      | -      | expression tag        | UNP P21218 |
| AJ    | 49      | MET      | -      | initiating methionine | UNP P21218 |
| AJ    | 50      | GLY      | -      | expression tag        | UNP P21218 |
| AJ    | 51      | SER      | -      | expression tag        | UNP P21218 |
| AJ    | 52      | SER      | -      | expression tag        | UNP P21218 |
| AJ    | 53      | HIS      | -      | expression tag        | UNP P21218 |
| AJ    | 54      | HIS      | -      | expression tag        | UNP P21218 |
| AJ    | 55      | HIS      | -      | expression tag        | UNP P21218 |
| AJ    | 56      | HIS      | -      | expression tag        | UNP P21218 |
| AJ    | 57      | HIS      | -      | expression tag        | UNP P21218 |
| AJ    | 58      | HIS      | -      | expression tag        | UNP P21218 |
| AJ    | 59      | SER      | -      | expression tag        | UNP P21218 |
| AJ    | 60      | SER      | -      | expression tag        | UNP P21218 |
| AJ    | 61      | GLY      | -      | expression tag        | UNP P21218 |
| AJ    | 62      | LEU      | -      | expression tag        | UNP P21218 |
| AJ    | 63      | VAL      | -      | expression tag        | UNP P21218 |
| AJ    | 64      | PRO      | -      | expression tag        | UNP P21218 |
| AJ    | 65      | ARG      | -      | expression tag        | UNP P21218 |
| AJ    | 66      | GLY      | -      | expression tag        | UNP P21218 |
| AJ    | 67      | SER      | -      | expression tag        | UNP P21218 |
| AK    | 49      | MET      | -      | initiating methionine | UNP P21218 |
| AK    | 50      | GLY      | -      | expression tag        | UNP P21218 |
| AK    | 51      | SER      | -      | expression tag        | UNP P21218 |
| AK    | 52      | SER      | -      | expression tag        | UNP P21218 |
| AK    | 53      | HIS      | -      | expression tag        | UNP P21218 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| AK    | 54      | HIS      | -      | expression tag        | UNP P21218 |
| AK    | 55      | HIS      | -      | expression tag        | UNP P21218 |
| AK    | 56      | HIS      | -      | expression tag        | UNP P21218 |
| AK    | 57      | HIS      | -      | expression tag        | UNP P21218 |
| AK    | 58      | HIS      | -      | expression tag        | UNP P21218 |
| AK    | 59      | SER      | -      | expression tag        | UNP P21218 |
| AK    | 60      | SER      | -      | expression tag        | UNP P21218 |
| AK    | 61      | GLY      | -      | expression tag        | UNP P21218 |
| AK    | 62      | LEU      | -      | expression tag        | UNP P21218 |
| AK    | 63      | VAL      | -      | expression tag        | UNP P21218 |
| AK    | 64      | PRO      | -      | expression tag        | UNP P21218 |
| AK    | 65      | ARG      | -      | expression tag        | UNP P21218 |
| AK    | 66      | GLY      | -      | expression tag        | UNP P21218 |
| AK    | 67      | SER      | -      | expression tag        | UNP P21218 |
| AL    | 49      | MET      | -      | initiating methionine | UNP P21218 |
| AL    | 50      | GLY      | -      | expression tag        | UNP P21218 |
| AL    | 51      | SER      | -      | expression tag        | UNP P21218 |
| AL    | 52      | SER      | -      | expression tag        | UNP P21218 |
| AL    | 53      | HIS      | -      | expression tag        | UNP P21218 |
| AL    | 54      | HIS      | -      | expression tag        | UNP P21218 |
| AL    | 55      | HIS      | -      | expression tag        | UNP P21218 |
| AL    | 56      | HIS      | -      | expression tag        | UNP P21218 |
| AL    | 57      | HIS      | -      | expression tag        | UNP P21218 |
| AL    | 58      | HIS      | -      | expression tag        | UNP P21218 |
| AL    | 59      | SER      | -      | expression tag        | UNP P21218 |
| AL    | 60      | SER      | -      | expression tag        | UNP P21218 |
| AL    | 61      | GLY      | -      | expression tag        | UNP P21218 |
| AL    | 62      | LEU      | -      | expression tag        | UNP P21218 |
| AL    | 63      | VAL      | -      | expression tag        | UNP P21218 |
| AL    | 64      | PRO      | -      | expression tag        | UNP P21218 |
| AL    | 65      | ARG      | -      | expression tag        | UNP P21218 |
| AL    | 66      | GLY      | -      | expression tag        | UNP P21218 |
| AL    | 67      | SER      | -      | expression tag        | UNP P21218 |
| BA    | 49      | MET      | -      | initiating methionine | UNP P21218 |
| BA    | 50      | GLY      | -      | expression tag        | UNP P21218 |
| BA    | 51      | SER      | -      | expression tag        | UNP P21218 |
| BA    | 52      | SER      | -      | expression tag        | UNP P21218 |
| BA    | 53      | HIS      | -      | expression tag        | UNP P21218 |
| BA    | 54      | HIS      | -      | expression tag        | UNP P21218 |
| BA    | 55      | HIS      | -      | expression tag        | UNP P21218 |
| BA    | 56      | HIS      | -      | expression tag        | UNP P21218 |
| BA    | 57      | HIS      | -      | expression tag        | UNP P21218 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| BA    | 58      | HIS      | -      | expression tag        | UNP P21218 |
| BA    | 59      | SER      | -      | expression tag        | UNP P21218 |
| BA    | 60      | SER      | -      | expression tag        | UNP P21218 |
| BA    | 61      | GLY      | -      | expression tag        | UNP P21218 |
| BA    | 62      | LEU      | -      | expression tag        | UNP P21218 |
| BA    | 63      | VAL      | -      | expression tag        | UNP P21218 |
| BA    | 64      | PRO      | -      | expression tag        | UNP P21218 |
| BA    | 65      | ARG      | -      | expression tag        | UNP P21218 |
| BA    | 66      | GLY      | -      | expression tag        | UNP P21218 |
| BA    | 67      | SER      | -      | expression tag        | UNP P21218 |
| BB    | 49      | MET      | -      | initiating methionine | UNP P21218 |
| BB    | 50      | GLY      | -      | expression tag        | UNP P21218 |
| BB    | 51      | SER      | -      | expression tag        | UNP P21218 |
| BB    | 52      | SER      | -      | expression tag        | UNP P21218 |
| BB    | 53      | HIS      | -      | expression tag        | UNP P21218 |
| BB    | 54      | HIS      | -      | expression tag        | UNP P21218 |
| BB    | 55      | HIS      | -      | expression tag        | UNP P21218 |
| BB    | 56      | HIS      | -      | expression tag        | UNP P21218 |
| BB    | 57      | HIS      | -      | expression tag        | UNP P21218 |
| BB    | 58      | HIS      | -      | expression tag        | UNP P21218 |
| BB    | 59      | SER      | -      | expression tag        | UNP P21218 |
| BB    | 60      | SER      | -      | expression tag        | UNP P21218 |
| BB    | 61      | GLY      | -      | expression tag        | UNP P21218 |
| BB    | 62      | LEU      | -      | expression tag        | UNP P21218 |
| BB    | 63      | VAL      | -      | expression tag        | UNP P21218 |
| BB    | 64      | PRO      | -      | expression tag        | UNP P21218 |
| BB    | 65      | ARG      | -      | expression tag        | UNP P21218 |
| BB    | 66      | GLY      | -      | expression tag        | UNP P21218 |
| BB    | 67      | SER      | -      | expression tag        | UNP P21218 |
| BC    | 49      | MET      | -      | initiating methionine | UNP P21218 |
| BC    | 50      | GLY      | -      | expression tag        | UNP P21218 |
| BC    | 51      | SER      | -      | expression tag        | UNP P21218 |
| BC    | 52      | SER      | -      | expression tag        | UNP P21218 |
| BC    | 53      | HIS      | -      | expression tag        | UNP P21218 |
| BC    | 54      | HIS      | -      | expression tag        | UNP P21218 |
| BC    | 55      | HIS      | -      | expression tag        | UNP P21218 |
| BC    | 56      | HIS      | -      | expression tag        | UNP P21218 |
| BC    | 57      | HIS      | -      | expression tag        | UNP P21218 |
| BC    | 58      | HIS      | -      | expression tag        | UNP P21218 |
| BC    | 59      | SER      | -      | expression tag        | UNP P21218 |
| BC    | 60      | SER      | -      | expression tag        | UNP P21218 |
| BC    | 61      | GLY      | -      | expression tag        | UNP P21218 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| BC    | 62      | LEU      | -      | expression tag        | UNP P21218 |
| BC    | 63      | VAL      | -      | expression tag        | UNP P21218 |
| BC    | 64      | PRO      | -      | expression tag        | UNP P21218 |
| BC    | 65      | ARG      | -      | expression tag        | UNP P21218 |
| BC    | 66      | GLY      | -      | expression tag        | UNP P21218 |
| BC    | 67      | SER      | -      | expression tag        | UNP P21218 |
| BD    | 49      | MET      | -      | initiating methionine | UNP P21218 |
| BD    | 50      | GLY      | -      | expression tag        | UNP P21218 |
| BD    | 51      | SER      | -      | expression tag        | UNP P21218 |
| BD    | 52      | SER      | -      | expression tag        | UNP P21218 |
| BD    | 53      | HIS      | -      | expression tag        | UNP P21218 |
| BD    | 54      | HIS      | -      | expression tag        | UNP P21218 |
| BD    | 55      | HIS      | -      | expression tag        | UNP P21218 |
| BD    | 56      | HIS      | -      | expression tag        | UNP P21218 |
| BD    | 57      | HIS      | -      | expression tag        | UNP P21218 |
| BD    | 58      | HIS      | -      | expression tag        | UNP P21218 |
| BD    | 59      | SER      | -      | expression tag        | UNP P21218 |
| BD    | 60      | SER      | -      | expression tag        | UNP P21218 |
| BD    | 61      | GLY      | -      | expression tag        | UNP P21218 |
| BD    | 62      | LEU      | -      | expression tag        | UNP P21218 |
| BD    | 63      | VAL      | -      | expression tag        | UNP P21218 |
| BD    | 64      | PRO      | -      | expression tag        | UNP P21218 |
| BD    | 65      | ARG      | -      | expression tag        | UNP P21218 |
| BD    | 66      | GLY      | -      | expression tag        | UNP P21218 |
| BD    | 67      | SER      | -      | expression tag        | UNP P21218 |
| BE    | 49      | MET      | -      | initiating methionine | UNP P21218 |
| BE    | 50      | GLY      | -      | expression tag        | UNP P21218 |
| BE    | 51      | SER      | -      | expression tag        | UNP P21218 |
| BE    | 52      | SER      | -      | expression tag        | UNP P21218 |
| BE    | 53      | HIS      | -      | expression tag        | UNP P21218 |
| BE    | 54      | HIS      | -      | expression tag        | UNP P21218 |
| BE    | 55      | HIS      | -      | expression tag        | UNP P21218 |
| BE    | 56      | HIS      | -      | expression tag        | UNP P21218 |
| BE    | 57      | HIS      | -      | expression tag        | UNP P21218 |
| BE    | 58      | HIS      | -      | expression tag        | UNP P21218 |
| BE    | 59      | SER      | -      | expression tag        | UNP P21218 |
| BE    | 60      | SER      | -      | expression tag        | UNP P21218 |
| BE    | 61      | GLY      | -      | expression tag        | UNP P21218 |
| BE    | 62      | LEU      | -      | expression tag        | UNP P21218 |
| BE    | 63      | VAL      | -      | expression tag        | UNP P21218 |
| BE    | 64      | PRO      | -      | expression tag        | UNP P21218 |
| BE    | 65      | ARG      | -      | expression tag        | UNP P21218 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| BE    | 66      | GLY      | -      | expression tag        | UNP P21218 |
| BE    | 67      | SER      | -      | expression tag        | UNP P21218 |
| BF    | 49      | MET      | -      | initiating methionine | UNP P21218 |
| BF    | 50      | GLY      | -      | expression tag        | UNP P21218 |
| BF    | 51      | SER      | -      | expression tag        | UNP P21218 |
| BF    | 52      | SER      | -      | expression tag        | UNP P21218 |
| BF    | 53      | HIS      | -      | expression tag        | UNP P21218 |
| BF    | 54      | HIS      | -      | expression tag        | UNP P21218 |
| BF    | 55      | HIS      | -      | expression tag        | UNP P21218 |
| BF    | 56      | HIS      | -      | expression tag        | UNP P21218 |
| BF    | 57      | HIS      | -      | expression tag        | UNP P21218 |
| BF    | 58      | HIS      | -      | expression tag        | UNP P21218 |
| BF    | 59      | SER      | -      | expression tag        | UNP P21218 |
| BF    | 60      | SER      | -      | expression tag        | UNP P21218 |
| BF    | 61      | GLY      | -      | expression tag        | UNP P21218 |
| BF    | 62      | LEU      | -      | expression tag        | UNP P21218 |
| BF    | 63      | VAL      | -      | expression tag        | UNP P21218 |
| BF    | 64      | PRO      | -      | expression tag        | UNP P21218 |
| BF    | 65      | ARG      | -      | expression tag        | UNP P21218 |
| BF    | 66      | GLY      | -      | expression tag        | UNP P21218 |
| BF    | 67      | SER      | -      | expression tag        | UNP P21218 |
| BG    | 49      | MET      | -      | initiating methionine | UNP P21218 |
| BG    | 50      | GLY      | -      | expression tag        | UNP P21218 |
| BG    | 51      | SER      | -      | expression tag        | UNP P21218 |
| BG    | 52      | SER      | -      | expression tag        | UNP P21218 |
| BG    | 53      | HIS      | -      | expression tag        | UNP P21218 |
| BG    | 54      | HIS      | -      | expression tag        | UNP P21218 |
| BG    | 55      | HIS      | -      | expression tag        | UNP P21218 |
| BG    | 56      | HIS      | -      | expression tag        | UNP P21218 |
| BG    | 57      | HIS      | -      | expression tag        | UNP P21218 |
| BG    | 58      | HIS      | -      | expression tag        | UNP P21218 |
| BG    | 59      | SER      | -      | expression tag        | UNP P21218 |
| BG    | 60      | SER      | -      | expression tag        | UNP P21218 |
| BG    | 61      | GLY      | -      | expression tag        | UNP P21218 |
| BG    | 62      | LEU      | -      | expression tag        | UNP P21218 |
| BG    | 63      | VAL      | -      | expression tag        | UNP P21218 |
| BG    | 64      | PRO      | -      | expression tag        | UNP P21218 |
| BG    | 65      | ARG      | -      | expression tag        | UNP P21218 |
| BG    | 66      | GLY      | -      | expression tag        | UNP P21218 |
| BG    | 67      | SER      | -      | expression tag        | UNP P21218 |
| BH    | 49      | MET      | -      | initiating methionine | UNP P21218 |
| BH    | 50      | GLY      | -      | expression tag        | UNP P21218 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| BH    | 51      | SER      | -      | expression tag        | UNP P21218 |
| BH    | 52      | SER      | -      | expression tag        | UNP P21218 |
| BH    | 53      | HIS      | -      | expression tag        | UNP P21218 |
| BH    | 54      | HIS      | -      | expression tag        | UNP P21218 |
| BH    | 55      | HIS      | -      | expression tag        | UNP P21218 |
| BH    | 56      | HIS      | -      | expression tag        | UNP P21218 |
| BH    | 57      | HIS      | -      | expression tag        | UNP P21218 |
| BH    | 58      | HIS      | -      | expression tag        | UNP P21218 |
| BH    | 59      | SER      | -      | expression tag        | UNP P21218 |
| BH    | 60      | SER      | -      | expression tag        | UNP P21218 |
| BH    | 61      | GLY      | -      | expression tag        | UNP P21218 |
| BH    | 62      | LEU      | -      | expression tag        | UNP P21218 |
| BH    | 63      | VAL      | -      | expression tag        | UNP P21218 |
| BH    | 64      | PRO      | -      | expression tag        | UNP P21218 |
| BH    | 65      | ARG      | -      | expression tag        | UNP P21218 |
| BH    | 66      | GLY      | -      | expression tag        | UNP P21218 |
| BH    | 67      | SER      | -      | expression tag        | UNP P21218 |
| BI    | 49      | MET      | -      | initiating methionine | UNP P21218 |
| BI    | 50      | GLY      | -      | expression tag        | UNP P21218 |
| BI    | 51      | SER      | -      | expression tag        | UNP P21218 |
| BI    | 52      | SER      | -      | expression tag        | UNP P21218 |
| BI    | 53      | HIS      | -      | expression tag        | UNP P21218 |
| BI    | 54      | HIS      | -      | expression tag        | UNP P21218 |
| BI    | 55      | HIS      | -      | expression tag        | UNP P21218 |
| BI    | 56      | HIS      | -      | expression tag        | UNP P21218 |
| BI    | 57      | HIS      | -      | expression tag        | UNP P21218 |
| BI    | 58      | HIS      | -      | expression tag        | UNP P21218 |
| BI    | 59      | SER      | -      | expression tag        | UNP P21218 |
| BI    | 60      | SER      | -      | expression tag        | UNP P21218 |
| BI    | 61      | GLY      | -      | expression tag        | UNP P21218 |
| BI    | 62      | LEU      | -      | expression tag        | UNP P21218 |
| BI    | 63      | VAL      | -      | expression tag        | UNP P21218 |
| BI    | 64      | PRO      | -      | expression tag        | UNP P21218 |
| BI    | 65      | ARG      | -      | expression tag        | UNP P21218 |
| BI    | 66      | GLY      | -      | expression tag        | UNP P21218 |
| BI    | 67      | SER      | -      | expression tag        | UNP P21218 |
| BJ    | 49      | MET      | -      | initiating methionine | UNP P21218 |
| BJ    | 50      | GLY      | -      | expression tag        | UNP P21218 |
| BJ    | 51      | SER      | -      | expression tag        | UNP P21218 |
| BJ    | 52      | SER      | -      | expression tag        | UNP P21218 |
| BJ    | 53      | HIS      | -      | expression tag        | UNP P21218 |
| BJ    | 54      | HIS      | -      | expression tag        | UNP P21218 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| BJ    | 55      | HIS      | -      | expression tag        | UNP P21218 |
| BJ    | 56      | HIS      | -      | expression tag        | UNP P21218 |
| BJ    | 57      | HIS      | -      | expression tag        | UNP P21218 |
| BJ    | 58      | HIS      | -      | expression tag        | UNP P21218 |
| BJ    | 59      | SER      | -      | expression tag        | UNP P21218 |
| BJ    | 60      | SER      | -      | expression tag        | UNP P21218 |
| BJ    | 61      | GLY      | -      | expression tag        | UNP P21218 |
| BJ    | 62      | LEU      | -      | expression tag        | UNP P21218 |
| BJ    | 63      | VAL      | -      | expression tag        | UNP P21218 |
| BJ    | 64      | PRO      | -      | expression tag        | UNP P21218 |
| BJ    | 65      | ARG      | -      | expression tag        | UNP P21218 |
| BJ    | 66      | GLY      | -      | expression tag        | UNP P21218 |
| BJ    | 67      | SER      | -      | expression tag        | UNP P21218 |
| BK    | 49      | MET      | -      | initiating methionine | UNP P21218 |
| BK    | 50      | GLY      | -      | expression tag        | UNP P21218 |
| BK    | 51      | SER      | -      | expression tag        | UNP P21218 |
| BK    | 52      | SER      | -      | expression tag        | UNP P21218 |
| BK    | 53      | HIS      | -      | expression tag        | UNP P21218 |
| BK    | 54      | HIS      | -      | expression tag        | UNP P21218 |
| BK    | 55      | HIS      | -      | expression tag        | UNP P21218 |
| BK    | 56      | HIS      | -      | expression tag        | UNP P21218 |
| BK    | 57      | HIS      | -      | expression tag        | UNP P21218 |
| BK    | 58      | HIS      | -      | expression tag        | UNP P21218 |
| BK    | 59      | SER      | -      | expression tag        | UNP P21218 |
| BK    | 60      | SER      | -      | expression tag        | UNP P21218 |
| BK    | 61      | GLY      | -      | expression tag        | UNP P21218 |
| BK    | 62      | LEU      | -      | expression tag        | UNP P21218 |
| BK    | 63      | VAL      | -      | expression tag        | UNP P21218 |
| BK    | 64      | PRO      | -      | expression tag        | UNP P21218 |
| BK    | 65      | ARG      | -      | expression tag        | UNP P21218 |
| BK    | 66      | GLY      | -      | expression tag        | UNP P21218 |
| BK    | 67      | SER      | -      | expression tag        | UNP P21218 |
| BL    | 49      | MET      | -      | initiating methionine | UNP P21218 |
| BL    | 50      | GLY      | -      | expression tag        | UNP P21218 |
| BL    | 51      | SER      | -      | expression tag        | UNP P21218 |
| BL    | 52      | SER      | -      | expression tag        | UNP P21218 |
| BL    | 53      | HIS      | -      | expression tag        | UNP P21218 |
| BL    | 54      | HIS      | -      | expression tag        | UNP P21218 |
| BL    | 55      | HIS      | -      | expression tag        | UNP P21218 |
| BL    | 56      | HIS      | -      | expression tag        | UNP P21218 |
| BL    | 57      | HIS      | -      | expression tag        | UNP P21218 |
| BL    | 58      | HIS      | -      | expression tag        | UNP P21218 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| BL    | 59      | SER      | -      | expression tag        | UNP P21218 |
| BL    | 60      | SER      | -      | expression tag        | UNP P21218 |
| BL    | 61      | GLY      | -      | expression tag        | UNP P21218 |
| BL    | 62      | LEU      | -      | expression tag        | UNP P21218 |
| BL    | 63      | VAL      | -      | expression tag        | UNP P21218 |
| BL    | 64      | PRO      | -      | expression tag        | UNP P21218 |
| BL    | 65      | ARG      | -      | expression tag        | UNP P21218 |
| BL    | 66      | GLY      | -      | expression tag        | UNP P21218 |
| BL    | 67      | SER      | -      | expression tag        | UNP P21218 |
| CA    | 49      | MET      | -      | initiating methionine | UNP P21218 |
| CA    | 50      | GLY      | -      | expression tag        | UNP P21218 |
| CA    | 51      | SER      | -      | expression tag        | UNP P21218 |
| CA    | 52      | SER      | -      | expression tag        | UNP P21218 |
| CA    | 53      | HIS      | -      | expression tag        | UNP P21218 |
| CA    | 54      | HIS      | -      | expression tag        | UNP P21218 |
| CA    | 55      | HIS      | -      | expression tag        | UNP P21218 |
| CA    | 56      | HIS      | -      | expression tag        | UNP P21218 |
| CA    | 57      | HIS      | -      | expression tag        | UNP P21218 |
| CA    | 58      | HIS      | -      | expression tag        | UNP P21218 |
| CA    | 59      | SER      | -      | expression tag        | UNP P21218 |
| CA    | 60      | SER      | -      | expression tag        | UNP P21218 |
| CA    | 61      | GLY      | -      | expression tag        | UNP P21218 |
| CA    | 62      | LEU      | -      | expression tag        | UNP P21218 |
| CA    | 63      | VAL      | -      | expression tag        | UNP P21218 |
| CA    | 64      | PRO      | -      | expression tag        | UNP P21218 |
| CA    | 65      | ARG      | -      | expression tag        | UNP P21218 |
| CA    | 66      | GLY      | -      | expression tag        | UNP P21218 |
| CA    | 67      | SER      | -      | expression tag        | UNP P21218 |
| CB    | 49      | MET      | -      | initiating methionine | UNP P21218 |
| CB    | 50      | GLY      | -      | expression tag        | UNP P21218 |
| CB    | 51      | SER      | -      | expression tag        | UNP P21218 |
| CB    | 52      | SER      | -      | expression tag        | UNP P21218 |
| CB    | 53      | HIS      | -      | expression tag        | UNP P21218 |
| CB    | 54      | HIS      | -      | expression tag        | UNP P21218 |
| CB    | 55      | HIS      | -      | expression tag        | UNP P21218 |
| CB    | 56      | HIS      | -      | expression tag        | UNP P21218 |
| CB    | 57      | HIS      | -      | expression tag        | UNP P21218 |
| CB    | 58      | HIS      | -      | expression tag        | UNP P21218 |
| CB    | 59      | SER      | -      | expression tag        | UNP P21218 |
| CB    | 60      | SER      | -      | expression tag        | UNP P21218 |
| CB    | 61      | GLY      | -      | expression tag        | UNP P21218 |
| CB    | 62      | LEU      | -      | expression tag        | UNP P21218 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| CB    | 63      | VAL      | -      | expression tag        | UNP P21218 |
| CB    | 64      | PRO      | -      | expression tag        | UNP P21218 |
| CB    | 65      | ARG      | -      | expression tag        | UNP P21218 |
| CB    | 66      | GLY      | -      | expression tag        | UNP P21218 |
| CB    | 67      | SER      | -      | expression tag        | UNP P21218 |
| CC    | 49      | MET      | -      | initiating methionine | UNP P21218 |
| CC    | 50      | GLY      | -      | expression tag        | UNP P21218 |
| CC    | 51      | SER      | -      | expression tag        | UNP P21218 |
| CC    | 52      | SER      | -      | expression tag        | UNP P21218 |
| CC    | 53      | HIS      | -      | expression tag        | UNP P21218 |
| CC    | 54      | HIS      | -      | expression tag        | UNP P21218 |
| CC    | 55      | HIS      | -      | expression tag        | UNP P21218 |
| CC    | 56      | HIS      | -      | expression tag        | UNP P21218 |
| CC    | 57      | HIS      | -      | expression tag        | UNP P21218 |
| CC    | 58      | HIS      | -      | expression tag        | UNP P21218 |
| CC    | 59      | SER      | -      | expression tag        | UNP P21218 |
| CC    | 60      | SER      | -      | expression tag        | UNP P21218 |
| CC    | 61      | GLY      | -      | expression tag        | UNP P21218 |
| CC    | 62      | LEU      | -      | expression tag        | UNP P21218 |
| CC    | 63      | VAL      | -      | expression tag        | UNP P21218 |
| CC    | 64      | PRO      | -      | expression tag        | UNP P21218 |
| CC    | 65      | ARG      | -      | expression tag        | UNP P21218 |
| CC    | 66      | GLY      | -      | expression tag        | UNP P21218 |
| CC    | 67      | SER      | -      | expression tag        | UNP P21218 |
| CD    | 49      | MET      | -      | initiating methionine | UNP P21218 |
| CD    | 50      | GLY      | -      | expression tag        | UNP P21218 |
| CD    | 51      | SER      | -      | expression tag        | UNP P21218 |
| CD    | 52      | SER      | -      | expression tag        | UNP P21218 |
| CD    | 53      | HIS      | -      | expression tag        | UNP P21218 |
| CD    | 54      | HIS      | -      | expression tag        | UNP P21218 |
| CD    | 55      | HIS      | -      | expression tag        | UNP P21218 |
| CD    | 56      | HIS      | -      | expression tag        | UNP P21218 |
| CD    | 57      | HIS      | -      | expression tag        | UNP P21218 |
| CD    | 58      | HIS      | -      | expression tag        | UNP P21218 |
| CD    | 59      | SER      | -      | expression tag        | UNP P21218 |
| CD    | 60      | SER      | -      | expression tag        | UNP P21218 |
| CD    | 61      | GLY      | -      | expression tag        | UNP P21218 |
| CD    | 62      | LEU      | -      | expression tag        | UNP P21218 |
| CD    | 63      | VAL      | -      | expression tag        | UNP P21218 |
| CD    | 64      | PRO      | -      | expression tag        | UNP P21218 |
| CD    | 65      | ARG      | -      | expression tag        | UNP P21218 |
| CD    | 66      | GLY      | -      | expression tag        | UNP P21218 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| CD    | 67      | SER      | -      | expression tag        | UNP P21218 |
| CE    | 49      | MET      | -      | initiating methionine | UNP P21218 |
| CE    | 50      | GLY      | -      | expression tag        | UNP P21218 |
| CE    | 51      | SER      | -      | expression tag        | UNP P21218 |
| CE    | 52      | SER      | -      | expression tag        | UNP P21218 |
| CE    | 53      | HIS      | -      | expression tag        | UNP P21218 |
| CE    | 54      | HIS      | -      | expression tag        | UNP P21218 |
| CE    | 55      | HIS      | -      | expression tag        | UNP P21218 |
| CE    | 56      | HIS      | -      | expression tag        | UNP P21218 |
| CE    | 57      | HIS      | -      | expression tag        | UNP P21218 |
| CE    | 58      | HIS      | -      | expression tag        | UNP P21218 |
| CE    | 59      | SER      | -      | expression tag        | UNP P21218 |
| CE    | 60      | SER      | -      | expression tag        | UNP P21218 |
| CE    | 61      | GLY      | -      | expression tag        | UNP P21218 |
| CE    | 62      | LEU      | -      | expression tag        | UNP P21218 |
| CE    | 63      | VAL      | -      | expression tag        | UNP P21218 |
| CE    | 64      | PRO      | -      | expression tag        | UNP P21218 |
| CE    | 65      | ARG      | -      | expression tag        | UNP P21218 |
| CE    | 66      | GLY      | -      | expression tag        | UNP P21218 |
| CE    | 67      | SER      | -      | expression tag        | UNP P21218 |
| CF    | 49      | MET      | -      | initiating methionine | UNP P21218 |
| CF    | 50      | GLY      | -      | expression tag        | UNP P21218 |
| CF    | 51      | SER      | -      | expression tag        | UNP P21218 |
| CF    | 52      | SER      | -      | expression tag        | UNP P21218 |
| CF    | 53      | HIS      | -      | expression tag        | UNP P21218 |
| CF    | 54      | HIS      | -      | expression tag        | UNP P21218 |
| CF    | 55      | HIS      | -      | expression tag        | UNP P21218 |
| CF    | 56      | HIS      | -      | expression tag        | UNP P21218 |
| CF    | 57      | HIS      | -      | expression tag        | UNP P21218 |
| CF    | 58      | HIS      | -      | expression tag        | UNP P21218 |
| CF    | 59      | SER      | -      | expression tag        | UNP P21218 |
| CF    | 60      | SER      | -      | expression tag        | UNP P21218 |
| CF    | 61      | GLY      | -      | expression tag        | UNP P21218 |
| CF    | 62      | LEU      | -      | expression tag        | UNP P21218 |
| CF    | 63      | VAL      | -      | expression tag        | UNP P21218 |
| CF    | 64      | PRO      | -      | expression tag        | UNP P21218 |
| CF    | 65      | ARG      | -      | expression tag        | UNP P21218 |
| CF    | 66      | GLY      | -      | expression tag        | UNP P21218 |
| CF    | 67      | SER      | -      | expression tag        | UNP P21218 |
| CG    | 49      | MET      | -      | initiating methionine | UNP P21218 |
| CG    | 50      | GLY      | -      | expression tag        | UNP P21218 |
| CG    | 51      | SER      | -      | expression tag        | UNP P21218 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| CG    | 52      | SER      | -      | expression tag        | UNP P21218 |
| CG    | 53      | HIS      | -      | expression tag        | UNP P21218 |
| CG    | 54      | HIS      | -      | expression tag        | UNP P21218 |
| CG    | 55      | HIS      | -      | expression tag        | UNP P21218 |
| CG    | 56      | HIS      | -      | expression tag        | UNP P21218 |
| CG    | 57      | HIS      | -      | expression tag        | UNP P21218 |
| CG    | 58      | HIS      | -      | expression tag        | UNP P21218 |
| CG    | 59      | SER      | -      | expression tag        | UNP P21218 |
| CG    | 60      | SER      | -      | expression tag        | UNP P21218 |
| CG    | 61      | GLY      | -      | expression tag        | UNP P21218 |
| CG    | 62      | LEU      | -      | expression tag        | UNP P21218 |
| CG    | 63      | VAL      | -      | expression tag        | UNP P21218 |
| CG    | 64      | PRO      | -      | expression tag        | UNP P21218 |
| CG    | 65      | ARG      | -      | expression tag        | UNP P21218 |
| CG    | 66      | GLY      | -      | expression tag        | UNP P21218 |
| CG    | 67      | SER      | -      | expression tag        | UNP P21218 |
| CH    | 49      | MET      | -      | initiating methionine | UNP P21218 |
| CH    | 50      | GLY      | -      | expression tag        | UNP P21218 |
| CH    | 51      | SER      | -      | expression tag        | UNP P21218 |
| CH    | 52      | SER      | -      | expression tag        | UNP P21218 |
| CH    | 53      | HIS      | -      | expression tag        | UNP P21218 |
| CH    | 54      | HIS      | -      | expression tag        | UNP P21218 |
| CH    | 55      | HIS      | -      | expression tag        | UNP P21218 |
| CH    | 56      | HIS      | -      | expression tag        | UNP P21218 |
| CH    | 57      | HIS      | -      | expression tag        | UNP P21218 |
| CH    | 58      | HIS      | -      | expression tag        | UNP P21218 |
| CH    | 59      | SER      | -      | expression tag        | UNP P21218 |
| CH    | 60      | SER      | -      | expression tag        | UNP P21218 |
| CH    | 61      | GLY      | -      | expression tag        | UNP P21218 |
| CH    | 62      | LEU      | -      | expression tag        | UNP P21218 |
| CH    | 63      | VAL      | -      | expression tag        | UNP P21218 |
| CH    | 64      | PRO      | -      | expression tag        | UNP P21218 |
| CH    | 65      | ARG      | -      | expression tag        | UNP P21218 |
| CH    | 66      | GLY      | -      | expression tag        | UNP P21218 |
| CH    | 67      | SER      | -      | expression tag        | UNP P21218 |
| CI    | 49      | MET      | -      | initiating methionine | UNP P21218 |
| CI    | 50      | GLY      | -      | expression tag        | UNP P21218 |
| CI    | 51      | SER      | -      | expression tag        | UNP P21218 |
| CI    | 52      | SER      | -      | expression tag        | UNP P21218 |
| CI    | 53      | HIS      | -      | expression tag        | UNP P21218 |
| CI    | 54      | HIS      | -      | expression tag        | UNP P21218 |
| CI    | 55      | HIS      | -      | expression tag        | UNP P21218 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| CI    | 56      | HIS      | -      | expression tag        | UNP P21218 |
| CI    | 57      | HIS      | -      | expression tag        | UNP P21218 |
| CI    | 58      | HIS      | -      | expression tag        | UNP P21218 |
| CI    | 59      | SER      | -      | expression tag        | UNP P21218 |
| CI    | 60      | SER      | -      | expression tag        | UNP P21218 |
| CI    | 61      | GLY      | -      | expression tag        | UNP P21218 |
| CI    | 62      | LEU      | -      | expression tag        | UNP P21218 |
| CI    | 63      | VAL      | -      | expression tag        | UNP P21218 |
| CI    | 64      | PRO      | -      | expression tag        | UNP P21218 |
| CI    | 65      | ARG      | -      | expression tag        | UNP P21218 |
| CI    | 66      | GLY      | -      | expression tag        | UNP P21218 |
| CI    | 67      | SER      | -      | expression tag        | UNP P21218 |
| CJ    | 49      | MET      | -      | initiating methionine | UNP P21218 |
| CJ    | 50      | GLY      | -      | expression tag        | UNP P21218 |
| CJ    | 51      | SER      | -      | expression tag        | UNP P21218 |
| CJ    | 52      | SER      | -      | expression tag        | UNP P21218 |
| CJ    | 53      | HIS      | -      | expression tag        | UNP P21218 |
| CJ    | 54      | HIS      | -      | expression tag        | UNP P21218 |
| CJ    | 55      | HIS      | -      | expression tag        | UNP P21218 |
| CJ    | 56      | HIS      | -      | expression tag        | UNP P21218 |
| CJ    | 57      | HIS      | -      | expression tag        | UNP P21218 |
| CJ    | 58      | HIS      | -      | expression tag        | UNP P21218 |
| CJ    | 59      | SER      | -      | expression tag        | UNP P21218 |
| CJ    | 60      | SER      | -      | expression tag        | UNP P21218 |
| CJ    | 61      | GLY      | -      | expression tag        | UNP P21218 |
| CJ    | 62      | LEU      | -      | expression tag        | UNP P21218 |
| CJ    | 63      | VAL      | -      | expression tag        | UNP P21218 |
| CJ    | 64      | PRO      | -      | expression tag        | UNP P21218 |
| CJ    | 65      | ARG      | -      | expression tag        | UNP P21218 |
| CJ    | 66      | GLY      | -      | expression tag        | UNP P21218 |
| CJ    | 67      | SER      | -      | expression tag        | UNP P21218 |
| CK    | 49      | MET      | -      | initiating methionine | UNP P21218 |
| CK    | 50      | GLY      | -      | expression tag        | UNP P21218 |
| CK    | 51      | SER      | -      | expression tag        | UNP P21218 |
| CK    | 52      | SER      | -      | expression tag        | UNP P21218 |
| CK    | 53      | HIS      | -      | expression tag        | UNP P21218 |
| CK    | 54      | HIS      | -      | expression tag        | UNP P21218 |
| CK    | 55      | HIS      | -      | expression tag        | UNP P21218 |
| CK    | 56      | HIS      | -      | expression tag        | UNP P21218 |
| CK    | 57      | HIS      | -      | expression tag        | UNP P21218 |
| CK    | 58      | HIS      | -      | expression tag        | UNP P21218 |
| CK    | 59      | SER      | -      | expression tag        | UNP P21218 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| CK    | 60      | SER      | -      | expression tag        | UNP P21218 |
| CK    | 61      | GLY      | -      | expression tag        | UNP P21218 |
| CK    | 62      | LEU      | -      | expression tag        | UNP P21218 |
| CK    | 63      | VAL      | -      | expression tag        | UNP P21218 |
| CK    | 64      | PRO      | -      | expression tag        | UNP P21218 |
| CK    | 65      | ARG      | -      | expression tag        | UNP P21218 |
| CK    | 66      | GLY      | -      | expression tag        | UNP P21218 |
| CK    | 67      | SER      | -      | expression tag        | UNP P21218 |
| CL    | 49      | MET      | -      | initiating methionine | UNP P21218 |
| CL    | 50      | GLY      | -      | expression tag        | UNP P21218 |
| CL    | 51      | SER      | -      | expression tag        | UNP P21218 |
| CL    | 52      | SER      | -      | expression tag        | UNP P21218 |
| CL    | 53      | HIS      | -      | expression tag        | UNP P21218 |
| CL    | 54      | HIS      | -      | expression tag        | UNP P21218 |
| CL    | 55      | HIS      | -      | expression tag        | UNP P21218 |
| CL    | 56      | HIS      | -      | expression tag        | UNP P21218 |
| CL    | 57      | HIS      | -      | expression tag        | UNP P21218 |
| CL    | 58      | HIS      | -      | expression tag        | UNP P21218 |
| CL    | 59      | SER      | -      | expression tag        | UNP P21218 |
| CL    | 60      | SER      | -      | expression tag        | UNP P21218 |
| CL    | 61      | GLY      | -      | expression tag        | UNP P21218 |
| CL    | 62      | LEU      | -      | expression tag        | UNP P21218 |
| CL    | 63      | VAL      | -      | expression tag        | UNP P21218 |
| CL    | 64      | PRO      | -      | expression tag        | UNP P21218 |
| CL    | 65      | ARG      | -      | expression tag        | UNP P21218 |
| CL    | 66      | GLY      | -      | expression tag        | UNP P21218 |
| CL    | 67      | SER      | -      | expression tag        | UNP P21218 |
| DA    | 49      | MET      | -      | initiating methionine | UNP P21218 |
| DA    | 50      | GLY      | -      | expression tag        | UNP P21218 |
| DA    | 51      | SER      | -      | expression tag        | UNP P21218 |
| DA    | 52      | SER      | -      | expression tag        | UNP P21218 |
| DA    | 53      | HIS      | -      | expression tag        | UNP P21218 |
| DA    | 54      | HIS      | -      | expression tag        | UNP P21218 |
| DA    | 55      | HIS      | -      | expression tag        | UNP P21218 |
| DA    | 56      | HIS      | -      | expression tag        | UNP P21218 |
| DA    | 57      | HIS      | -      | expression tag        | UNP P21218 |
| DA    | 58      | HIS      | -      | expression tag        | UNP P21218 |
| DA    | 59      | SER      | -      | expression tag        | UNP P21218 |
| DA    | 60      | SER      | -      | expression tag        | UNP P21218 |
| DA    | 61      | GLY      | -      | expression tag        | UNP P21218 |
| DA    | 62      | LEU      | -      | expression tag        | UNP P21218 |
| DA    | 63      | VAL      | -      | expression tag        | UNP P21218 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| DA    | 64      | PRO      | -      | expression tag        | UNP P21218 |
| DA    | 65      | ARG      | -      | expression tag        | UNP P21218 |
| DA    | 66      | GLY      | -      | expression tag        | UNP P21218 |
| DA    | 67      | SER      | -      | expression tag        | UNP P21218 |
| DB    | 49      | MET      | -      | initiating methionine | UNP P21218 |
| DB    | 50      | GLY      | -      | expression tag        | UNP P21218 |
| DB    | 51      | SER      | -      | expression tag        | UNP P21218 |
| DB    | 52      | SER      | -      | expression tag        | UNP P21218 |
| DB    | 53      | HIS      | -      | expression tag        | UNP P21218 |
| DB    | 54      | HIS      | -      | expression tag        | UNP P21218 |
| DB    | 55      | HIS      | -      | expression tag        | UNP P21218 |
| DB    | 56      | HIS      | -      | expression tag        | UNP P21218 |
| DB    | 57      | HIS      | -      | expression tag        | UNP P21218 |
| DB    | 58      | HIS      | -      | expression tag        | UNP P21218 |
| DB    | 59      | SER      | -      | expression tag        | UNP P21218 |
| DB    | 60      | SER      | -      | expression tag        | UNP P21218 |
| DB    | 61      | GLY      | -      | expression tag        | UNP P21218 |
| DB    | 62      | LEU      | -      | expression tag        | UNP P21218 |
| DB    | 63      | VAL      | -      | expression tag        | UNP P21218 |
| DB    | 64      | PRO      | -      | expression tag        | UNP P21218 |
| DB    | 65      | ARG      | -      | expression tag        | UNP P21218 |
| DB    | 66      | GLY      | -      | expression tag        | UNP P21218 |
| DB    | 67      | SER      | -      | expression tag        | UNP P21218 |
| DC    | 49      | MET      | -      | initiating methionine | UNP P21218 |
| DC    | 50      | GLY      | -      | expression tag        | UNP P21218 |
| DC    | 51      | SER      | -      | expression tag        | UNP P21218 |
| DC    | 52      | SER      | -      | expression tag        | UNP P21218 |
| DC    | 53      | HIS      | -      | expression tag        | UNP P21218 |
| DC    | 54      | HIS      | -      | expression tag        | UNP P21218 |
| DC    | 55      | HIS      | -      | expression tag        | UNP P21218 |
| DC    | 56      | HIS      | -      | expression tag        | UNP P21218 |
| DC    | 57      | HIS      | -      | expression tag        | UNP P21218 |
| DC    | 58      | HIS      | -      | expression tag        | UNP P21218 |
| DC    | 59      | SER      | -      | expression tag        | UNP P21218 |
| DC    | 60      | SER      | -      | expression tag        | UNP P21218 |
| DC    | 61      | GLY      | -      | expression tag        | UNP P21218 |
| DC    | 62      | LEU      | -      | expression tag        | UNP P21218 |
| DC    | 63      | VAL      | -      | expression tag        | UNP P21218 |
| DC    | 64      | PRO      | -      | expression tag        | UNP P21218 |
| DC    | 65      | ARG      | -      | expression tag        | UNP P21218 |
| DC    | 66      | GLY      | -      | expression tag        | UNP P21218 |
| DC    | 67      | SER      | -      | expression tag        | UNP P21218 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| DD    | 49      | MET      | -      | initiating methionine | UNP P21218 |
| DD    | 50      | GLY      | -      | expression tag        | UNP P21218 |
| DD    | 51      | SER      | -      | expression tag        | UNP P21218 |
| DD    | 52      | SER      | -      | expression tag        | UNP P21218 |
| DD    | 53      | HIS      | -      | expression tag        | UNP P21218 |
| DD    | 54      | HIS      | -      | expression tag        | UNP P21218 |
| DD    | 55      | HIS      | -      | expression tag        | UNP P21218 |
| DD    | 56      | HIS      | -      | expression tag        | UNP P21218 |
| DD    | 57      | HIS      | -      | expression tag        | UNP P21218 |
| DD    | 58      | HIS      | -      | expression tag        | UNP P21218 |
| DD    | 59      | SER      | -      | expression tag        | UNP P21218 |
| DD    | 60      | SER      | -      | expression tag        | UNP P21218 |
| DD    | 61      | GLY      | -      | expression tag        | UNP P21218 |
| DD    | 62      | LEU      | -      | expression tag        | UNP P21218 |
| DD    | 63      | VAL      | -      | expression tag        | UNP P21218 |
| DD    | 64      | PRO      | -      | expression tag        | UNP P21218 |
| DD    | 65      | ARG      | -      | expression tag        | UNP P21218 |
| DD    | 66      | GLY      | -      | expression tag        | UNP P21218 |
| DD    | 67      | SER      | -      | expression tag        | UNP P21218 |
| DE    | 49      | MET      | -      | initiating methionine | UNP P21218 |
| DE    | 50      | GLY      | -      | expression tag        | UNP P21218 |
| DE    | 51      | SER      | -      | expression tag        | UNP P21218 |
| DE    | 52      | SER      | -      | expression tag        | UNP P21218 |
| DE    | 53      | HIS      | -      | expression tag        | UNP P21218 |
| DE    | 54      | HIS      | -      | expression tag        | UNP P21218 |
| DE    | 55      | HIS      | -      | expression tag        | UNP P21218 |
| DE    | 56      | HIS      | -      | expression tag        | UNP P21218 |
| DE    | 57      | HIS      | -      | expression tag        | UNP P21218 |
| DE    | 58      | HIS      | -      | expression tag        | UNP P21218 |
| DE    | 59      | SER      | -      | expression tag        | UNP P21218 |
| DE    | 60      | SER      | -      | expression tag        | UNP P21218 |
| DE    | 61      | GLY      | -      | expression tag        | UNP P21218 |
| DE    | 62      | LEU      | -      | expression tag        | UNP P21218 |
| DE    | 63      | VAL      | -      | expression tag        | UNP P21218 |
| DE    | 64      | PRO      | -      | expression tag        | UNP P21218 |
| DE    | 65      | ARG      | -      | expression tag        | UNP P21218 |
| DE    | 66      | GLY      | -      | expression tag        | UNP P21218 |
| DE    | 67      | SER      | -      | expression tag        | UNP P21218 |
| DF    | 49      | MET      | -      | initiating methionine | UNP P21218 |
| DF    | 50      | GLY      | -      | expression tag        | UNP P21218 |
| DF    | 51      | SER      | -      | expression tag        | UNP P21218 |
| DF    | 52      | SER      | -      | expression tag        | UNP P21218 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| DF    | 53      | HIS      | -      | expression tag        | UNP P21218 |
| DF    | 54      | HIS      | -      | expression tag        | UNP P21218 |
| DF    | 55      | HIS      | -      | expression tag        | UNP P21218 |
| DF    | 56      | HIS      | -      | expression tag        | UNP P21218 |
| DF    | 57      | HIS      | -      | expression tag        | UNP P21218 |
| DF    | 58      | HIS      | -      | expression tag        | UNP P21218 |
| DF    | 59      | SER      | -      | expression tag        | UNP P21218 |
| DF    | 60      | SER      | -      | expression tag        | UNP P21218 |
| DF    | 61      | GLY      | -      | expression tag        | UNP P21218 |
| DF    | 62      | LEU      | -      | expression tag        | UNP P21218 |
| DF    | 63      | VAL      | -      | expression tag        | UNP P21218 |
| DF    | 64      | PRO      | -      | expression tag        | UNP P21218 |
| DF    | 65      | ARG      | -      | expression tag        | UNP P21218 |
| DF    | 66      | GLY      | -      | expression tag        | UNP P21218 |
| DF    | 67      | SER      | -      | expression tag        | UNP P21218 |
| DG    | 49      | MET      | -      | initiating methionine | UNP P21218 |
| DG    | 50      | GLY      | -      | expression tag        | UNP P21218 |
| DG    | 51      | SER      | -      | expression tag        | UNP P21218 |
| DG    | 52      | SER      | -      | expression tag        | UNP P21218 |
| DG    | 53      | HIS      | -      | expression tag        | UNP P21218 |
| DG    | 54      | HIS      | -      | expression tag        | UNP P21218 |
| DG    | 55      | HIS      | -      | expression tag        | UNP P21218 |
| DG    | 56      | HIS      | -      | expression tag        | UNP P21218 |
| DG    | 57      | HIS      | -      | expression tag        | UNP P21218 |
| DG    | 58      | HIS      | -      | expression tag        | UNP P21218 |
| DG    | 59      | SER      | -      | expression tag        | UNP P21218 |
| DG    | 60      | SER      | -      | expression tag        | UNP P21218 |
| DG    | 61      | GLY      | -      | expression tag        | UNP P21218 |
| DG    | 62      | LEU      | -      | expression tag        | UNP P21218 |
| DG    | 63      | VAL      | -      | expression tag        | UNP P21218 |
| DG    | 64      | PRO      | -      | expression tag        | UNP P21218 |
| DG    | 65      | ARG      | -      | expression tag        | UNP P21218 |
| DG    | 66      | GLY      | -      | expression tag        | UNP P21218 |
| DG    | 67      | SER      | -      | expression tag        | UNP P21218 |
| DH    | 49      | MET      | -      | initiating methionine | UNP P21218 |
| DH    | 50      | GLY      | -      | expression tag        | UNP P21218 |
| DH    | 51      | SER      | -      | expression tag        | UNP P21218 |
| DH    | 52      | SER      | -      | expression tag        | UNP P21218 |
| DH    | 53      | HIS      | -      | expression tag        | UNP P21218 |
| DH    | 54      | HIS      | -      | expression tag        | UNP P21218 |
| DH    | 55      | HIS      | -      | expression tag        | UNP P21218 |
| DH    | 56      | HIS      | -      | expression tag        | UNP P21218 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| DH    | 57      | HIS      | -      | expression tag | UNP P21218 |
| DH    | 58      | HIS      | -      | expression tag | UNP P21218 |
| DH    | 59      | SER      | -      | expression tag | UNP P21218 |
| DH    | 60      | SER      | -      | expression tag | UNP P21218 |
| DH    | 61      | GLY      | -      | expression tag | UNP P21218 |
| DH    | 62      | LEU      | -      | expression tag | UNP P21218 |
| DH    | 63      | VAL      | -      | expression tag | UNP P21218 |
| DH    | 64      | PRO      | -      | expression tag | UNP P21218 |
| DH    | 65      | ARG      | -      | expression tag | UNP P21218 |
| DH    | 66      | GLY      | -      | expression tag | UNP P21218 |
| DH    | 67      | SER      | -      | expression tag | UNP P21218 |

- # NDP



WORLD WIDE  
PDB  
PROTEIN DATA BANK

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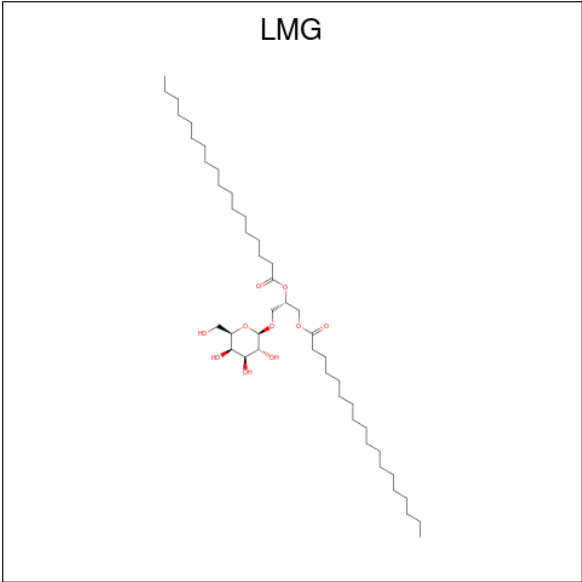
| Mol | Chain | Residues | Atoms       |         |        |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 2   | AF    | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       |
| 2   | AG    | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       |
| 2   | AH    | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       |
| 2   | AI    | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       |
| 2   | AJ    | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       |
| 2   | AK    | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       |
| 2   | AL    | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       |
| 2   | BA    | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       |
| 2   | BB    | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       |
| 2   | BC    | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       |
| 2   | BD    | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       |
| 2   | BE    | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       |
| 2   | BF    | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       |
| 2   | BG    | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       |
| 2   | BH    | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       |
| 2   | BI    | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       |
| 2   | BJ    | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       |
| 2   | BK    | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       |
| 2   | BL    | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       |
| 2   | CA    | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       |
| 2   | CB    | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       |

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| Mol | Chain | Residues | Atoms       |         |        |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 2   | CC    | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       |
| 2   | CD    | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       |
| 2   | CE    | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       |
| 2   | CF    | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       |
| 2   | CG    | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       |
| 2   | CH    | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       |
| 2   | CI    | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       |
| 2   | CJ    | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       |
| 2   | CK    | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       |
| 2   | CL    | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       |
| 2   | DA    | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       |
| 2   | DB    | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       |
| 2   | DC    | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       |
| 2   | DD    | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       |
| 2   | DE    | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       |
| 2   | DF    | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       |
| 2   | DG    | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       |
| 2   | DH    | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       |

- Molecule 3 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 3   | AA    | 1        | Total | C  | O  | 0       |
|     |       |          | 23    | 13 | 10 |         |
| 3   | AB    | 1        | Total | C  | O  | 0       |
|     |       |          | 23    | 13 | 10 |         |
| 3   | AC    | 1        | Total | C  | O  | 0       |
|     |       |          | 23    | 13 | 10 |         |
| 3   | AD    | 1        | Total | C  | O  | 0       |
|     |       |          | 23    | 13 | 10 |         |
| 3   | AE    | 1        | Total | C  | O  | 0       |
|     |       |          | 23    | 13 | 10 |         |
| 3   | AF    | 1        | Total | C  | O  | 0       |
|     |       |          | 23    | 13 | 10 |         |
| 3   | AG    | 1        | Total | C  | O  | 0       |
|     |       |          | 23    | 13 | 10 |         |
| 3   | AH    | 1        | Total | C  | O  | 0       |
|     |       |          | 23    | 13 | 10 |         |
| 3   | AI    | 1        | Total | C  | O  | 0       |
|     |       |          | 23    | 13 | 10 |         |
| 3   | AJ    | 1        | Total | C  | O  | 0       |
|     |       |          | 23    | 13 | 10 |         |
| 3   | AK    | 1        | Total | C  | O  | 0       |
|     |       |          | 23    | 13 | 10 |         |
| 3   | AL    | 1        | Total | C  | O  | 0       |
|     |       |          | 23    | 13 | 10 |         |
| 3   | BA    | 1        | Total | C  | O  | 0       |
|     |       |          | 23    | 13 | 10 |         |
| 3   | BB    | 1        | Total | C  | O  | 0       |
|     |       |          | 23    | 13 | 10 |         |

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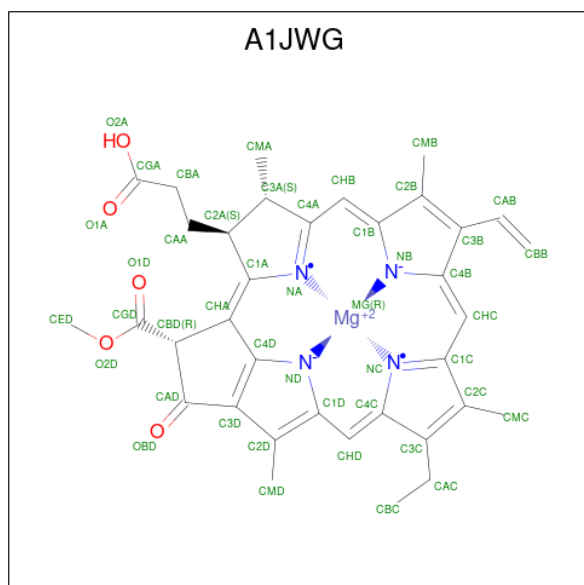
| Mol | Chain | Residues | Atoms       |         |         | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 3   | BC    | 1        | Total<br>23 | C<br>13 | O<br>10 | 0       |
| 3   | BD    | 1        | Total<br>23 | C<br>13 | O<br>10 | 0       |
| 3   | BE    | 1        | Total<br>23 | C<br>13 | O<br>10 | 0       |
| 3   | BF    | 1        | Total<br>23 | C<br>13 | O<br>10 | 0       |
| 3   | BG    | 1        | Total<br>23 | C<br>13 | O<br>10 | 0       |
| 3   | BH    | 1        | Total<br>23 | C<br>13 | O<br>10 | 0       |
| 3   | BI    | 1        | Total<br>23 | C<br>13 | O<br>10 | 0       |
| 3   | BJ    | 1        | Total<br>23 | C<br>13 | O<br>10 | 0       |
| 3   | BK    | 1        | Total<br>23 | C<br>13 | O<br>10 | 0       |
| 3   | BL    | 1        | Total<br>23 | C<br>13 | O<br>10 | 0       |
| 3   | CA    | 1        | Total<br>23 | C<br>13 | O<br>10 | 0       |
| 3   | CB    | 1        | Total<br>23 | C<br>13 | O<br>10 | 0       |
| 3   | CC    | 1        | Total<br>23 | C<br>13 | O<br>10 | 0       |
| 3   | CD    | 1        | Total<br>23 | C<br>13 | O<br>10 | 0       |
| 3   | CE    | 1        | Total<br>23 | C<br>13 | O<br>10 | 0       |
| 3   | CF    | 1        | Total<br>23 | C<br>13 | O<br>10 | 0       |
| 3   | CG    | 1        | Total<br>23 | C<br>13 | O<br>10 | 0       |
| 3   | CH    | 1        | Total<br>23 | C<br>13 | O<br>10 | 0       |
| 3   | CI    | 1        | Total<br>23 | C<br>13 | O<br>10 | 0       |
| 3   | CJ    | 1        | Total<br>23 | C<br>13 | O<br>10 | 0       |
| 3   | CK    | 1        | Total<br>23 | C<br>13 | O<br>10 | 0       |

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| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 3   | CL    | 1        | Total | C  | O  | 0       |
|     |       |          | 23    | 13 | 10 |         |
| 3   | DA    | 1        | Total | C  | O  | 0       |
|     |       |          | 23    | 13 | 10 |         |
| 3   | DB    | 1        | Total | C  | O  | 0       |
|     |       |          | 23    | 13 | 10 |         |
| 3   | DC    | 1        | Total | C  | O  | 0       |
|     |       |          | 23    | 13 | 10 |         |
| 3   | DD    | 1        | Total | C  | O  | 0       |
|     |       |          | 23    | 13 | 10 |         |
| 3   | DE    | 1        | Total | C  | O  | 0       |
|     |       |          | 23    | 13 | 10 |         |
| 3   | DF    | 1        | Total | C  | O  | 0       |
|     |       |          | 23    | 13 | 10 |         |
| 3   | DG    | 1        | Total | C  | O  | 0       |
|     |       |          | 23    | 13 | 10 |         |
| 3   | DH    | 1        | Total | C  | O  | 0       |
|     |       |          | 23    | 13 | 10 |         |

- Molecule 4 is Chlorophyllide a (CCD ID: A1JWG) (formula:  $C_{35}H_{34}MgN_4O_5$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|----|---|---|---------|
| 4   | AA    | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 4   | AB    | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms |    |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|----|---|---|---------|
| 4   | AC    | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 4   | AD    | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 4   | AE    | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 4   | AF    | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 4   | AG    | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 4   | AH    | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 4   | AI    | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 4   | AJ    | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 4   | AK    | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 4   | AL    | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 4   | BA    | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 4   | BB    | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 4   | BC    | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 4   | BD    | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 4   | BE    | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 4   | BF    | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 4   | BG    | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 4   | BH    | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 4   | BI    | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 4   | BJ    | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 4   | BK    | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |

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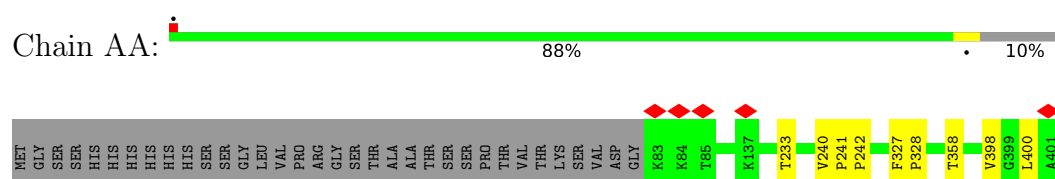
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| Mol | Chain | Residues | Atoms |    |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|----|---|---|---------|
| 4   | BL    | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 4   | CA    | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 4   | CB    | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 4   | CC    | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 4   | CD    | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 4   | CE    | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 4   | CF    | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 4   | CG    | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 4   | CH    | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 4   | CI    | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 4   | CJ    | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 4   | CK    | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 4   | CL    | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 4   | DA    | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 4   | DB    | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 4   | DC    | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 4   | DD    | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 4   | DE    | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 4   | DF    | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 4   | DG    | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |
| 4   | DH    | 1        | Total | C  | H  | Mg | N | O | 0       |
|     |       |          | 78    | 35 | 33 | 1  | 4 | 5 |         |

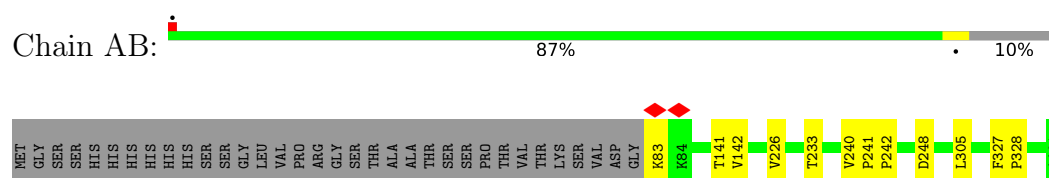
### 3 Residue-property plots [i](#)

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.

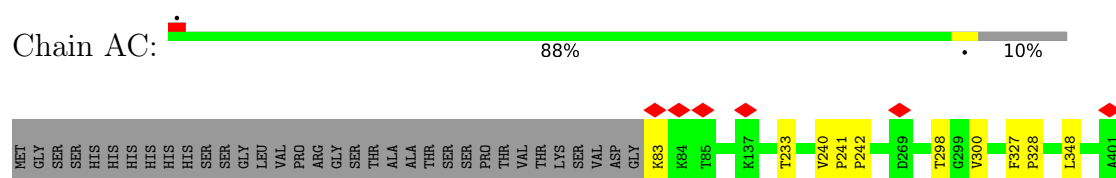
- Molecule 1: Protochlorophyllide reductase B, chloroplastic



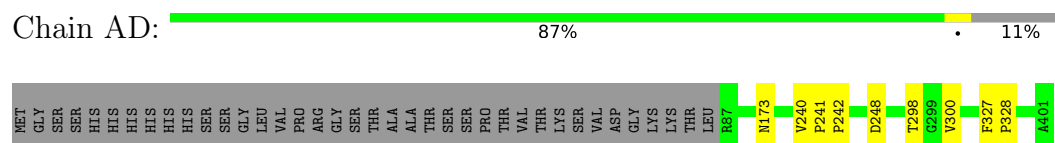
- Molecule 1: Protochlorophyllide reductase B, chloroplastic



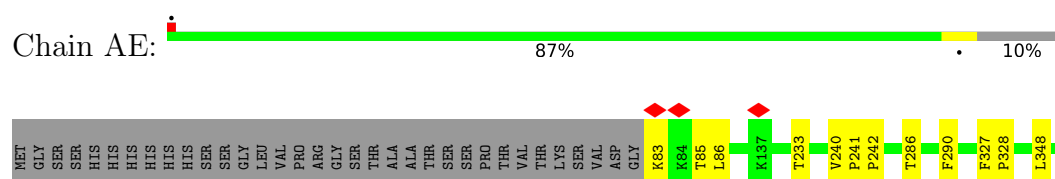
- Molecule 1: Protochlorophyllide reductase B, chloroplastic



- Molecule 1: Protochlorophyllide reductase B, chloroplastic

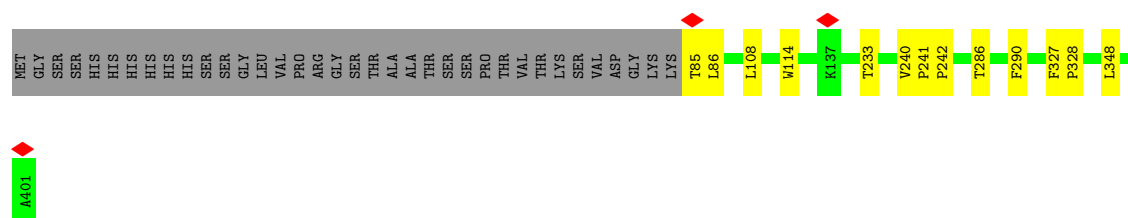


- Molecule 1: Protochlorophyllide reductase B, chloroplastic



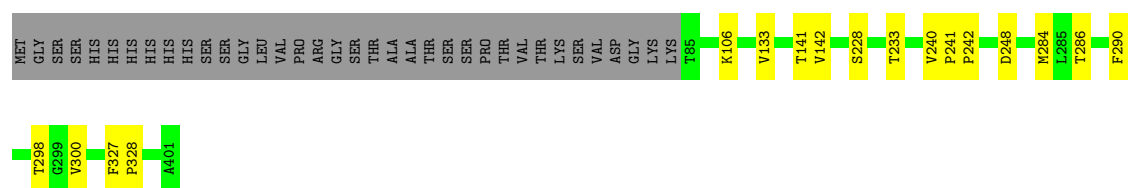
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain AF:  86% 10%



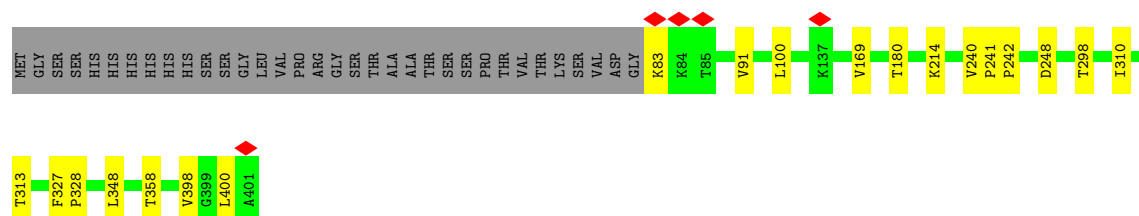
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain AG:  85% 5% 10%



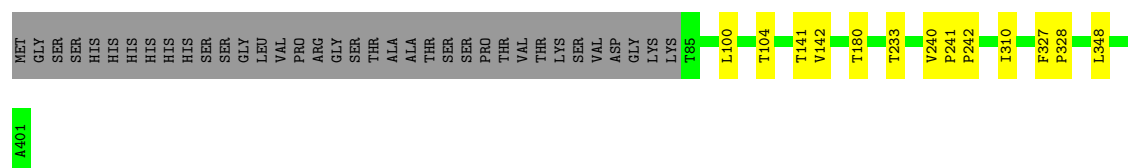
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain AH:  85% 5% 10%



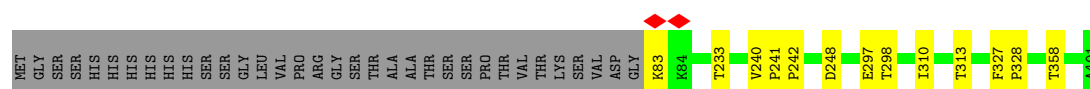
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain AI:  86% 10%



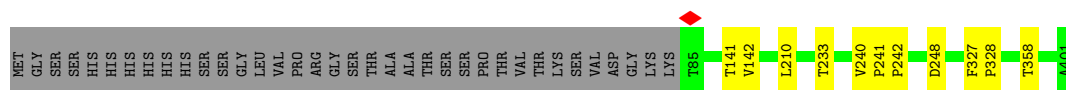
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain AJ:  87% 10%



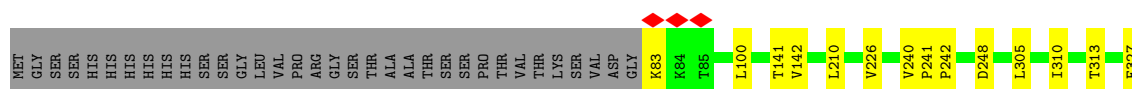
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain AK:  87% 10%



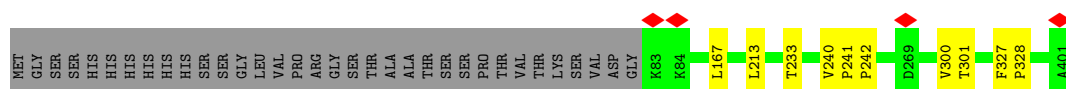
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain AL:  85% 5% 10%



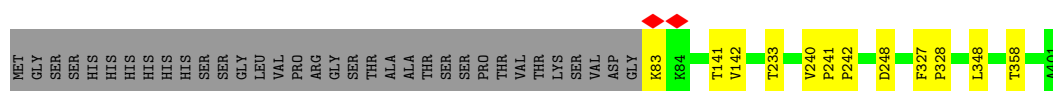
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain BA:  88% 10%



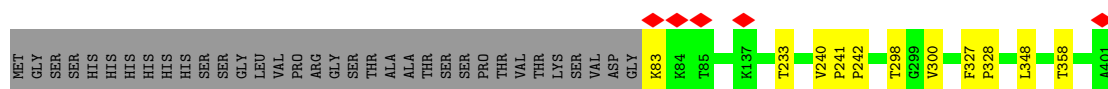
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain BB:  87% 10%



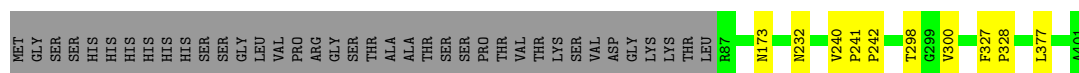
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain BC:  87% 10%



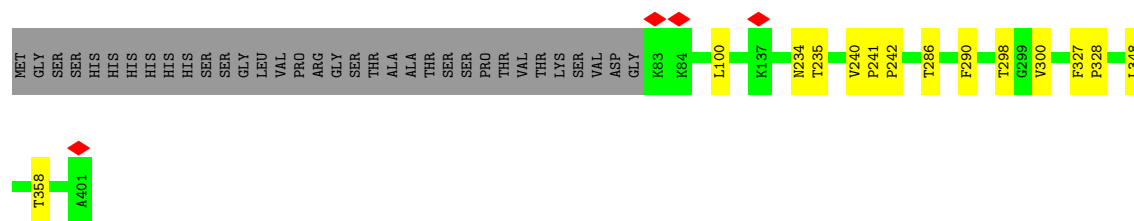
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain BD:  86% 11%



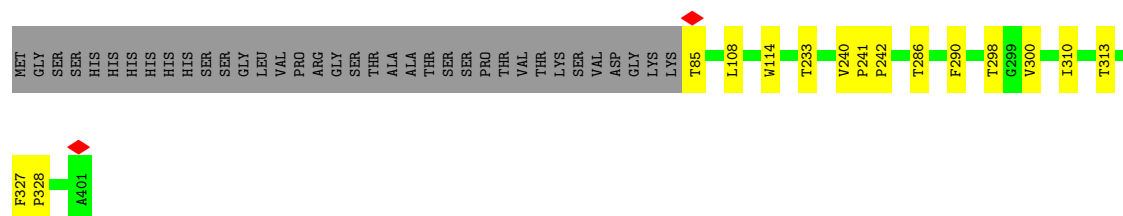
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain BE:  86% 10%



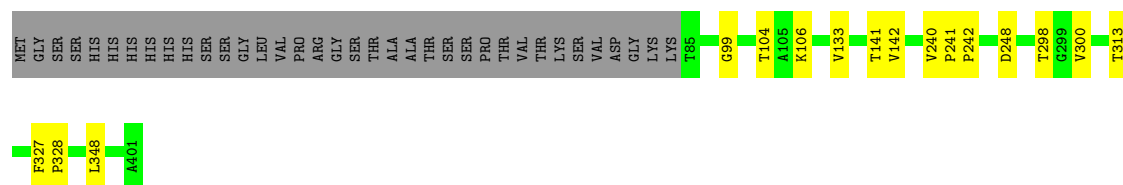
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain BF:  86% 10%



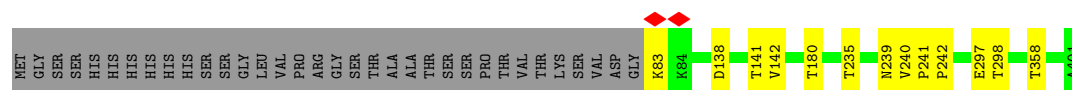
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain BG:  85% 5% 10%



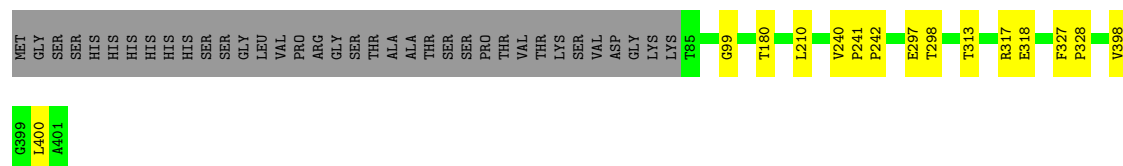
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain BH:  87% 10%



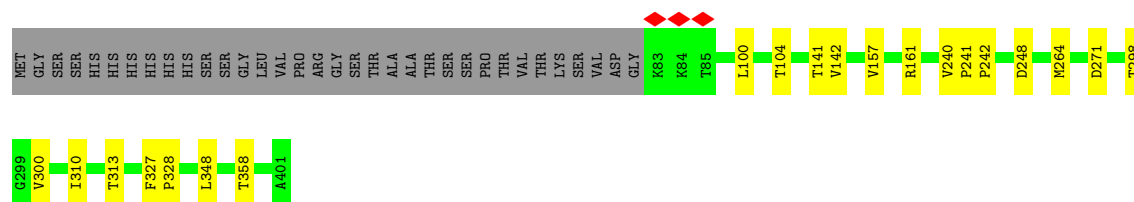
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain BI:  86% 10%



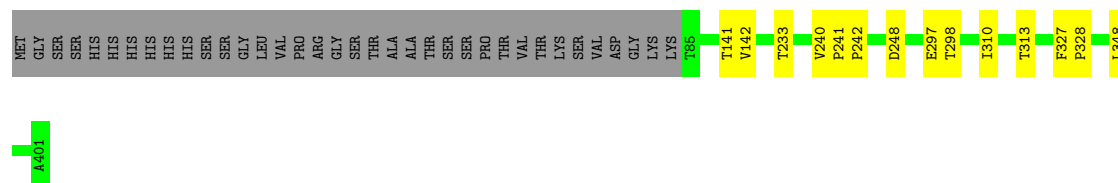
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain BJ:  85% 6% 10%



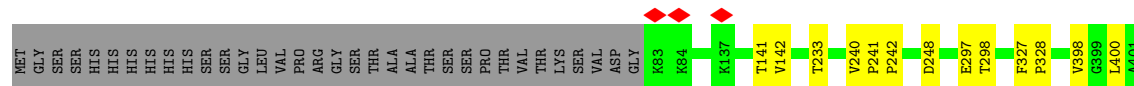
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain BK:  86% 10%



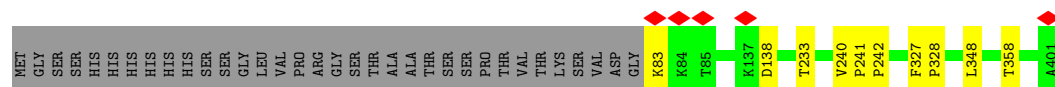
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain BL:  87% 10%



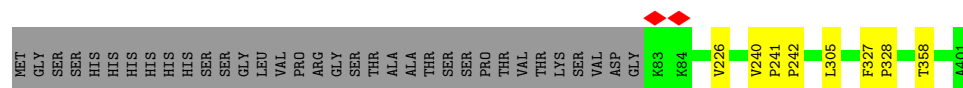
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain CA:  88% 10%



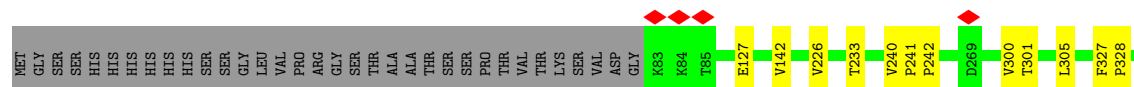
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain CB:  88% 10%



- Molecule 1: Protochlorophyllide reductase B, chloroplastic

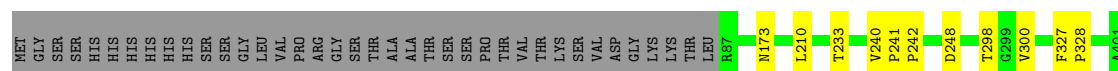
Chain CC:  87% 10%





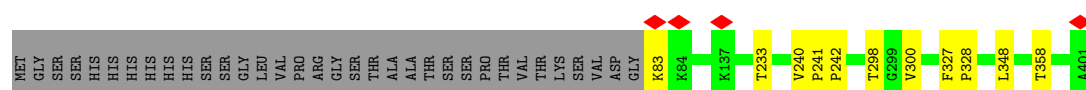
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain CD: 86% 11%



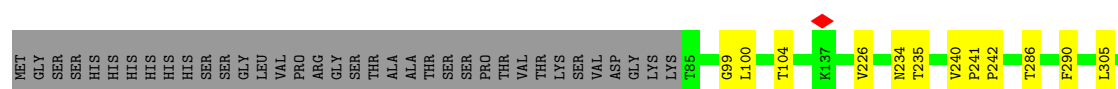
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain CE: 87% 10%



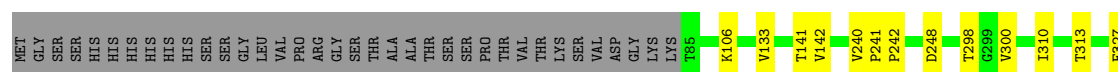
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain CF: 85% 5% 10%



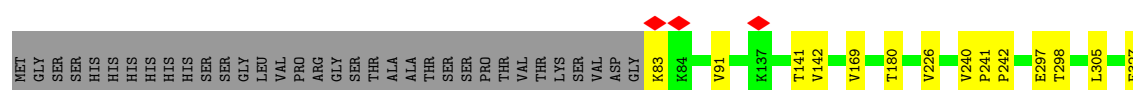
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain CG: 86% 10%



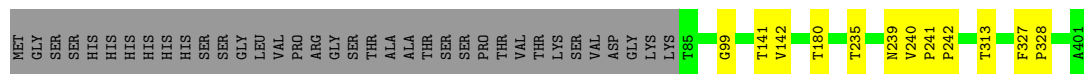
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain CH: 86% 10%



- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain CI:  86% 10%



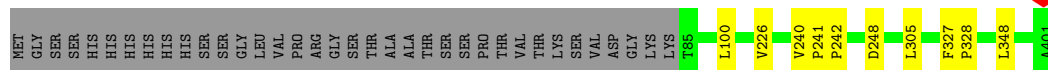
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain CJ:  86% 10%



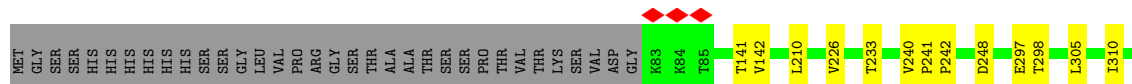
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain CK:  87% 10%



- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain CL:  86% 5% 10%



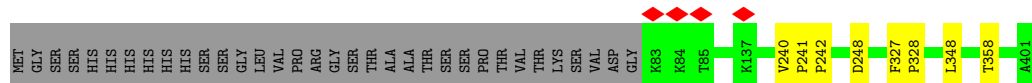
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain DA:  88% 10%



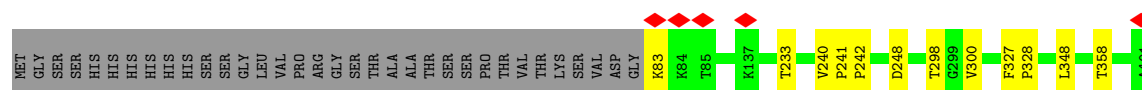
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain DB:  88% 10%



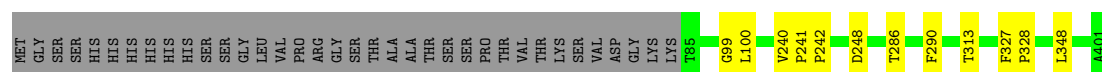
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain DC:  87% 10%



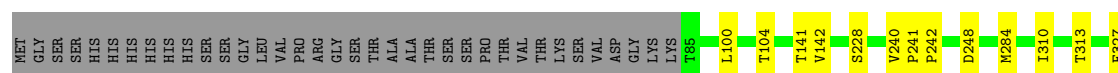
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain DD:  86% 10%



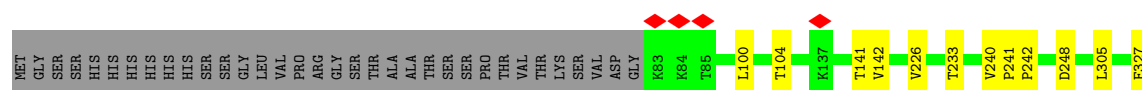
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain DE:  85% 5% 10%



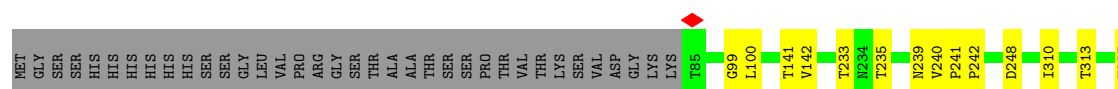
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain DF:  86% 10%



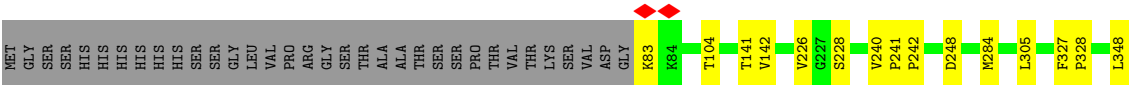
- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain DG:  86% 10%



- Molecule 1: Protochlorophyllide reductase B, chloroplastic

Chain DH:  86% 10%



## 4 Experimental information

| Property                             | Value                                               | Source    |
|--------------------------------------|-----------------------------------------------------|-----------|
| EM reconstruction method             | HELICAL                                             | Depositor |
| Imposed symmetry                     | HELICAL, twist=-96.375°, rise=6.857 Å, axial sym=D1 | Depositor |
| Number of segments used              | 70789                                               | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                                   | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION             | Depositor |
| Microscope                           | TFS KRIOS                                           | Depositor |
| Voltage (kV)                         | 300                                                 | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 40.39                                               | Depositor |
| Minimum defocus (nm)                 | 900                                                 | Depositor |
| Maximum defocus (nm)                 | 2100                                                | Depositor |
| Magnification                        | Not provided                                        |           |
| Image detector                       | GATAN K3 BIOCONTINUUM (6k x 4k)                     | Depositor |
| Maximum map value                    | 0.519                                               | Depositor |
| Minimum map value                    | -0.223                                              | Depositor |
| Average map value                    | 0.001                                               | Depositor |
| Map value standard deviation         | 0.024                                               | Depositor |
| Recommended contour level            | 0.11                                                | Depositor |
| Map size (Å)                         | 550.4, 550.4, 550.4                                 | wwPDB     |
| Map dimensions                       | 640, 640, 640                                       | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                                    | wwPDB     |
| Pixel spacing (Å)                    | 0.86, 0.86, 0.86                                    | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1JWG, NDP, LMG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |             | Bond angles |             |
|-----|-------|--------------|-------------|-------------|-------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$ |
| 1   | AA    | 0.13         | 0/2495      | 0.29        | 0/3374      |
| 1   | AB    | 0.15         | 0/2495      | 0.30        | 0/3374      |
| 1   | AC    | 0.13         | 0/2495      | 0.29        | 0/3374      |
| 1   | AD    | 0.15         | 0/2462      | 0.31        | 0/3331      |
| 1   | AE    | 0.14         | 0/2495      | 0.30        | 0/3374      |
| 1   | AF    | 0.14         | 0/2477      | 0.29        | 0/3352      |
| 1   | AG    | 0.15         | 0/2477      | 0.31        | 0/3352      |
| 1   | AH    | 0.15         | 0/2495      | 0.30        | 0/3374      |
| 1   | AI    | 0.14         | 0/2477      | 0.30        | 0/3352      |
| 1   | AJ    | 0.15         | 0/2495      | 0.31        | 0/3374      |
| 1   | AK    | 0.15         | 0/2477      | 0.31        | 0/3352      |
| 1   | AL    | 0.15         | 0/2495      | 0.30        | 0/3374      |
| 1   | BA    | 0.13         | 0/2495      | 0.29        | 0/3374      |
| 1   | BB    | 0.15         | 0/2495      | 0.32        | 0/3374      |
| 1   | BC    | 0.14         | 0/2495      | 0.29        | 0/3374      |
| 1   | BD    | 0.15         | 0/2462      | 0.31        | 0/3331      |
| 1   | BE    | 0.14         | 0/2495      | 0.29        | 0/3374      |
| 1   | BF    | 0.14         | 0/2477      | 0.30        | 0/3352      |
| 1   | BG    | 0.15         | 0/2477      | 0.31        | 0/3352      |
| 1   | BH    | 0.14         | 0/2495      | 0.29        | 0/3374      |
| 1   | BI    | 0.15         | 0/2477      | 0.31        | 0/3352      |
| 1   | BJ    | 0.15         | 0/2495      | 0.31        | 0/3374      |
| 1   | BK    | 0.15         | 0/2477      | 0.31        | 0/3352      |
| 1   | BL    | 0.15         | 0/2495      | 0.30        | 0/3374      |
| 1   | CA    | 0.14         | 0/2495      | 0.30        | 0/3374      |
| 1   | CB    | 0.15         | 0/2495      | 0.30        | 0/3374      |
| 1   | CC    | 0.13         | 0/2495      | 0.29        | 0/3374      |
| 1   | CD    | 0.15         | 0/2462      | 0.32        | 0/3331      |
| 1   | CE    | 0.14         | 0/2495      | 0.28        | 0/3374      |
| 1   | CF    | 0.14         | 0/2477      | 0.30        | 0/3352      |
| 1   | CG    | 0.15         | 0/2477      | 0.30        | 0/3352      |
| 1   | CH    | 0.15         | 0/2495      | 0.30        | 0/3374      |

| Mol | Chain | Bond lengths |          | Bond angles |          |
|-----|-------|--------------|----------|-------------|----------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5  |
| 1   | CI    | 0.14         | 0/2477   | 0.30        | 0/3352   |
| 1   | CJ    | 0.15         | 0/2495   | 0.31        | 0/3374   |
| 1   | CK    | 0.15         | 0/2477   | 0.31        | 0/3352   |
| 1   | CL    | 0.15         | 0/2495   | 0.31        | 0/3374   |
| 1   | DA    | 0.14         | 0/2495   | 0.29        | 0/3374   |
| 1   | DB    | 0.15         | 0/2495   | 0.30        | 0/3374   |
| 1   | DC    | 0.14         | 0/2495   | 0.30        | 0/3374   |
| 1   | DD    | 0.15         | 0/2477   | 0.30        | 0/3352   |
| 1   | DE    | 0.15         | 0/2477   | 0.30        | 0/3352   |
| 1   | DF    | 0.15         | 0/2495   | 0.30        | 0/3374   |
| 1   | DG    | 0.15         | 0/2477   | 0.30        | 0/3352   |
| 1   | DH    | 0.15         | 0/2495   | 0.31        | 0/3374   |
| All | All   | 0.15         | 0/109411 | 0.30        | 0/147997 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | AA    | 2446  | 2397     | 2450     | 11      | 0            |
| 1   | AB    | 2446  | 2397     | 2450     | 11      | 0            |
| 1   | AC    | 2446  | 2397     | 2450     | 14      | 0            |
| 1   | AD    | 2413  | 2387     | 2406     | 9       | 0            |
| 1   | AE    | 2446  | 2397     | 2450     | 13      | 0            |
| 1   | AF    | 2428  | 2397     | 2424     | 13      | 0            |
| 1   | AG    | 2428  | 2397     | 2424     | 12      | 0            |
| 1   | AH    | 2446  | 2397     | 2450     | 18      | 0            |
| 1   | AI    | 2428  | 2397     | 2424     | 15      | 0            |
| 1   | AJ    | 2446  | 2397     | 2450     | 14      | 0            |
| 1   | AK    | 2428  | 2397     | 2424     | 11      | 0            |
| 1   | AL    | 2446  | 2397     | 2450     | 15      | 0            |
| 1   | BA    | 2446  | 2397     | 2450     | 12      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | BB    | 2446  | 2397     | 2450     | 13      | 0            |
| 1   | BC    | 2446  | 2397     | 2450     | 11      | 0            |
| 1   | BD    | 2413  | 2387     | 2406     | 8       | 0            |
| 1   | BE    | 2446  | 2397     | 2450     | 15      | 0            |
| 1   | BF    | 2428  | 2397     | 2424     | 14      | 0            |
| 1   | BG    | 2428  | 2397     | 2424     | 12      | 0            |
| 1   | BH    | 2446  | 2397     | 2450     | 13      | 0            |
| 1   | BI    | 2428  | 2397     | 2424     | 13      | 0            |
| 1   | BJ    | 2446  | 2397     | 2450     | 14      | 0            |
| 1   | BK    | 2428  | 2397     | 2424     | 14      | 0            |
| 1   | BL    | 2446  | 2397     | 2450     | 12      | 0            |
| 1   | CA    | 2446  | 2397     | 2450     | 12      | 0            |
| 1   | CB    | 2446  | 2397     | 2450     | 8       | 0            |
| 1   | CC    | 2446  | 2397     | 2450     | 10      | 0            |
| 1   | CD    | 2413  | 2387     | 2406     | 13      | 0            |
| 1   | CE    | 2446  | 2397     | 2450     | 13      | 0            |
| 1   | CF    | 2428  | 2397     | 2424     | 16      | 0            |
| 1   | CG    | 2428  | 2397     | 2424     | 12      | 0            |
| 1   | CH    | 2446  | 2397     | 2450     | 13      | 0            |
| 1   | CI    | 2428  | 2397     | 2424     | 14      | 0            |
| 1   | CJ    | 2446  | 2397     | 2450     | 15      | 0            |
| 1   | CK    | 2428  | 2397     | 2424     | 9       | 0            |
| 1   | CL    | 2446  | 2397     | 2450     | 15      | 0            |
| 1   | DA    | 2446  | 2397     | 2450     | 11      | 0            |
| 1   | DB    | 2446  | 2397     | 2450     | 9       | 0            |
| 1   | DC    | 2446  | 2397     | 2450     | 14      | 0            |
| 1   | DD    | 2428  | 2397     | 2424     | 12      | 0            |
| 1   | DE    | 2428  | 2397     | 2424     | 15      | 0            |
| 1   | DF    | 2446  | 2397     | 2450     | 14      | 0            |
| 1   | DG    | 2428  | 2397     | 2424     | 12      | 0            |
| 1   | DH    | 2446  | 2397     | 2450     | 13      | 0            |
| 2   | AA    | 48    | 0        | 26       | 0       | 0            |
| 2   | AB    | 48    | 0        | 26       | 0       | 0            |
| 2   | AC    | 48    | 0        | 26       | 0       | 0            |
| 2   | AD    | 48    | 0        | 26       | 1       | 0            |
| 2   | AE    | 48    | 0        | 26       | 0       | 0            |
| 2   | AF    | 48    | 0        | 26       | 1       | 0            |
| 2   | AG    | 48    | 0        | 26       | 1       | 0            |
| 2   | AH    | 48    | 0        | 26       | 1       | 0            |
| 2   | AI    | 48    | 0        | 26       | 1       | 0            |
| 2   | AJ    | 48    | 0        | 26       | 0       | 0            |
| 2   | AK    | 48    | 0        | 26       | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | AL    | 48    | 0        | 26       | 0       | 0            |
| 2   | BA    | 48    | 0        | 26       | 0       | 0            |
| 2   | BB    | 48    | 0        | 26       | 0       | 0            |
| 2   | BC    | 48    | 0        | 26       | 0       | 0            |
| 2   | BD    | 48    | 0        | 26       | 1       | 0            |
| 2   | BE    | 48    | 0        | 26       | 1       | 0            |
| 2   | BF    | 48    | 0        | 26       | 2       | 0            |
| 2   | BG    | 48    | 0        | 26       | 0       | 0            |
| 2   | BH    | 48    | 0        | 26       | 0       | 0            |
| 2   | BI    | 48    | 0        | 26       | 0       | 0            |
| 2   | BJ    | 48    | 0        | 26       | 0       | 0            |
| 2   | BK    | 48    | 0        | 26       | 0       | 0            |
| 2   | BL    | 48    | 0        | 26       | 0       | 0            |
| 2   | CA    | 48    | 0        | 26       | 0       | 0            |
| 2   | CB    | 48    | 0        | 26       | 0       | 0            |
| 2   | CC    | 48    | 0        | 26       | 0       | 0            |
| 2   | CD    | 48    | 0        | 26       | 1       | 0            |
| 2   | CE    | 48    | 0        | 26       | 0       | 0            |
| 2   | CF    | 48    | 0        | 26       | 2       | 0            |
| 2   | CG    | 48    | 0        | 26       | 1       | 0            |
| 2   | CH    | 48    | 0        | 26       | 0       | 0            |
| 2   | CI    | 48    | 0        | 26       | 0       | 0            |
| 2   | CJ    | 48    | 0        | 26       | 0       | 0            |
| 2   | CK    | 48    | 0        | 26       | 0       | 0            |
| 2   | CL    | 48    | 0        | 26       | 0       | 0            |
| 2   | DA    | 48    | 0        | 26       | 0       | 0            |
| 2   | DB    | 48    | 0        | 26       | 0       | 0            |
| 2   | DC    | 48    | 0        | 26       | 0       | 0            |
| 2   | DD    | 48    | 0        | 26       | 1       | 0            |
| 2   | DE    | 48    | 0        | 26       | 1       | 0            |
| 2   | DF    | 48    | 0        | 26       | 0       | 0            |
| 2   | DG    | 48    | 0        | 26       | 0       | 0            |
| 2   | DH    | 48    | 0        | 26       | 0       | 0            |
| 3   | AA    | 23    | 0        | 16       | 2       | 0            |
| 3   | AB    | 23    | 0        | 16       | 0       | 0            |
| 3   | AC    | 23    | 0        | 16       | 2       | 0            |
| 3   | AD    | 23    | 0        | 16       | 0       | 0            |
| 3   | AE    | 23    | 0        | 16       | 1       | 0            |
| 3   | AF    | 23    | 0        | 16       | 1       | 0            |
| 3   | AG    | 23    | 0        | 16       | 0       | 0            |
| 3   | AH    | 23    | 0        | 16       | 1       | 0            |
| 3   | AI    | 23    | 0        | 16       | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | AJ    | 23    | 0        | 16       | 1       | 0            |
| 3   | AK    | 23    | 0        | 16       | 1       | 0            |
| 3   | AL    | 23    | 0        | 16       | 1       | 0            |
| 3   | BA    | 23    | 0        | 16       | 3       | 0            |
| 3   | BB    | 23    | 0        | 16       | 0       | 0            |
| 3   | BC    | 23    | 0        | 16       | 0       | 0            |
| 3   | BD    | 23    | 0        | 16       | 0       | 0            |
| 3   | BE    | 23    | 0        | 16       | 1       | 0            |
| 3   | BF    | 23    | 0        | 16       | 1       | 0            |
| 3   | BG    | 23    | 0        | 16       | 1       | 0            |
| 3   | BH    | 23    | 0        | 16       | 1       | 0            |
| 3   | BI    | 23    | 0        | 16       | 1       | 0            |
| 3   | BJ    | 23    | 0        | 16       | 0       | 0            |
| 3   | BK    | 23    | 0        | 16       | 2       | 0            |
| 3   | BL    | 23    | 0        | 16       | 1       | 0            |
| 3   | CA    | 23    | 0        | 16       | 1       | 0            |
| 3   | CB    | 23    | 0        | 16       | 1       | 0            |
| 3   | CC    | 23    | 0        | 16       | 0       | 0            |
| 3   | CD    | 23    | 0        | 16       | 1       | 0            |
| 3   | CE    | 23    | 0        | 16       | 1       | 0            |
| 3   | CF    | 23    | 0        | 16       | 1       | 0            |
| 3   | CG    | 23    | 0        | 16       | 1       | 0            |
| 3   | CH    | 23    | 0        | 16       | 0       | 0            |
| 3   | CI    | 23    | 0        | 16       | 4       | 0            |
| 3   | CJ    | 23    | 0        | 16       | 2       | 0            |
| 3   | CK    | 23    | 0        | 16       | 1       | 0            |
| 3   | CL    | 23    | 0        | 16       | 1       | 0            |
| 3   | DA    | 23    | 0        | 16       | 0       | 0            |
| 3   | DB    | 23    | 0        | 16       | 1       | 0            |
| 3   | DC    | 23    | 0        | 16       | 1       | 0            |
| 3   | DD    | 23    | 0        | 16       | 1       | 0            |
| 3   | DE    | 23    | 0        | 16       | 1       | 0            |
| 3   | DF    | 23    | 0        | 16       | 1       | 0            |
| 3   | DG    | 23    | 0        | 16       | 1       | 0            |
| 3   | DH    | 23    | 0        | 16       | 1       | 0            |
| 4   | AA    | 45    | 33       | 0        | 0       | 0            |
| 4   | AB    | 45    | 33       | 0        | 0       | 0            |
| 4   | AC    | 45    | 33       | 0        | 0       | 0            |
| 4   | AD    | 45    | 33       | 0        | 0       | 0            |
| 4   | AE    | 45    | 33       | 0        | 0       | 0            |
| 4   | AF    | 45    | 33       | 0        | 1       | 0            |
| 4   | AG    | 45    | 33       | 0        | 1       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 4   | AH    | 45     | 33       | 0        | 1       | 0            |
| 4   | AI    | 45     | 33       | 0        | 1       | 0            |
| 4   | AJ    | 45     | 33       | 0        | 0       | 0            |
| 4   | AK    | 45     | 33       | 0        | 0       | 0            |
| 4   | AL    | 45     | 33       | 0        | 0       | 0            |
| 4   | BA    | 45     | 33       | 0        | 0       | 0            |
| 4   | BB    | 45     | 33       | 0        | 0       | 0            |
| 4   | BC    | 45     | 33       | 0        | 0       | 0            |
| 4   | BD    | 45     | 33       | 0        | 0       | 0            |
| 4   | BE    | 45     | 33       | 0        | 1       | 0            |
| 4   | BF    | 45     | 33       | 0        | 2       | 0            |
| 4   | BG    | 45     | 33       | 0        | 0       | 0            |
| 4   | BH    | 45     | 33       | 0        | 0       | 0            |
| 4   | BI    | 45     | 33       | 0        | 0       | 0            |
| 4   | BJ    | 45     | 33       | 0        | 0       | 0            |
| 4   | BK    | 45     | 33       | 0        | 0       | 0            |
| 4   | BL    | 45     | 33       | 0        | 0       | 0            |
| 4   | CA    | 45     | 33       | 0        | 0       | 0            |
| 4   | CB    | 45     | 33       | 0        | 0       | 0            |
| 4   | CC    | 45     | 33       | 0        | 0       | 0            |
| 4   | CD    | 45     | 33       | 0        | 0       | 0            |
| 4   | CE    | 45     | 33       | 0        | 0       | 0            |
| 4   | CF    | 45     | 33       | 0        | 1       | 0            |
| 4   | CG    | 45     | 33       | 0        | 1       | 0            |
| 4   | CH    | 45     | 33       | 0        | 0       | 0            |
| 4   | CI    | 45     | 33       | 0        | 0       | 0            |
| 4   | CJ    | 45     | 33       | 0        | 0       | 0            |
| 4   | CK    | 45     | 33       | 0        | 0       | 0            |
| 4   | CL    | 45     | 33       | 0        | 0       | 0            |
| 4   | DA    | 45     | 33       | 0        | 0       | 0            |
| 4   | DB    | 45     | 33       | 0        | 0       | 0            |
| 4   | DC    | 45     | 33       | 0        | 0       | 0            |
| 4   | DD    | 45     | 33       | 0        | 1       | 0            |
| 4   | DE    | 45     | 33       | 0        | 0       | 0            |
| 4   | DF    | 45     | 33       | 0        | 0       | 0            |
| 4   | DG    | 45     | 33       | 0        | 0       | 0            |
| 4   | DH    | 45     | 33       | 0        | 0       | 0            |
| All | All   | 112359 | 106890   | 109126   | 570     | 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 3.

The worst 5 of 570 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) |
|------------------|------------------|--------------------------|-------------------|
| 1:AC:241:PRO:HG2 | 3:AC:501:LMG:HC8 | 1.51                     | 0.93              |
| 1:BE:241:PRO:HG2 | 3:BE:502:LMG:HC8 | 1.49                     | 0.91              |
| 1:AI:241:PRO:HG2 | 3:AI:502:LMG:HC8 | 1.51                     | 0.90              |
| 1:CB:241:PRO:HG2 | 3:CB:503:LMG:HC8 | 1.54                     | 0.88              |
| 1:DD:241:PRO:HG2 | 3:DD:702:LMG:HC8 | 1.59                     | 0.85              |

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   | AA    | 317/353 (90%) | 308 (97%) | 9 (3%)  | 0        | 100         | 100 |
| 1   | AB    | 317/353 (90%) | 307 (97%) | 10 (3%) | 0        | 100         | 100 |
| 1   | AC    | 317/353 (90%) | 308 (97%) | 9 (3%)  | 0        | 100         | 100 |
| 1   | AD    | 313/353 (89%) | 304 (97%) | 9 (3%)  | 0        | 100         | 100 |
| 1   | AE    | 317/353 (90%) | 310 (98%) | 7 (2%)  | 0        | 100         | 100 |
| 1   | AF    | 315/353 (89%) | 307 (98%) | 8 (2%)  | 0        | 100         | 100 |
| 1   | AG    | 315/353 (89%) | 308 (98%) | 7 (2%)  | 0        | 100         | 100 |
| 1   | AH    | 317/353 (90%) | 310 (98%) | 7 (2%)  | 0        | 100         | 100 |
| 1   | AI    | 315/353 (89%) | 308 (98%) | 7 (2%)  | 0        | 100         | 100 |
| 1   | AJ    | 317/353 (90%) | 310 (98%) | 7 (2%)  | 0        | 100         | 100 |
| 1   | AK    | 315/353 (89%) | 308 (98%) | 7 (2%)  | 0        | 100         | 100 |
| 1   | AL    | 317/353 (90%) | 311 (98%) | 6 (2%)  | 0        | 100         | 100 |
| 1   | BA    | 317/353 (90%) | 309 (98%) | 8 (2%)  | 0        | 100         | 100 |
| 1   | BB    | 317/353 (90%) | 309 (98%) | 8 (2%)  | 0        | 100         | 100 |
| 1   | BC    | 317/353 (90%) | 309 (98%) | 8 (2%)  | 0        | 100         | 100 |
| 1   | BD    | 313/353 (89%) | 306 (98%) | 7 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 1   | BE    | 317/353 (90%)     | 309 (98%)   | 8 (2%)   | 0        | 100         | 100 |
| 1   | BF    | 315/353 (89%)     | 307 (98%)   | 8 (2%)   | 0        | 100         | 100 |
| 1   | BG    | 315/353 (89%)     | 306 (97%)   | 9 (3%)   | 0        | 100         | 100 |
| 1   | BH    | 317/353 (90%)     | 310 (98%)   | 7 (2%)   | 0        | 100         | 100 |
| 1   | BI    | 315/353 (89%)     | 308 (98%)   | 7 (2%)   | 0        | 100         | 100 |
| 1   | BJ    | 317/353 (90%)     | 308 (97%)   | 9 (3%)   | 0        | 100         | 100 |
| 1   | BK    | 315/353 (89%)     | 307 (98%)   | 8 (2%)   | 0        | 100         | 100 |
| 1   | BL    | 317/353 (90%)     | 310 (98%)   | 7 (2%)   | 0        | 100         | 100 |
| 1   | CA    | 317/353 (90%)     | 307 (97%)   | 10 (3%)  | 0        | 100         | 100 |
| 1   | CB    | 317/353 (90%)     | 309 (98%)   | 8 (2%)   | 0        | 100         | 100 |
| 1   | CC    | 317/353 (90%)     | 309 (98%)   | 8 (2%)   | 0        | 100         | 100 |
| 1   | CD    | 313/353 (89%)     | 306 (98%)   | 7 (2%)   | 0        | 100         | 100 |
| 1   | CE    | 317/353 (90%)     | 310 (98%)   | 7 (2%)   | 0        | 100         | 100 |
| 1   | CF    | 315/353 (89%)     | 307 (98%)   | 8 (2%)   | 0        | 100         | 100 |
| 1   | CG    | 315/353 (89%)     | 306 (97%)   | 9 (3%)   | 0        | 100         | 100 |
| 1   | CH    | 317/353 (90%)     | 309 (98%)   | 8 (2%)   | 0        | 100         | 100 |
| 1   | CI    | 315/353 (89%)     | 310 (98%)   | 5 (2%)   | 0        | 100         | 100 |
| 1   | CJ    | 317/353 (90%)     | 311 (98%)   | 6 (2%)   | 0        | 100         | 100 |
| 1   | CK    | 315/353 (89%)     | 307 (98%)   | 8 (2%)   | 0        | 100         | 100 |
| 1   | CL    | 317/353 (90%)     | 309 (98%)   | 8 (2%)   | 0        | 100         | 100 |
| 1   | DA    | 317/353 (90%)     | 306 (96%)   | 11 (4%)  | 0        | 100         | 100 |
| 1   | DB    | 317/353 (90%)     | 308 (97%)   | 9 (3%)   | 0        | 100         | 100 |
| 1   | DC    | 317/353 (90%)     | 309 (98%)   | 8 (2%)   | 0        | 100         | 100 |
| 1   | DD    | 315/353 (89%)     | 306 (97%)   | 9 (3%)   | 0        | 100         | 100 |
| 1   | DE    | 315/353 (89%)     | 307 (98%)   | 8 (2%)   | 0        | 100         | 100 |
| 1   | DF    | 317/353 (90%)     | 308 (97%)   | 9 (3%)   | 0        | 100         | 100 |
| 1   | DG    | 315/353 (89%)     | 308 (98%)   | 7 (2%)   | 0        | 100         | 100 |
| 1   | DH    | 317/353 (90%)     | 310 (98%)   | 7 (2%)   | 0        | 100         | 100 |
| All | All   | 13906/15532 (90%) | 13559 (98%) | 347 (2%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 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   | AA    | 262/290 (90%) | 262 (100%) | 0        | 100         | 100 |
| 1   | AB    | 262/290 (90%) | 262 (100%) | 0        | 100         | 100 |
| 1   | AC    | 262/290 (90%) | 262 (100%) | 0        | 100         | 100 |
| 1   | AD    | 258/290 (89%) | 258 (100%) | 0        | 100         | 100 |
| 1   | AE    | 262/290 (90%) | 262 (100%) | 0        | 100         | 100 |
| 1   | AF    | 260/290 (90%) | 260 (100%) | 0        | 100         | 100 |
| 1   | AG    | 260/290 (90%) | 260 (100%) | 0        | 100         | 100 |
| 1   | AH    | 262/290 (90%) | 262 (100%) | 0        | 100         | 100 |
| 1   | AI    | 260/290 (90%) | 260 (100%) | 0        | 100         | 100 |
| 1   | AJ    | 262/290 (90%) | 262 (100%) | 0        | 100         | 100 |
| 1   | AK    | 260/290 (90%) | 260 (100%) | 0        | 100         | 100 |
| 1   | AL    | 262/290 (90%) | 262 (100%) | 0        | 100         | 100 |
| 1   | BA    | 262/290 (90%) | 262 (100%) | 0        | 100         | 100 |
| 1   | BB    | 262/290 (90%) | 262 (100%) | 0        | 100         | 100 |
| 1   | BC    | 262/290 (90%) | 262 (100%) | 0        | 100         | 100 |
| 1   | BD    | 258/290 (89%) | 258 (100%) | 0        | 100         | 100 |
| 1   | BE    | 262/290 (90%) | 262 (100%) | 0        | 100         | 100 |
| 1   | BF    | 260/290 (90%) | 260 (100%) | 0        | 100         | 100 |
| 1   | BG    | 260/290 (90%) | 260 (100%) | 0        | 100         | 100 |
| 1   | BH    | 262/290 (90%) | 262 (100%) | 0        | 100         | 100 |
| 1   | BI    | 260/290 (90%) | 260 (100%) | 0        | 100         | 100 |
| 1   | BJ    | 262/290 (90%) | 262 (100%) | 0        | 100         | 100 |
| 1   | BK    | 260/290 (90%) | 260 (100%) | 0        | 100         | 100 |
| 1   | BL    | 262/290 (90%) | 262 (100%) | 0        | 100         | 100 |
| 1   | CA    | 262/290 (90%) | 262 (100%) | 0        | 100         | 100 |
| 1   | CB    | 262/290 (90%) | 262 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Rotameric    | Outliers | Percentiles |     |
|-----|-------|-------------------|--------------|----------|-------------|-----|
| 1   | CC    | 262/290 (90%)     | 262 (100%)   | 0        | 100         | 100 |
| 1   | CD    | 258/290 (89%)     | 258 (100%)   | 0        | 100         | 100 |
| 1   | CE    | 262/290 (90%)     | 262 (100%)   | 0        | 100         | 100 |
| 1   | CF    | 260/290 (90%)     | 260 (100%)   | 0        | 100         | 100 |
| 1   | CG    | 260/290 (90%)     | 260 (100%)   | 0        | 100         | 100 |
| 1   | CH    | 262/290 (90%)     | 262 (100%)   | 0        | 100         | 100 |
| 1   | CI    | 260/290 (90%)     | 260 (100%)   | 0        | 100         | 100 |
| 1   | CJ    | 262/290 (90%)     | 262 (100%)   | 0        | 100         | 100 |
| 1   | CK    | 260/290 (90%)     | 260 (100%)   | 0        | 100         | 100 |
| 1   | CL    | 262/290 (90%)     | 262 (100%)   | 0        | 100         | 100 |
| 1   | DA    | 262/290 (90%)     | 262 (100%)   | 0        | 100         | 100 |
| 1   | DB    | 262/290 (90%)     | 262 (100%)   | 0        | 100         | 100 |
| 1   | DC    | 262/290 (90%)     | 262 (100%)   | 0        | 100         | 100 |
| 1   | DD    | 260/290 (90%)     | 260 (100%)   | 0        | 100         | 100 |
| 1   | DE    | 260/290 (90%)     | 260 (100%)   | 0        | 100         | 100 |
| 1   | DF    | 262/290 (90%)     | 262 (100%)   | 0        | 100         | 100 |
| 1   | DG    | 260/290 (90%)     | 260 (100%)   | 0        | 100         | 100 |
| 1   | DH    | 262/290 (90%)     | 262 (100%)   | 0        | 100         | 100 |
| All | All   | 11486/12760 (90%) | 11486 (100%) | 0        | 100         | 100 |

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | CC    | 295 | HIS  |
| 1   | DA    | 283 | ASN  |
| 1   | CE    | 90  | ASN  |
| 1   | CI    | 288 | GLN  |
| 1   | DC    | 144 | HIS  |

### 5.3.3 RNA ⓘ

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](#)

132 ligands are modelled in this entry.

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$ |
| 3   | LMG   | AK    | 502 | -    | 23,23,55     | 0.74 | 0           | 31,31,63    | 0.81 | 0           |
| 4   | A1JWG | AF    | 503 | -    | 48,53,53     | 1.38 | 5 (10%)     | 62,89,89    | 1.17 | 3 (4%)      |
| 4   | A1JWG | BC    | 502 | -    | 48,53,53     | 1.39 | 5 (10%)     | 62,89,89    | 1.13 | 4 (6%)      |
| 2   | NDP   | CD    | 502 | -    | 49,52,52     | 2.16 | 4 (8%)      | 66,80,80    | 1.66 | 14 (21%)    |
| 2   | NDP   | CK    | 501 | -    | 49,52,52     | 2.14 | 4 (8%)      | 66,80,80    | 1.63 | 14 (21%)    |
| 2   | NDP   | AC    | 503 | -    | 49,52,52     | 2.18 | 5 (10%)     | 66,80,80    | 1.66 | 13 (19%)    |
| 3   | LMG   | AI    | 502 | -    | 23,23,55     | 0.74 | 0           | 31,31,63    | 0.79 | 0           |
| 4   | A1JWG | CE    | 502 | -    | 48,53,53     | 1.38 | 5 (10%)     | 62,89,89    | 1.10 | 3 (4%)      |
| 2   | NDP   | CL    | 501 | -    | 49,52,52     | 2.16 | 4 (8%)      | 66,80,80    | 1.63 | 14 (21%)    |
| 3   | LMG   | BF    | 502 | -    | 23,23,55     | 0.71 | 0           | 31,31,63    | 0.94 | 1 (3%)      |
| 3   | LMG   | BI    | 702 | -    | 23,23,55     | 0.73 | 0           | 31,31,63    | 0.83 | 0           |
| 3   | LMG   | AH    | 702 | -    | 23,23,55     | 0.73 | 0           | 31,31,63    | 0.81 | 0           |
| 3   | LMG   | CK    | 503 | -    | 23,23,55     | 0.73 | 0           | 31,31,63    | 0.79 | 0           |
| 2   | NDP   | CH    | 501 | -    | 49,52,52     | 2.15 | 4 (8%)      | 66,80,80    | 1.65 | 14 (21%)    |
| 4   | A1JWG | AD    | 503 | -    | 48,53,53     | 1.37 | 5 (10%)     | 62,89,89    | 1.12 | 2 (3%)      |
| 4   | A1JWG | AJ    | 502 | -    | 48,53,53     | 1.37 | 5 (10%)     | 62,89,89    | 1.12 | 3 (4%)      |
| 4   | A1JWG | CB    | 502 | -    | 48,53,53     | 1.38 | 5 (10%)     | 62,89,89    | 1.17 | 2 (3%)      |
| 2   | NDP   | AF    | 501 | -    | 49,52,52     | 2.16 | 4 (8%)      | 66,80,80    | 1.64 | 13 (19%)    |
| 4   | A1JWG | DA    | 502 | -    | 48,53,53     | 1.38 | 5 (10%)     | 62,89,89    | 1.16 | 2 (3%)      |

| Mol | Type  | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|-------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |       |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 4   | A1JWG | DH    | 503 | -    | 48,53,53     | 1.37 | 5 (10%)  | 62,89,89    | 1.15 | 3 (4%)   |
| 3   | LMG   | AC    | 501 | -    | 23,23,55     | 0.71 | 0        | 31,31,63    | 0.74 | 0        |
| 2   | NDP   | BH    | 702 | -    | 49,52,52     | 2.16 | 5 (10%)  | 66,80,80    | 1.65 | 14 (21%) |
| 3   | LMG   | BK    | 501 | -    | 23,23,55     | 0.73 | 0        | 31,31,63    | 0.84 | 0        |
| 4   | A1JWG | AH    | 701 | -    | 48,53,53     | 1.38 | 5 (10%)  | 62,89,89    | 1.12 | 2 (3%)   |
| 4   | A1JWG | CD    | 503 | -    | 48,53,53     | 1.38 | 5 (10%)  | 62,89,89    | 1.15 | 2 (3%)   |
| 4   | A1JWG | AI    | 503 | -    | 48,53,53     | 1.39 | 5 (10%)  | 62,89,89    | 1.16 | 3 (4%)   |
| 3   | LMG   | BC    | 503 | -    | 23,23,55     | 0.69 | 0        | 31,31,63    | 0.77 | 0        |
| 2   | NDP   | BC    | 501 | -    | 49,52,52     | 2.19 | 5 (10%)  | 66,80,80    | 1.66 | 13 (19%) |
| 3   | LMG   | AD    | 502 | -    | 23,23,55     | 0.74 | 0        | 31,31,63    | 0.90 | 1 (3%)   |
| 4   | A1JWG | BF    | 503 | -    | 48,53,53     | 1.39 | 5 (10%)  | 62,89,89    | 1.15 | 3 (4%)   |
| 4   | A1JWG | CJ    | 503 | -    | 48,53,53     | 1.37 | 5 (10%)  | 62,89,89    | 1.13 | 3 (4%)   |
| 2   | NDP   | AE    | 702 | -    | 49,52,52     | 2.15 | 4 (8%)   | 66,80,80    | 1.66 | 15 (22%) |
| 2   | NDP   | DE    | 702 | -    | 49,52,52     | 2.15 | 5 (10%)  | 66,80,80    | 1.65 | 15 (22%) |
| 2   | NDP   | DD    | 703 | -    | 49,52,52     | 2.17 | 4 (8%)   | 66,80,80    | 1.67 | 14 (21%) |
| 4   | A1JWG | BI    | 701 | -    | 48,53,53     | 1.39 | 5 (10%)  | 62,89,89    | 1.16 | 2 (3%)   |
| 4   | A1JWG | AG    | 701 | -    | 48,53,53     | 1.39 | 5 (10%)  | 62,89,89    | 1.20 | 3 (4%)   |
| 2   | NDP   | CI    | 503 | -    | 49,52,52     | 2.16 | 5 (10%)  | 66,80,80    | 1.66 | 14 (21%) |
| 3   | LMG   | DG    | 503 | -    | 23,23,55     | 0.75 | 0        | 31,31,63    | 0.79 | 0        |
| 2   | NDP   | BA    | 501 | -    | 49,52,52     | 2.22 | 5 (10%)  | 66,80,80    | 1.65 | 12 (18%) |
| 2   | NDP   | DG    | 501 | -    | 49,52,52     | 2.14 | 4 (8%)   | 66,80,80    | 1.64 | 14 (21%) |
| 3   | LMG   | AE    | 703 | -    | 23,23,55     | 0.70 | 0        | 31,31,63    | 0.90 | 0        |
| 2   | NDP   | DH    | 501 | -    | 49,52,52     | 2.17 | 5 (10%)  | 66,80,80    | 1.64 | 13 (19%) |
| 2   | NDP   | BL    | 702 | -    | 49,52,52     | 2.15 | 4 (8%)   | 66,80,80    | 1.64 | 14 (21%) |
| 2   | NDP   | DC    | 702 | -    | 49,52,52     | 2.17 | 4 (8%)   | 66,80,80    | 1.66 | 13 (19%) |
| 2   | NDP   | DF    | 503 | -    | 49,52,52     | 2.14 | 4 (8%)   | 66,80,80    | 1.65 | 14 (21%) |
| 4   | A1JWG | CK    | 502 | -    | 48,53,53     | 1.38 | 5 (10%)  | 62,89,89    | 1.18 | 2 (3%)   |
| 4   | A1JWG | BJ    | 502 | -    | 48,53,53     | 1.37 | 5 (10%)  | 62,89,89    | 1.12 | 3 (4%)   |
| 3   | LMG   | AJ    | 501 | -    | 23,23,55     | 0.71 | 0        | 31,31,63    | 0.77 | 0        |
| 3   | LMG   | DC    | 703 | -    | 23,23,55     | 0.73 | 0        | 31,31,63    | 0.80 | 0        |
| 4   | A1JWG | AB    | 502 | -    | 48,53,53     | 1.38 | 5 (10%)  | 62,89,89    | 1.12 | 5 (8%)   |
| 2   | NDP   | AG    | 703 | -    | 49,52,52     | 2.15 | 4 (8%)   | 66,80,80    | 1.65 | 13 (19%) |
| 3   | LMG   | CD    | 501 | -    | 23,23,55     | 0.69 | 0        | 31,31,63    | 0.78 | 0        |
| 3   | LMG   | CG    | 502 | -    | 23,23,55     | 0.74 | 0        | 31,31,63    | 0.83 | 0        |
| 4   | A1JWG | DB    | 701 | -    | 48,53,53     | 1.37 | 5 (10%)  | 62,89,89    | 1.13 | 2 (3%)   |
| 3   | LMG   | BE    | 502 | -    | 23,23,55     | 0.72 | 0        | 31,31,63    | 0.77 | 0        |
| 2   | NDP   | DA    | 501 | -    | 49,52,52     | 2.17 | 4 (8%)   | 66,80,80    | 1.65 | 13 (19%) |

| Mol | Type  | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|-------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |       |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | LMG   | CB    | 503 | -    | 23,23,55     | 0.75 | 0        | 31,31,63    | 0.83 | 0        |
| 3   | LMG   | CC    | 501 | -    | 23,23,55     | 0.71 | 0        | 31,31,63    | 0.87 | 0        |
| 4   | A1JWG | BB    | 503 | -    | 48,53,53     | 1.37 | 5 (10%)  | 62,89,89    | 1.21 | 2 (3%)   |
| 3   | LMG   | CJ    | 502 | -    | 23,23,55     | 0.72 | 0        | 31,31,63    | 0.84 | 0        |
| 3   | LMG   | BH    | 703 | -    | 23,23,55     | 0.73 | 0        | 31,31,63    | 0.79 | 0        |
| 2   | NDP   | AL    | 503 | -    | 49,52,52     | 2.14 | 4 (8%)   | 66,80,80    | 1.64 | 15 (22%) |
| 4   | A1JWG | DF    | 502 | -    | 48,53,53     | 1.36 | 5 (10%)  | 62,89,89    | 1.03 | 2 (3%)   |
| 3   | LMG   | CL    | 502 | -    | 23,23,55     | 0.74 | 0        | 31,31,63    | 0.83 | 0        |
| 4   | A1JWG | DC    | 701 | -    | 48,53,53     | 1.38 | 5 (10%)  | 62,89,89    | 1.09 | 2 (3%)   |
| 3   | LMG   | DD    | 702 | -    | 23,23,55     | 0.72 | 0        | 31,31,63    | 0.81 | 0        |
| 4   | A1JWG | AC    | 502 | -    | 48,53,53     | 1.38 | 5 (10%)  | 62,89,89    | 1.06 | 3 (4%)   |
| 2   | NDP   | CF    | 502 | -    | 49,52,52     | 2.16 | 4 (8%)   | 66,80,80    | 1.66 | 14 (21%) |
| 4   | A1JWG | DE    | 701 | -    | 48,53,53     | 1.37 | 5 (10%)  | 62,89,89    | 1.16 | 3 (4%)   |
| 2   | NDP   | AA    | 501 | -    | 49,52,52     | 2.19 | 5 (10%)  | 66,80,80    | 1.66 | 13 (19%) |
| 2   | NDP   | BK    | 502 | -    | 49,52,52     | 2.16 | 4 (8%)   | 66,80,80    | 1.63 | 14 (21%) |
| 4   | A1JWG | BA    | 503 | -    | 48,53,53     | 1.39 | 5 (10%)  | 62,89,89    | 1.17 | 2 (3%)   |
| 2   | NDP   | BB    | 501 | -    | 49,52,52     | 2.16 | 4 (8%)   | 66,80,80    | 1.65 | 13 (19%) |
| 2   | NDP   | BD    | 502 | -    | 49,52,52     | 2.19 | 5 (10%)  | 66,80,80    | 1.65 | 14 (21%) |
| 3   | LMG   | CE    | 503 | -    | 23,23,55     | 0.72 | 0        | 31,31,63    | 0.78 | 0        |
| 3   | LMG   | BD    | 501 | -    | 23,23,55     | 0.71 | 0        | 31,31,63    | 0.85 | 0        |
| 2   | NDP   | AB    | 501 | -    | 49,52,52     | 2.15 | 4 (8%)   | 66,80,80    | 1.66 | 14 (21%) |
| 2   | NDP   | BJ    | 503 | -    | 49,52,52     | 2.15 | 5 (10%)  | 66,80,80    | 1.64 | 14 (21%) |
| 4   | A1JWG | AL    | 502 | -    | 48,53,53     | 1.38 | 5 (10%)  | 62,89,89    | 1.19 | 2 (3%)   |
| 4   | A1JWG | CC    | 503 | -    | 48,53,53     | 1.39 | 5 (10%)  | 62,89,89    | 1.12 | 2 (3%)   |
| 3   | LMG   | DA    | 503 | -    | 23,23,55     | 0.70 | 0        | 31,31,63    | 0.77 | 0        |
| 2   | NDP   | DB    | 702 | -    | 49,52,52     | 2.18 | 5 (10%)  | 66,80,80    | 1.63 | 12 (18%) |
| 4   | A1JWG | CL    | 503 | -    | 48,53,53     | 1.38 | 5 (10%)  | 62,89,89    | 1.13 | 2 (3%)   |
| 3   | LMG   | DF    | 501 | -    | 23,23,55     | 0.72 | 0        | 31,31,63    | 0.77 | 0        |
| 4   | A1JWG | CF    | 503 | -    | 48,53,53     | 1.39 | 5 (10%)  | 62,89,89    | 1.17 | 4 (6%)   |
| 4   | A1JWG | BD    | 503 | -    | 48,53,53     | 1.38 | 5 (10%)  | 62,89,89    | 1.13 | 3 (4%)   |
| 2   | NDP   | CB    | 501 | -    | 49,52,52     | 2.19 | 4 (8%)   | 66,80,80    | 1.64 | 14 (21%) |
| 4   | A1JWG | BK    | 503 | -    | 48,53,53     | 1.38 | 5 (10%)  | 62,89,89    | 1.13 | 1 (1%)   |
| 3   | LMG   | BL    | 703 | -    | 23,23,55     | 0.74 | 0        | 31,31,63    | 0.82 | 0        |
| 2   | NDP   | AH    | 703 | -    | 49,52,52     | 2.16 | 4 (8%)   | 66,80,80    | 1.64 | 13 (19%) |
| 2   | NDP   | CG    | 501 | -    | 49,52,52     | 2.17 | 5 (10%)  | 66,80,80    | 1.64 | 13 (19%) |
| 4   | A1JWG | BE    | 503 | -    | 48,53,53     | 1.40 | 5 (10%)  | 62,89,89    | 1.22 | 4 (6%)   |
| 3   | LMG   | CA    | 702 | -    | 23,23,55     | 0.71 | 0        | 31,31,63    | 0.75 | 0        |

| Mol | Type  | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|-------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |       |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | NDP   | AI    | 501 | -    | 49,52,52     | 2.16 | 4 (8%)   | 66,80,80    | 1.64 | 13 (19%) |
| 4   | A1JWG | CI    | 502 | -    | 48,53,53     | 1.39 | 5 (10%)  | 62,89,89    | 1.23 | 4 (6%)   |
| 4   | A1JWG | BH    | 701 | -    | 48,53,53     | 1.38 | 5 (10%)  | 62,89,89    | 1.21 | 3 (4%)   |
| 2   | NDP   | AK    | 501 | -    | 49,52,52     | 2.13 | 4 (8%)   | 66,80,80    | 1.64 | 15 (22%) |
| 3   | LMG   | BG    | 503 | -    | 23,23,55     | 0.72 | 0        | 31,31,63    | 0.79 | 0        |
| 3   | LMG   | AA    | 502 | -    | 23,23,55     | 0.72 | 0        | 31,31,63    | 0.86 | 0        |
| 2   | NDP   | BG    | 501 | -    | 49,52,52     | 2.14 | 4 (8%)   | 66,80,80    | 1.65 | 13 (19%) |
| 3   | LMG   | AG    | 702 | -    | 23,23,55     | 0.73 | 0        | 31,31,63    | 0.88 | 1 (3%)   |
| 2   | NDP   | CC    | 502 | -    | 49,52,52     | 2.18 | 5 (10%)  | 66,80,80    | 1.66 | 12 (18%) |
| 4   | A1JWG | AE    | 701 | -    | 48,53,53     | 1.37 | 5 (10%)  | 62,89,89    | 1.19 | 2 (3%)   |
| 4   | A1JWG | CH    | 503 | -    | 48,53,53     | 1.40 | 5 (10%)  | 62,89,89    | 1.11 | 2 (3%)   |
| 3   | LMG   | AL    | 501 | -    | 23,23,55     | 0.73 | 0        | 31,31,63    | 0.83 | 0        |
| 4   | A1JWG | AK    | 503 | -    | 48,53,53     | 1.37 | 5 (10%)  | 62,89,89    | 1.21 | 3 (4%)   |
| 2   | NDP   | AD    | 501 | -    | 49,52,52     | 2.16 | 5 (10%)  | 66,80,80    | 1.66 | 14 (21%) |
| 2   | NDP   | CA    | 703 | -    | 49,52,52     | 2.19 | 4 (8%)   | 66,80,80    | 1.66 | 13 (19%) |
| 3   | LMG   | BJ    | 501 | -    | 23,23,55     | 0.72 | 0        | 31,31,63    | 0.83 | 0        |
| 2   | NDP   | CJ    | 501 | -    | 49,52,52     | 2.13 | 4 (8%)   | 66,80,80    | 1.65 | 13 (19%) |
| 3   | LMG   | DH    | 502 | -    | 23,23,55     | 0.75 | 0        | 31,31,63    | 0.84 | 0        |
| 4   | A1JWG | DG    | 502 | -    | 48,53,53     | 1.38 | 5 (10%)  | 62,89,89    | 1.12 | 4 (6%)   |
| 4   | A1JWG | BL    | 701 | -    | 48,53,53     | 1.38 | 5 (10%)  | 62,89,89    | 1.12 | 4 (6%)   |
| 3   | LMG   | AB    | 503 | -    | 23,23,55     | 0.72 | 0        | 31,31,63    | 0.80 | 0        |
| 2   | NDP   | CE    | 501 | -    | 49,52,52     | 2.18 | 4 (8%)   | 66,80,80    | 1.66 | 14 (21%) |
| 3   | LMG   | BA    | 502 | -    | 23,23,55     | 0.71 | 0        | 31,31,63    | 0.80 | 0        |
| 3   | LMG   | CH    | 502 | -    | 23,23,55     | 0.77 | 0        | 31,31,63    | 0.86 | 0        |
| 2   | NDP   | BF    | 501 | -    | 49,52,52     | 2.19 | 4 (8%)   | 66,80,80    | 1.64 | 13 (19%) |
| 4   | A1JWG | CA    | 701 | -    | 48,53,53     | 1.38 | 5 (10%)  | 62,89,89    | 1.09 | 3 (4%)   |
| 3   | LMG   | DB    | 703 | -    | 23,23,55     | 0.71 | 0        | 31,31,63    | 0.79 | 0        |
| 2   | NDP   | BE    | 501 | -    | 49,52,52     | 2.16 | 4 (8%)   | 66,80,80    | 1.64 | 14 (21%) |
| 3   | LMG   | BB    | 502 | -    | 23,23,55     | 0.70 | 0        | 31,31,63    | 0.82 | 0        |
| 4   | A1JWG | AA    | 503 | -    | 48,53,53     | 1.39 | 5 (10%)  | 62,89,89    | 1.10 | 5 (8%)   |
| 2   | NDP   | AJ    | 503 | -    | 49,52,52     | 2.16 | 4 (8%)   | 66,80,80    | 1.64 | 14 (21%) |
| 4   | A1JWG | DD    | 701 | -    | 48,53,53     | 1.38 | 5 (10%)  | 62,89,89    | 1.25 | 2 (3%)   |
| 4   | A1JWG | BG    | 502 | -    | 48,53,53     | 1.37 | 5 (10%)  | 62,89,89    | 1.23 | 2 (3%)   |
| 4   | A1JWG | CG    | 503 | -    | 48,53,53     | 1.37 | 5 (10%)  | 62,89,89    | 1.19 | 3 (4%)   |
| 3   | LMG   | CF    | 501 | -    | 23,23,55     | 0.71 | 0        | 31,31,63    | 0.78 | 0        |
| 3   | LMG   | AF    | 502 | -    | 23,23,55     | 0.71 | 0        | 31,31,63    | 0.78 | 0        |
| 2   | NDP   | BI    | 703 | -    | 49,52,52     | 2.16 | 4 (8%)   | 66,80,80    | 1.65 | 14 (21%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | LMG  | DE    | 703 | -    | 23,23,55     | 0.73 | 0        | 31,31,63    | 0.84 | 0        |
| 3   | LMG  | CI    | 501 | -    | 23,23,55     | 0.74 | 0        | 31,31,63    | 0.73 | 0        |

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   |
|-----|-------|-------|-----|------|-----------|-------------|---------|
| 3   | LMG   | AK    | 502 | -    | -         | 3/16/36/70  | 0/1/1/1 |
| 4   | A1JWG | AF    | 503 | -    | 3/3/15/15 | 10/15/91/91 | -       |
| 4   | A1JWG | BC    | 502 | -    | 2/2/15/15 | 5/15/91/91  | -       |
| 2   | NDP   | CD    | 502 | -    | -         | 12/34/77/77 | 0/5/5/5 |
| 2   | NDP   | CK    | 501 | -    | -         | 11/34/77/77 | 0/5/5/5 |
| 2   | NDP   | AC    | 503 | -    | -         | 13/34/77/77 | 0/5/5/5 |
| 3   | LMG   | AI    | 502 | -    | -         | 4/16/36/70  | 0/1/1/1 |
| 4   | A1JWG | CE    | 502 | -    | 2/2/15/15 | 2/15/91/91  | -       |
| 2   | NDP   | CL    | 501 | -    | -         | 12/34/77/77 | 0/5/5/5 |
| 3   | LMG   | BF    | 502 | -    | -         | 8/16/36/70  | 0/1/1/1 |
| 3   | LMG   | BI    | 702 | -    | -         | 2/16/36/70  | 0/1/1/1 |
| 3   | LMG   | AH    | 702 | -    | -         | 2/16/36/70  | 0/1/1/1 |
| 3   | LMG   | CK    | 503 | -    | -         | 4/16/36/70  | 0/1/1/1 |
| 2   | NDP   | CH    | 501 | -    | -         | 12/34/77/77 | 0/5/5/5 |
| 4   | A1JWG | AD    | 503 | -    | 2/2/15/15 | 4/15/91/91  | -       |
| 4   | A1JWG | AJ    | 502 | -    | 2/2/15/15 | 4/15/91/91  | -       |
| 4   | A1JWG | CB    | 502 | -    | 3/3/15/15 | 4/15/91/91  | -       |
| 2   | NDP   | AF    | 501 | -    | -         | 12/34/77/77 | 0/5/5/5 |
| 4   | A1JWG | DA    | 502 | -    | 3/3/15/15 | 5/15/91/91  | -       |
| 4   | A1JWG | DH    | 503 | -    | 2/2/15/15 | 4/15/91/91  | -       |
| 3   | LMG   | AC    | 501 | -    | -         | 4/16/36/70  | 0/1/1/1 |
| 4   | A1JWG | AH    | 701 | -    | 2/2/15/15 | 3/15/91/91  | -       |
| 2   | NDP   | BH    | 702 | -    | -         | 12/34/77/77 | 0/5/5/5 |
| 3   | LMG   | BK    | 501 | -    | -         | 9/16/36/70  | 0/1/1/1 |
| 4   | A1JWG | CD    | 503 | -    | 3/3/15/15 | 8/15/91/91  | -       |
| 4   | A1JWG | AI    | 503 | -    | 2/2/15/15 | 4/15/91/91  | -       |
| 3   | LMG   | BC    | 503 | -    | -         | 4/16/36/70  | 0/1/1/1 |

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| Mol | Type  | Chain | Res | Link | Chirals   | Torsions    | Rings   |
|-----|-------|-------|-----|------|-----------|-------------|---------|
| 2   | NDP   | BC    | 501 | -    | -         | 12/34/77/77 | 0/5/5/5 |
| 3   | LMG   | AD    | 502 | -    | -         | 6/16/36/70  | 0/1/1/1 |
| 4   | A1JWG | BF    | 503 | -    | 2/2/15/15 | 9/15/91/91  | -       |
| 4   | A1JWG | CJ    | 503 | -    | 2/2/15/15 | 4/15/91/91  | -       |
| 2   | NDP   | AE    | 702 | -    | -         | 6/34/77/77  | 0/5/5/5 |
| 2   | NDP   | DE    | 702 | -    | -         | 13/34/77/77 | 0/5/5/5 |
| 2   | NDP   | DD    | 703 | -    | -         | 9/34/77/77  | 0/5/5/5 |
| 4   | A1JWG | BI    | 701 | -    | 3/3/15/15 | 4/15/91/91  | -       |
| 4   | A1JWG | AG    | 701 | -    | 3/3/15/15 | 11/15/91/91 | -       |
| 2   | NDP   | CI    | 503 | -    | -         | 12/34/77/77 | 0/5/5/5 |
| 3   | LMG   | DG    | 503 | -    | -         | 4/16/36/70  | 0/1/1/1 |
| 2   | NDP   | BA    | 501 | -    | -         | 6/34/77/77  | 0/5/5/5 |
| 2   | NDP   | DG    | 501 | -    | -         | 12/34/77/77 | 0/5/5/5 |
| 3   | LMG   | AE    | 703 | -    | -         | 3/16/36/70  | 0/1/1/1 |
| 2   | NDP   | DH    | 501 | -    | -         | 11/34/77/77 | 0/5/5/5 |
| 2   | NDP   | BL    | 702 | -    | -         | 10/34/77/77 | 0/5/5/5 |
| 2   | NDP   | DC    | 702 | -    | -         | 10/34/77/77 | 0/5/5/5 |
| 2   | NDP   | DF    | 503 | -    | -         | 12/34/77/77 | 0/5/5/5 |
| 4   | A1JWG | CK    | 502 | -    | 2/2/15/15 | 5/15/91/91  | -       |
| 4   | A1JWG | BJ    | 502 | -    | 2/2/15/15 | 3/15/91/91  | -       |
| 3   | LMG   | AJ    | 501 | -    | -         | 7/16/36/70  | 0/1/1/1 |
| 3   | LMG   | DC    | 703 | -    | -         | 0/16/36/70  | 0/1/1/1 |
| 4   | A1JWG | AB    | 502 | -    | 3/3/15/15 | 5/15/91/91  | -       |
| 2   | NDP   | AG    | 703 | -    | -         | 12/34/77/77 | 0/5/5/5 |
| 3   | LMG   | CD    | 501 | -    | -         | 6/16/36/70  | 0/1/1/1 |
| 3   | LMG   | CG    | 502 | -    | -         | 2/16/36/70  | 0/1/1/1 |
| 4   | A1JWG | DB    | 701 | -    | 3/3/15/15 | 3/15/91/91  | -       |
| 3   | LMG   | BE    | 502 | -    | -         | 1/16/36/70  | 0/1/1/1 |
| 2   | NDP   | DA    | 501 | -    | -         | 12/34/77/77 | 0/5/5/5 |
| 3   | LMG   | CB    | 503 | -    | -         | 4/16/36/70  | 0/1/1/1 |
| 4   | A1JWG | BB    | 503 | -    | 2/2/15/15 | 5/15/91/91  | -       |
| 3   | LMG   | CC    | 501 | -    | -         | 4/16/36/70  | 0/1/1/1 |
| 3   | LMG   | CJ    | 502 | -    | -         | 4/16/36/70  | 0/1/1/1 |
| 3   | LMG   | BH    | 703 | -    | -         | 5/16/36/70  | 0/1/1/1 |

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| Mol | Type  | Chain | Res | Link | Chirals   | Torsions    | Rings   |
|-----|-------|-------|-----|------|-----------|-------------|---------|
| 2   | NDP   | AL    | 503 | -    | -         | 14/34/77/77 | 0/5/5/5 |
| 4   | A1JWG | DF    | 502 | -    | 3/3/15/15 | 6/15/91/91  | -       |
| 3   | LMG   | CL    | 502 | -    | -         | 2/16/36/70  | 0/1/1/1 |
| 4   | A1JWG | DC    | 701 | -    | 2/2/15/15 | 5/15/91/91  | -       |
| 3   | LMG   | DD    | 702 | -    | -         | 4/16/36/70  | 0/1/1/1 |
| 4   | A1JWG | AC    | 502 | -    | 2/2/15/15 | 6/15/91/91  | -       |
| 4   | A1JWG | DE    | 701 | -    | 3/3/15/15 | 5/15/91/91  | -       |
| 2   | NDP   | CF    | 502 | -    | -         | 14/34/77/77 | 0/5/5/5 |
| 2   | NDP   | AA    | 501 | -    | -         | 10/34/77/77 | 0/5/5/5 |
| 2   | NDP   | BK    | 502 | -    | -         | 12/34/77/77 | 0/5/5/5 |
| 4   | A1JWG | BA    | 503 | -    | 2/2/15/15 | 7/15/91/91  | -       |
| 2   | NDP   | BB    | 501 | -    | -         | 12/34/77/77 | 0/5/5/5 |
| 2   | NDP   | BD    | 502 | -    | -         | 12/34/77/77 | 0/5/5/5 |
| 3   | LMG   | CE    | 503 | -    | -         | 4/16/36/70  | 0/1/1/1 |
| 3   | LMG   | BD    | 501 | -    | -         | 4/16/36/70  | 0/1/1/1 |
| 2   | NDP   | AB    | 501 | -    | -         | 12/34/77/77 | 0/5/5/5 |
| 4   | A1JWG | AL    | 502 | -    | 3/3/15/15 | 4/15/91/91  | -       |
| 2   | NDP   | BJ    | 503 | -    | -         | 12/34/77/77 | 0/5/5/5 |
| 4   | A1JWG | CC    | 503 | -    | 3/3/15/15 | 5/15/91/91  | -       |
| 3   | LMG   | DA    | 503 | -    | -         | 6/16/36/70  | 0/1/1/1 |
| 2   | NDP   | DB    | 702 | -    | -         | 5/34/77/77  | 0/5/5/5 |
| 4   | A1JWG | CL    | 503 | -    | 2/2/15/15 | 4/15/91/91  | -       |
| 4   | A1JWG | CF    | 503 | -    | 3/3/15/15 | 6/15/91/91  | -       |
| 3   | LMG   | DF    | 501 | -    | -         | 4/16/36/70  | 0/1/1/1 |
| 4   | A1JWG | BD    | 503 | -    | 2/2/15/15 | 7/15/91/91  | -       |
| 2   | NDP   | CB    | 501 | -    | -         | 12/34/77/77 | 0/5/5/5 |
| 4   | A1JWG | BK    | 503 | -    | 3/3/15/15 | 2/15/91/91  | -       |
| 3   | LMG   | BL    | 703 | -    | -         | 6/16/36/70  | 0/1/1/1 |
| 4   | A1JWG | BE    | 503 | -    | 3/3/15/15 | 8/15/91/91  | -       |
| 2   | NDP   | AH    | 703 | -    | -         | 12/34/77/77 | 0/5/5/5 |
| 2   | NDP   | CG    | 501 | -    | -         | 12/34/77/77 | 0/5/5/5 |
| 3   | LMG   | CA    | 702 | -    | -         | 2/16/36/70  | 0/1/1/1 |
| 2   | NDP   | AI    | 501 | -    | -         | 12/34/77/77 | 0/5/5/5 |
| 4   | A1JWG | CI    | 502 | -    | 3/3/15/15 | 7/15/91/91  | -       |

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| Mol | Type  | Chain | Res | Link | Chirals   | Torsions    | Rings   |
|-----|-------|-------|-----|------|-----------|-------------|---------|
| 4   | A1JWG | BH    | 701 | -    | 3/3/15/15 | 6/15/91/91  | -       |
| 2   | NDP   | AK    | 501 | -    | -         | 14/34/77/77 | 0/5/5/5 |
| 3   | LMG   | AA    | 502 | -    | -         | 6/16/36/70  | 0/1/1/1 |
| 3   | LMG   | BG    | 503 | -    | -         | 6/16/36/70  | 0/1/1/1 |
| 2   | NDP   | BG    | 501 | -    | -         | 12/34/77/77 | 0/5/5/5 |
| 3   | LMG   | AG    | 702 | -    | -         | 6/16/36/70  | 0/1/1/1 |
| 2   | NDP   | CC    | 502 | -    | -         | 12/34/77/77 | 0/5/5/5 |
| 4   | A1JWG | AE    | 701 | -    | 2/2/15/15 | 4/15/91/91  | -       |
| 4   | A1JWG | CH    | 503 | -    | 2/2/15/15 | 6/15/91/91  | -       |
| 3   | LMG   | AL    | 501 | -    | -         | 5/16/36/70  | 0/1/1/1 |
| 4   | A1JWG | AK    | 503 | -    | 3/3/15/15 | 6/15/91/91  | -       |
| 2   | NDP   | AD    | 501 | -    | -         | 12/34/77/77 | 0/5/5/5 |
| 2   | NDP   | CA    | 703 | -    | -         | 12/34/77/77 | 0/5/5/5 |
| 3   | LMG   | BJ    | 501 | -    | -         | 6/16/36/70  | 0/1/1/1 |
| 2   | NDP   | CJ    | 501 | -    | -         | 12/34/77/77 | 0/5/5/5 |
| 4   | A1JWG | DG    | 502 | -    | 3/3/15/15 | 6/15/91/91  | -       |
| 3   | LMG   | DH    | 502 | -    | -         | 3/16/36/70  | 0/1/1/1 |
| 4   | A1JWG | BL    | 701 | -    | 2/2/15/15 | 3/15/91/91  | -       |
| 3   | LMG   | AB    | 503 | -    | -         | 7/16/36/70  | 0/1/1/1 |
| 2   | NDP   | CE    | 501 | -    | -         | 8/34/77/77  | 0/5/5/5 |
| 3   | LMG   | BA    | 502 | -    | -         | 3/16/36/70  | 0/1/1/1 |
| 3   | LMG   | CH    | 502 | -    | -         | 8/16/36/70  | 0/1/1/1 |
| 4   | A1JWG | CA    | 701 | -    | 2/2/15/15 | 6/15/91/91  | -       |
| 2   | NDP   | BF    | 501 | -    | -         | 12/34/77/77 | 0/5/5/5 |
| 3   | LMG   | DB    | 703 | -    | -         | 2/16/36/70  | 0/1/1/1 |
| 2   | NDP   | BE    | 501 | -    | -         | 13/34/77/77 | 0/5/5/5 |
| 3   | LMG   | BB    | 502 | -    | -         | 5/16/36/70  | 0/1/1/1 |
| 4   | A1JWG | AA    | 503 | -    | 2/2/15/15 | 5/15/91/91  | -       |
| 2   | NDP   | AJ    | 503 | -    | -         | 11/34/77/77 | 0/5/5/5 |
| 4   | A1JWG | DD    | 701 | -    | 3/3/15/15 | 6/15/91/91  | -       |
| 4   | A1JWG | BG    | 502 | -    | 2/2/15/15 | 9/15/91/91  | -       |
| 4   | A1JWG | CG    | 503 | -    | 3/3/15/15 | 6/15/91/91  | -       |
| 3   | LMG   | CF    | 501 | -    | -         | 5/16/36/70  | 0/1/1/1 |
| 3   | LMG   | AF    | 502 | -    | -         | 7/16/36/70  | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions    | Rings   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 2   | NDP  | BI    | 703 | -    | -       | 12/34/77/77 | 0/5/5/5 |
| 3   | LMG  | DE    | 703 | -    | -       | 6/16/36/70  | 0/1/1/1 |
| 3   | LMG  | CI    | 501 | -    | -       | 2/16/36/70  | 0/1/1/1 |

The worst 5 of 410 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | BA    | 501 | NDP  | P2B-O2B | 12.53 | 1.83        | 1.59     |
| 2   | BF    | 501 | NDP  | P2B-O2B | 12.48 | 1.82        | 1.59     |
| 2   | CE    | 501 | NDP  | P2B-O2B | 12.46 | 1.82        | 1.59     |
| 2   | BC    | 501 | NDP  | P2B-O2B | 12.45 | 1.82        | 1.59     |
| 2   | CA    | 703 | NDP  | P2B-O2B | 12.44 | 1.82        | 1.59     |

The worst 5 of 722 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | CC    | 502 | NDP  | PN-O3-PA | -7.15 | 108.29      | 132.83   |
| 2   | CE    | 501 | NDP  | PN-O3-PA | -7.15 | 108.31      | 132.83   |
| 2   | AC    | 503 | NDP  | PN-O3-PA | -7.12 | 108.38      | 132.83   |
| 2   | AE    | 702 | NDP  | PN-O3-PA | -7.11 | 108.43      | 132.83   |
| 2   | CA    | 703 | NDP  | PN-O3-PA | -7.09 | 108.49      | 132.83   |

5 of 109 chirality outliers are listed below:

| Mol | Chain | Res | Type  | Atom |
|-----|-------|-----|-------|------|
| 4   | AA    | 503 | A1JWG | NC   |
| 4   | AA    | 503 | A1JWG | NB   |
| 4   | AB    | 502 | A1JWG | NA   |
| 4   | AB    | 502 | A1JWG | NC   |
| 4   | AB    | 502 | A1JWG | NB   |

5 of 934 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | AA    | 501 | NDP  | C5B-O5B-PA-O1A  |
| 2   | AA    | 501 | NDP  | C3D-C4D-C5D-O5D |
| 2   | AB    | 501 | NDP  | C5B-O5B-PA-O1A  |
| 2   | AB    | 501 | NDP  | C5B-O5B-PA-O2A  |
| 2   | AB    | 501 | NDP  | PN-O3-PA-O5B    |

There are no ring outliers.

56 monomers are involved in 58 short contacts:

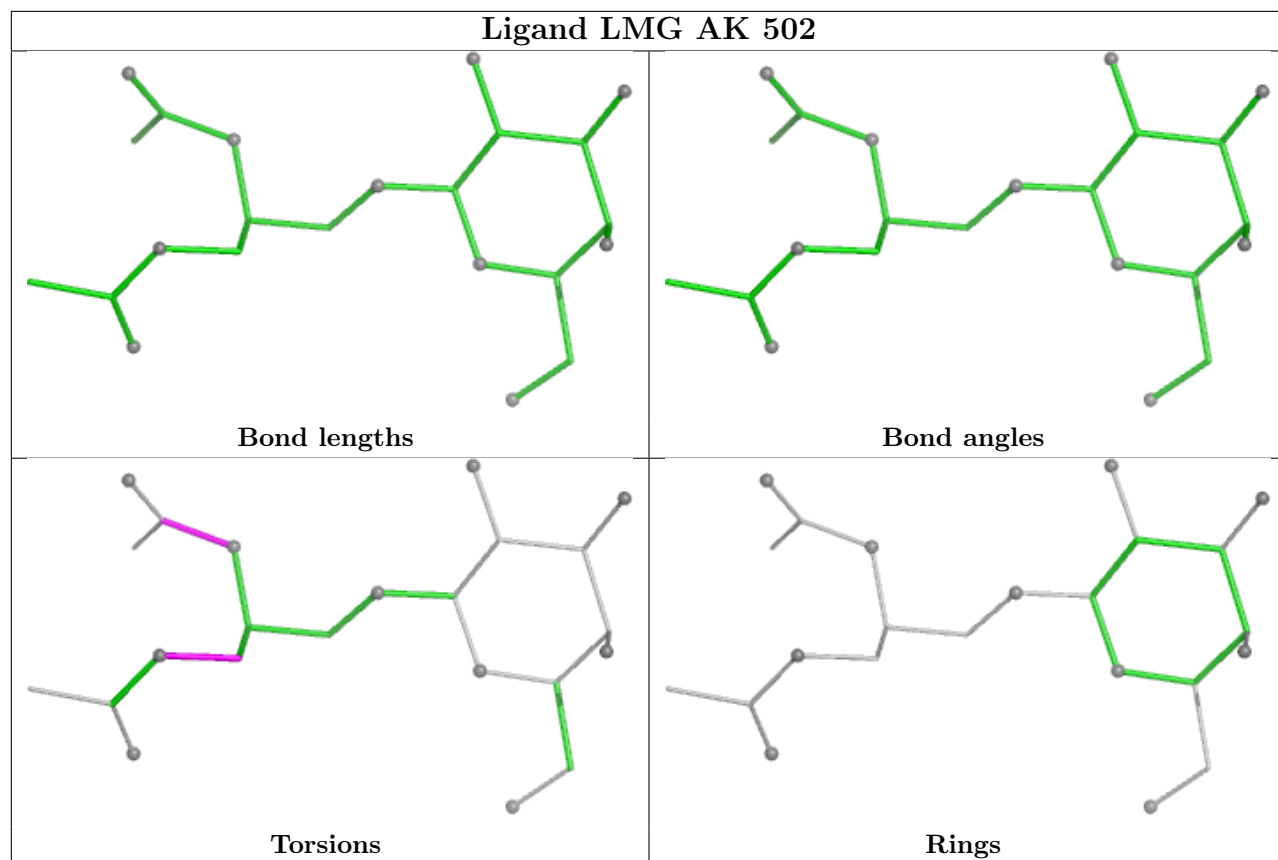
| Mol | Chain | Res | Type  | Clashes | Symm-Clashes |
|-----|-------|-----|-------|---------|--------------|
| 3   | AK    | 502 | LMG   | 1       | 0            |
| 4   | AF    | 503 | A1JWG | 1       | 0            |
| 2   | CD    | 502 | NDP   | 1       | 0            |
| 3   | AI    | 502 | LMG   | 1       | 0            |
| 3   | BF    | 502 | LMG   | 1       | 0            |
| 3   | BI    | 702 | LMG   | 1       | 0            |
| 3   | AH    | 702 | LMG   | 1       | 0            |
| 3   | CK    | 503 | LMG   | 1       | 0            |
| 2   | AF    | 501 | NDP   | 1       | 0            |
| 3   | AC    | 501 | LMG   | 2       | 0            |
| 3   | BK    | 501 | LMG   | 2       | 0            |
| 4   | AH    | 701 | A1JWG | 1       | 0            |
| 4   | AI    | 503 | A1JWG | 1       | 0            |
| 4   | BF    | 503 | A1JWG | 2       | 0            |
| 2   | DE    | 702 | NDP   | 1       | 0            |
| 2   | DD    | 703 | NDP   | 1       | 0            |
| 4   | AG    | 701 | A1JWG | 1       | 0            |
| 3   | DG    | 503 | LMG   | 1       | 0            |
| 3   | AE    | 703 | LMG   | 1       | 0            |
| 3   | AJ    | 501 | LMG   | 1       | 0            |
| 3   | DC    | 703 | LMG   | 1       | 0            |
| 2   | AG    | 703 | NDP   | 1       | 0            |
| 3   | CD    | 501 | LMG   | 1       | 0            |
| 3   | CG    | 502 | LMG   | 1       | 0            |
| 3   | BE    | 502 | LMG   | 1       | 0            |
| 3   | CB    | 503 | LMG   | 1       | 0            |
| 3   | CJ    | 502 | LMG   | 2       | 0            |
| 3   | BH    | 703 | LMG   | 1       | 0            |
| 3   | CL    | 502 | LMG   | 1       | 0            |
| 3   | DD    | 702 | LMG   | 1       | 0            |
| 2   | CF    | 502 | NDP   | 2       | 0            |
| 2   | BD    | 502 | NDP   | 1       | 0            |
| 3   | CE    | 503 | LMG   | 1       | 0            |
| 3   | DF    | 501 | LMG   | 1       | 0            |
| 4   | CF    | 503 | A1JWG | 1       | 0            |
| 3   | BL    | 703 | LMG   | 1       | 0            |
| 2   | AH    | 703 | NDP   | 1       | 0            |
| 2   | CG    | 501 | NDP   | 1       | 0            |
| 4   | BE    | 503 | A1JWG | 1       | 0            |
| 3   | CA    | 702 | LMG   | 1       | 0            |
| 2   | AI    | 501 | NDP   | 1       | 0            |
| 3   | BG    | 503 | LMG   | 1       | 0            |

*Continued on next page...*

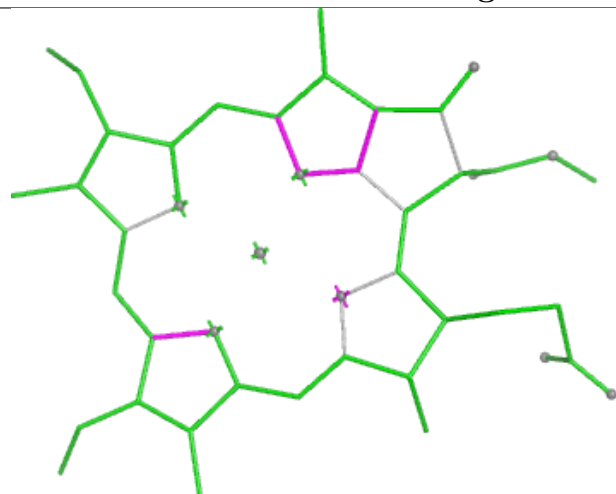
*Continued from previous page...*

| Mol | Chain | Res | Type  | Clashes | Symm-Clashes |
|-----|-------|-----|-------|---------|--------------|
| 3   | AA    | 502 | LMG   | 2       | 0            |
| 3   | AL    | 501 | LMG   | 1       | 0            |
| 2   | AD    | 501 | NDP   | 1       | 0            |
| 3   | DH    | 502 | LMG   | 1       | 0            |
| 3   | BA    | 502 | LMG   | 3       | 0            |
| 2   | BF    | 501 | NDP   | 2       | 0            |
| 3   | DB    | 703 | LMG   | 1       | 0            |
| 2   | BE    | 501 | NDP   | 1       | 0            |
| 4   | DD    | 701 | A1JWG | 1       | 0            |
| 4   | CG    | 503 | A1JWG | 1       | 0            |
| 3   | CF    | 501 | LMG   | 1       | 0            |
| 3   | AF    | 502 | LMG   | 1       | 0            |
| 3   | DE    | 703 | LMG   | 1       | 0            |
| 3   | CI    | 501 | LMG   | 4       | 0            |

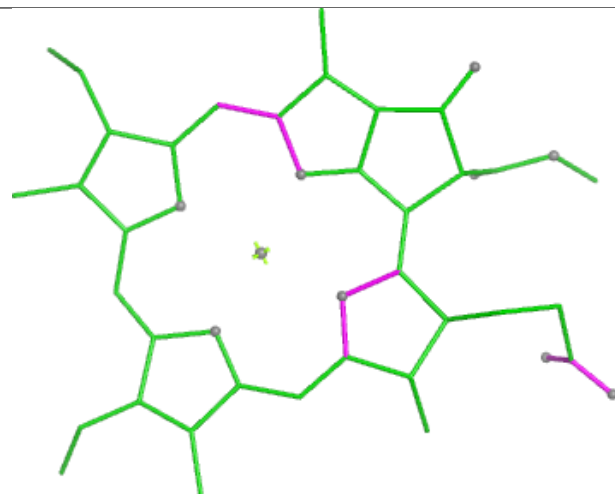
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



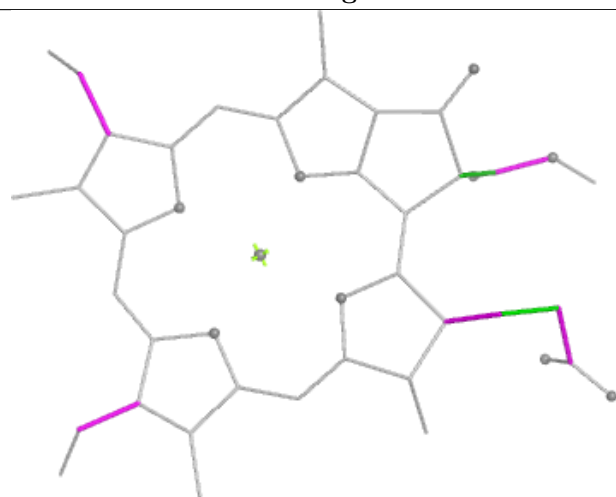
## Ligand A1JWG AF 503



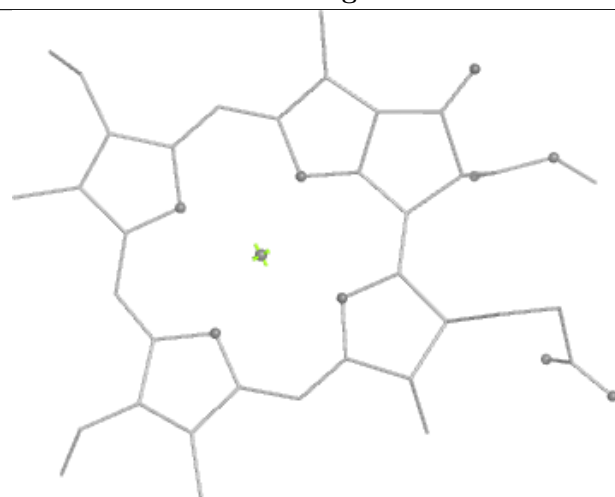
Bond lengths



Bond angles

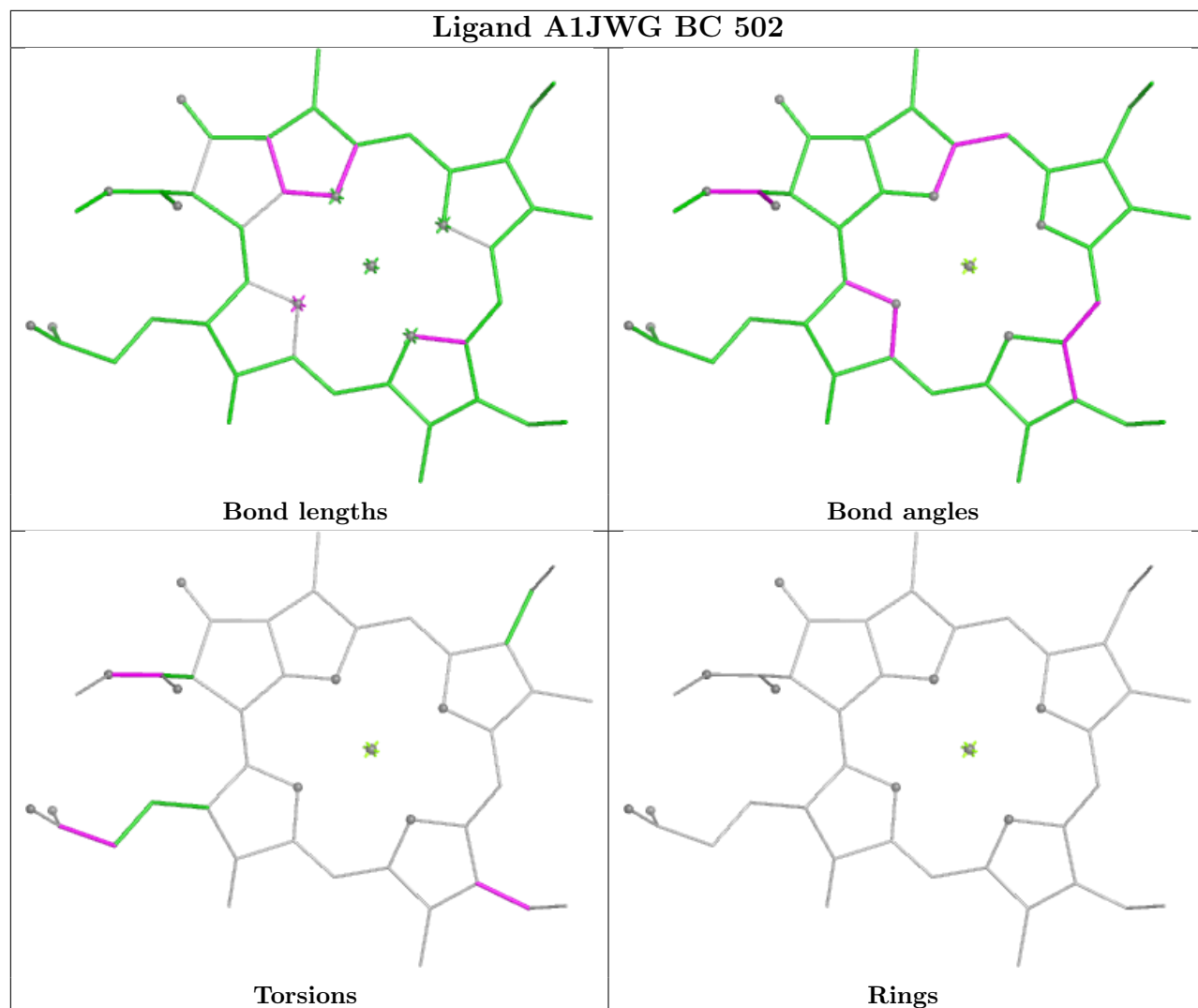


Torsions

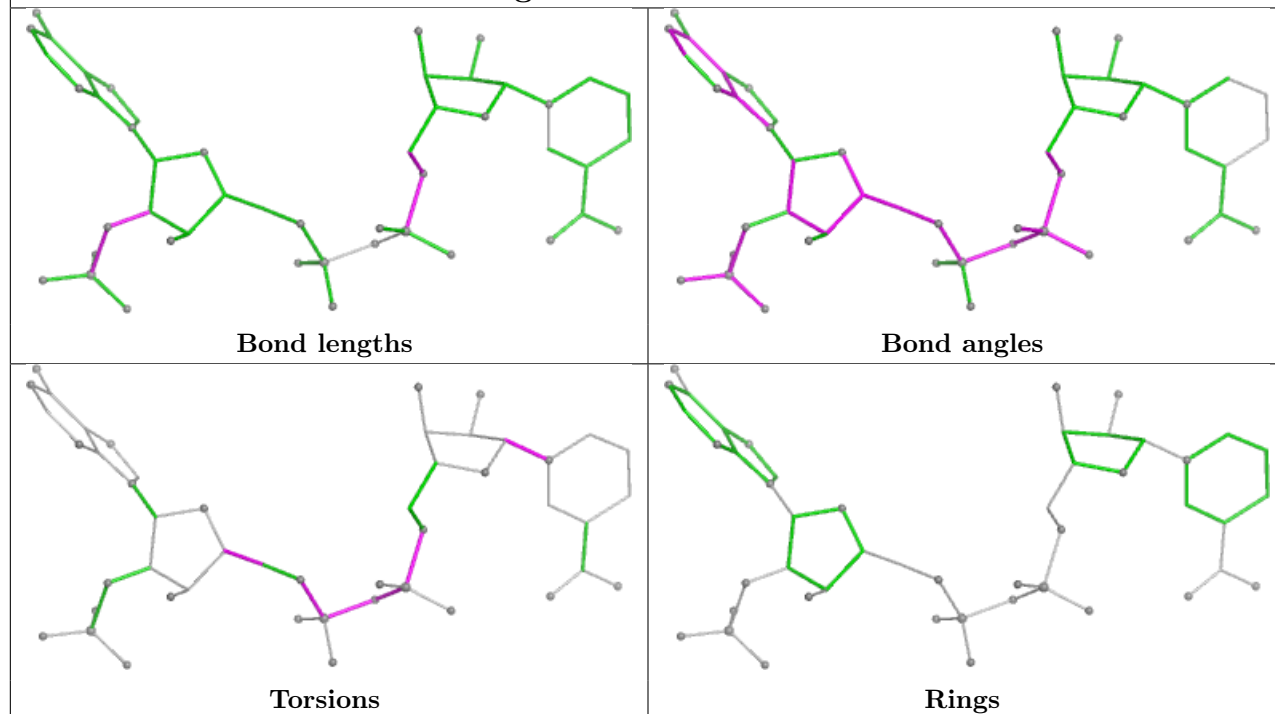


Rings

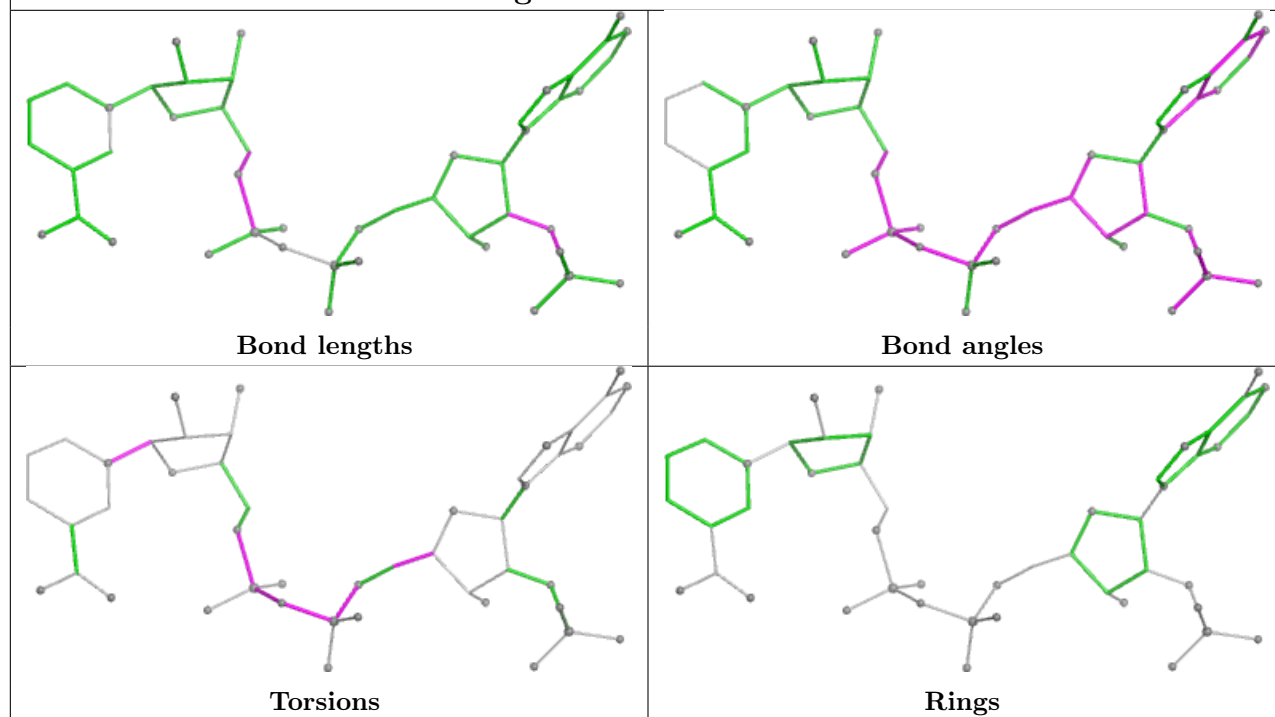
## Ligand A1JWG BC 502

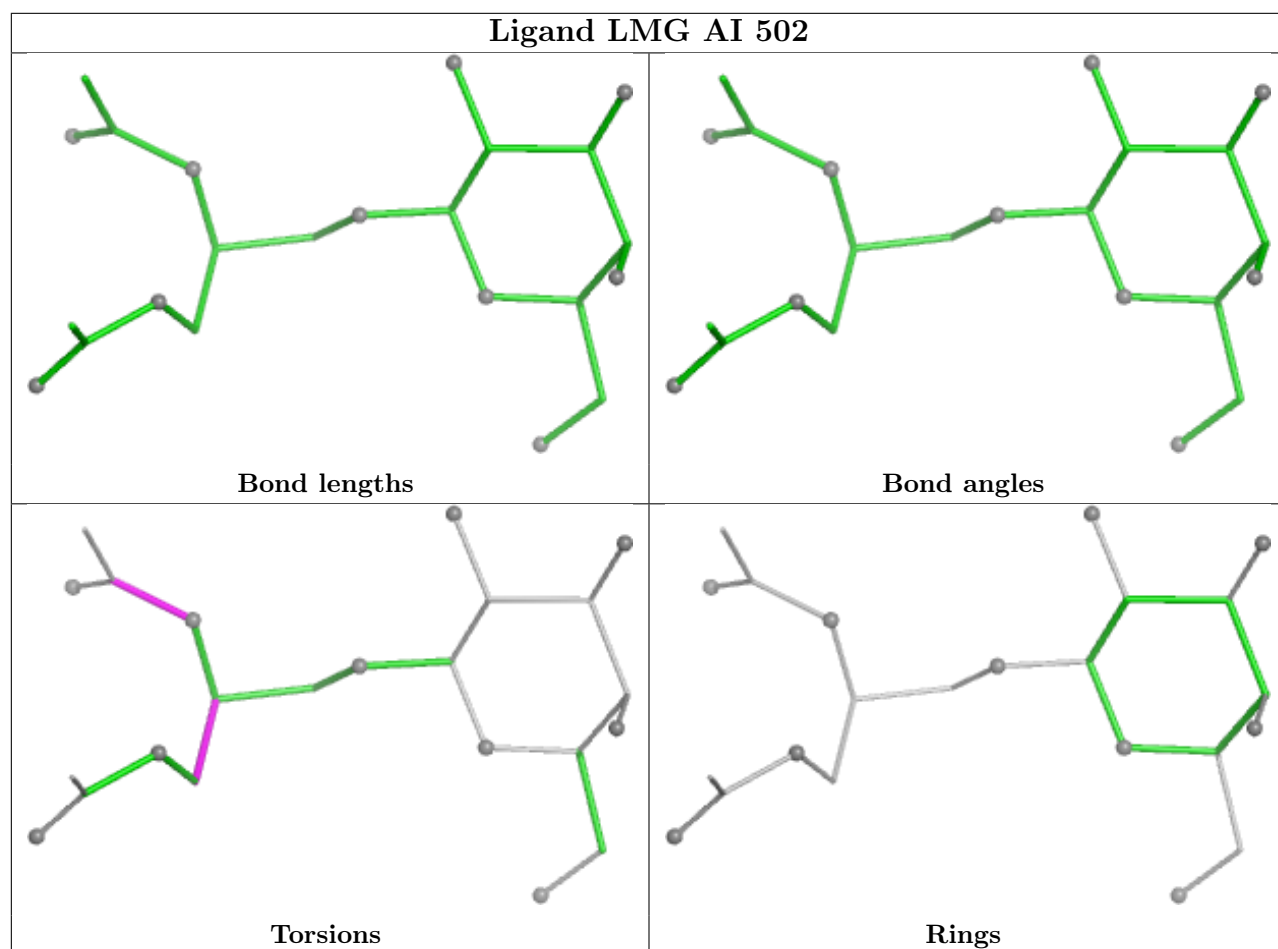
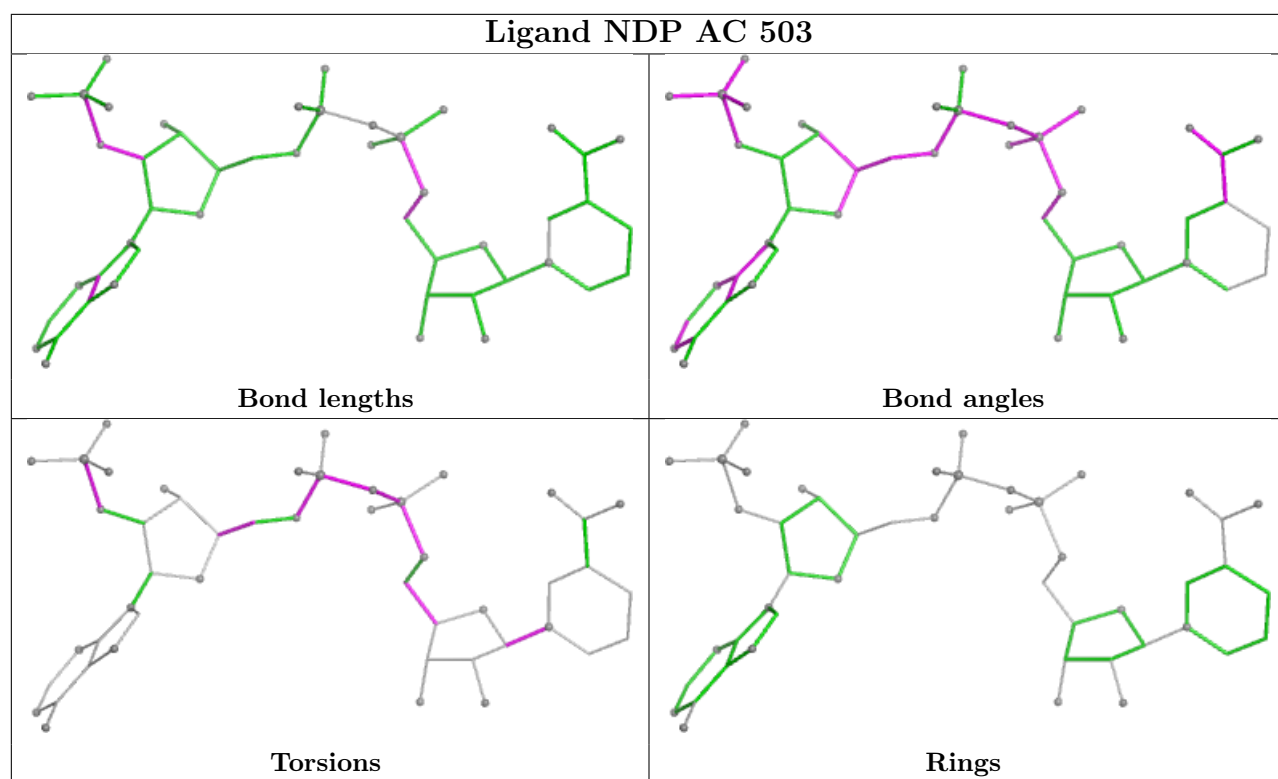


## Ligand NDP CD 502

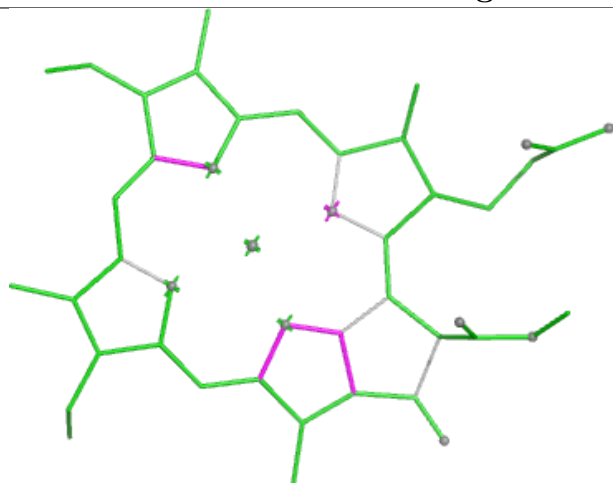


## Ligand NDP CK 501

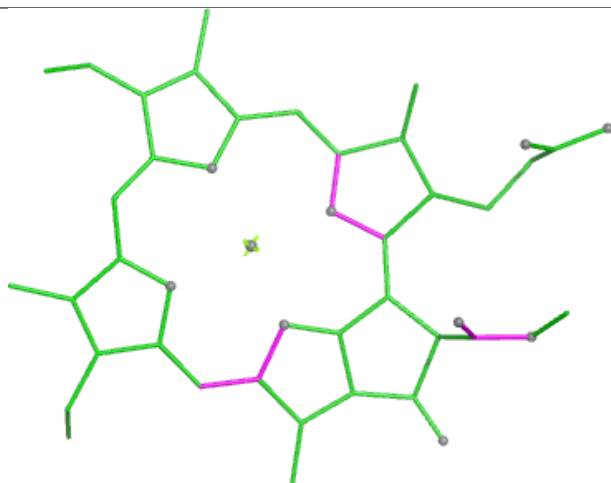




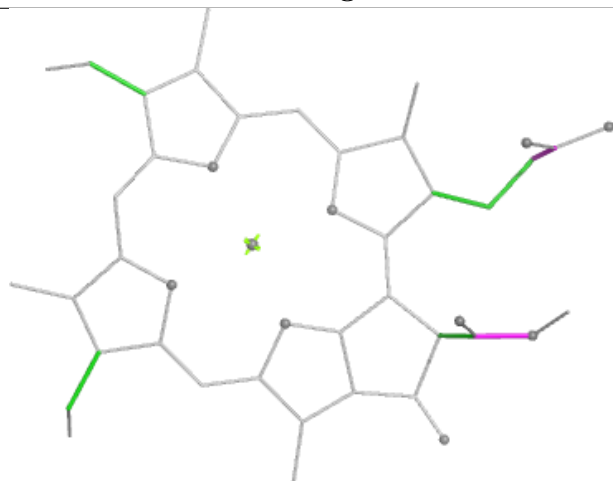
## Ligand A1JWG CE 502



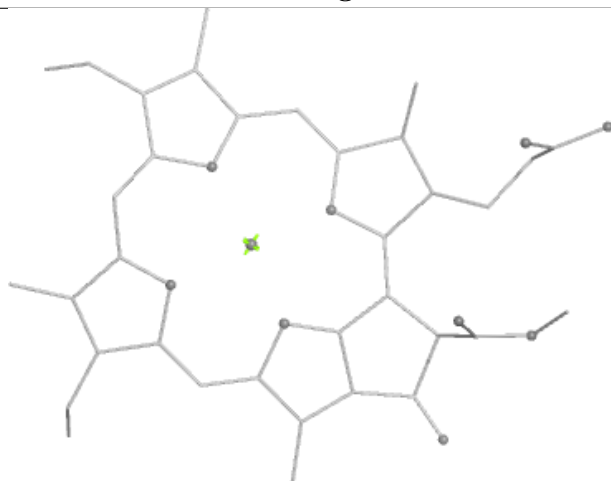
Bond lengths



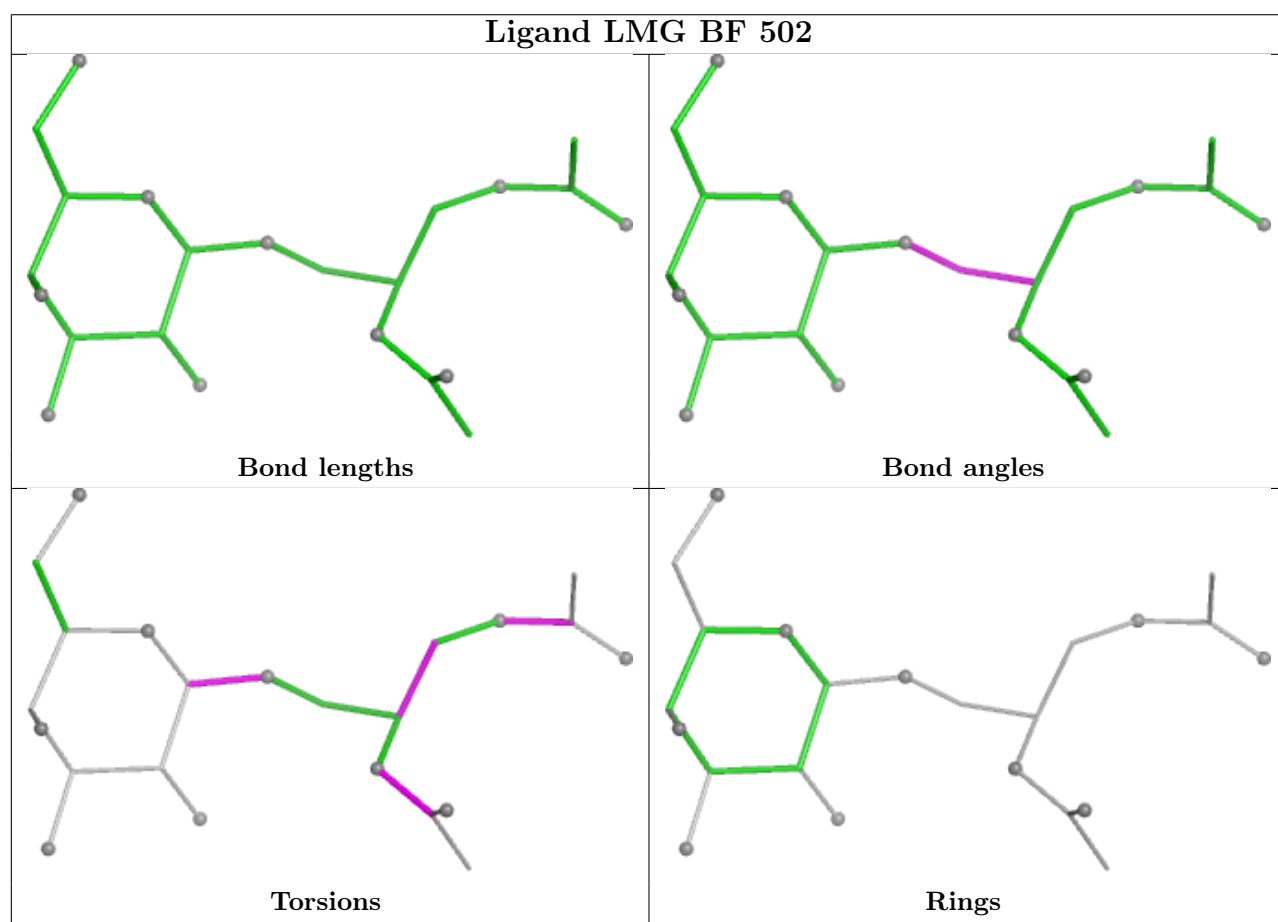
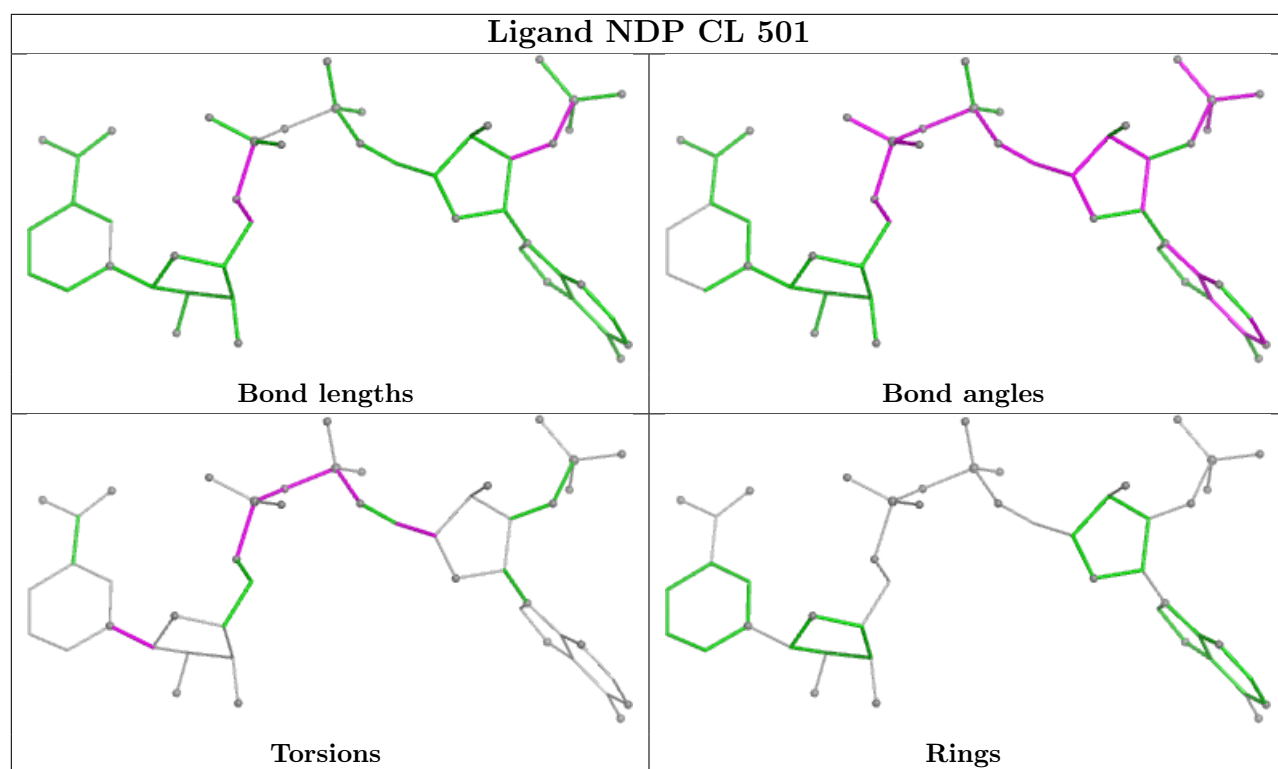
Bond angles

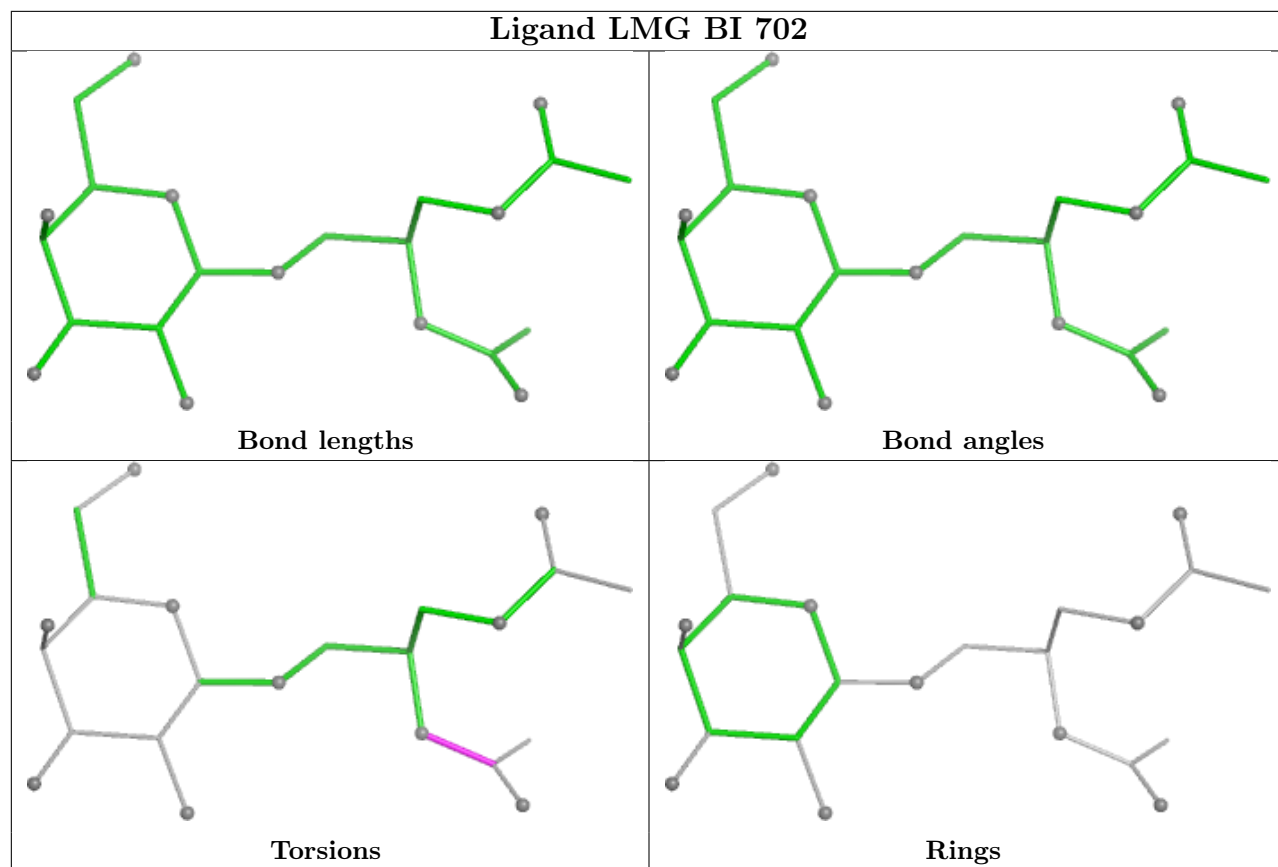


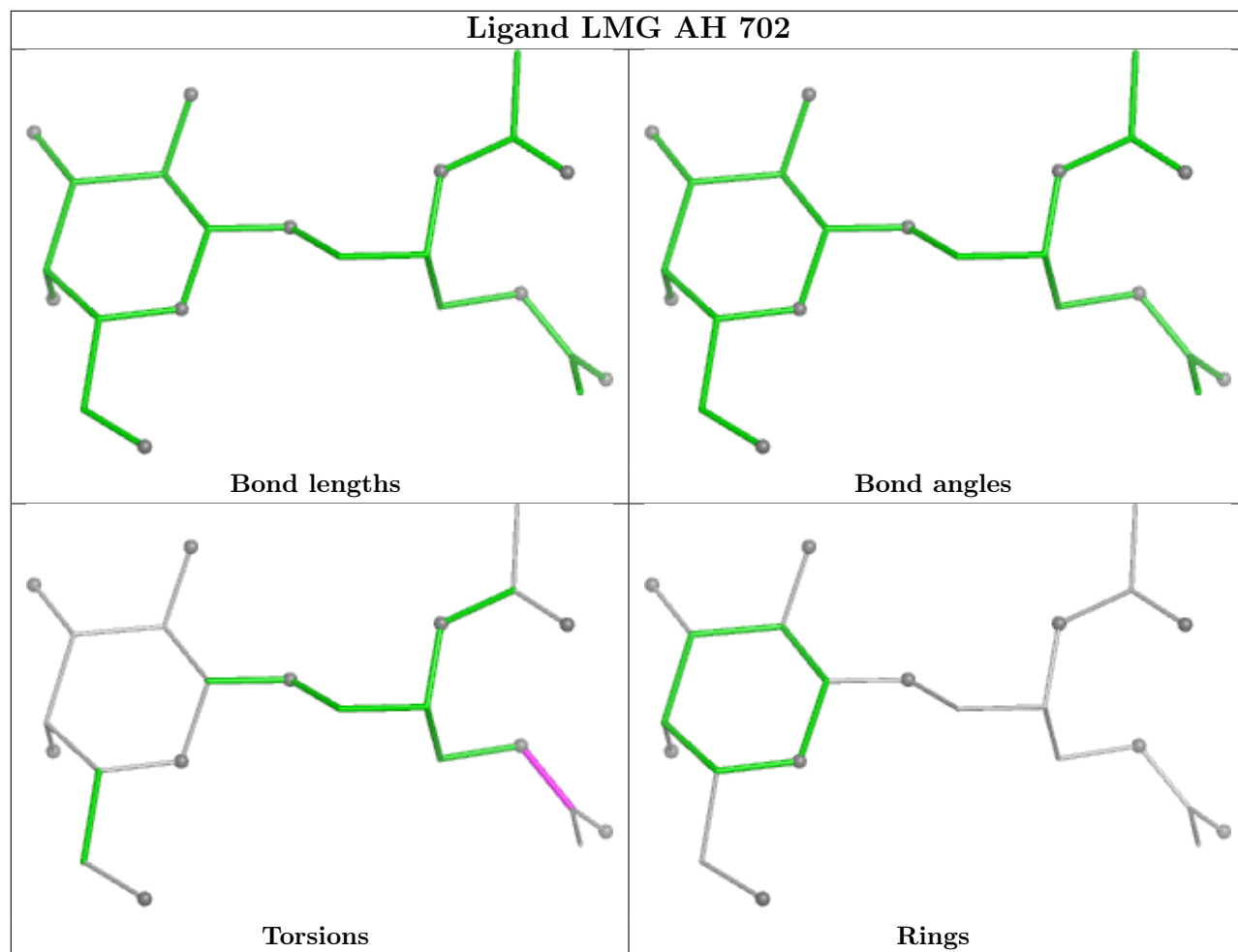
Torsions

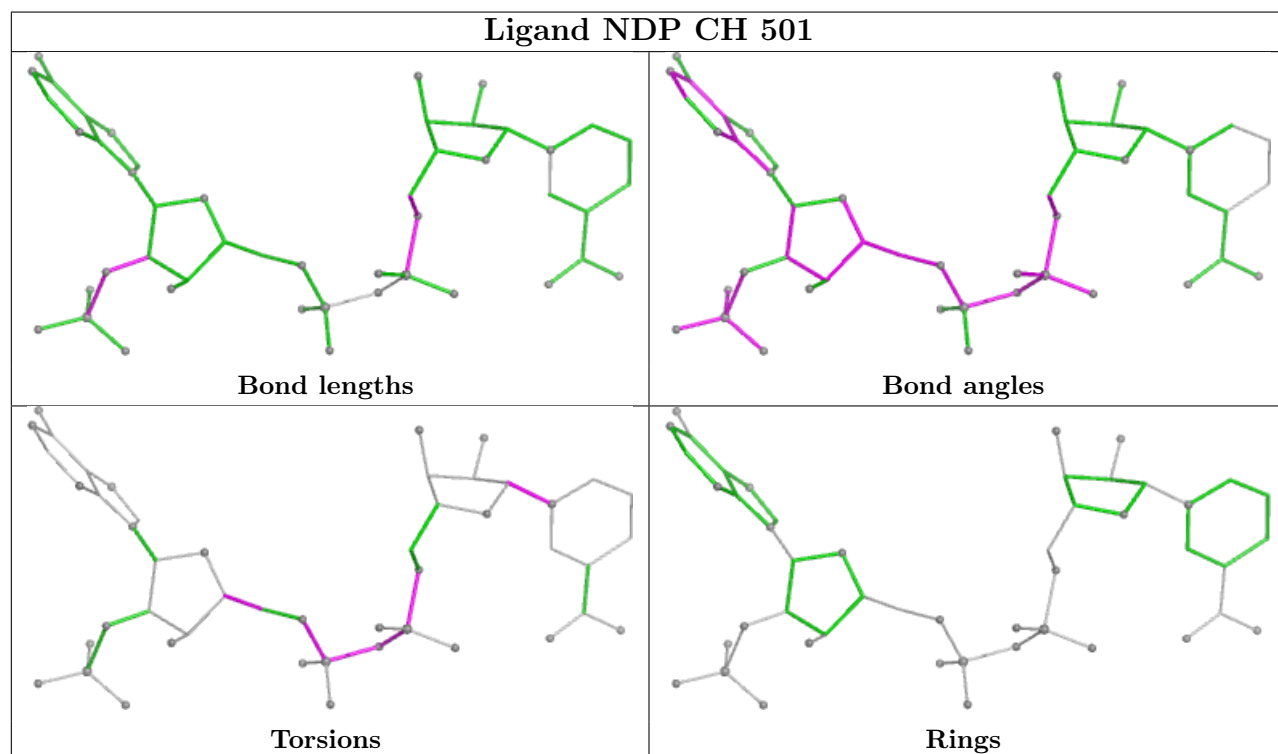
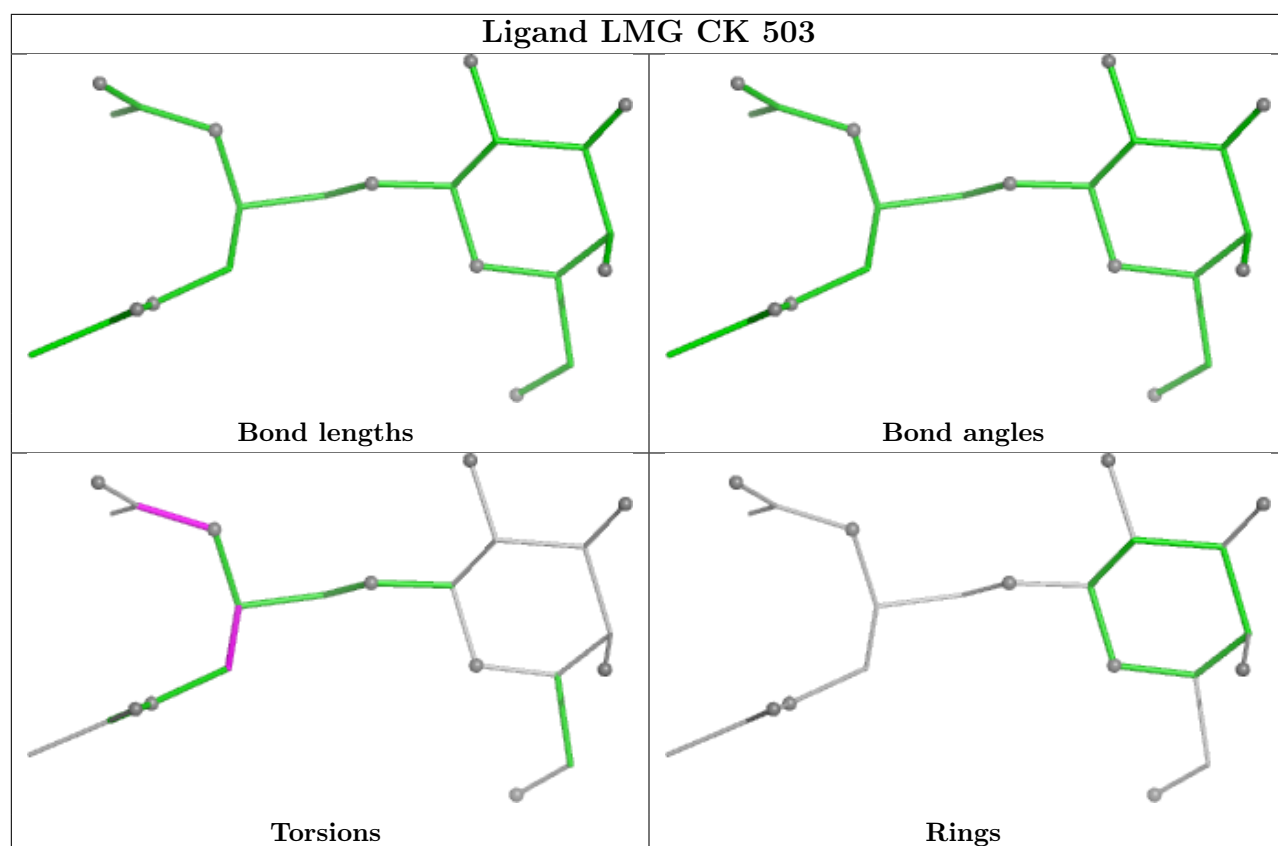


Rings

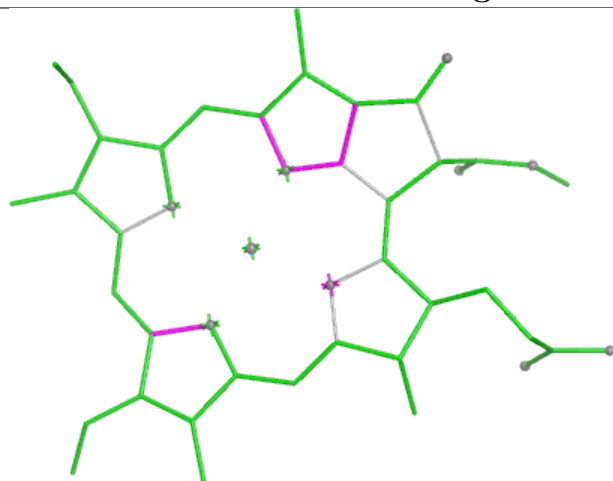




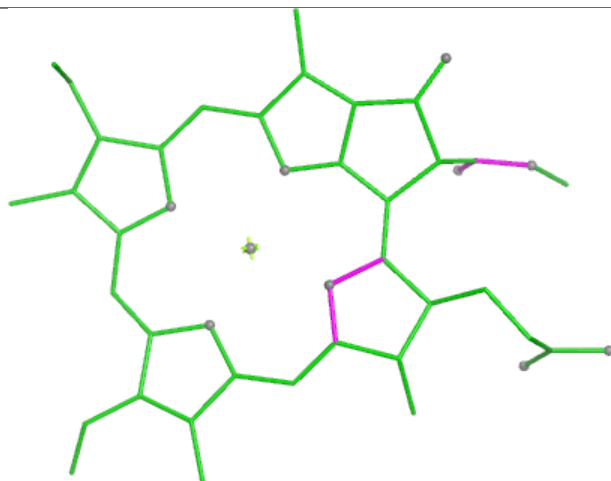




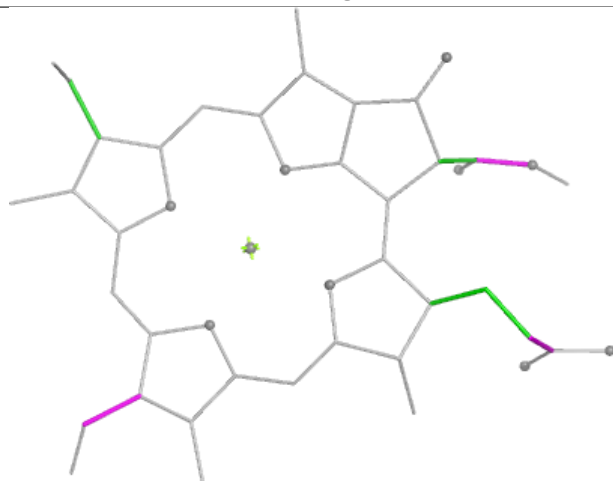
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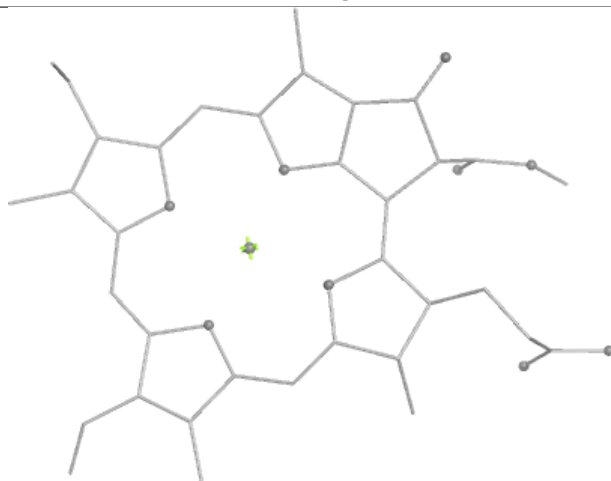
Bond lengths



Bond angles

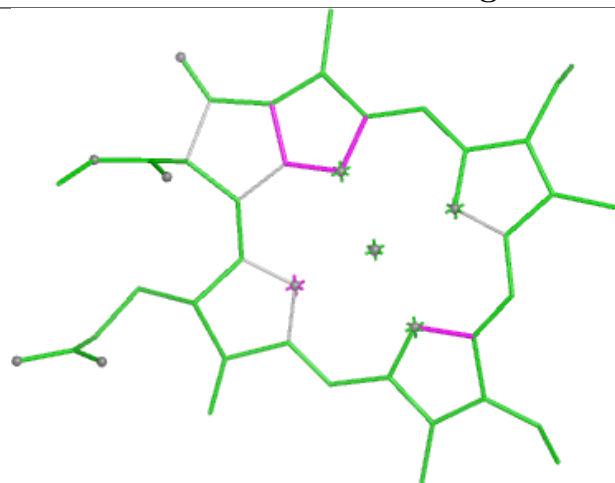


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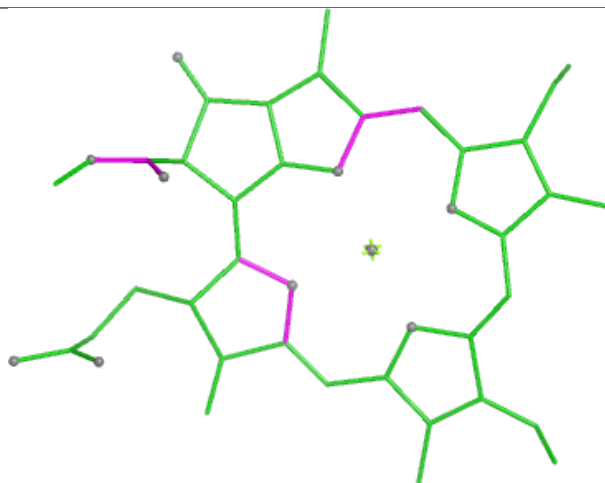


Rings

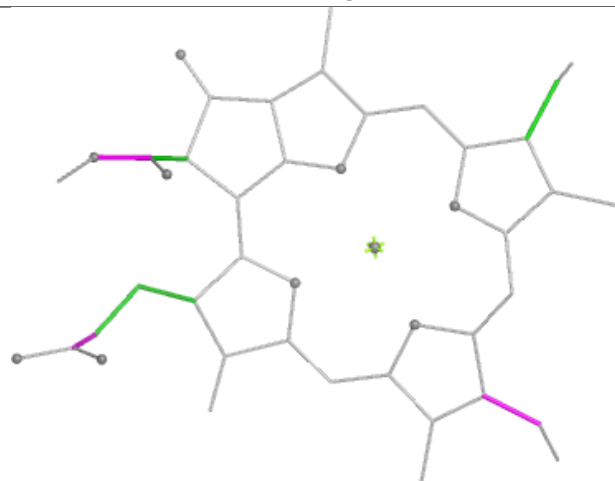
## Ligand A1JWG AJ 502



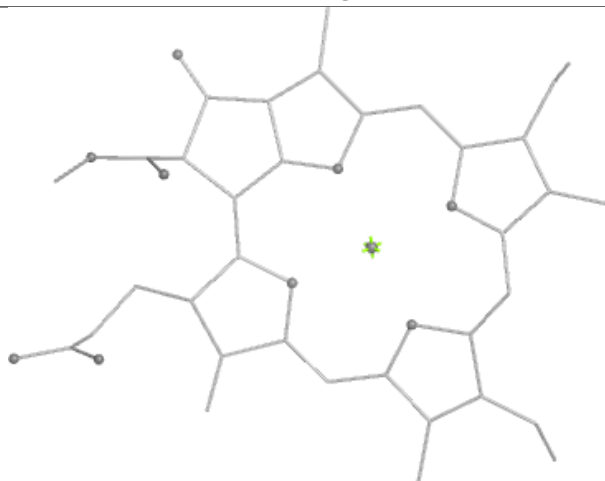
Bond lengths



Bond angles

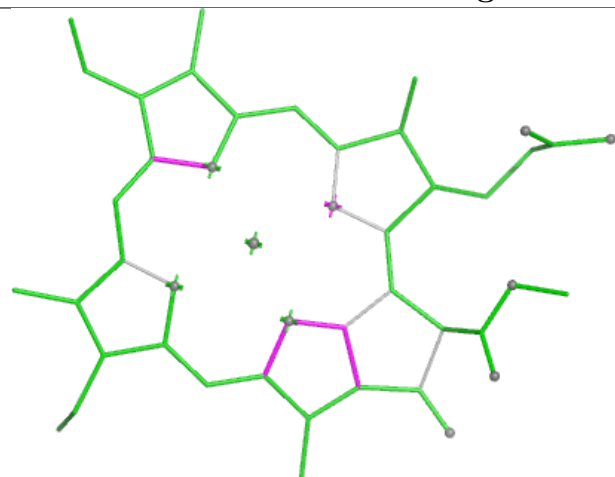


Torsions

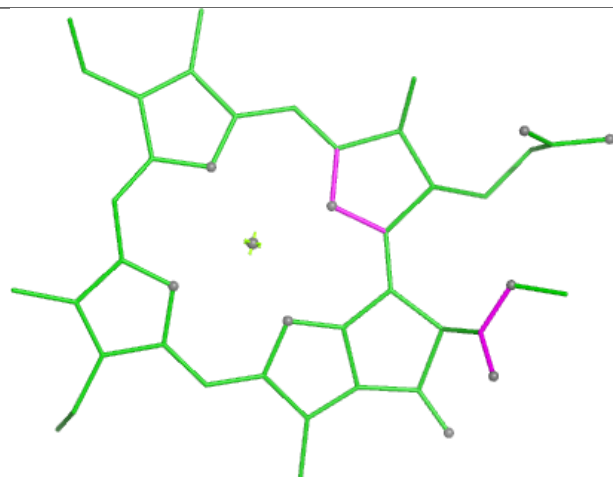


Rings

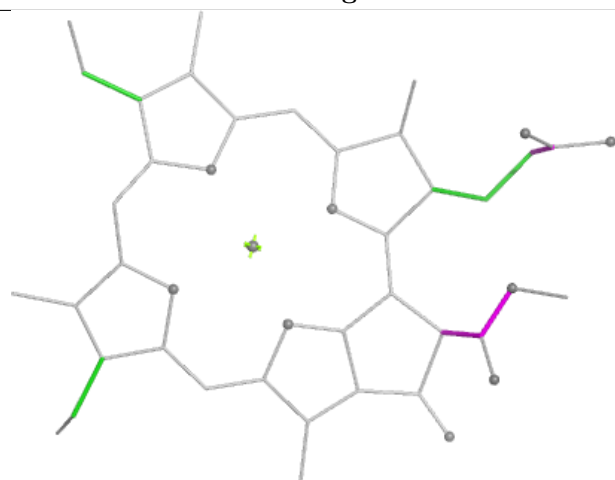
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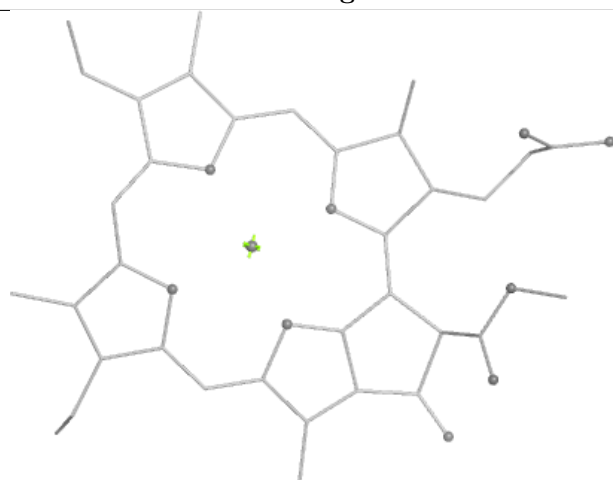
Bond lengths



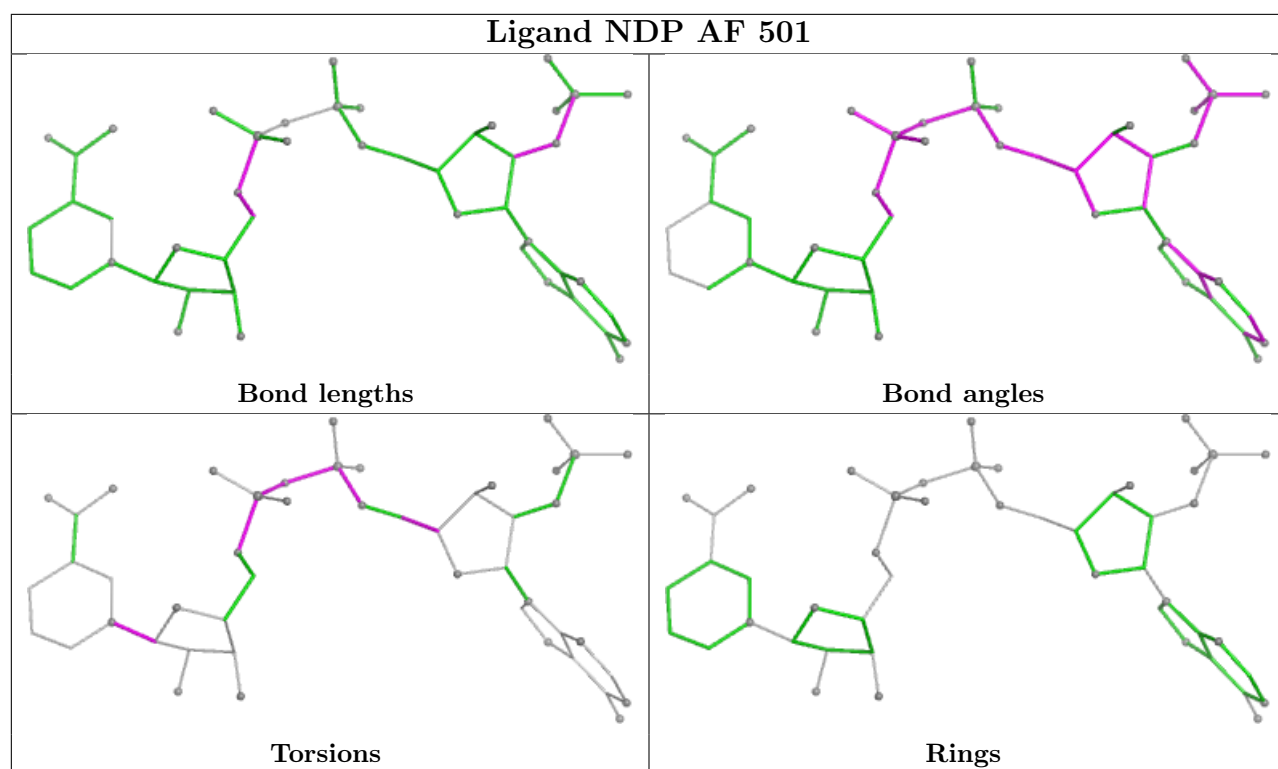
Bond angles



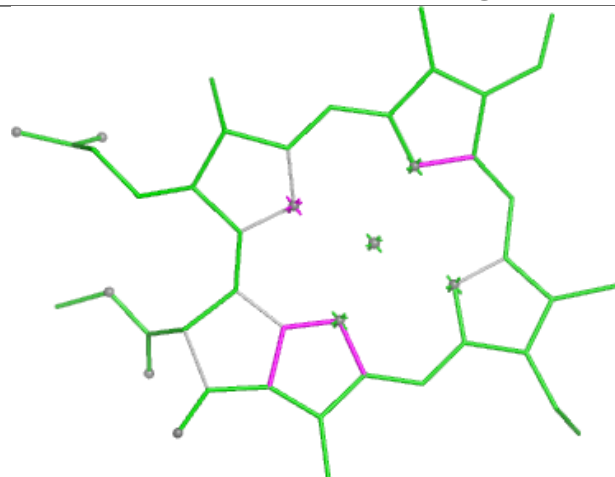
Torsions



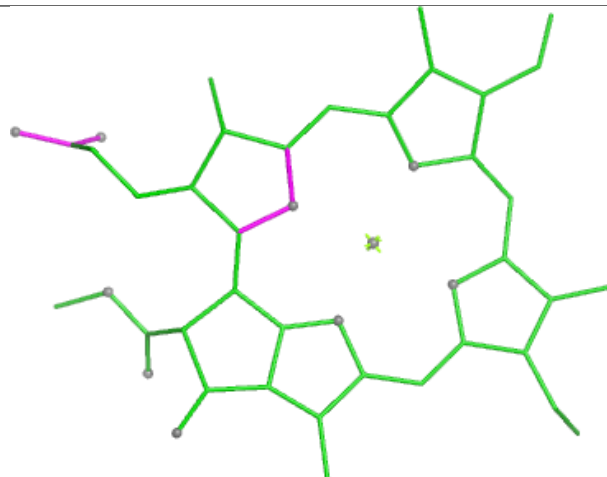
Rings



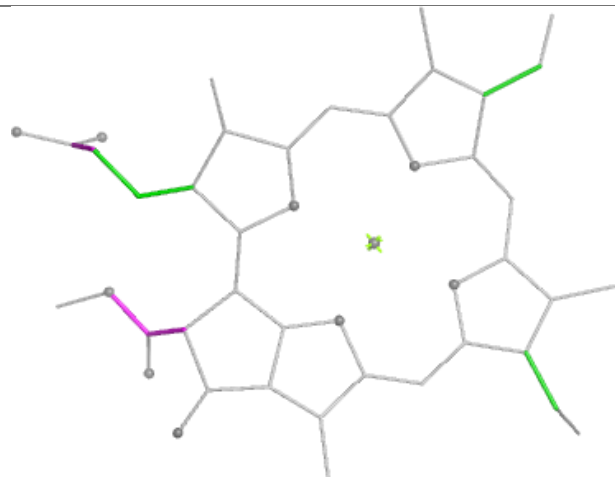
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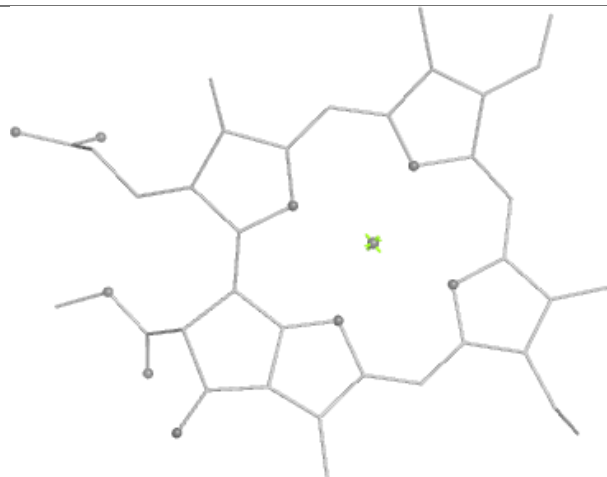
Bond lengths



Bond angles

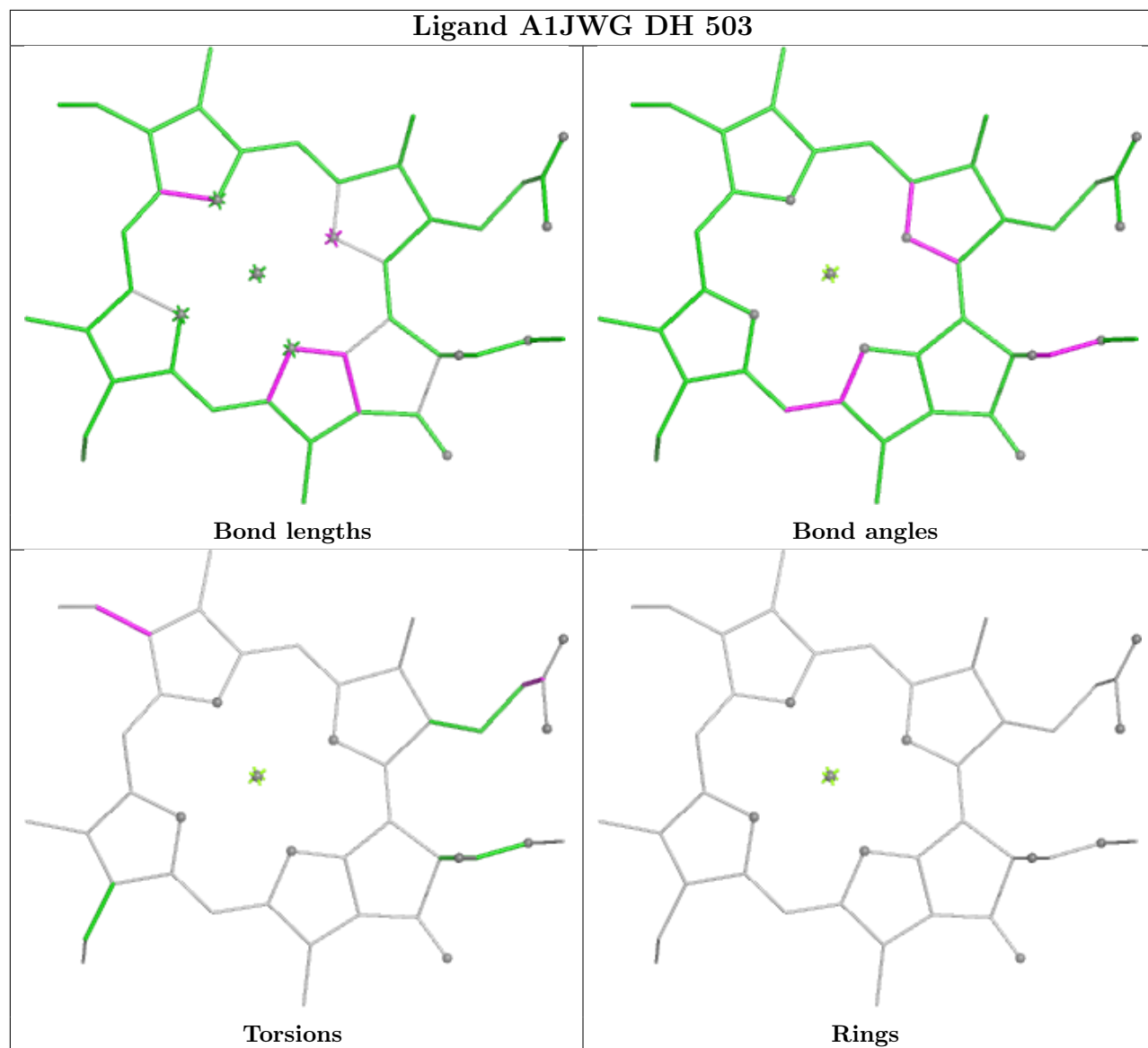


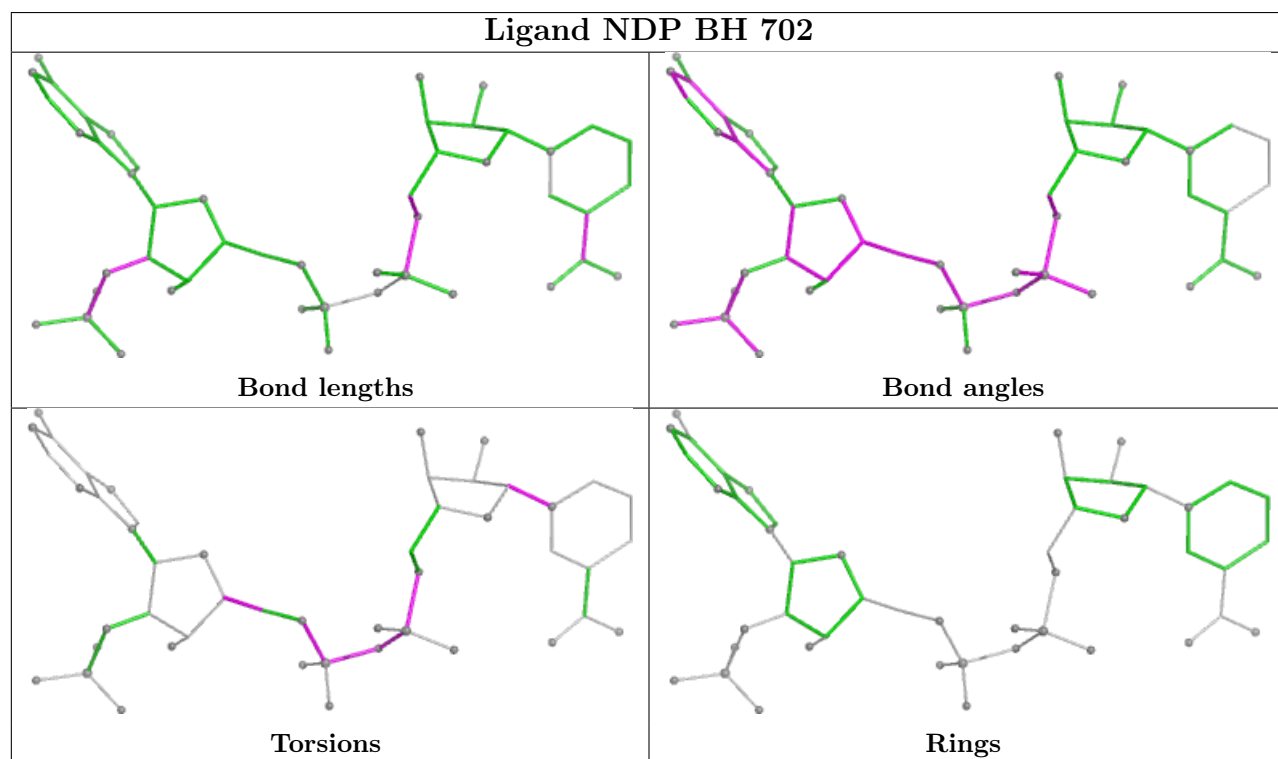
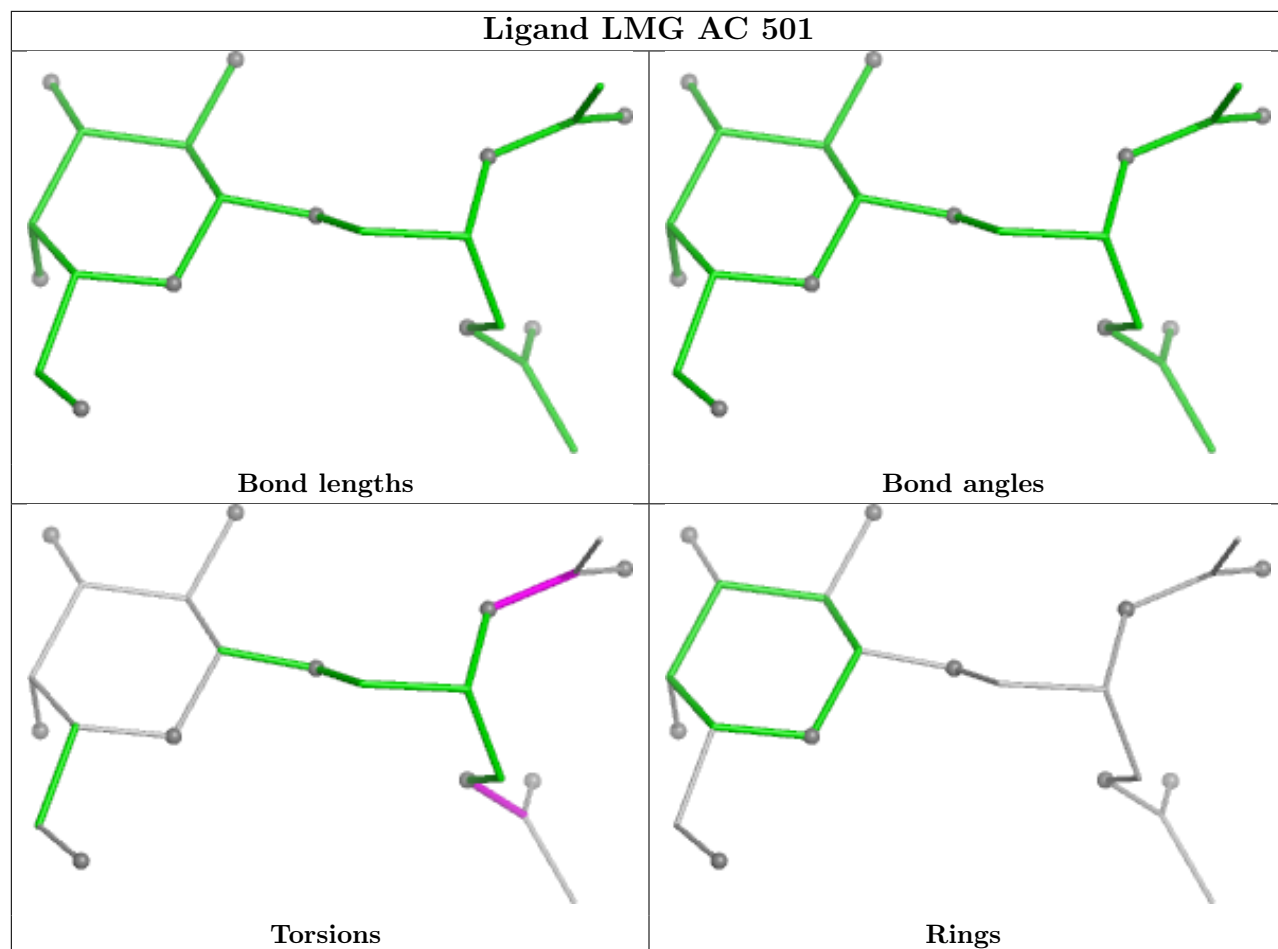
Torsions

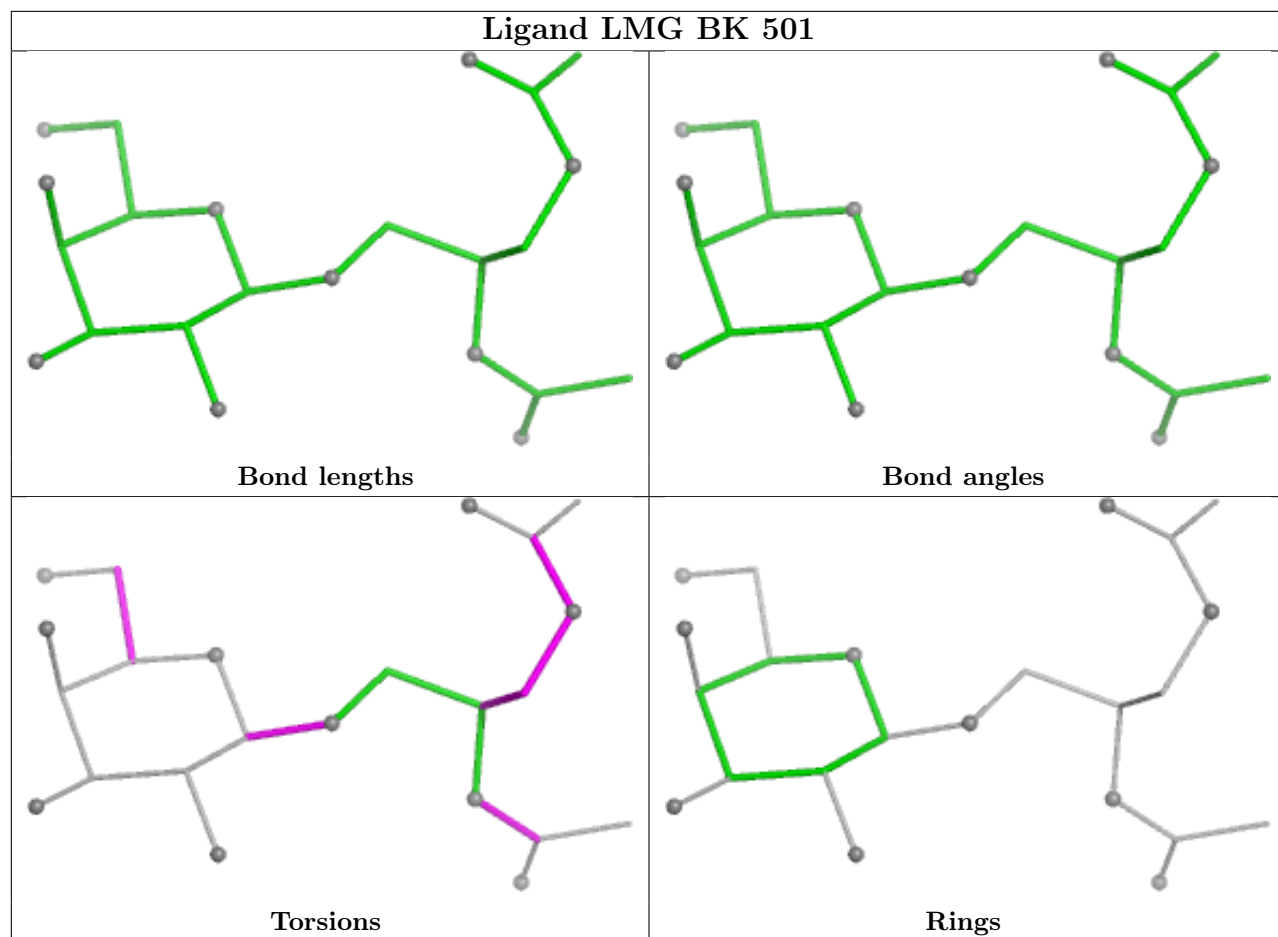


Rings

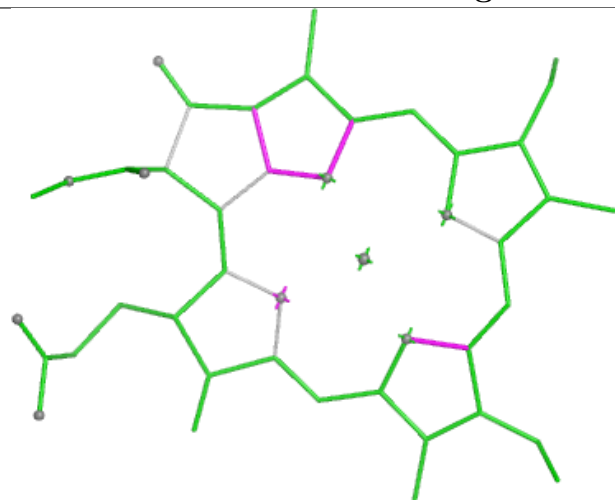
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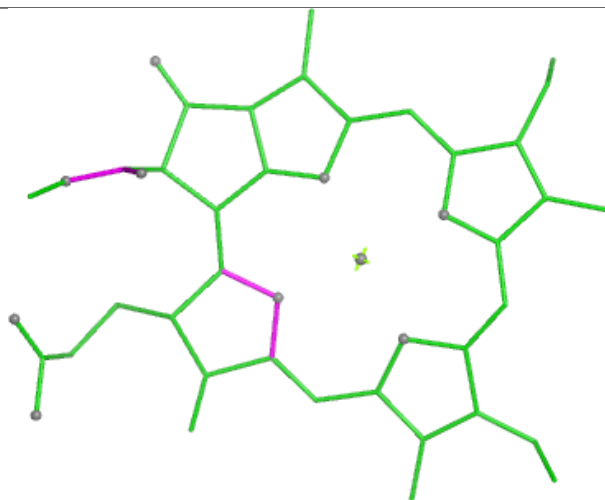




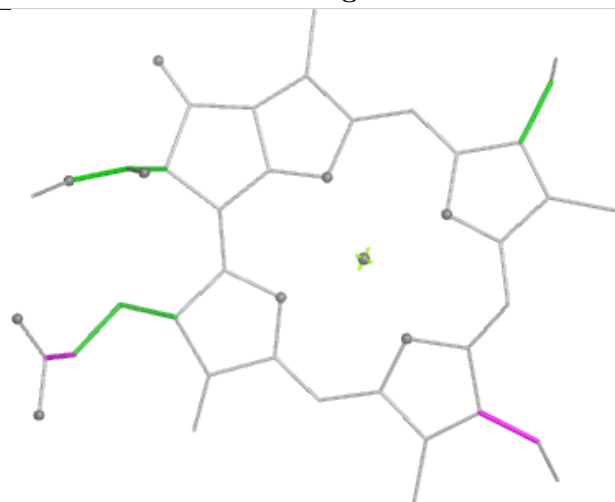
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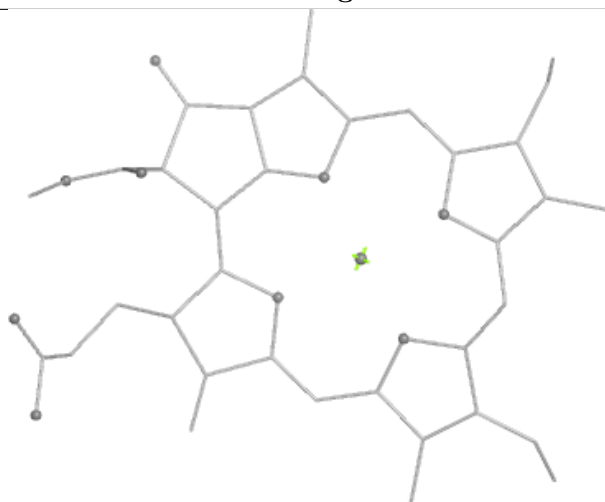
Bond lengths



Bond angles

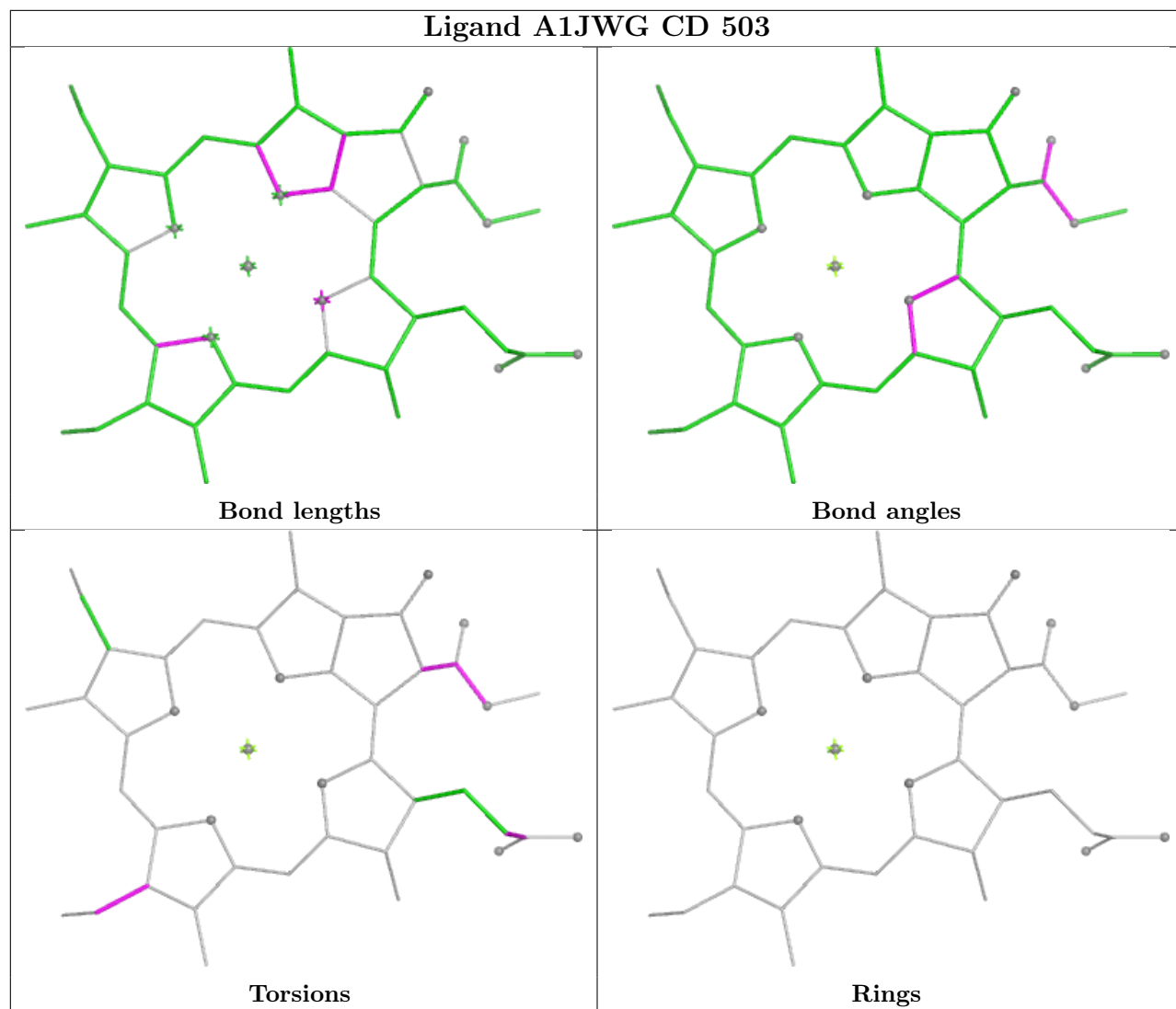


Torsions

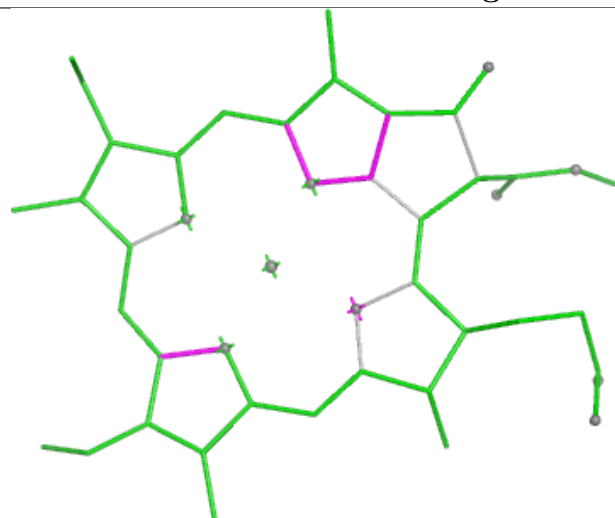


Rings

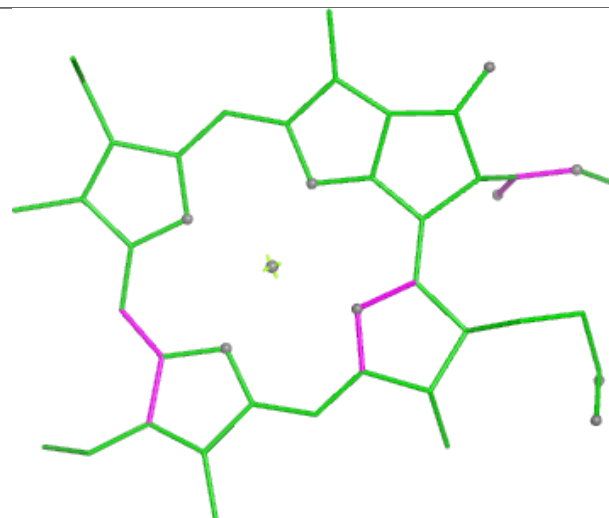
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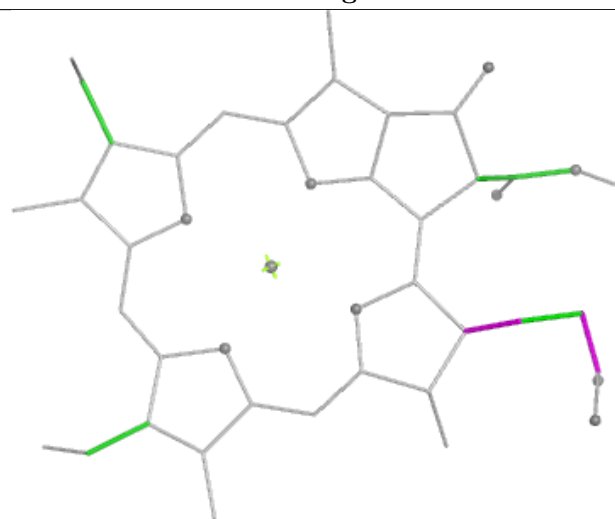
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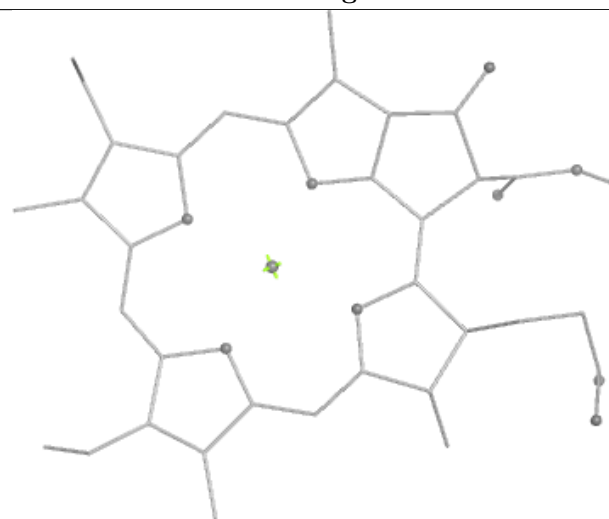
Bond lengths



Bond angles

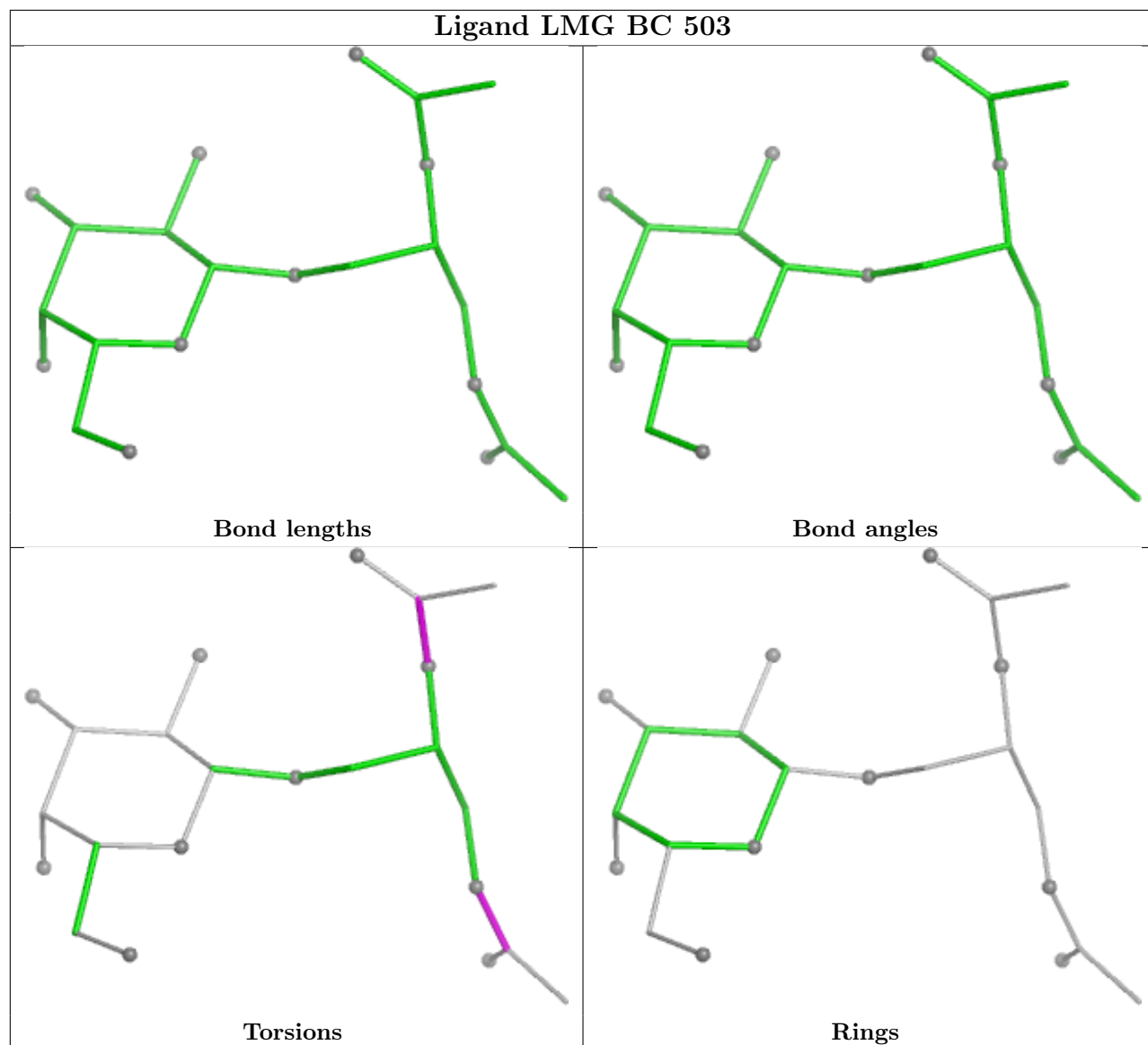


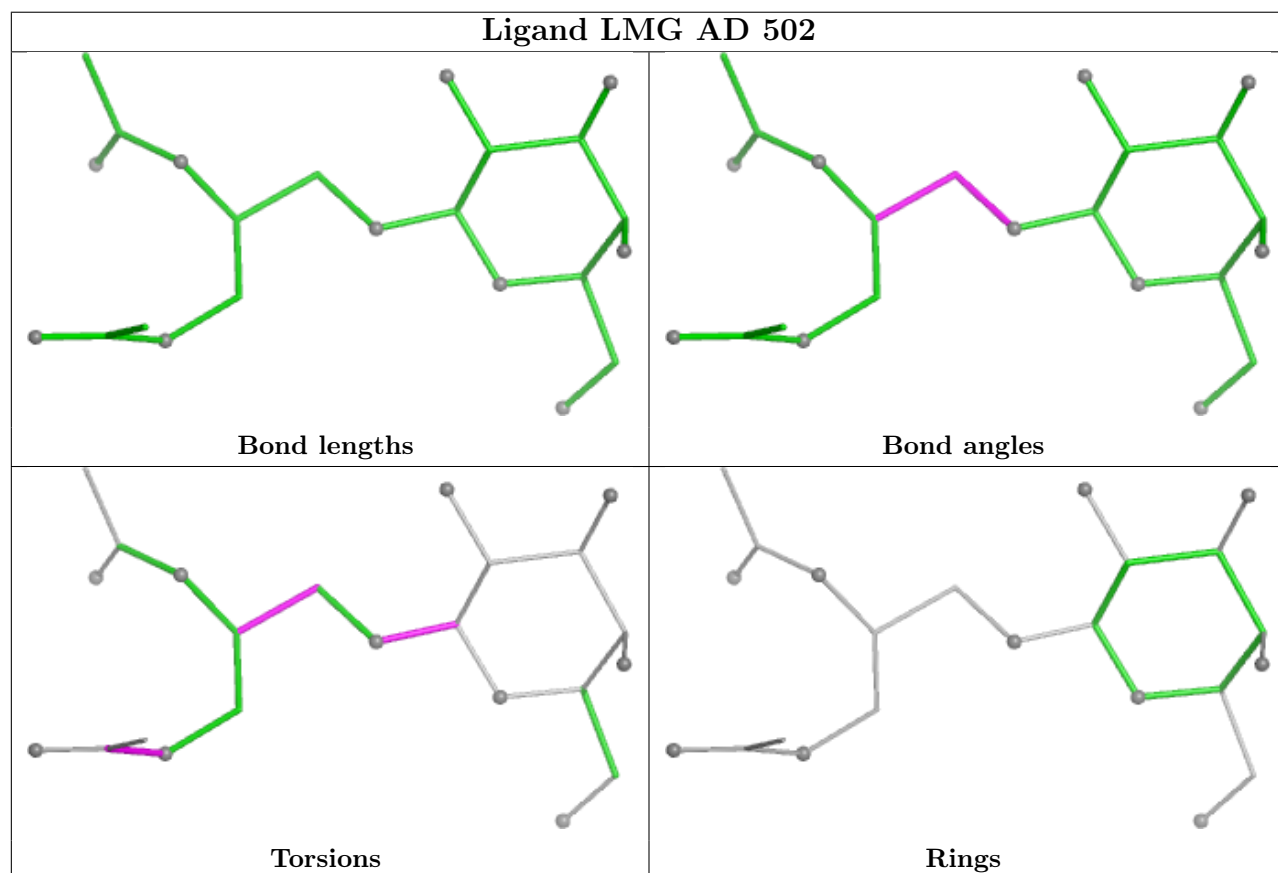
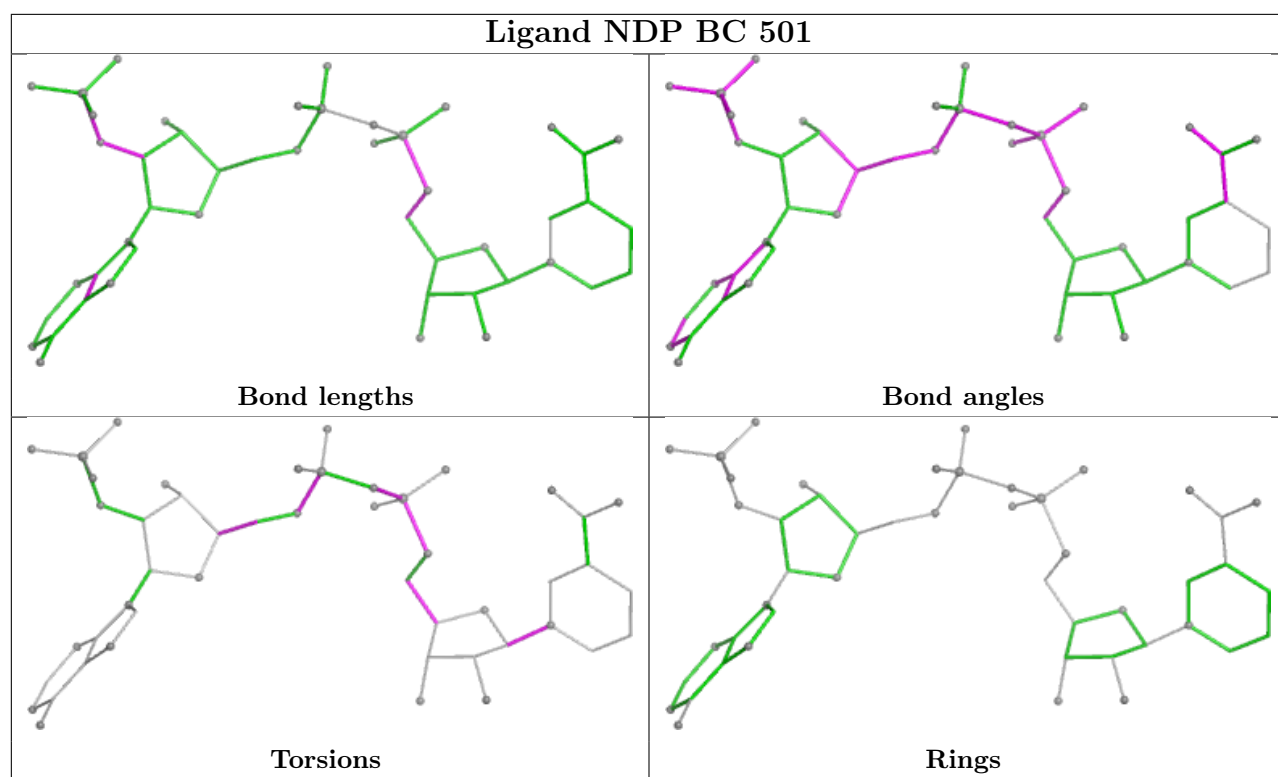
Torsions



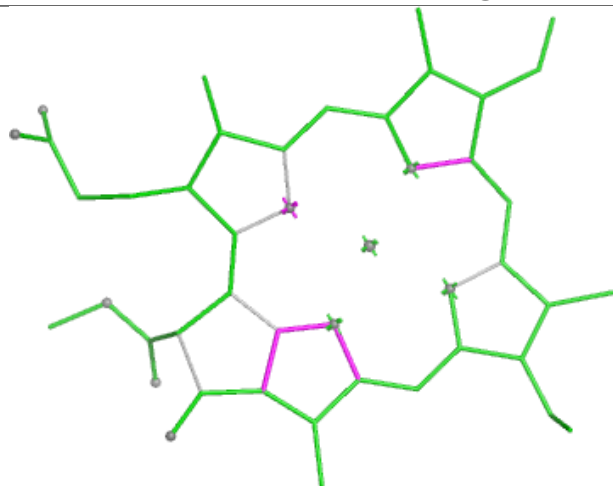
Rings

## Ligand LMG BC 503

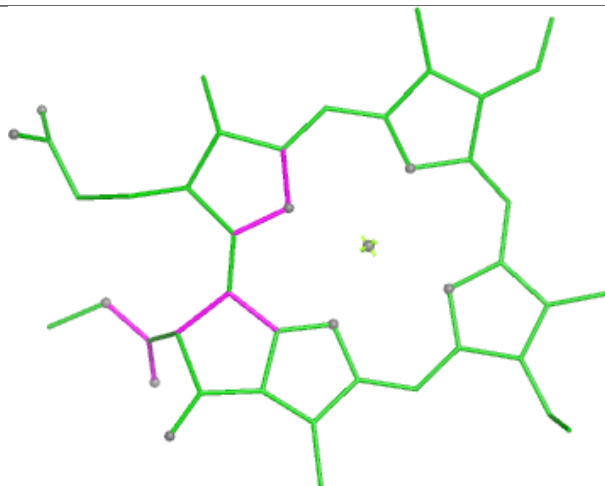




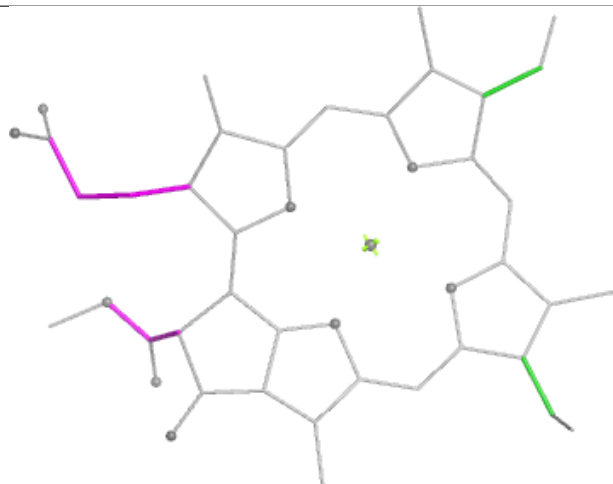
## Ligand A1JWG BF 503



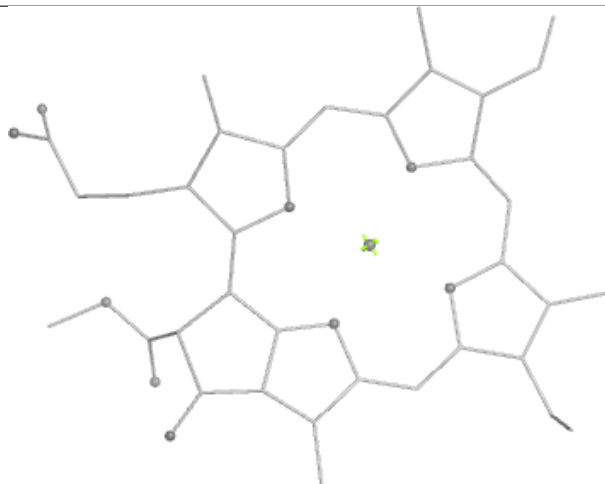
Bond lengths



Bond angles

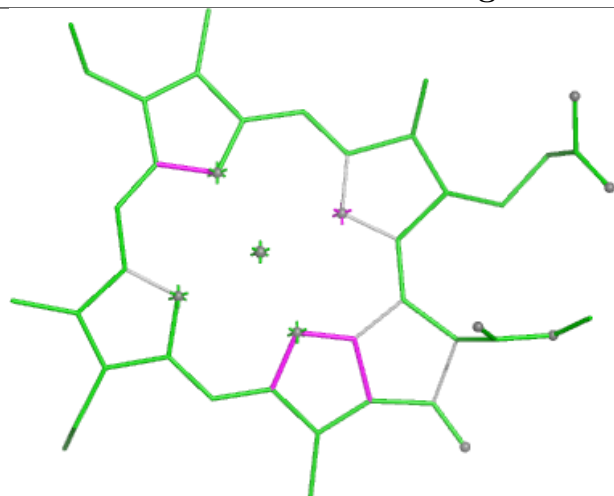


Torsions

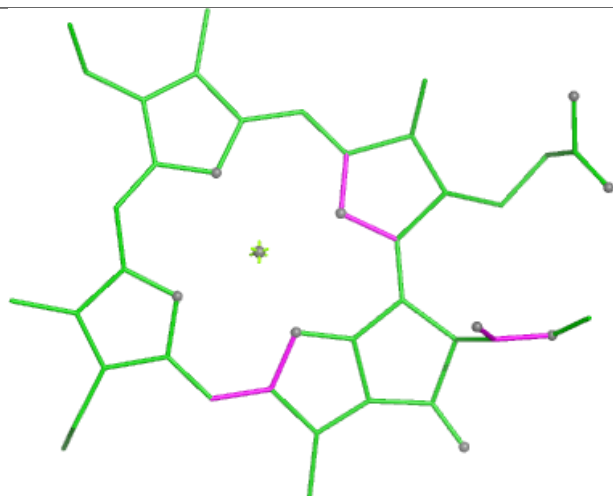


Rings

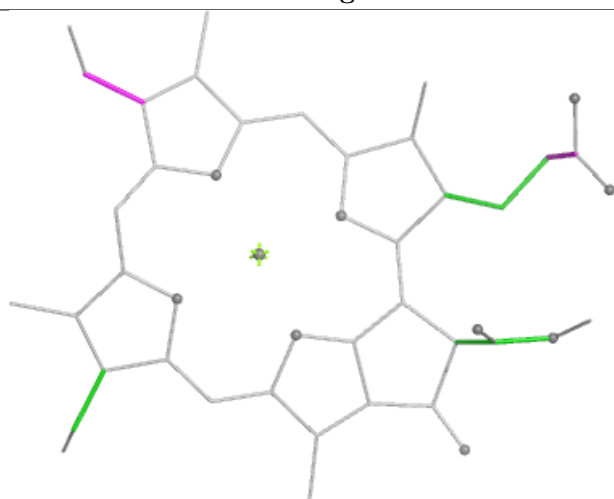
## Ligand A1JWG CJ 503



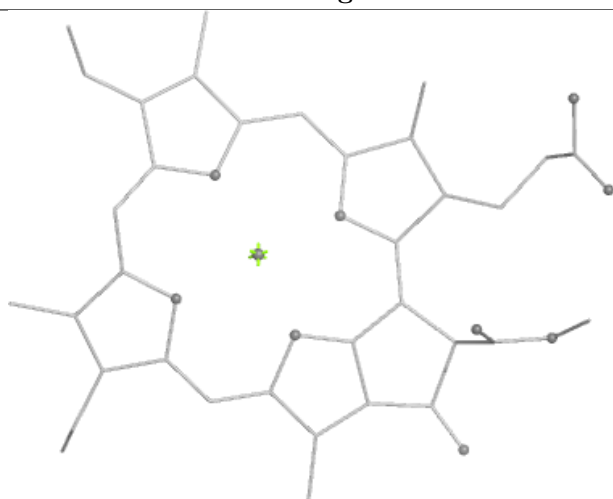
Bond lengths



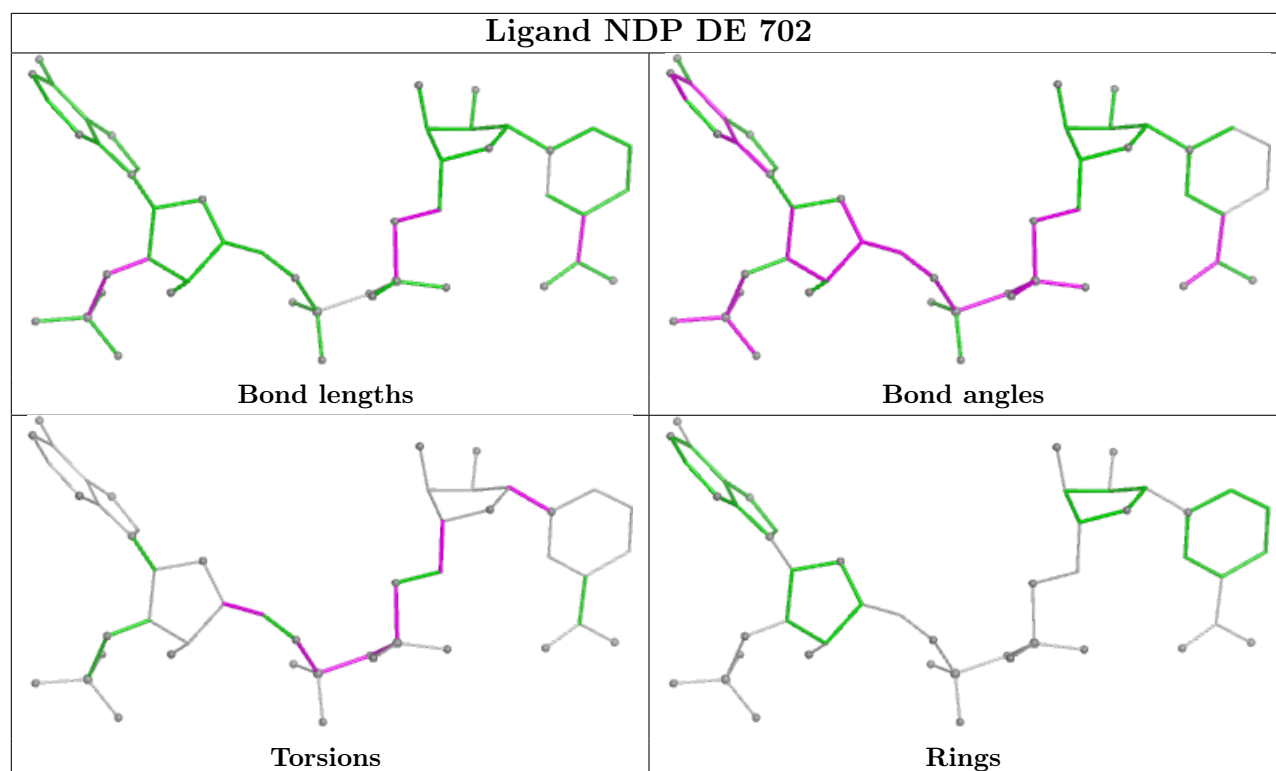
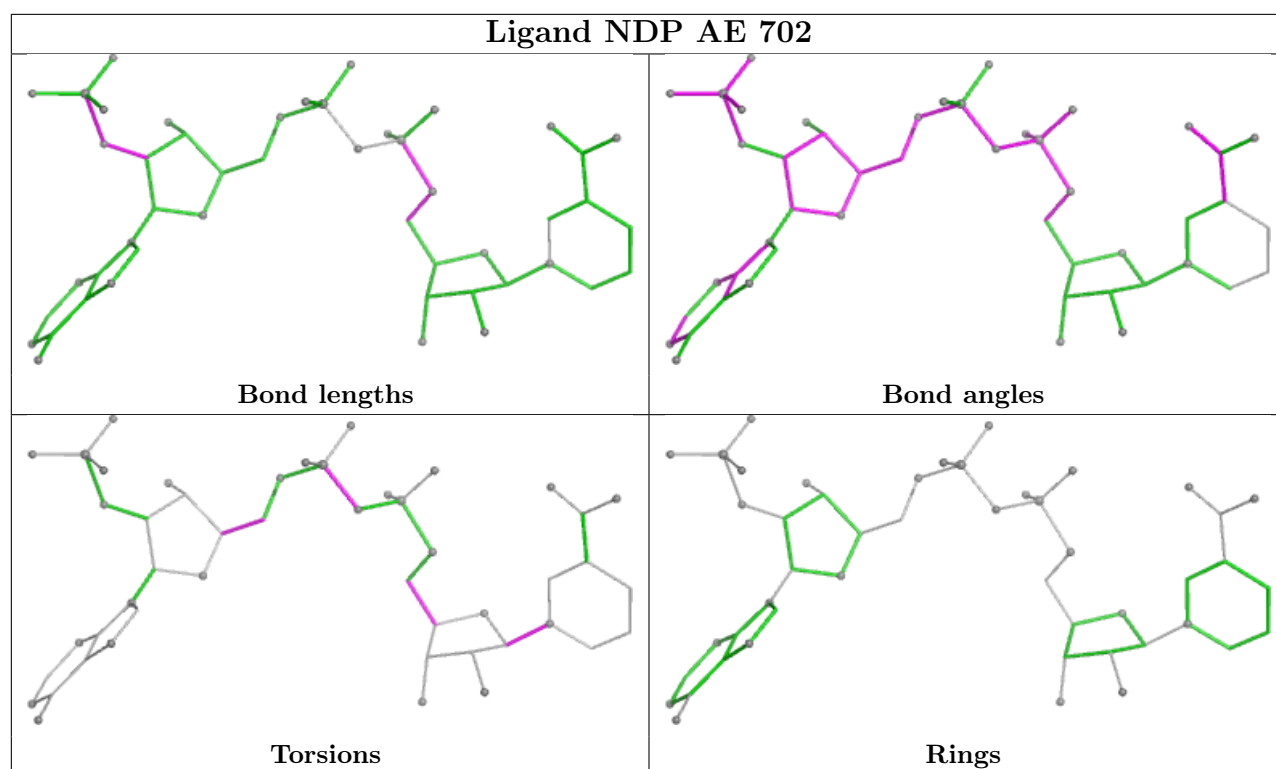
Bond angles

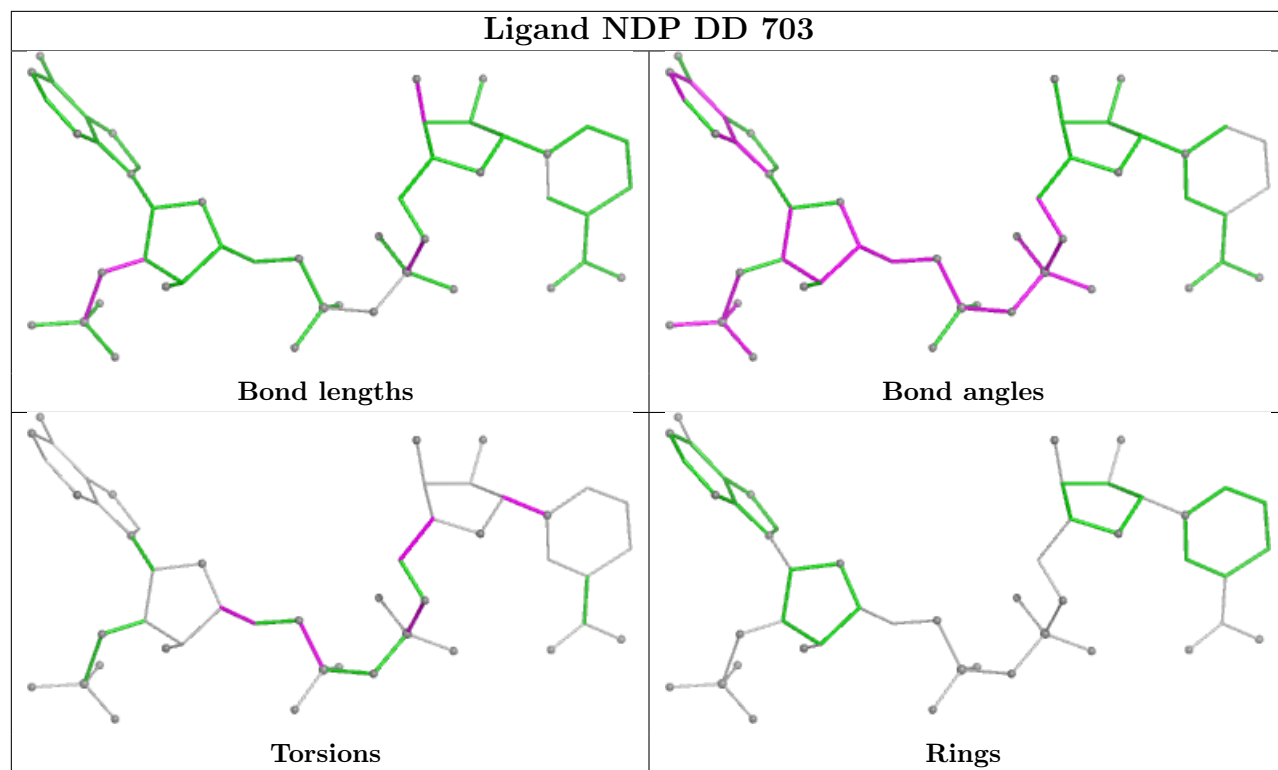


Torsions

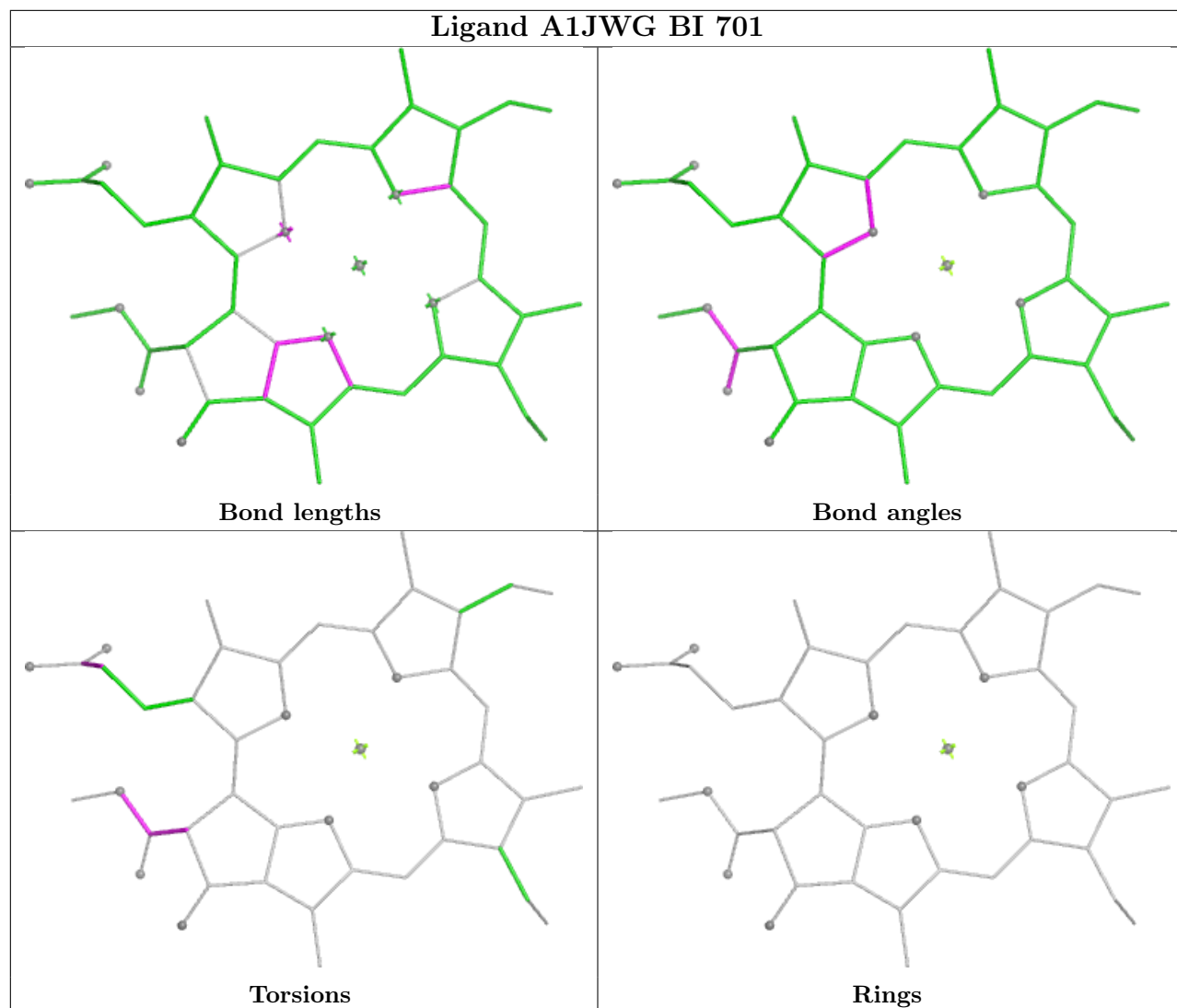


Rings

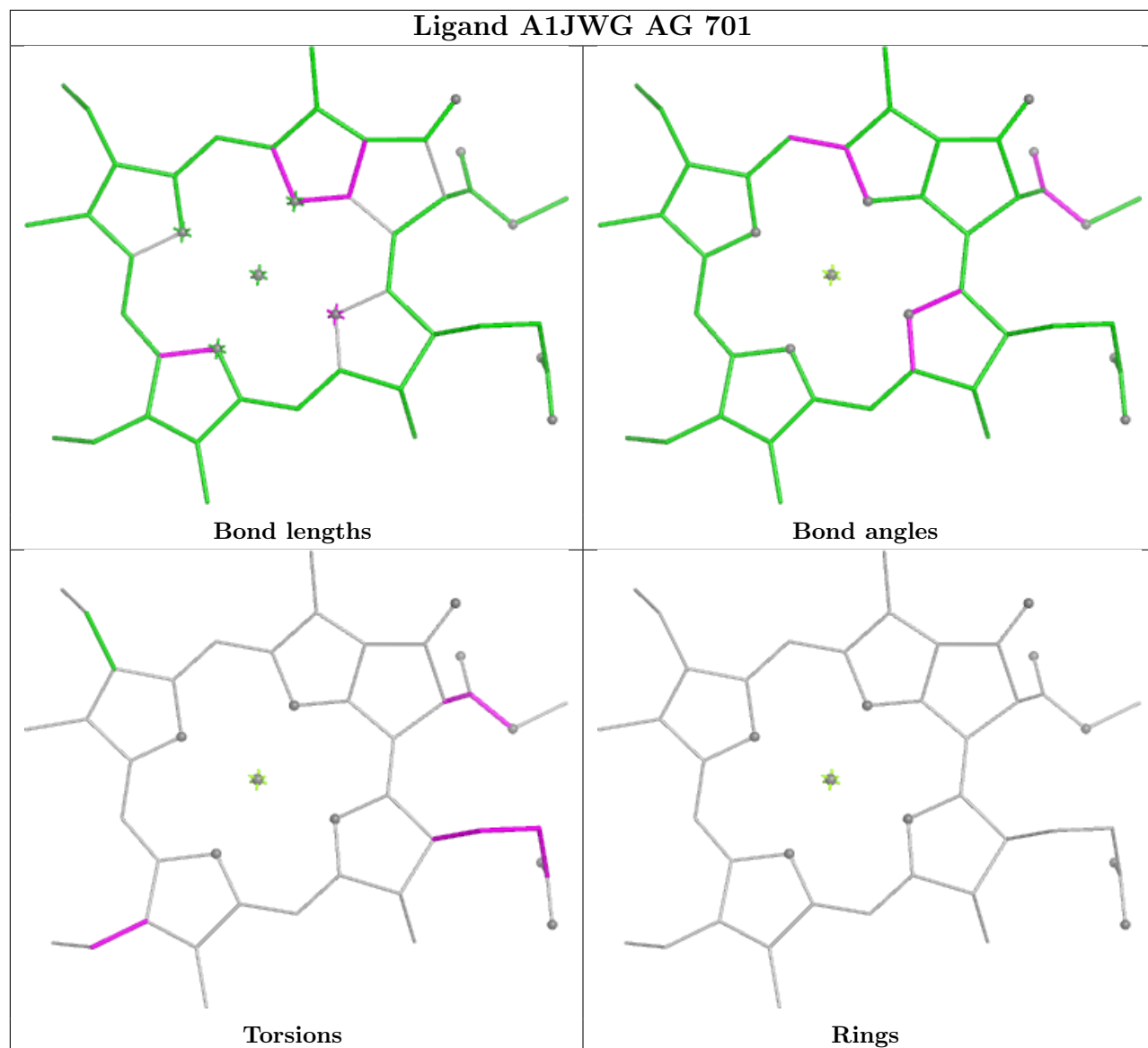




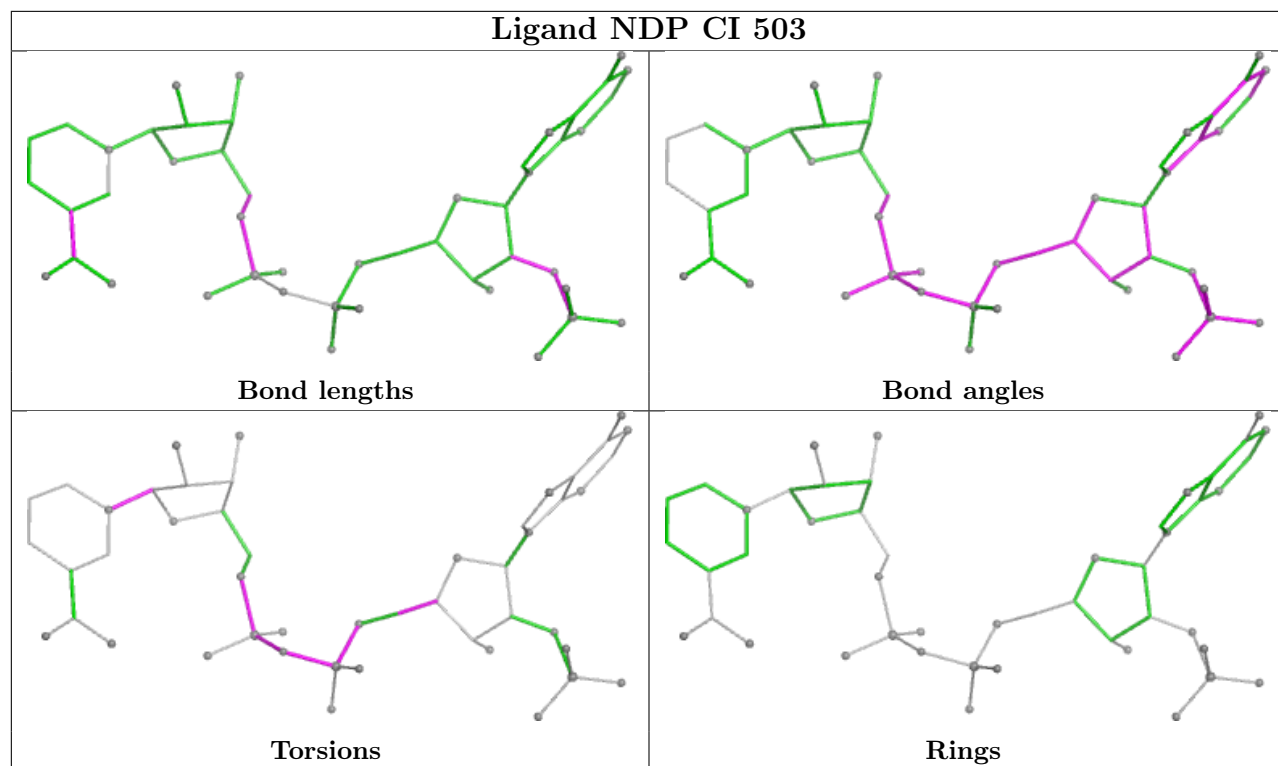
## Ligand A1JWG BI 701



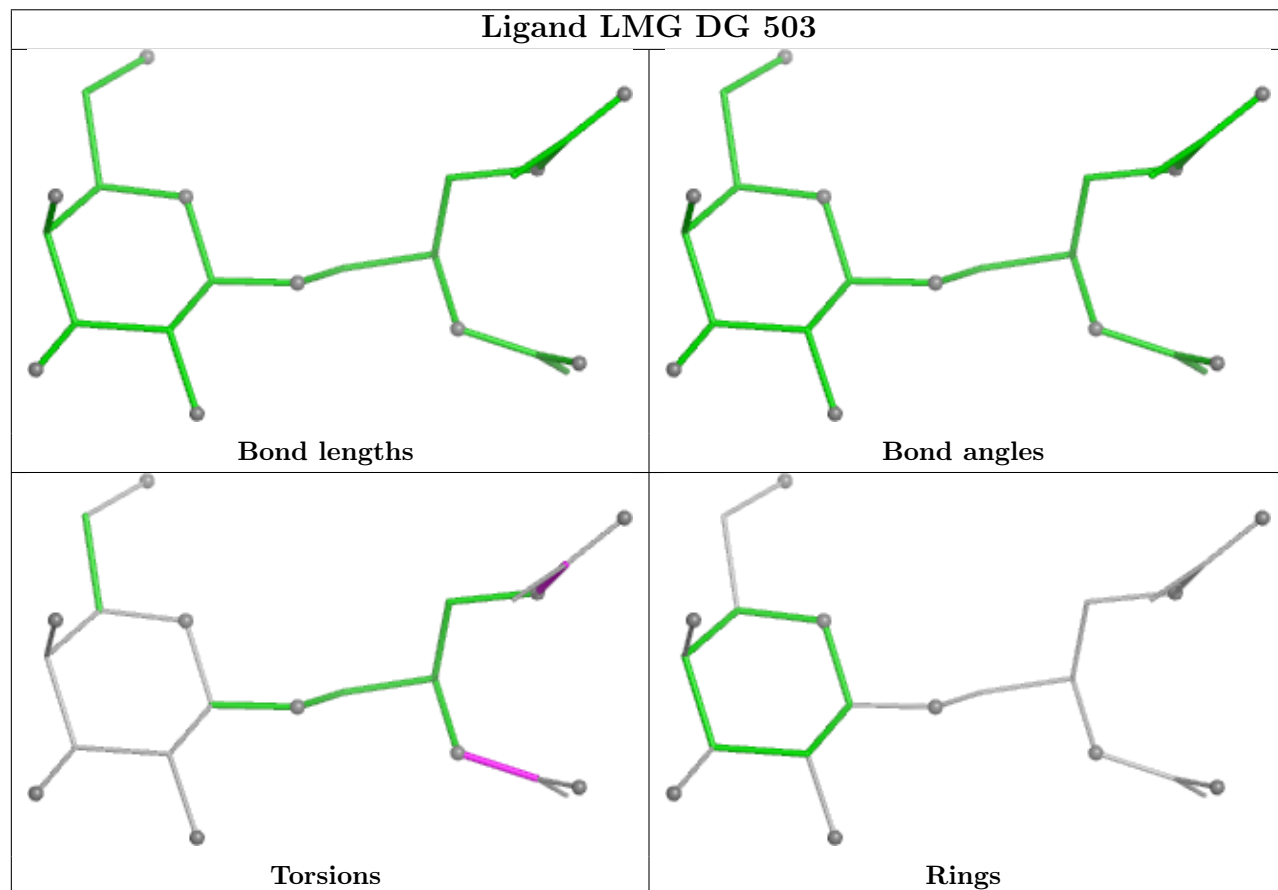
## Ligand A1JWG AG 701



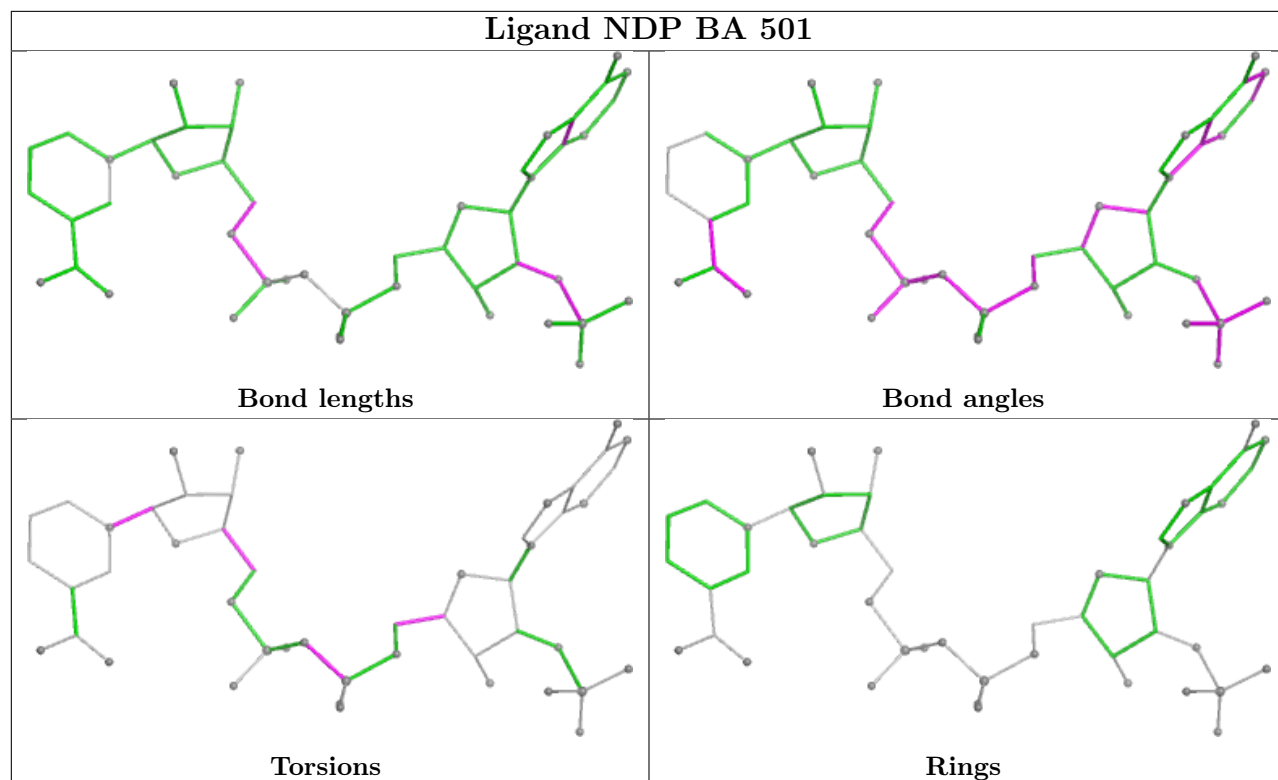
## Ligand NDP CI 503



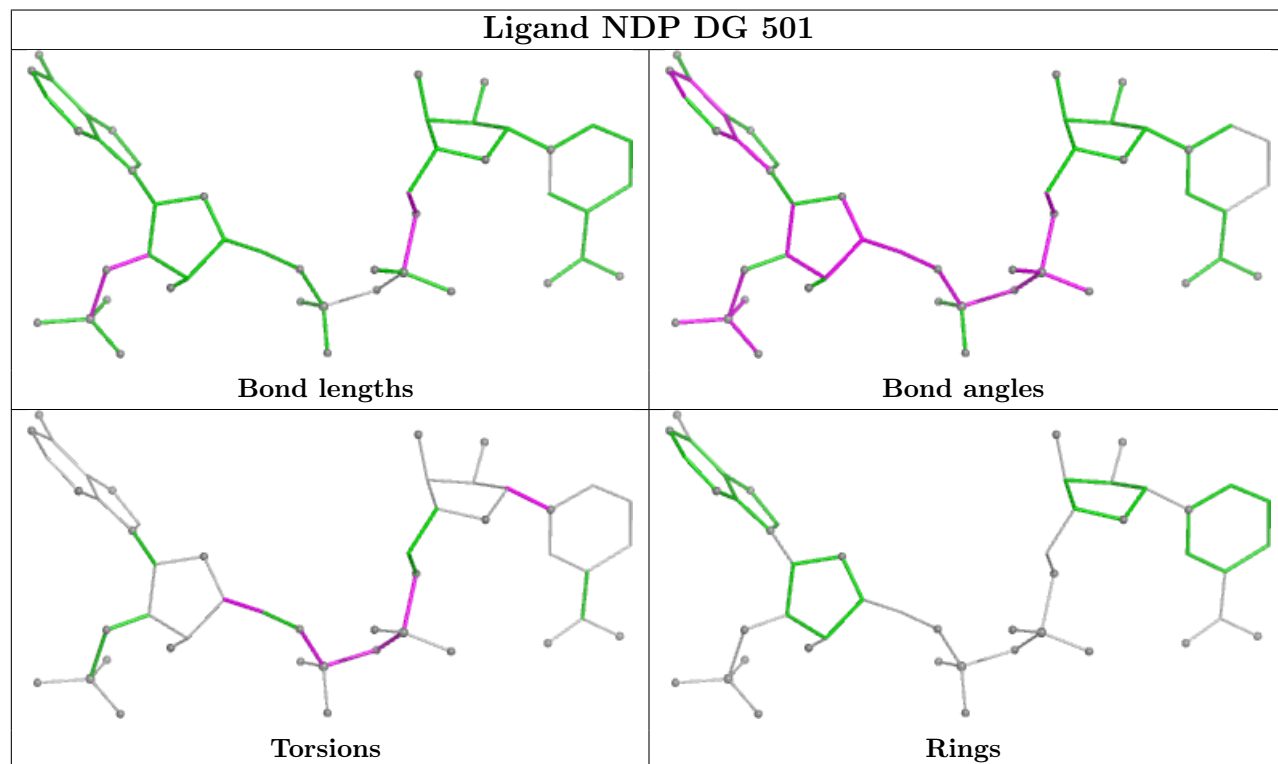
## Ligand LMG DG 503



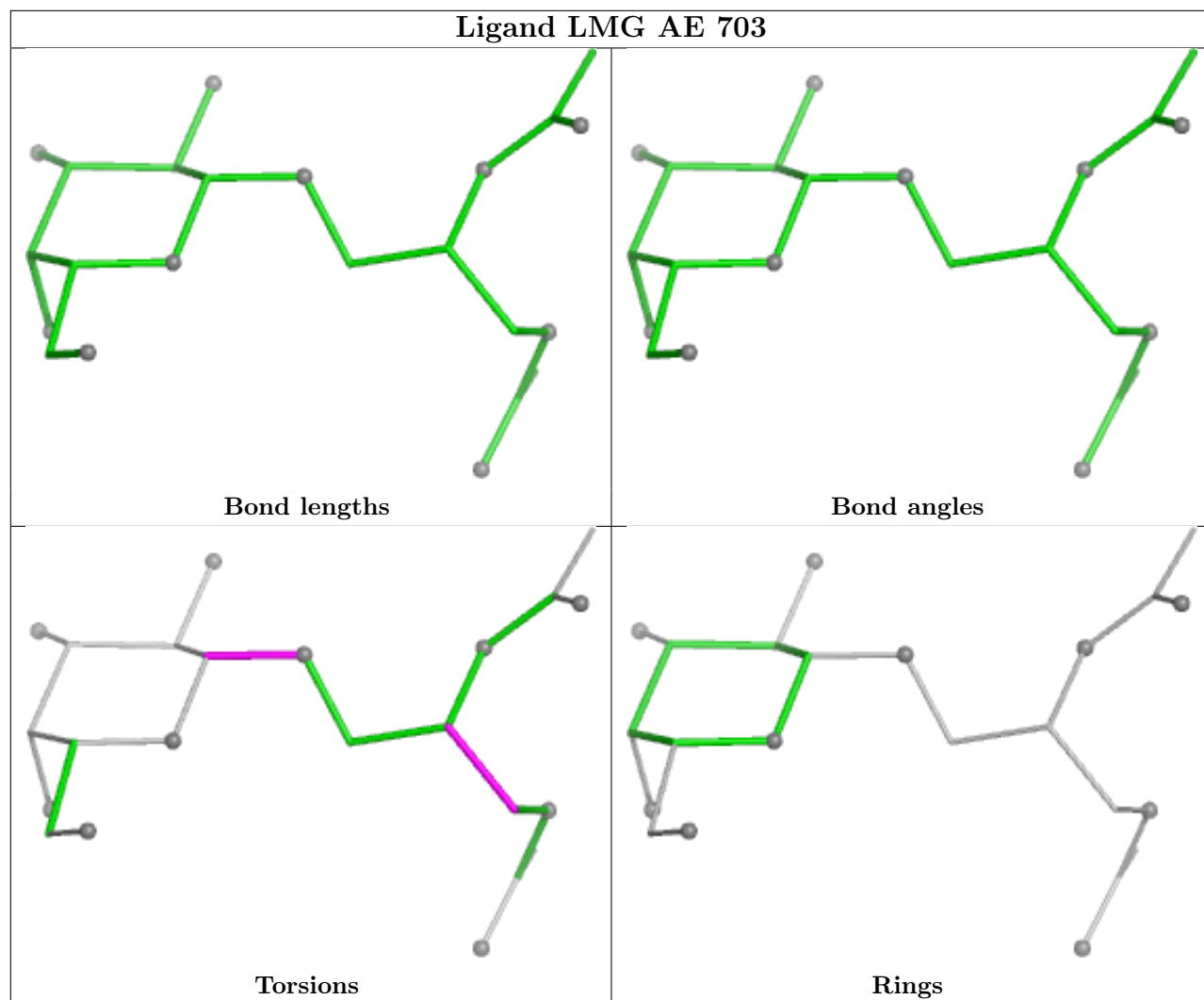
## Ligand NDP BA 501



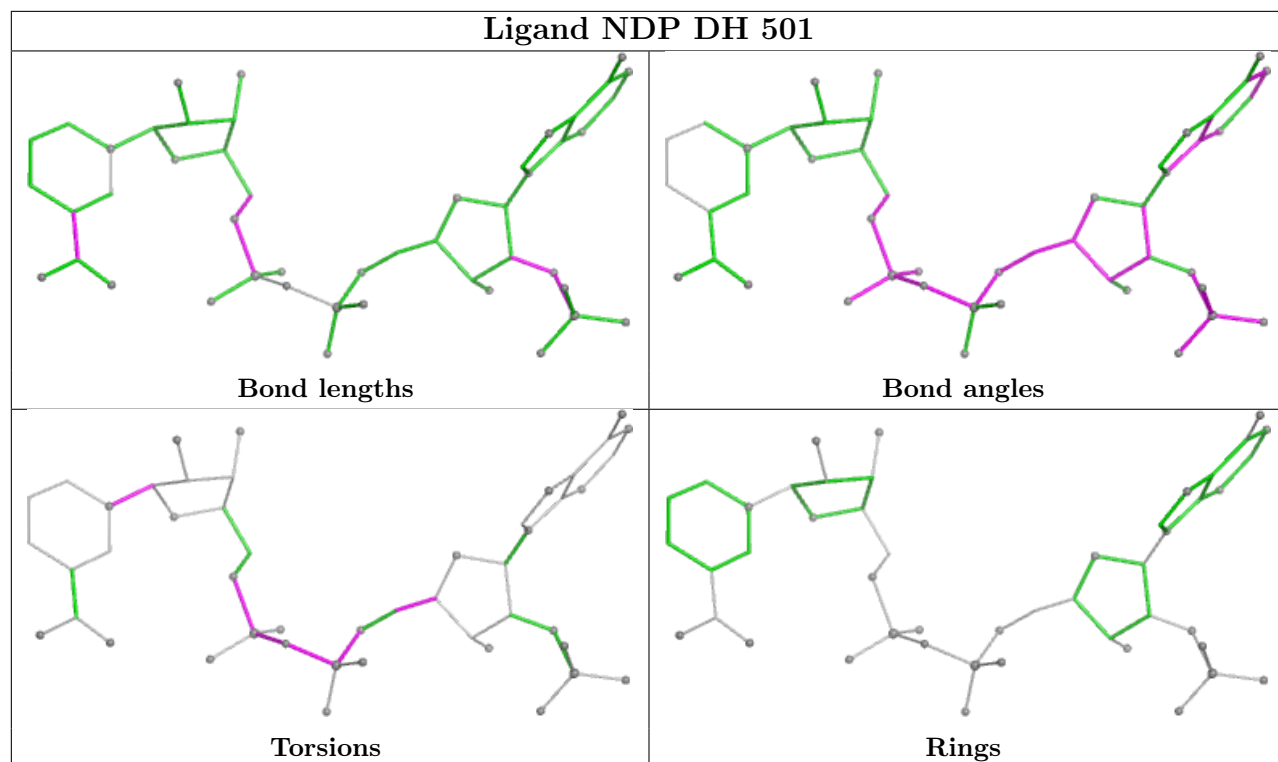
## Ligand NDP DG 501



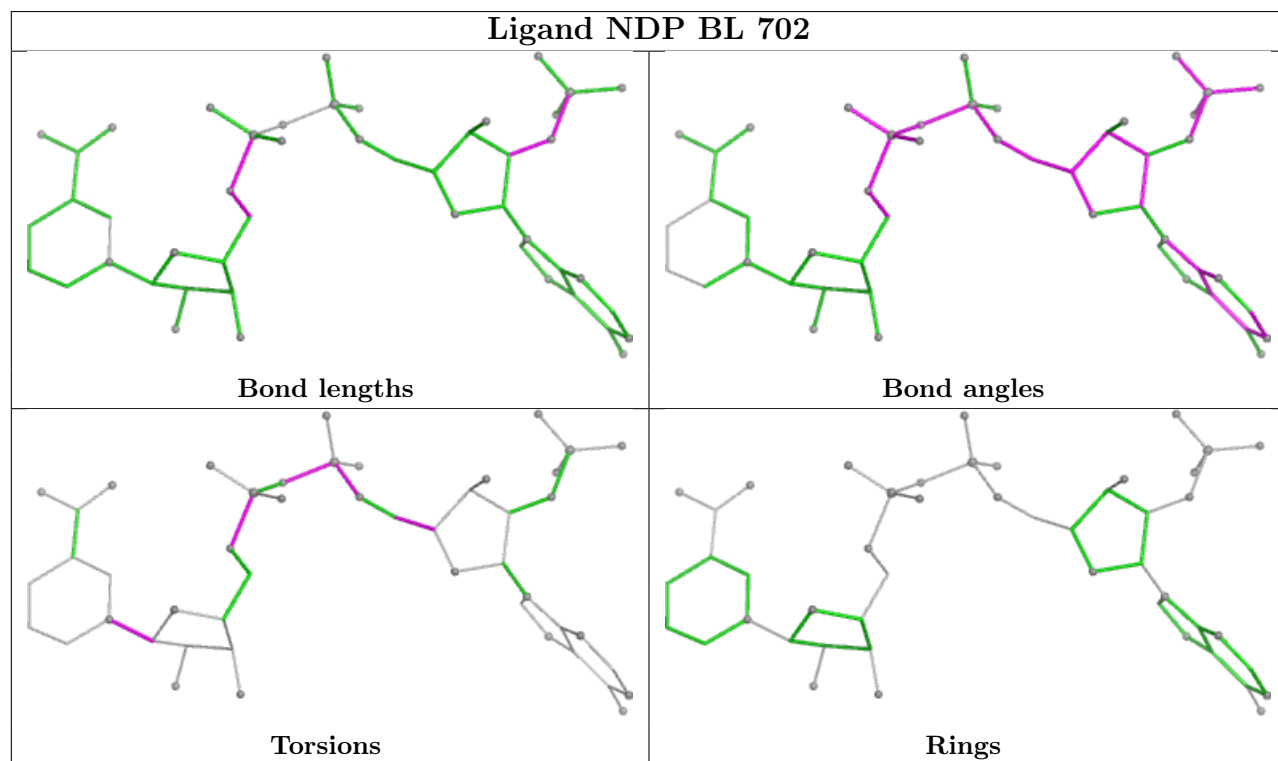
## Ligand LMG AE 703



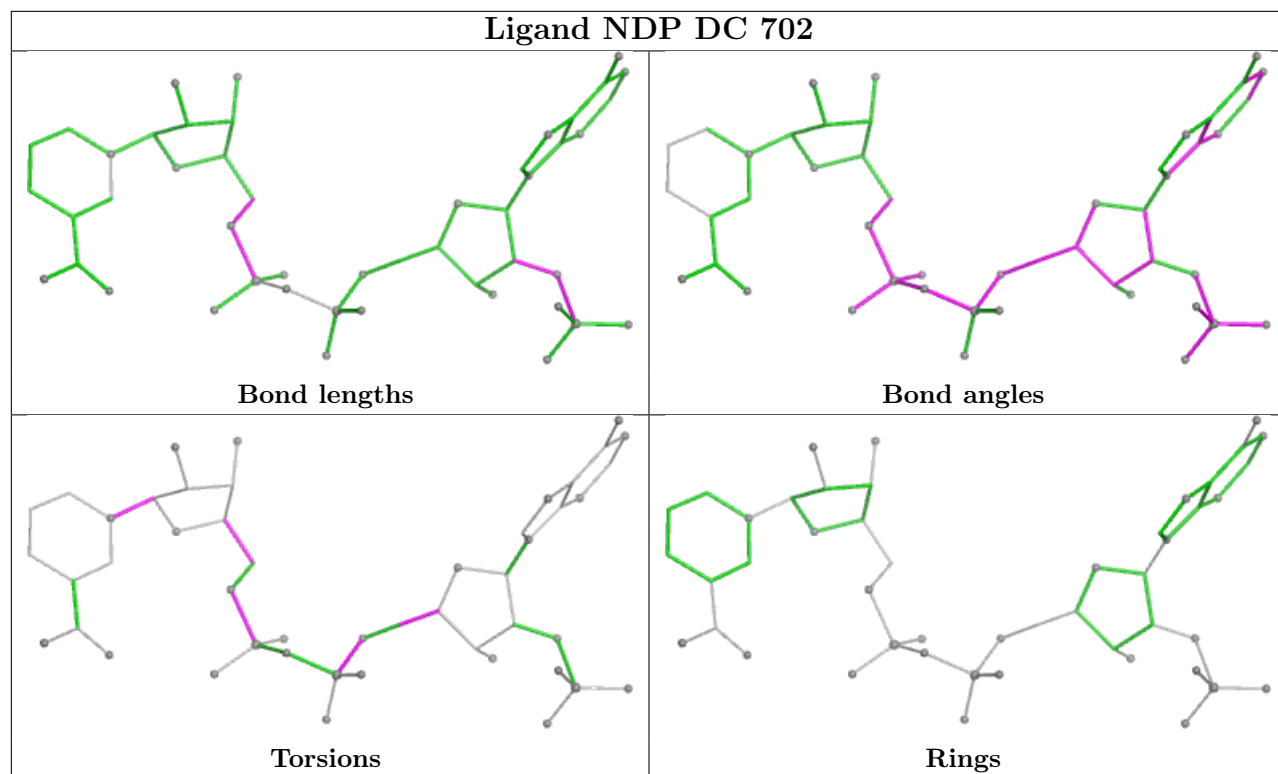
## Ligand NDP DH 501



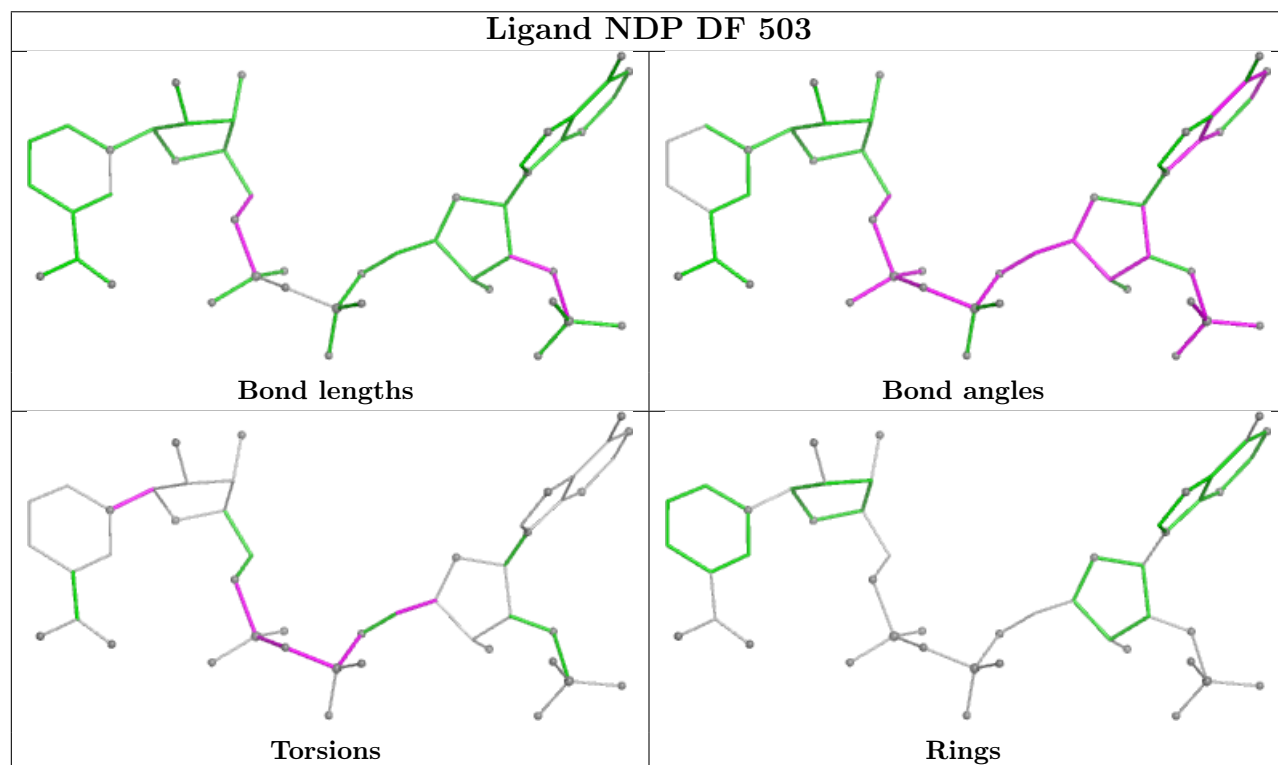
## Ligand NDP BL 702



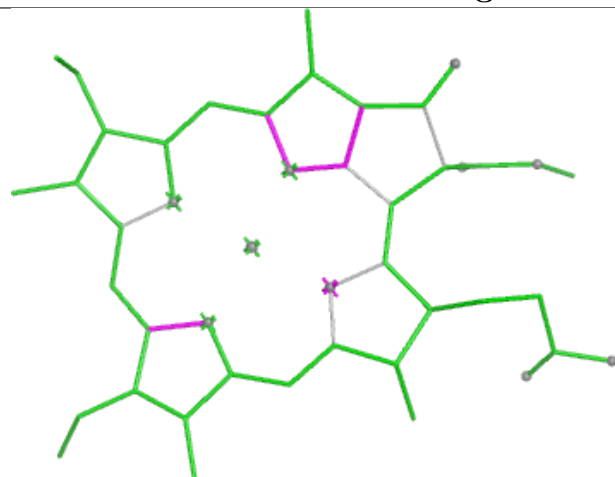
## Ligand NDP DC 702



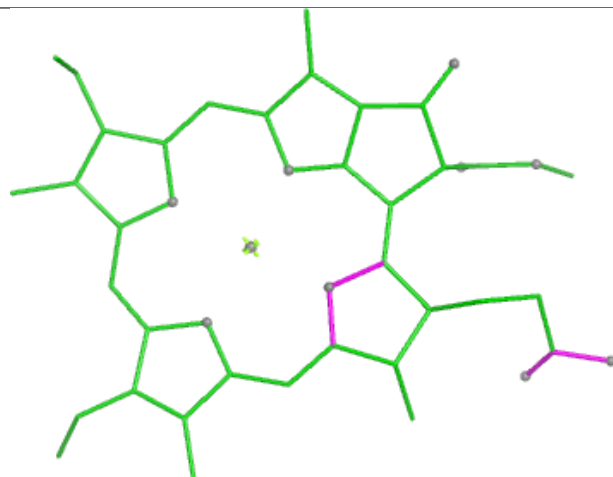
## Ligand NDP DF 503



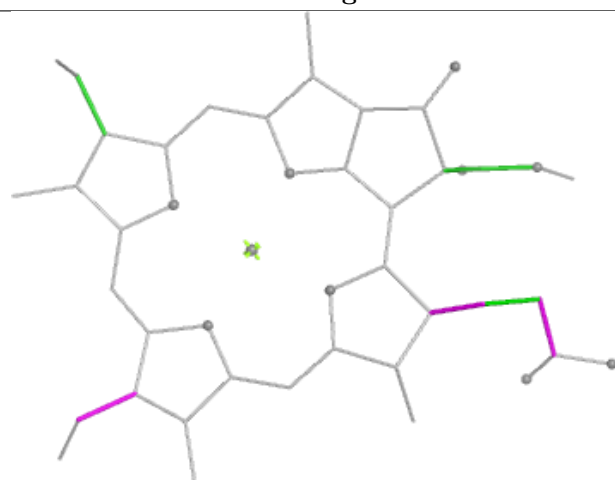
## Ligand A1JWG CK 502



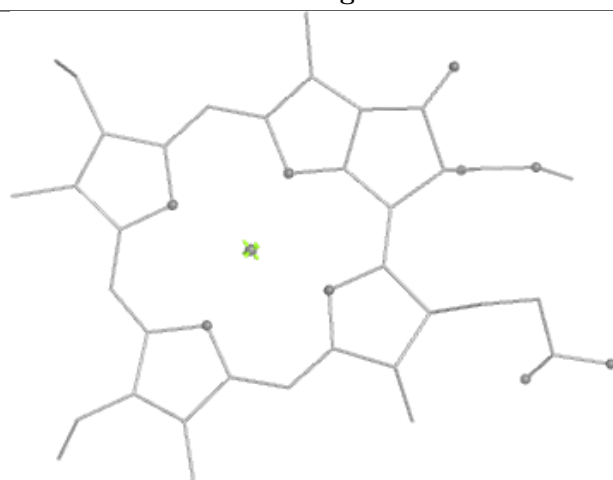
Bond lengths



Bond angles

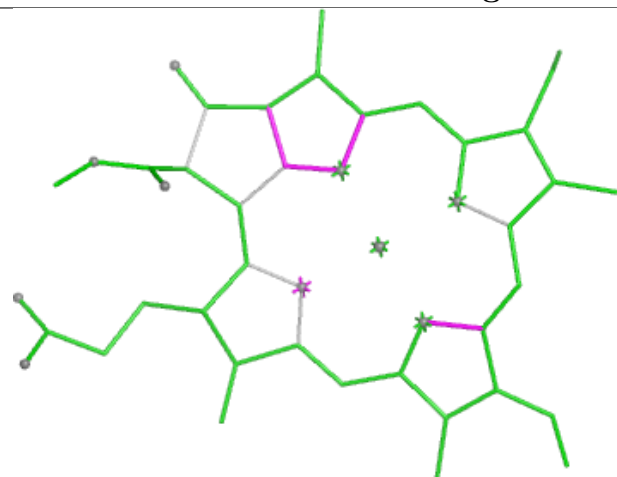


Torsions

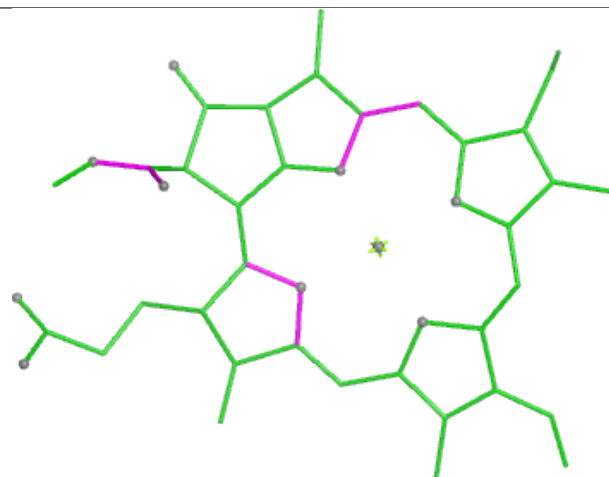


Rings

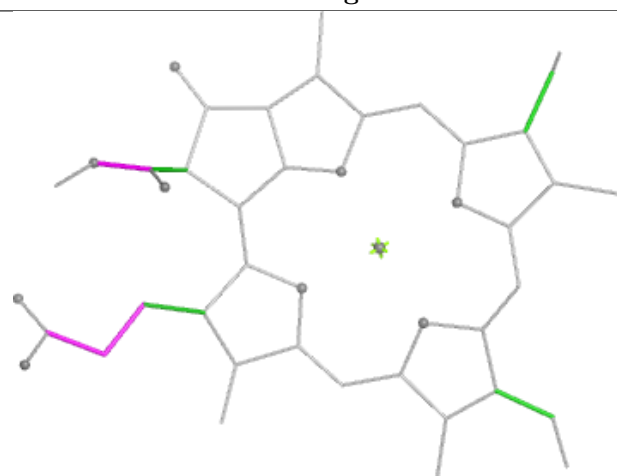
## Ligand A1JWG BJ 502



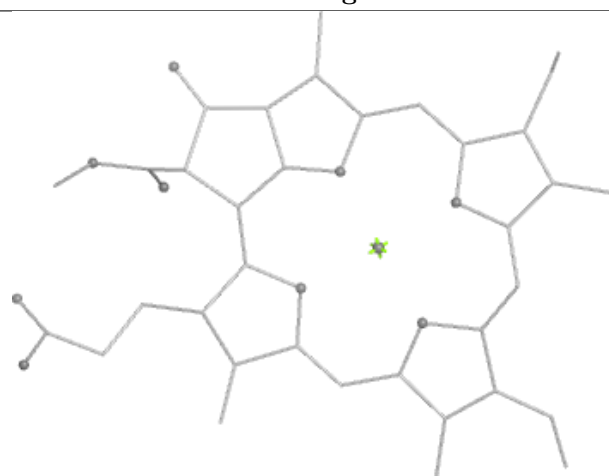
Bond lengths



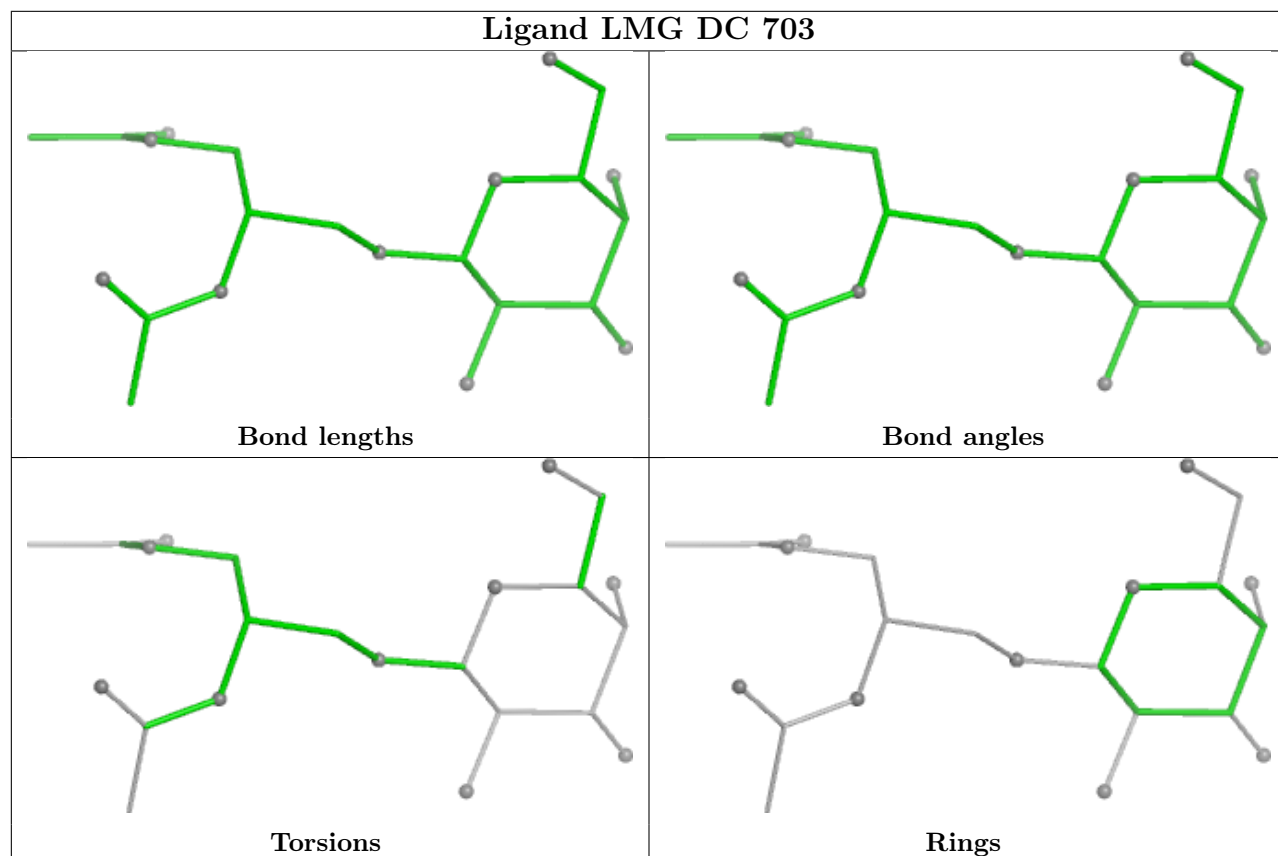
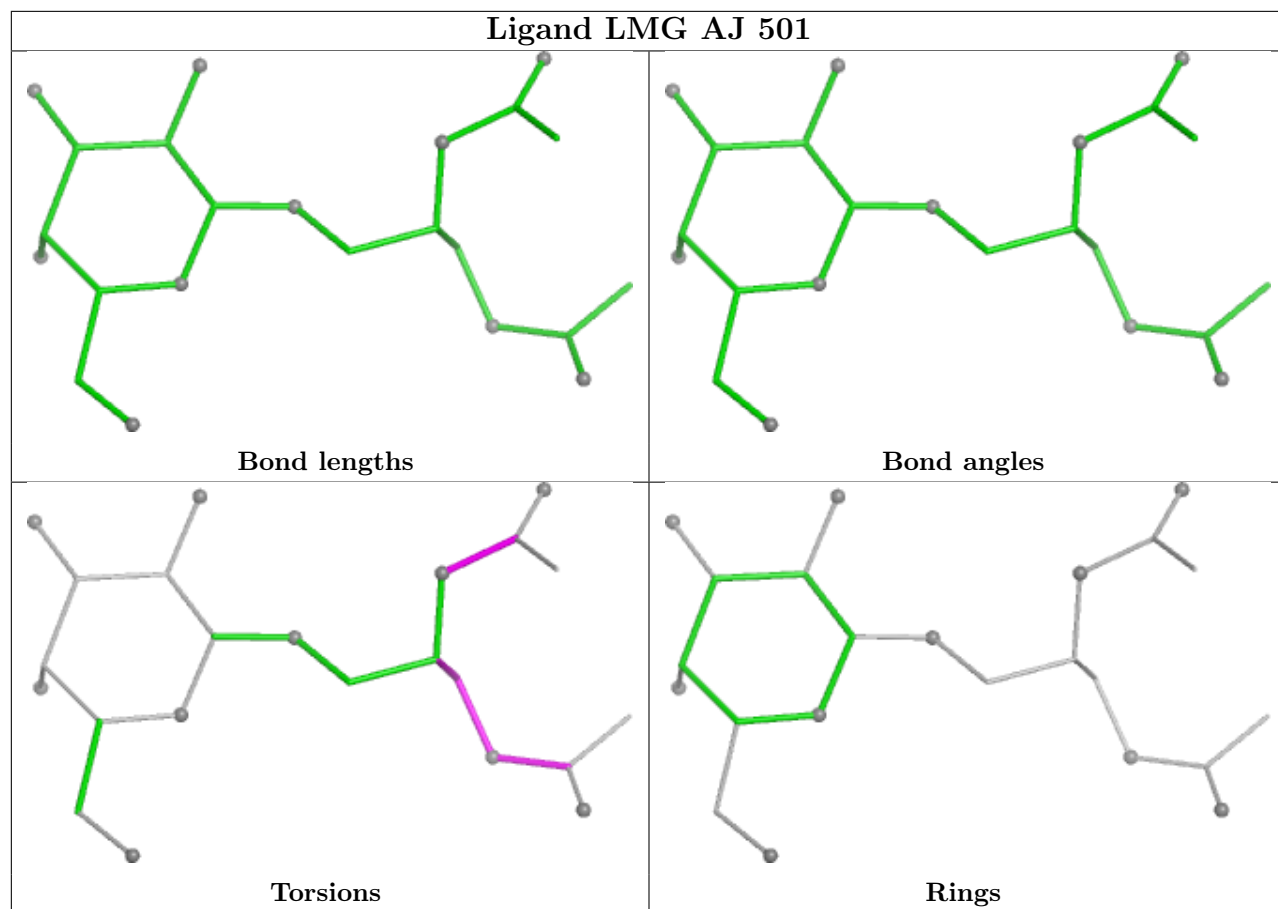
Bond angles



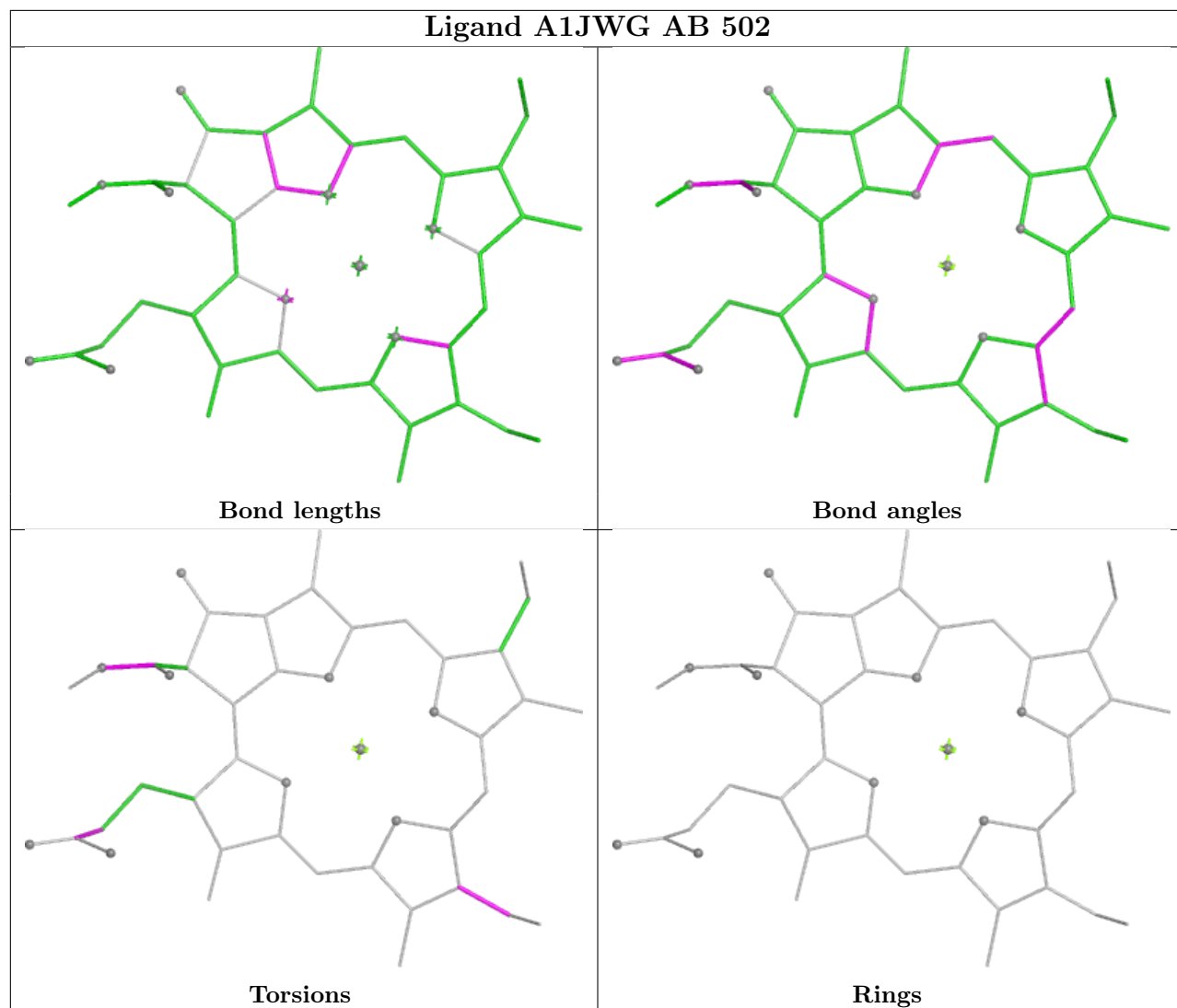
Torsions



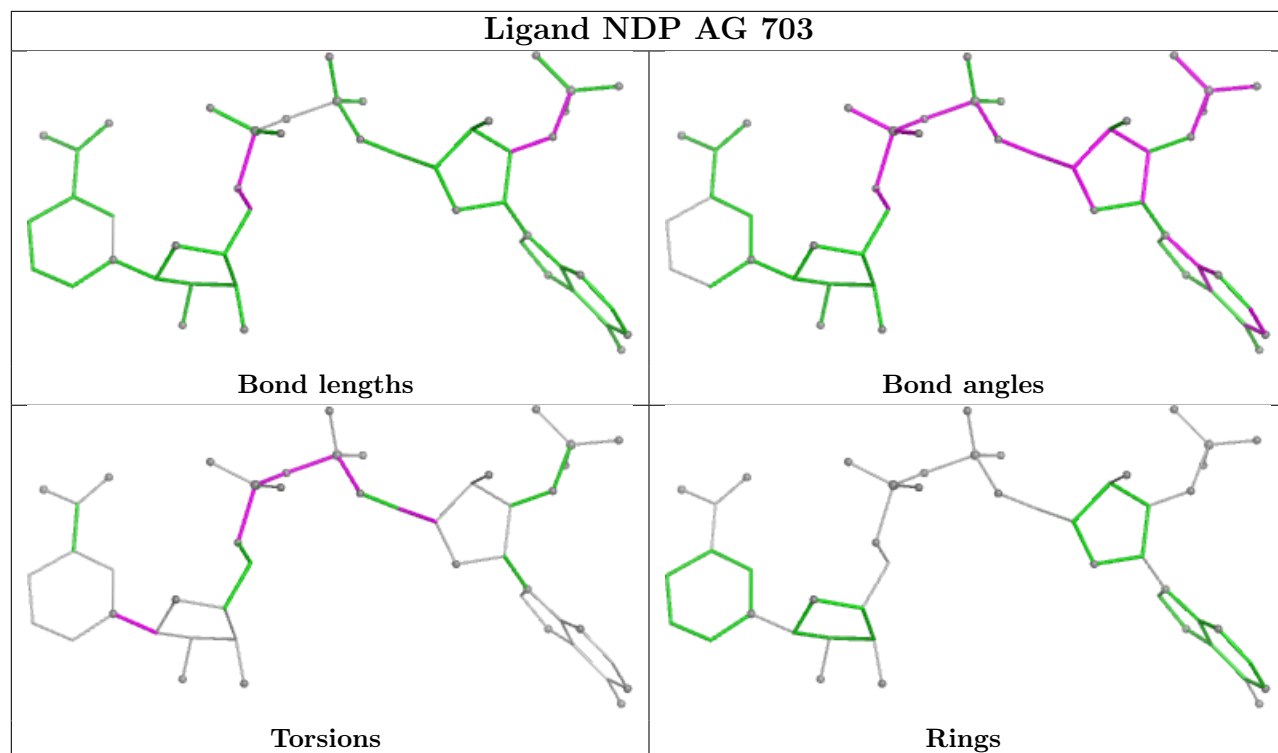
Rings



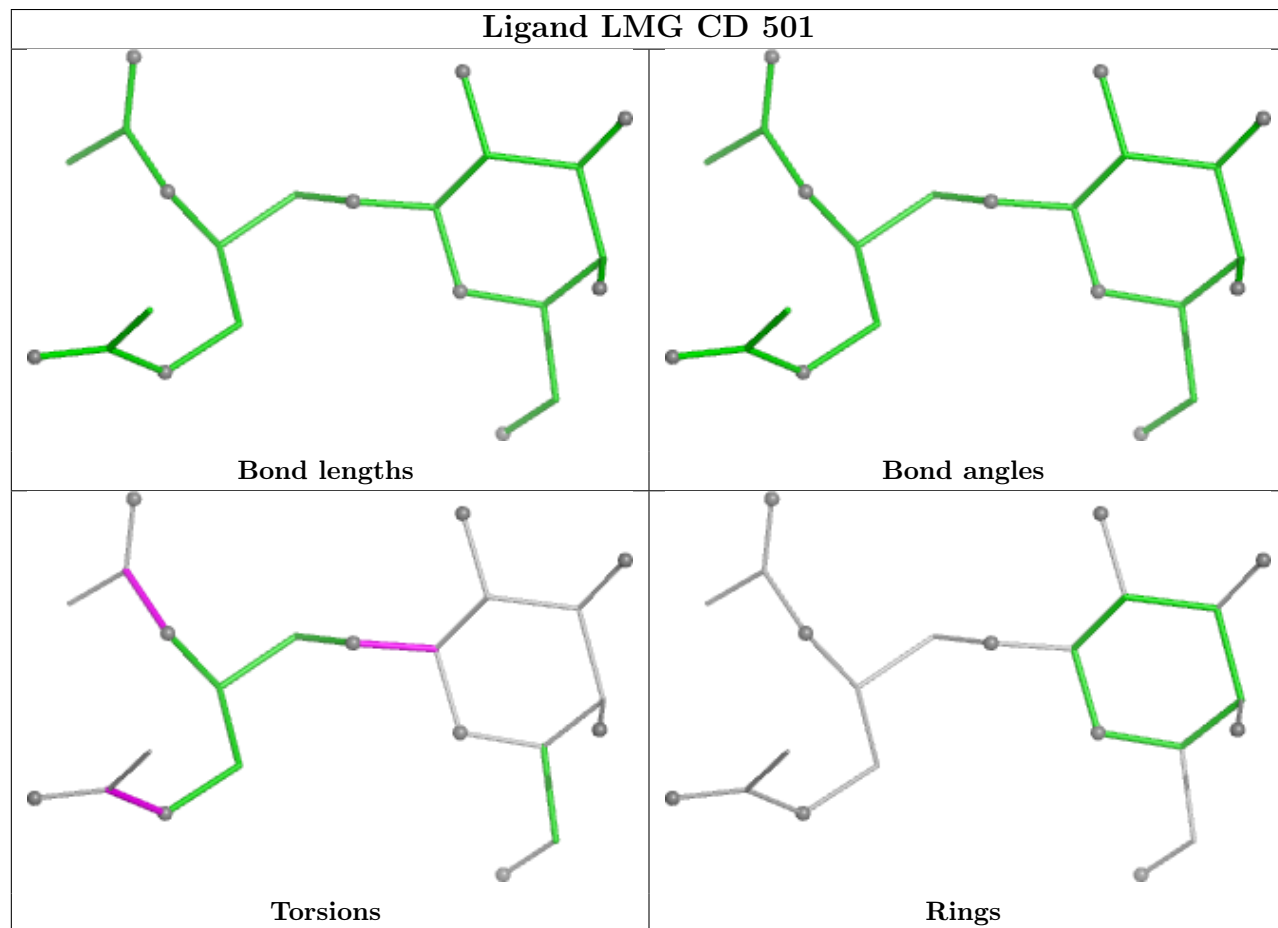
## Ligand A1JWG AB 502

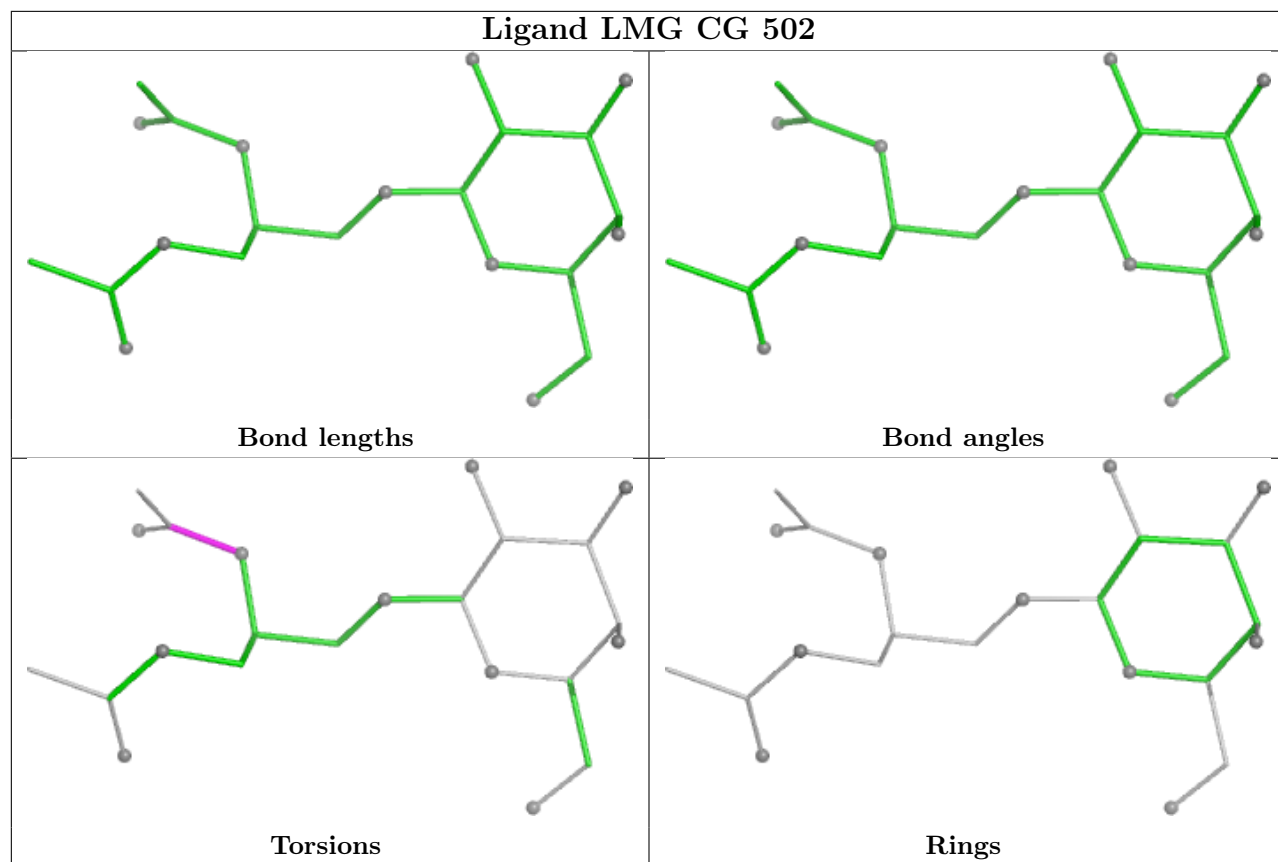


## Ligand NDP AG 703

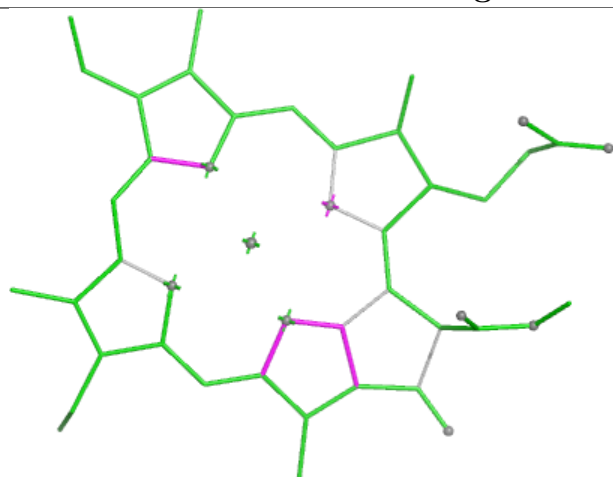


## Ligand LMG CD 501

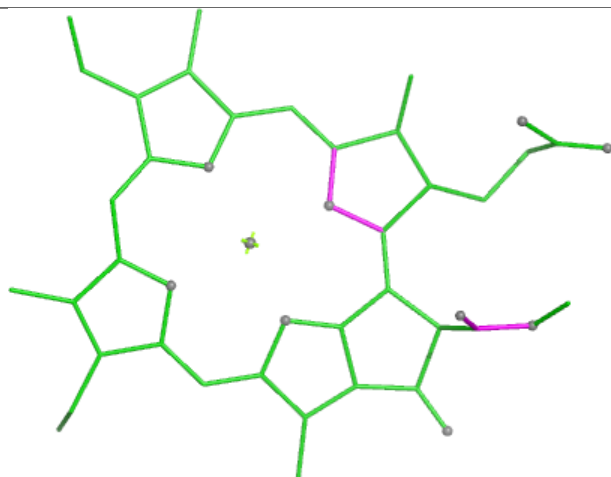




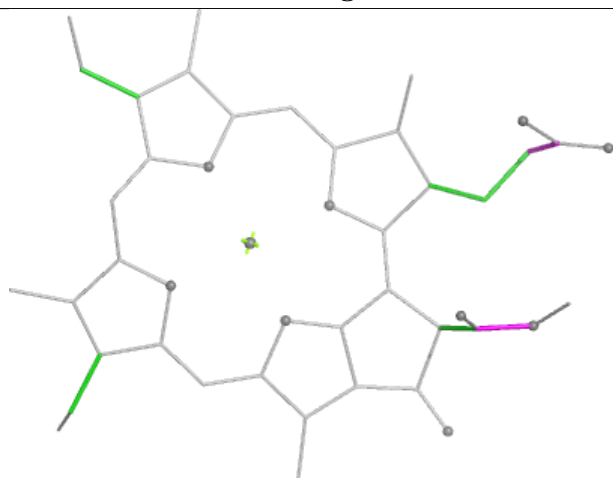
## Ligand A1JWG DB 701



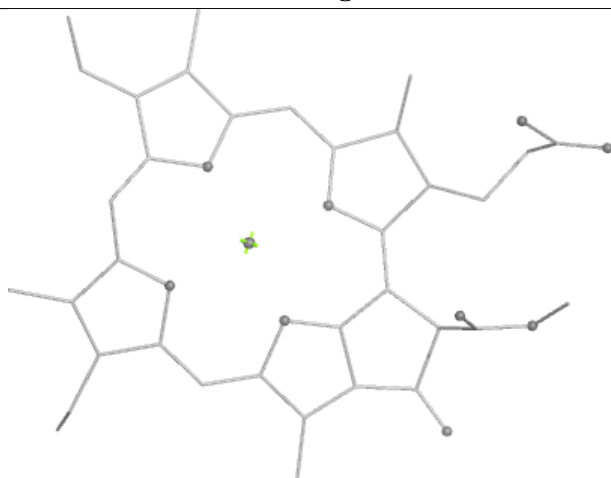
Bond lengths



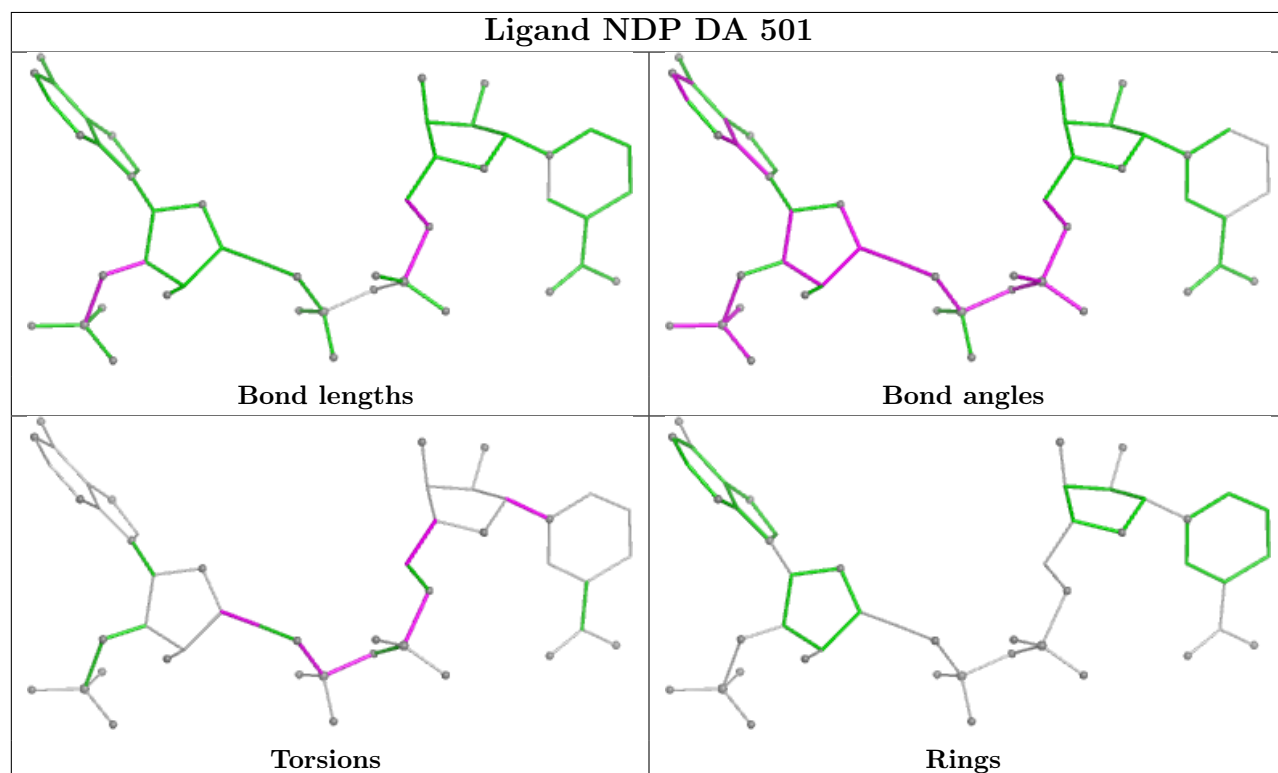
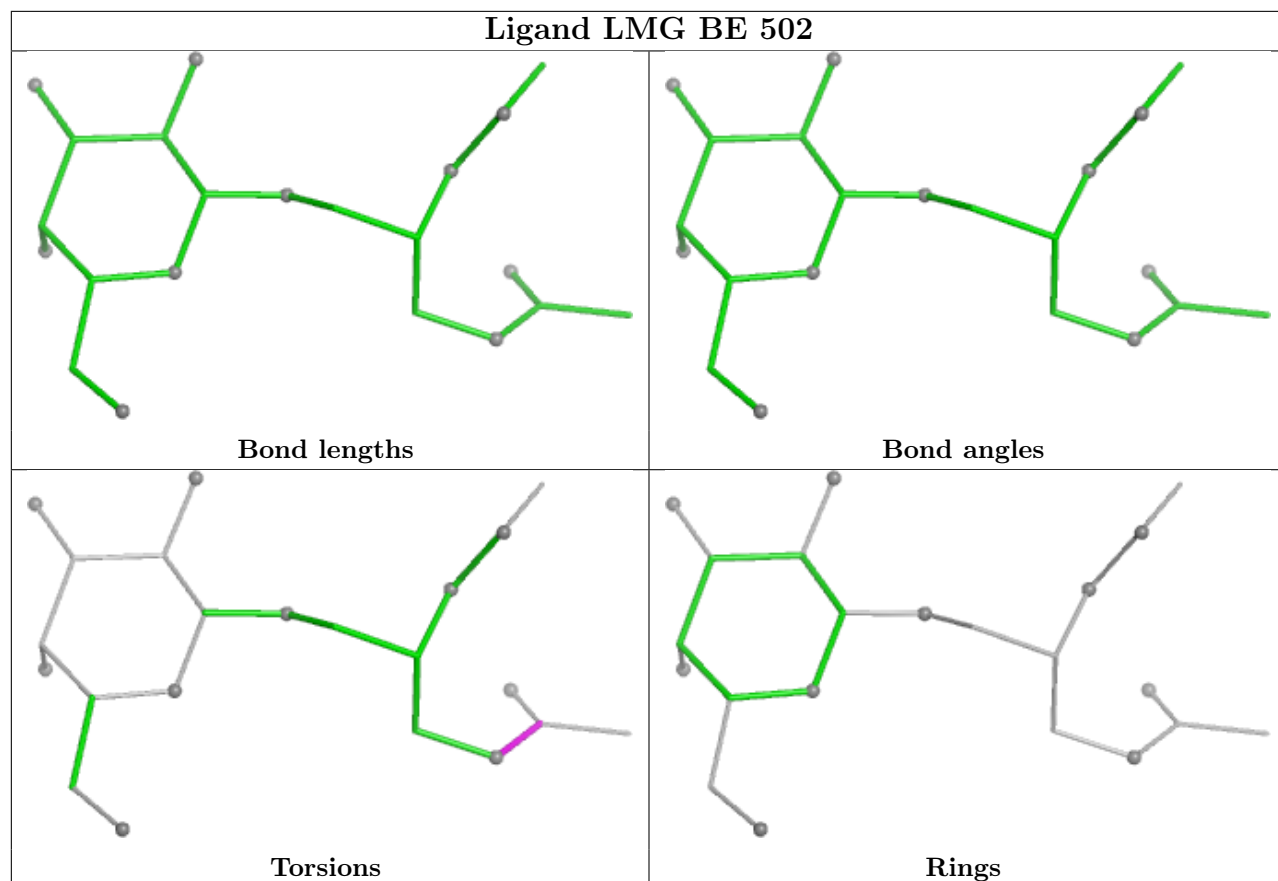
Bond angles

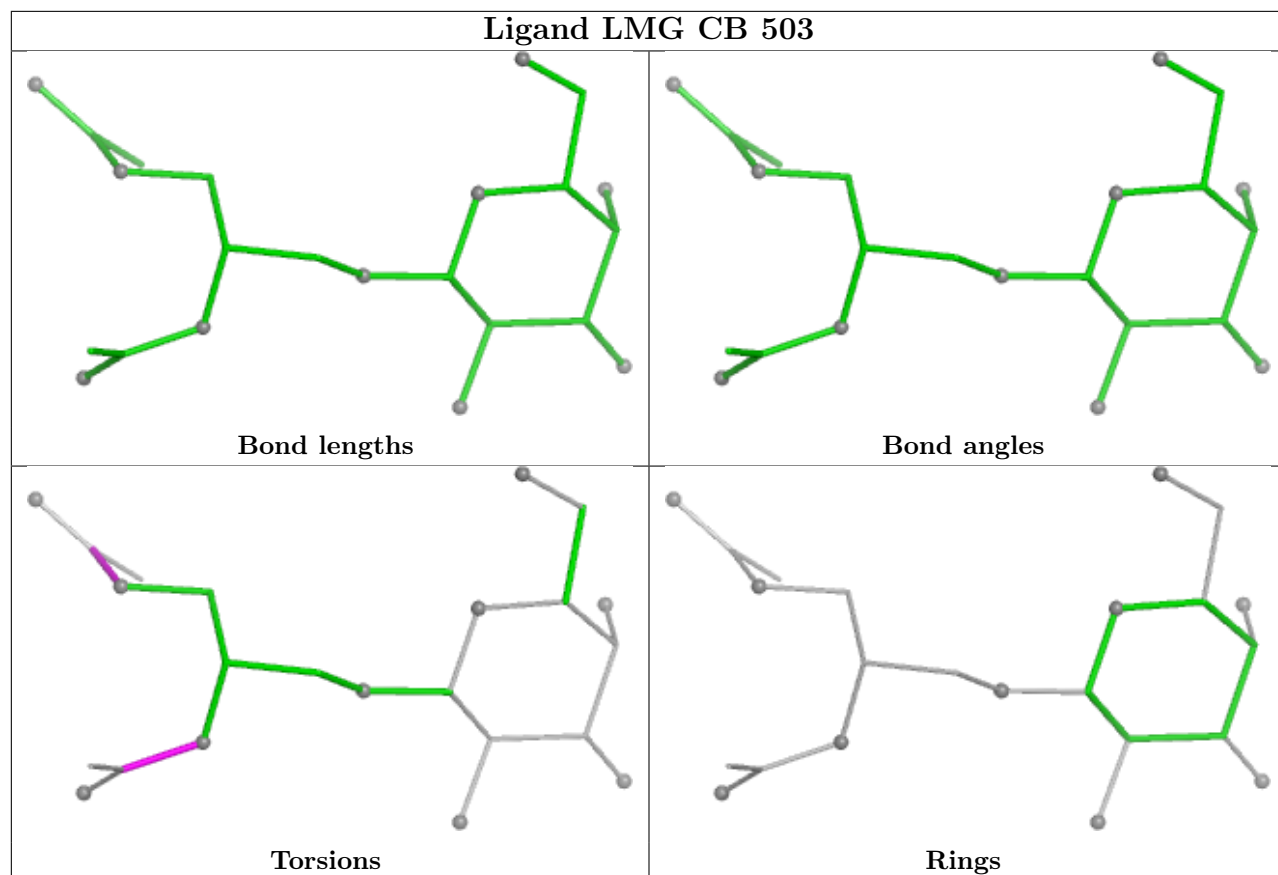


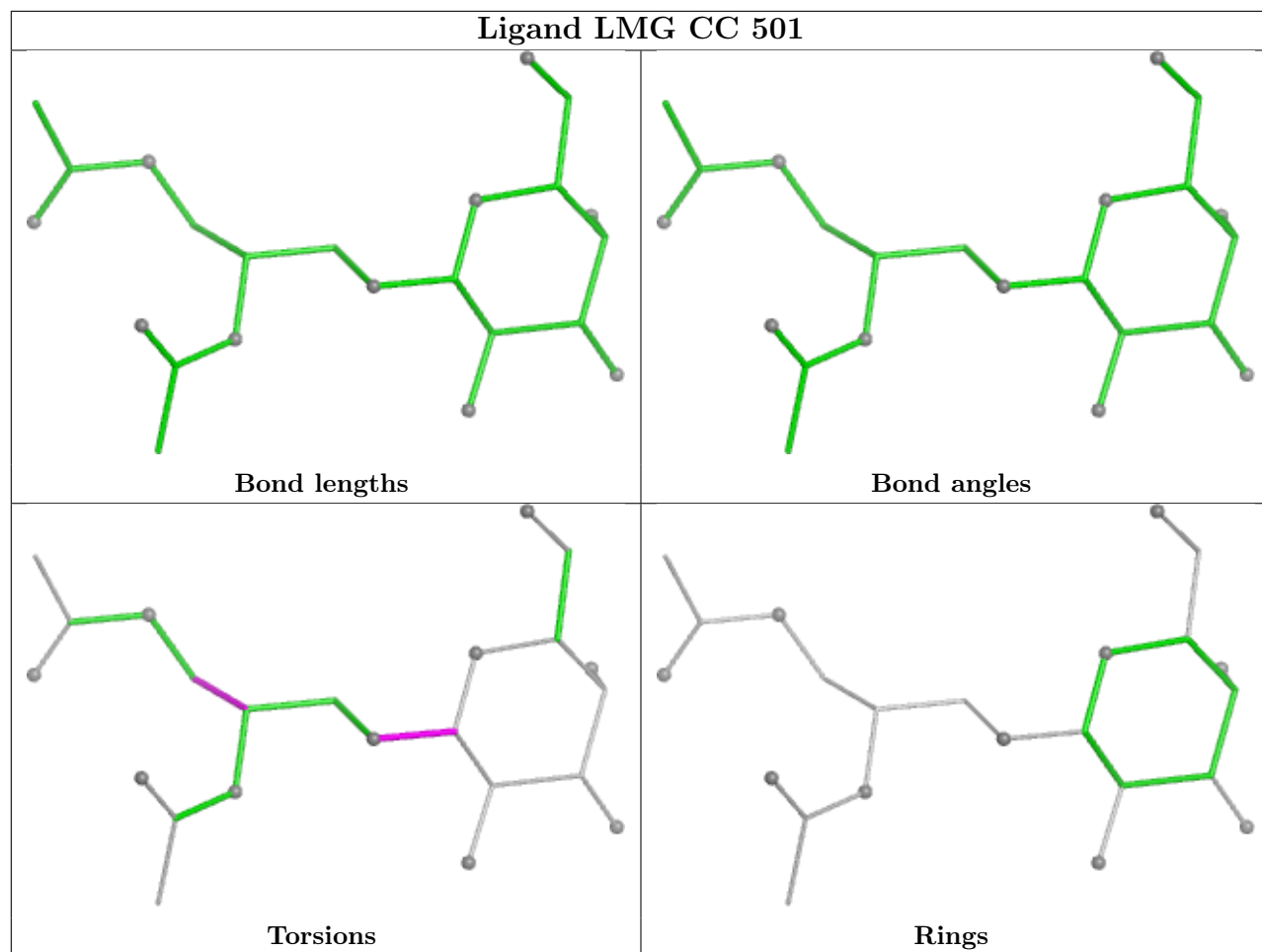
Torsions



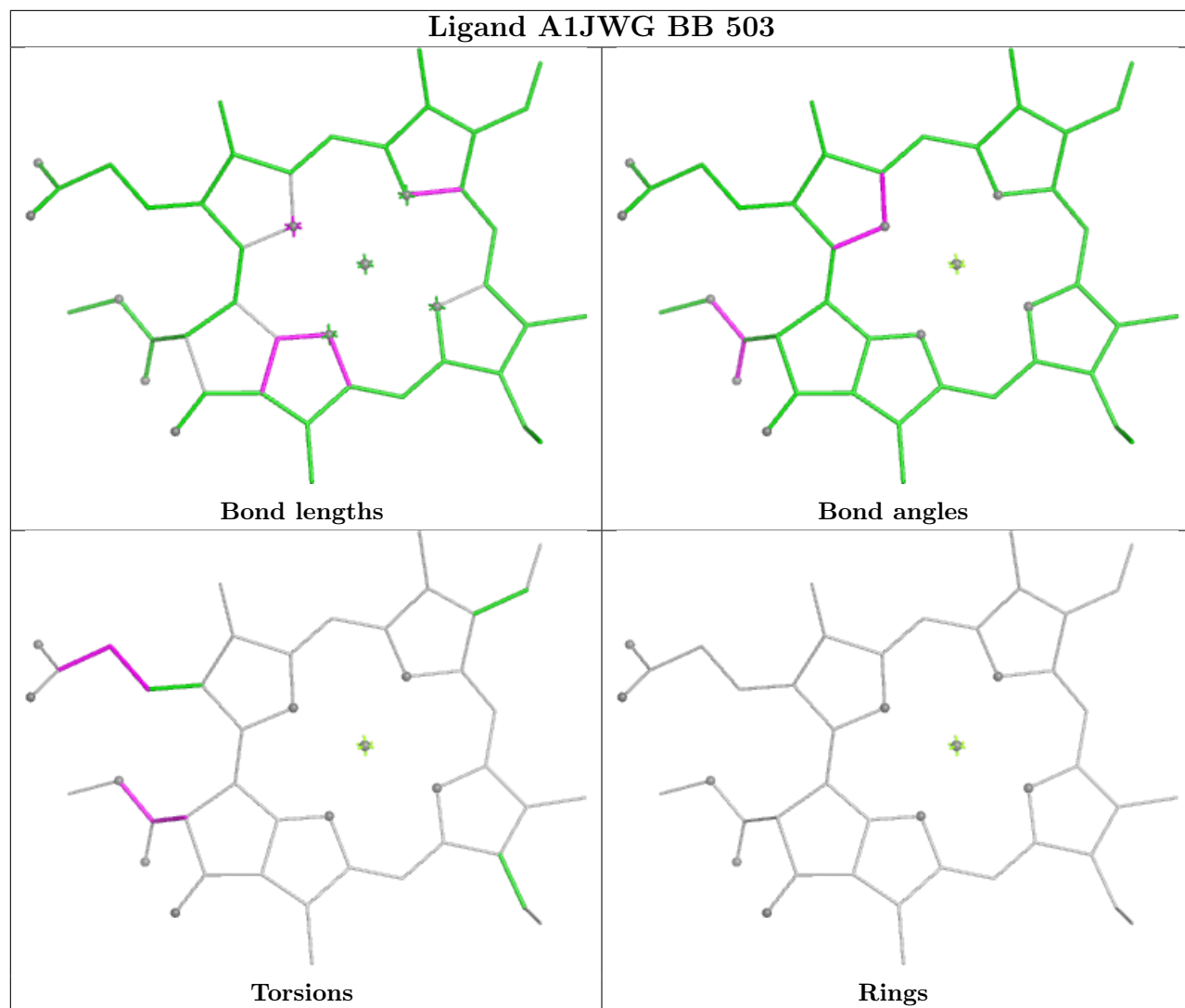
Rings

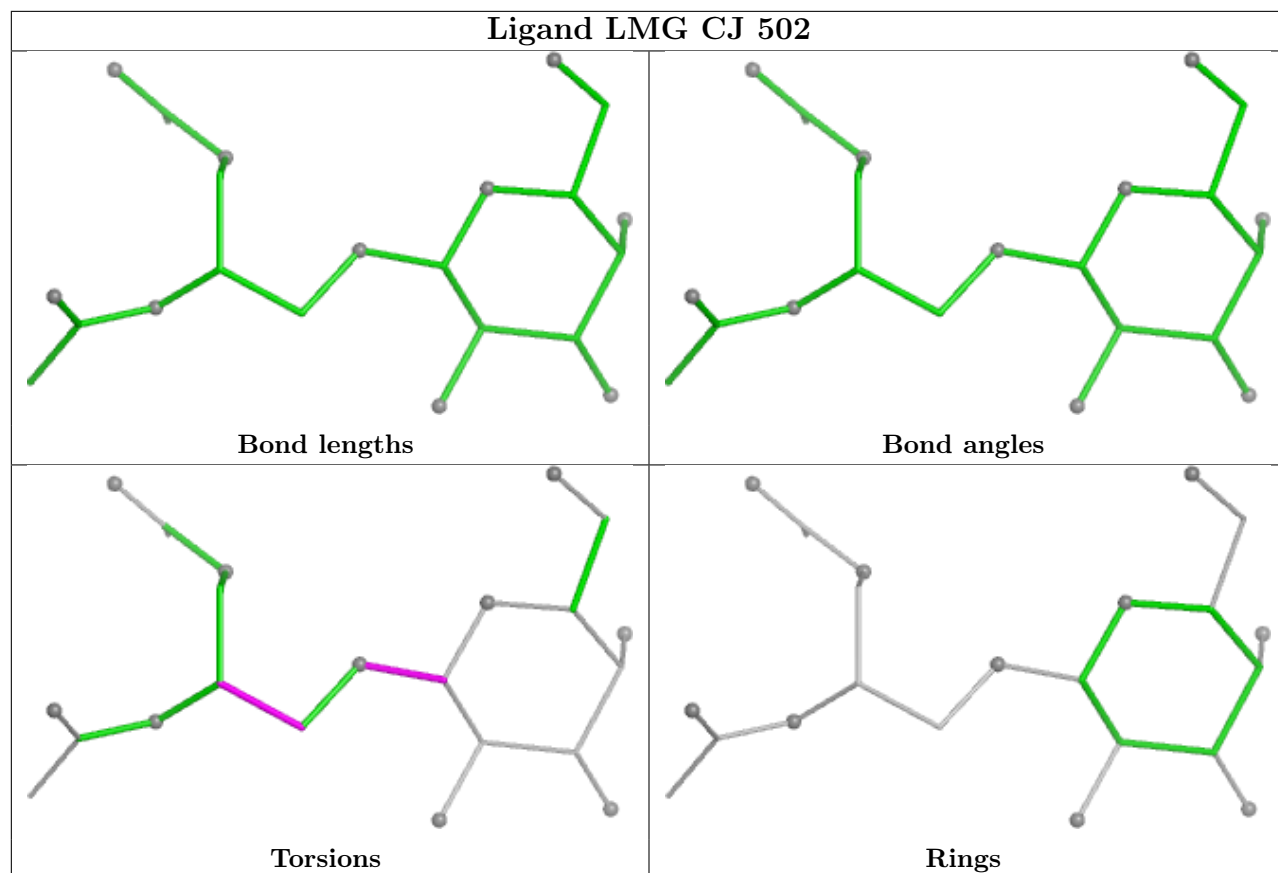




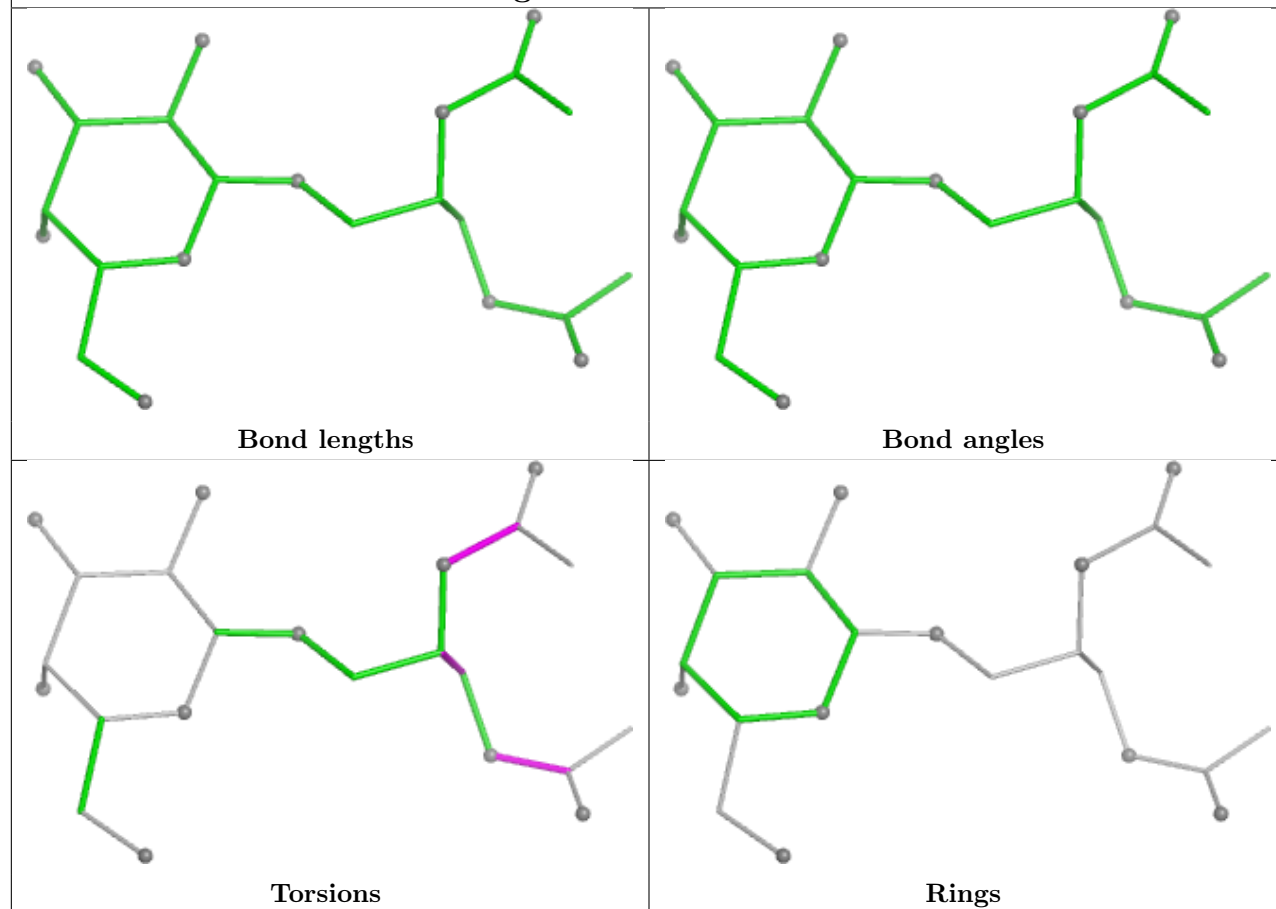


## Ligand A1JWG BB 503

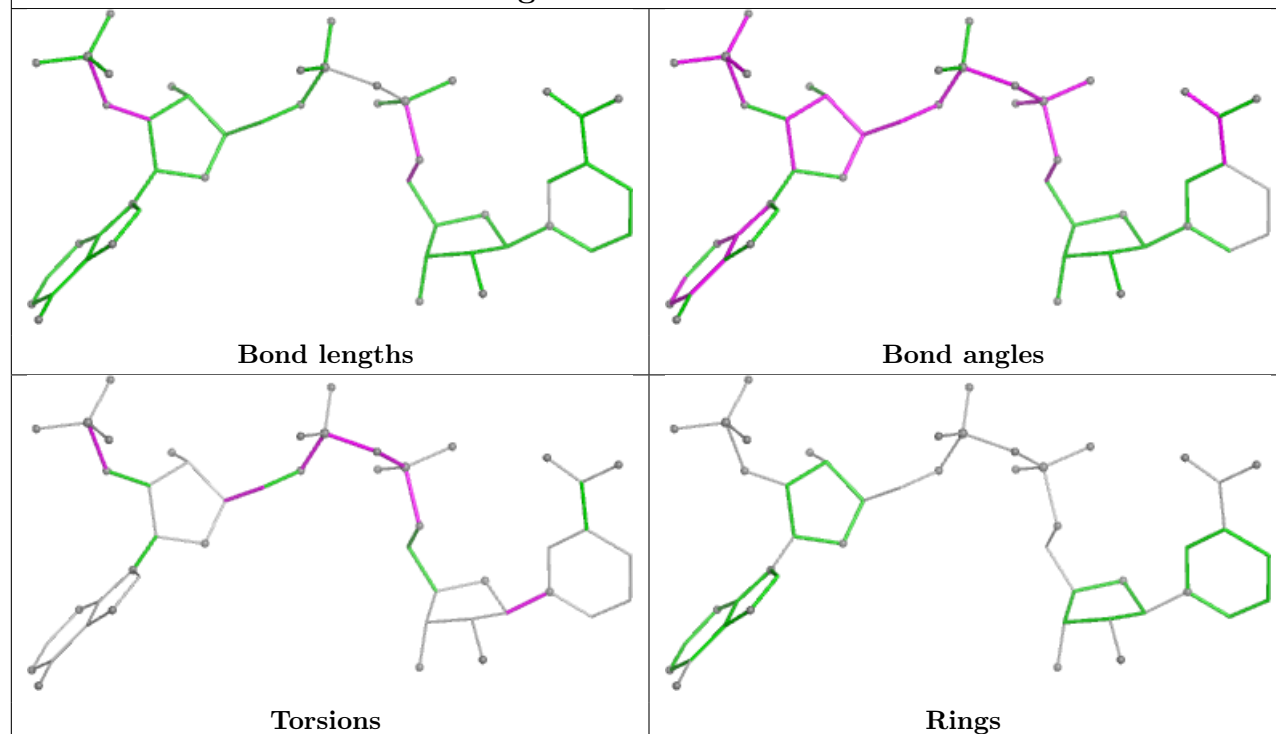




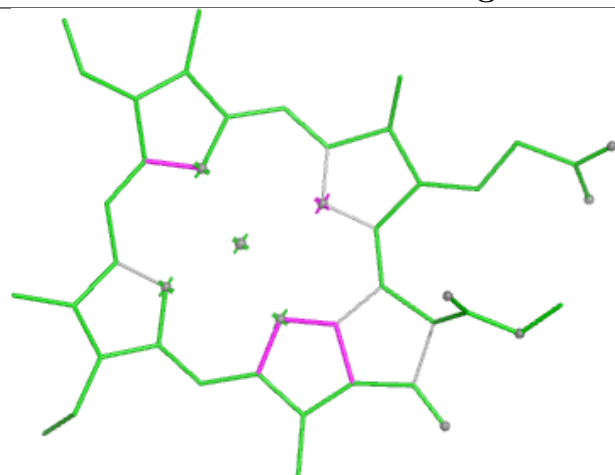
## Ligand LMG BH 703



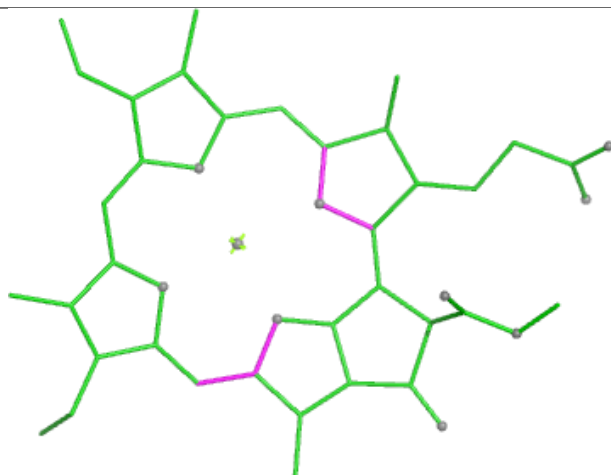
## Ligand NDP AL 503



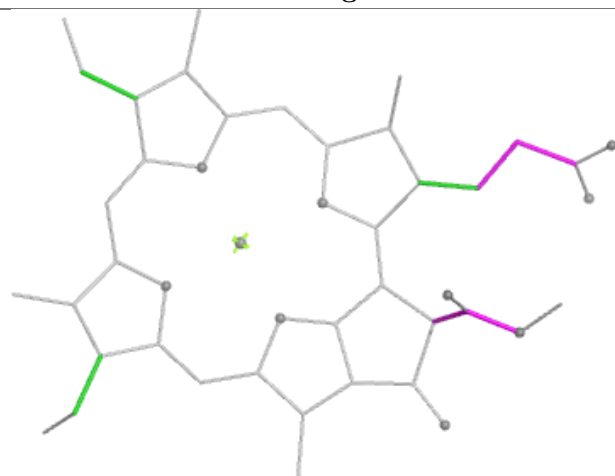
## Ligand A1JWG DF 502



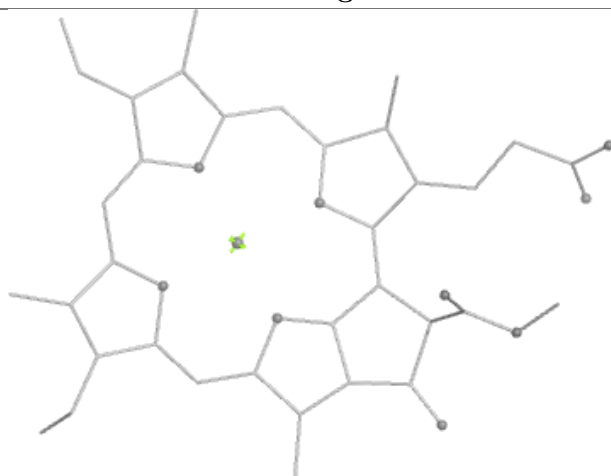
Bond lengths



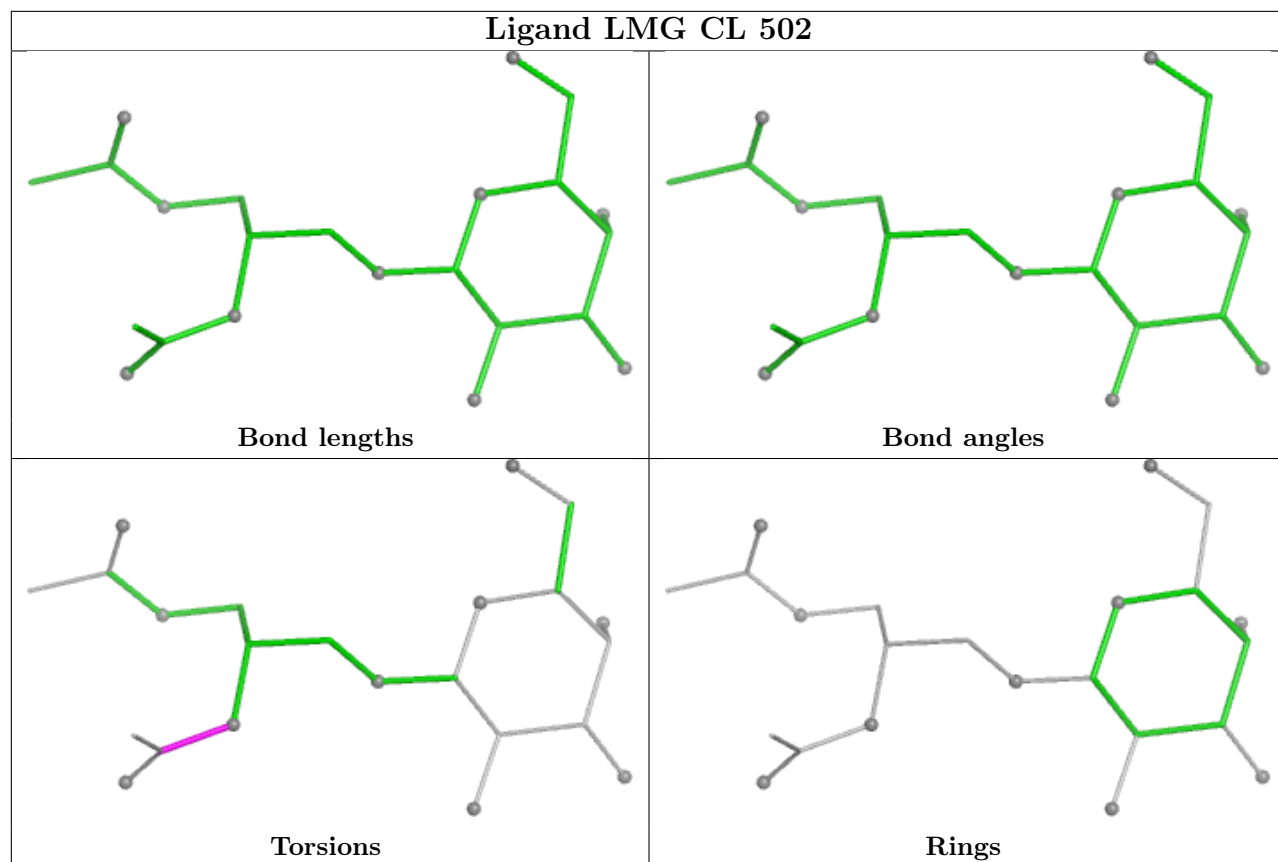
Bond angles



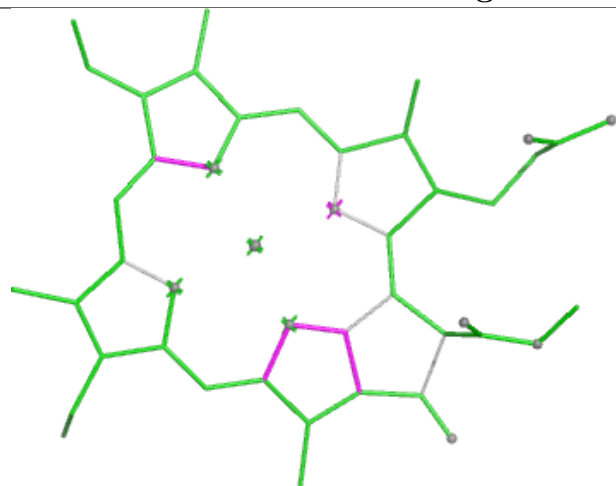
Torsions



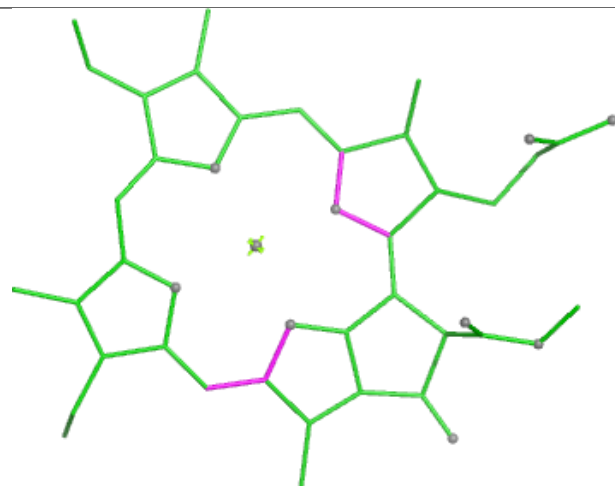
Rings



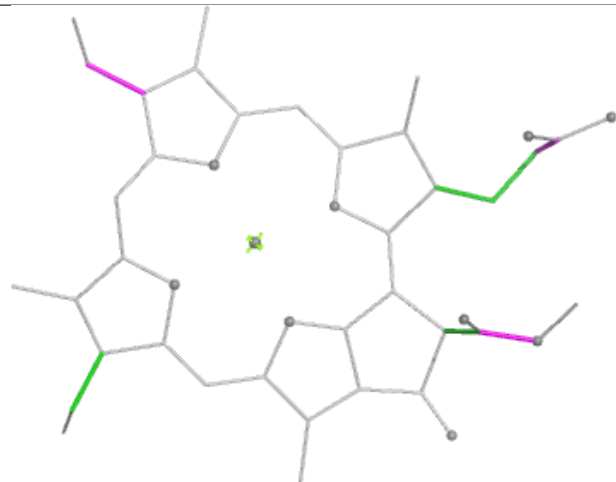
## Ligand A1JWG DC 701



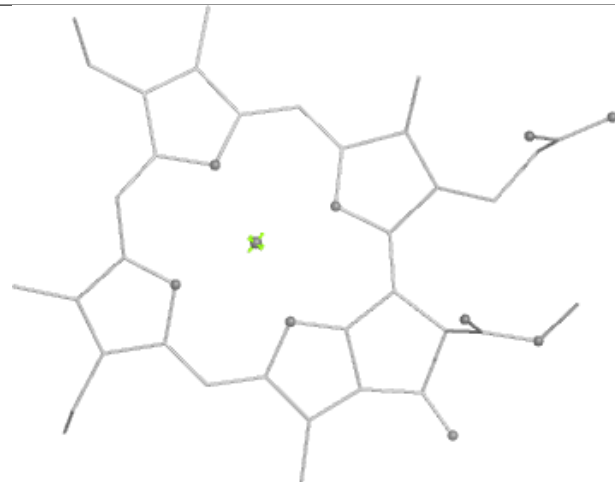
Bond lengths



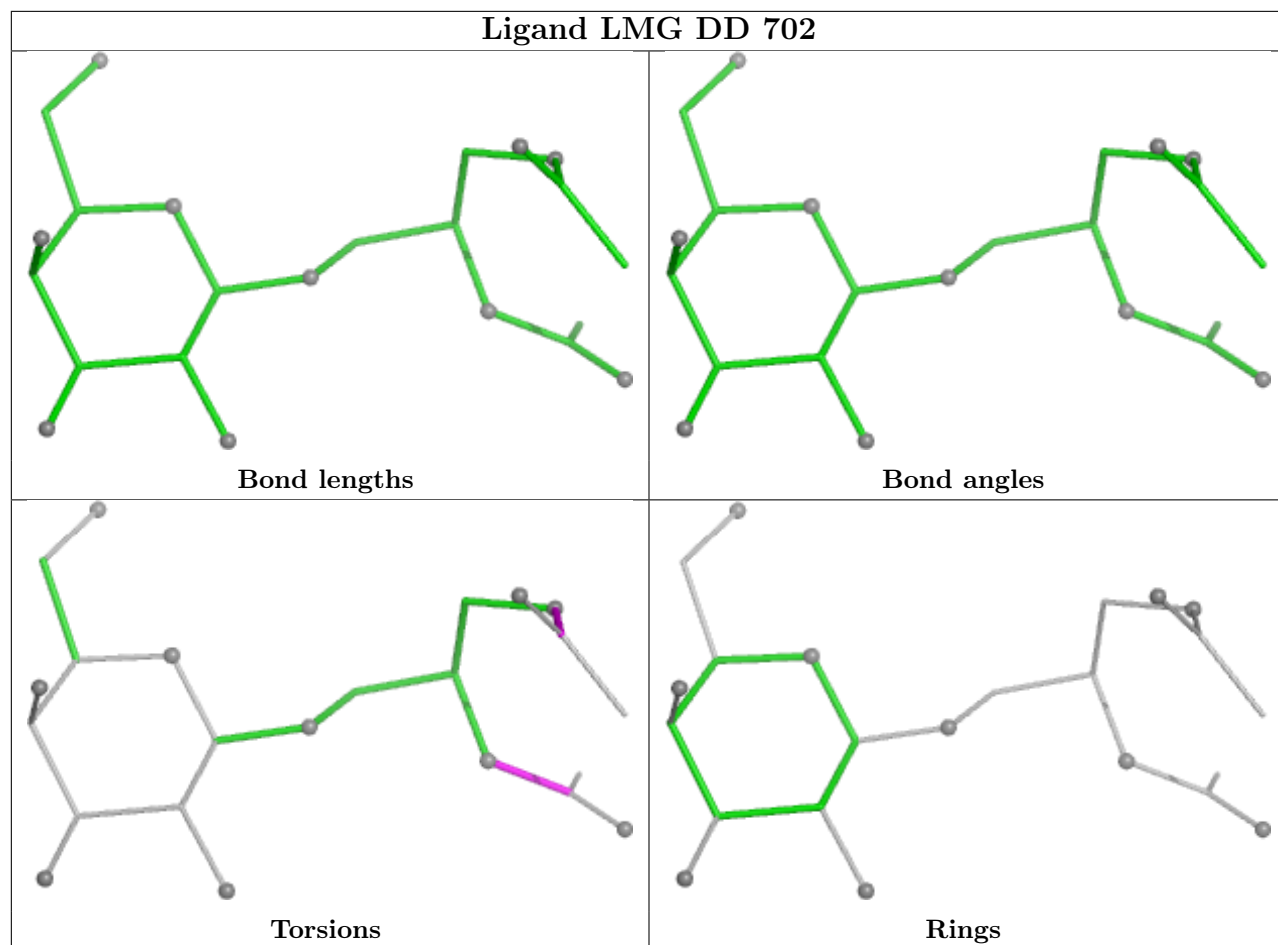
Bond angles



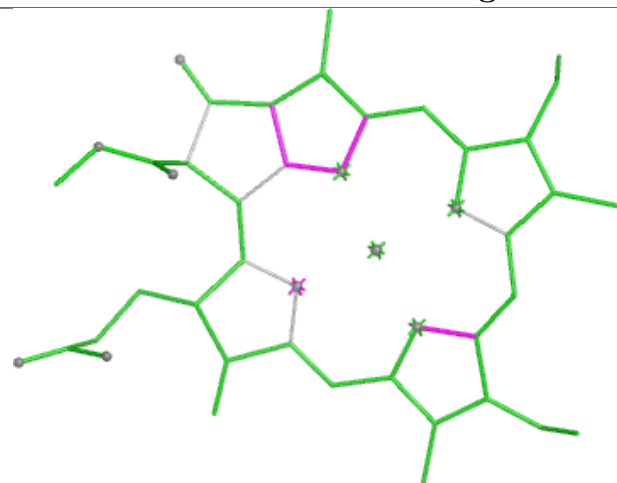
Torsions



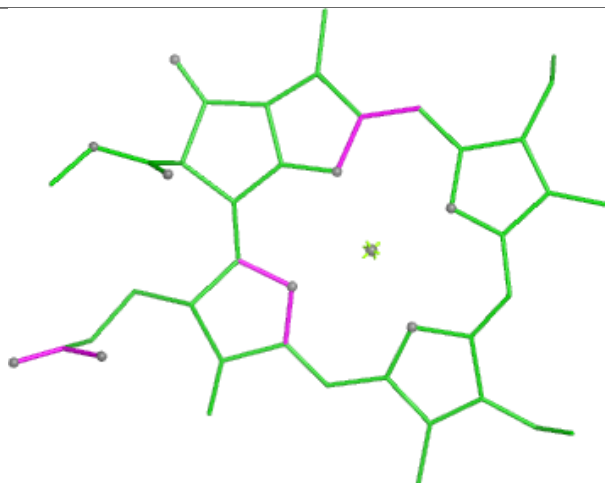
Rings



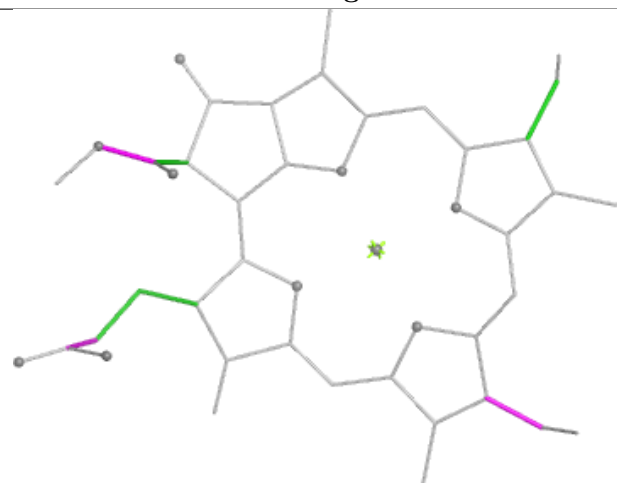
## Ligand A1JWG AC 502



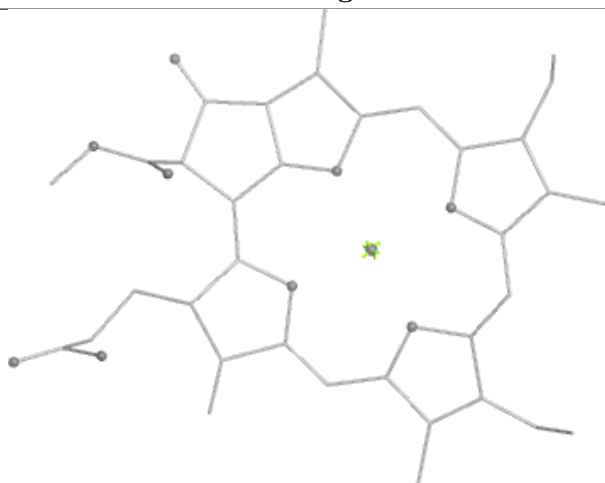
Bond lengths



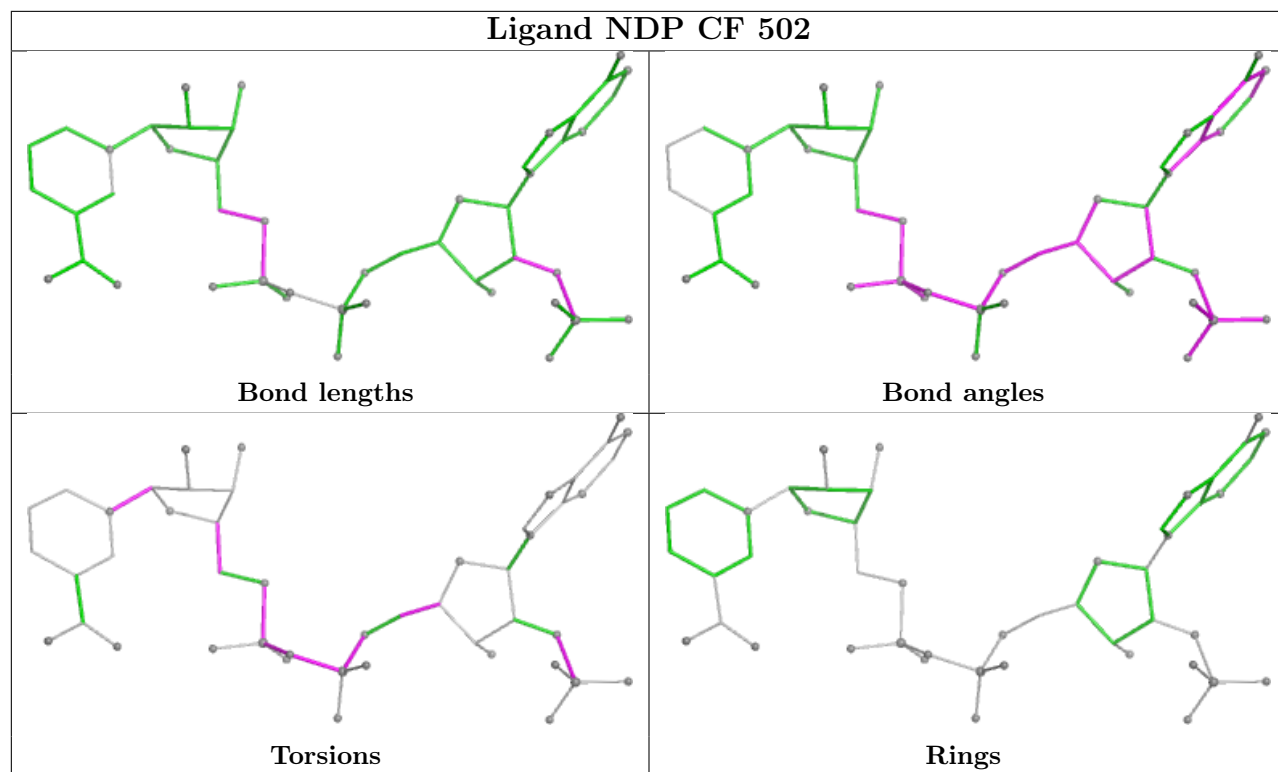
Bond angles



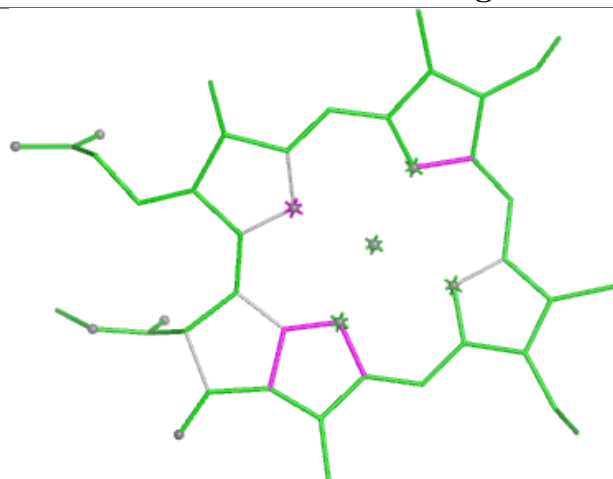
Torsions



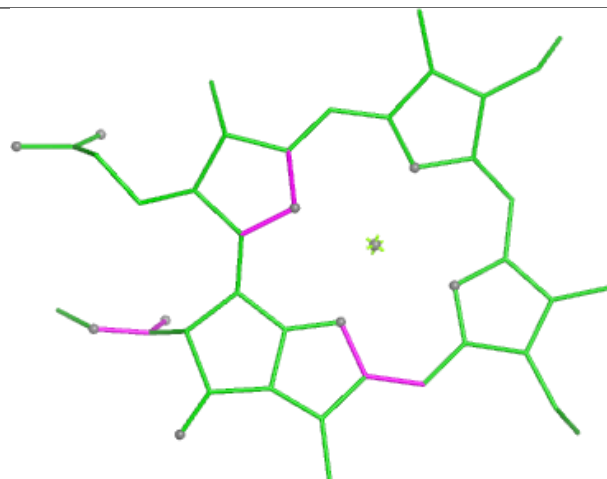
Rings



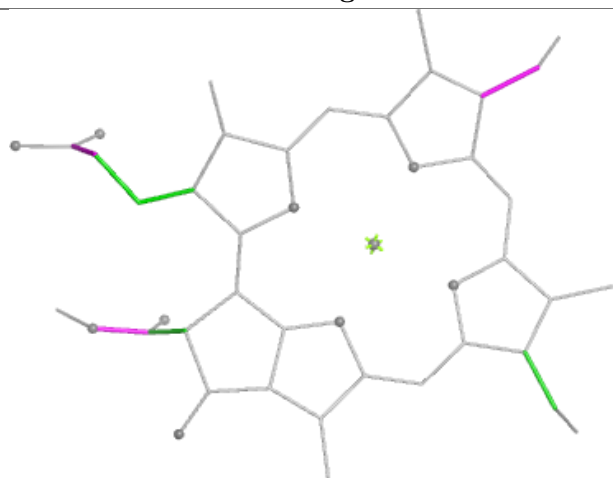
## Ligand A1JWG DE 701



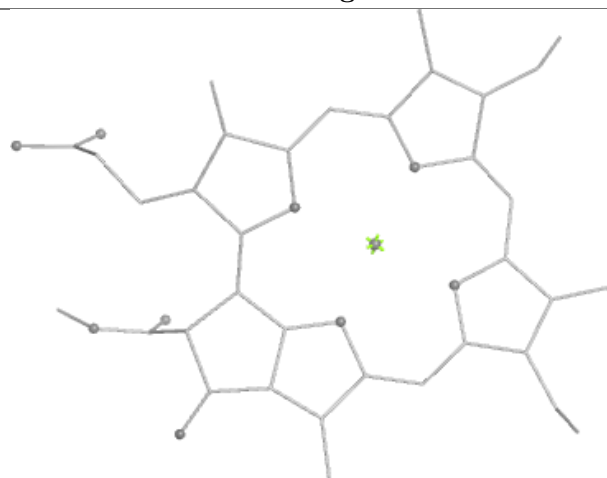
Bond lengths



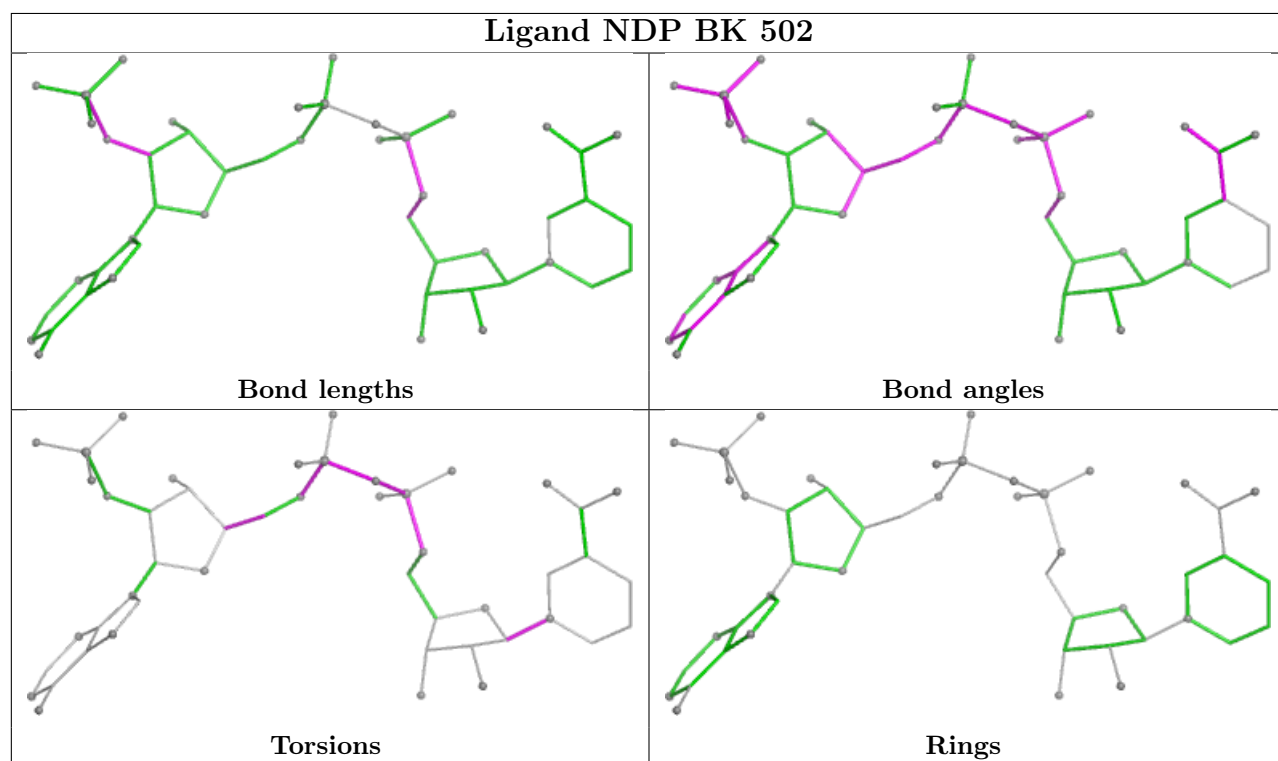
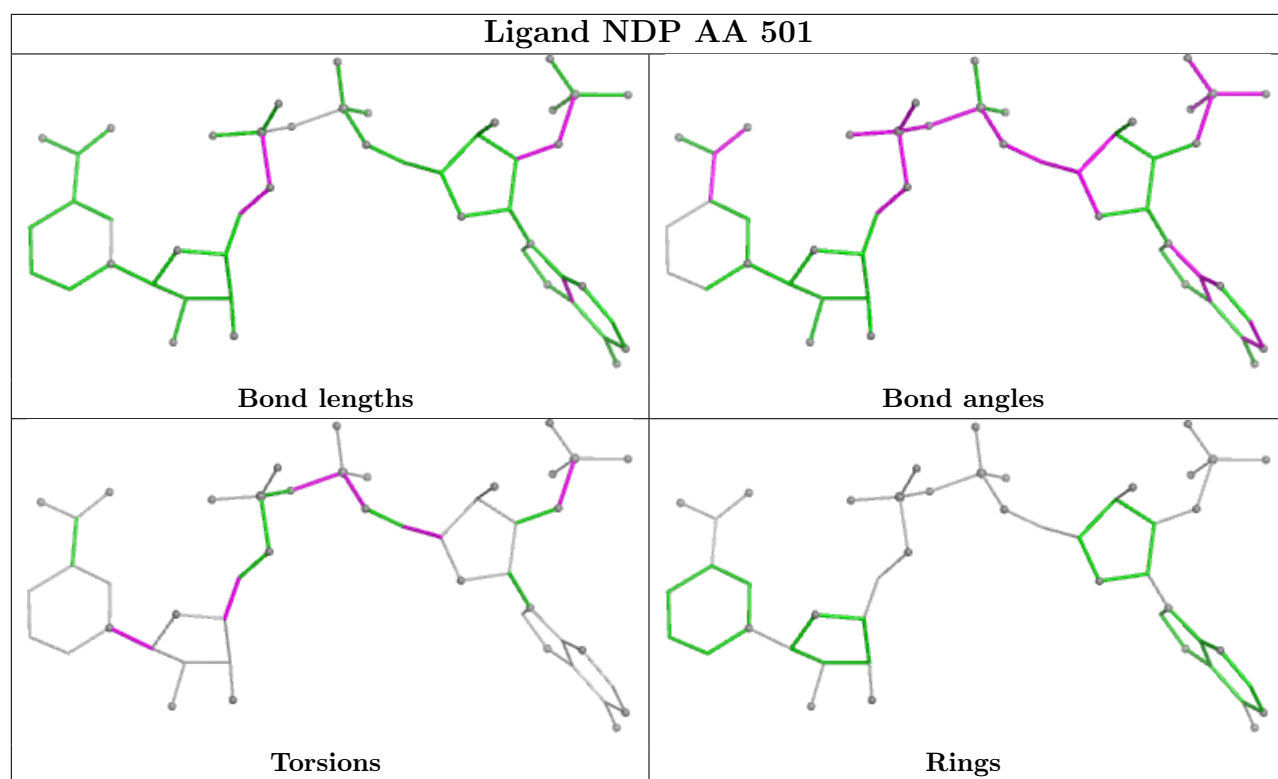
Bond angles



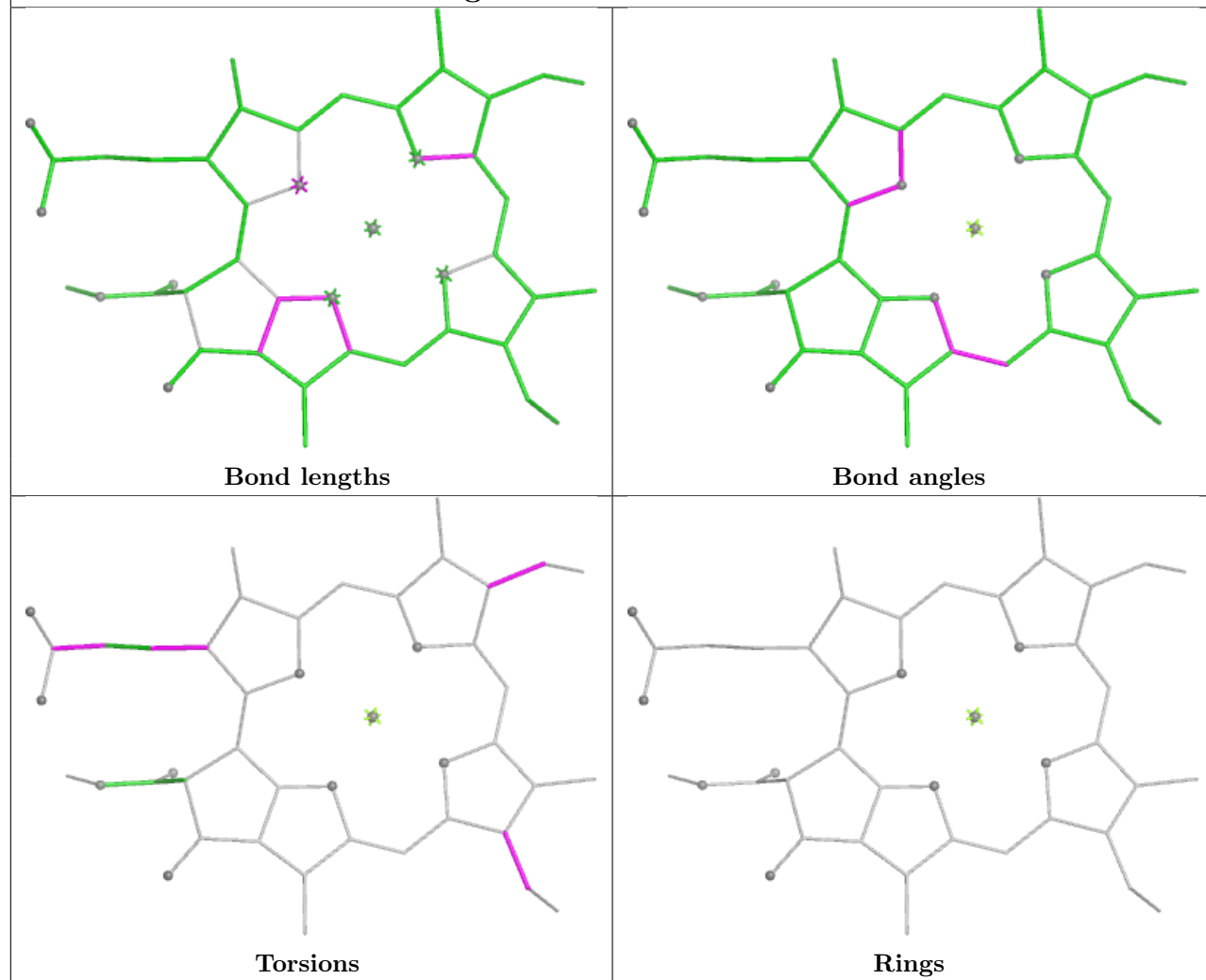
Torsions



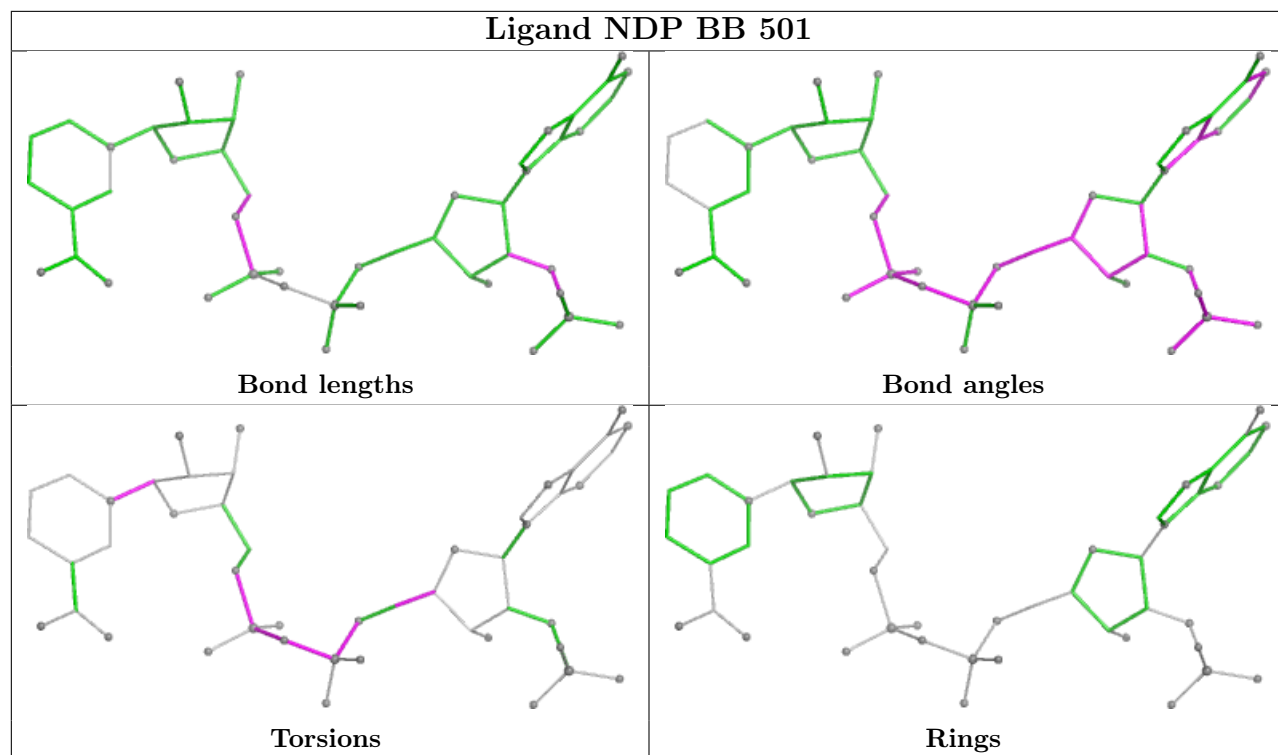
Rings



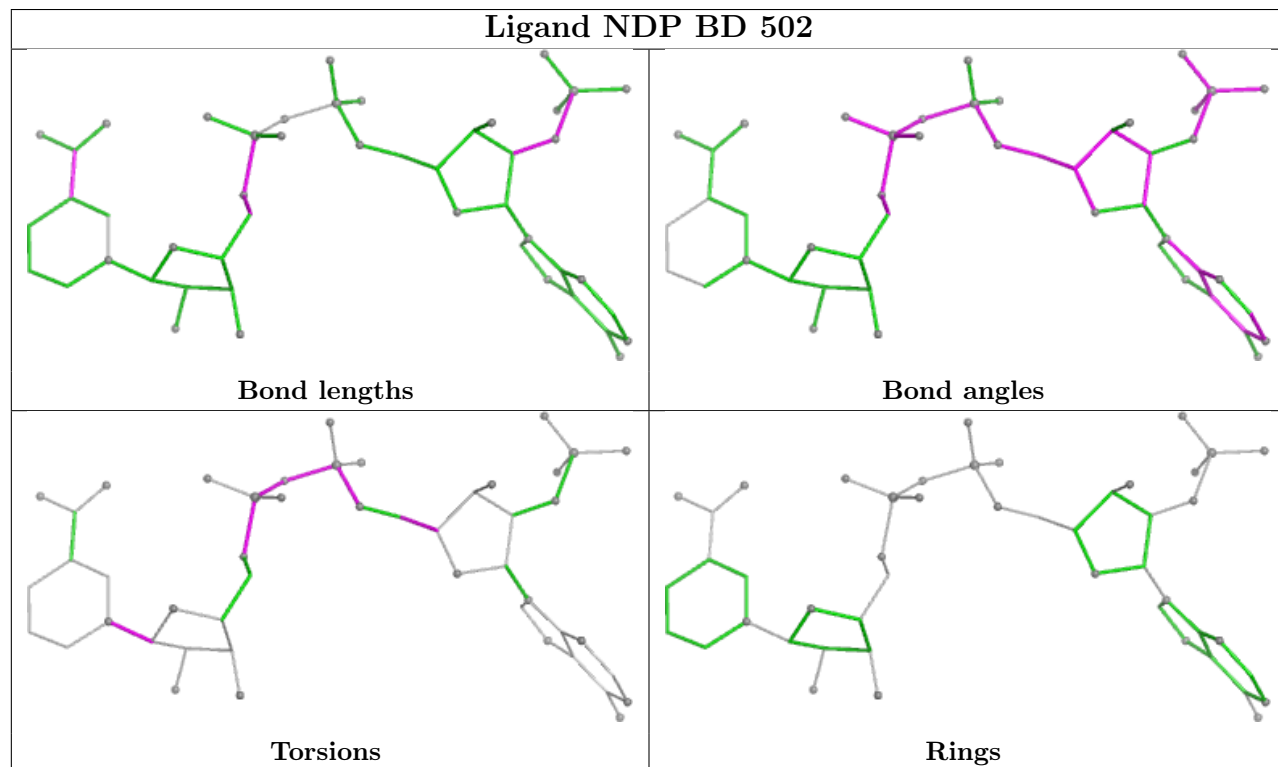
## Ligand A1JWG BA 503

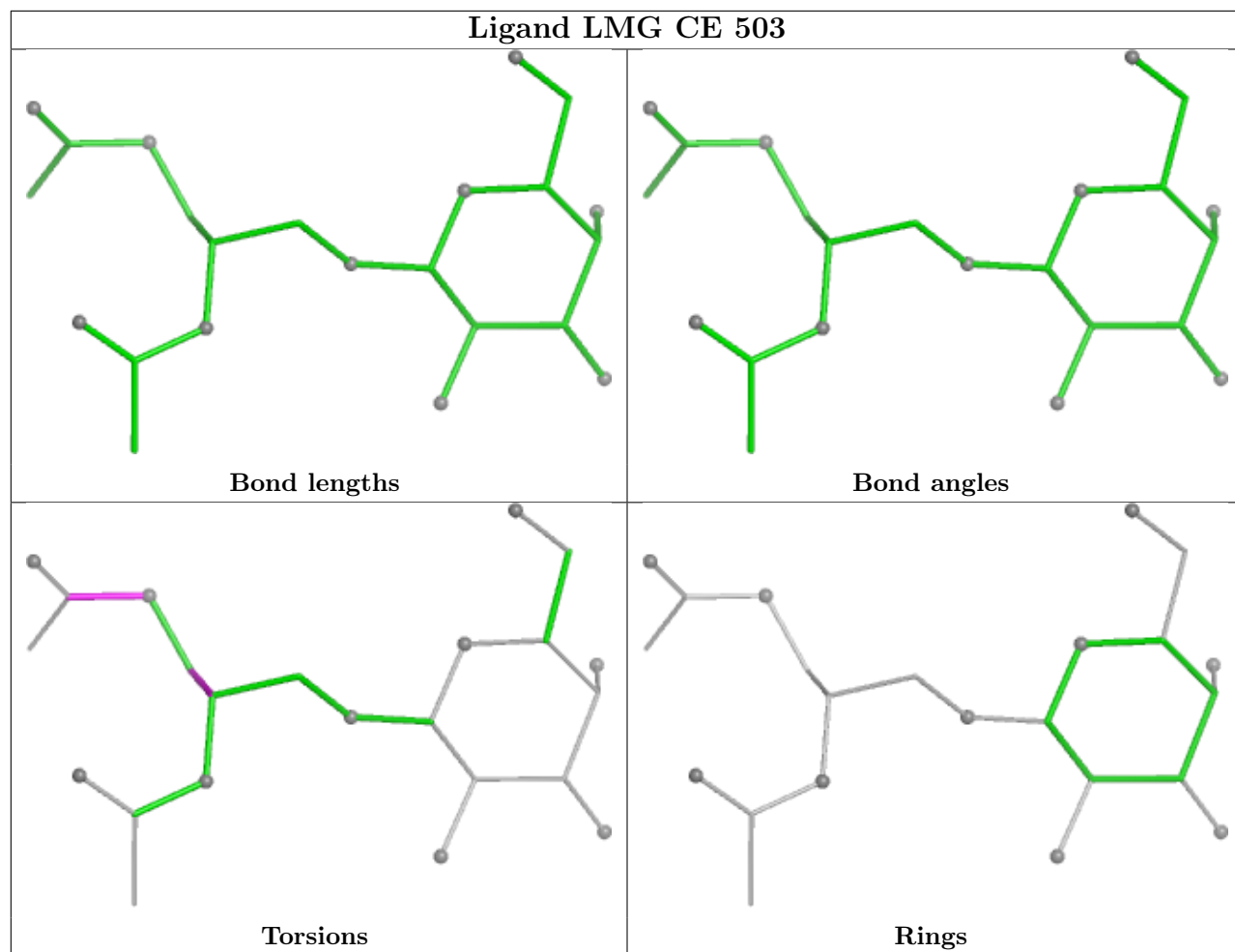


## Ligand NDP BB 501

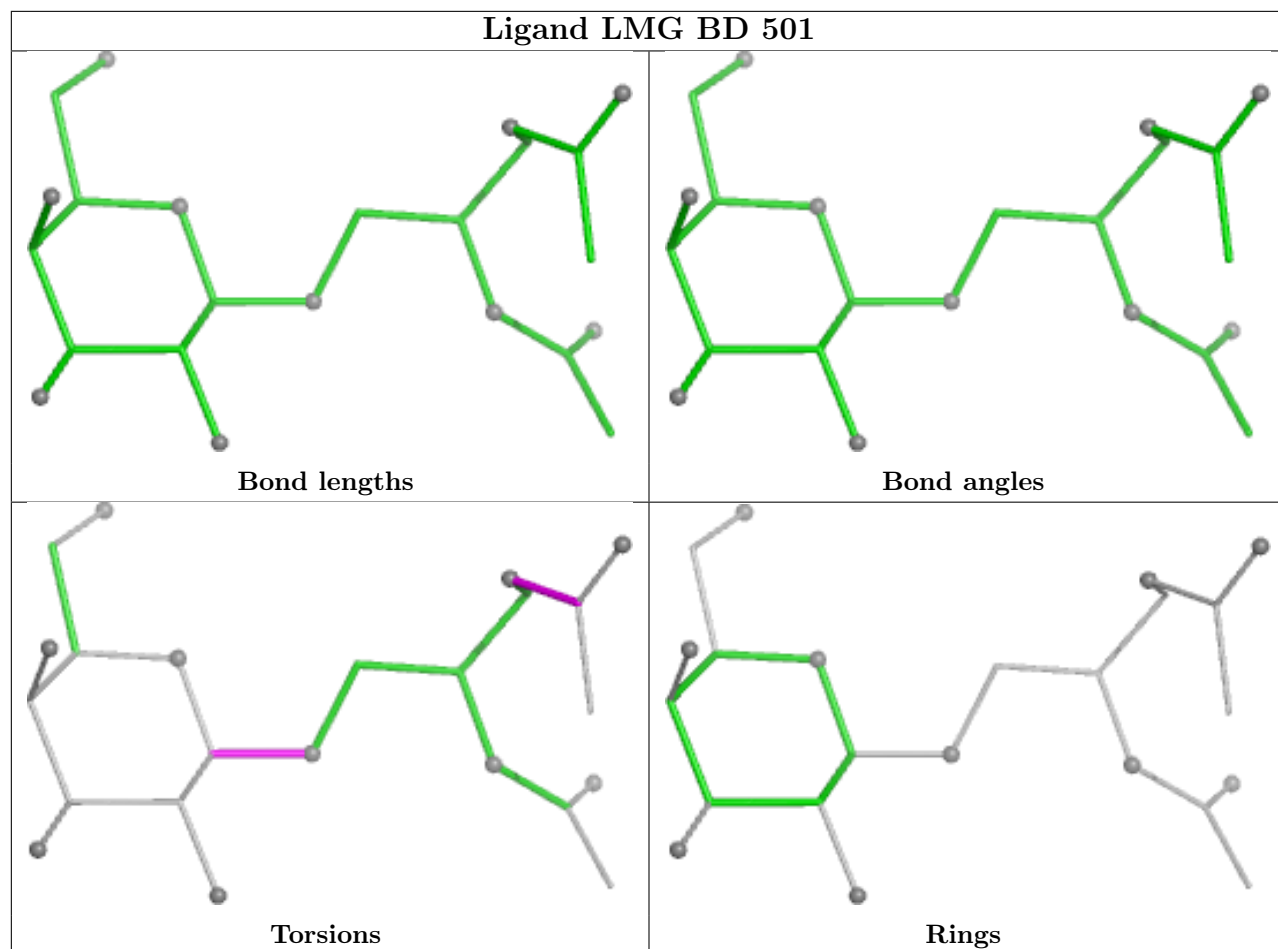


## Ligand NDP BD 502

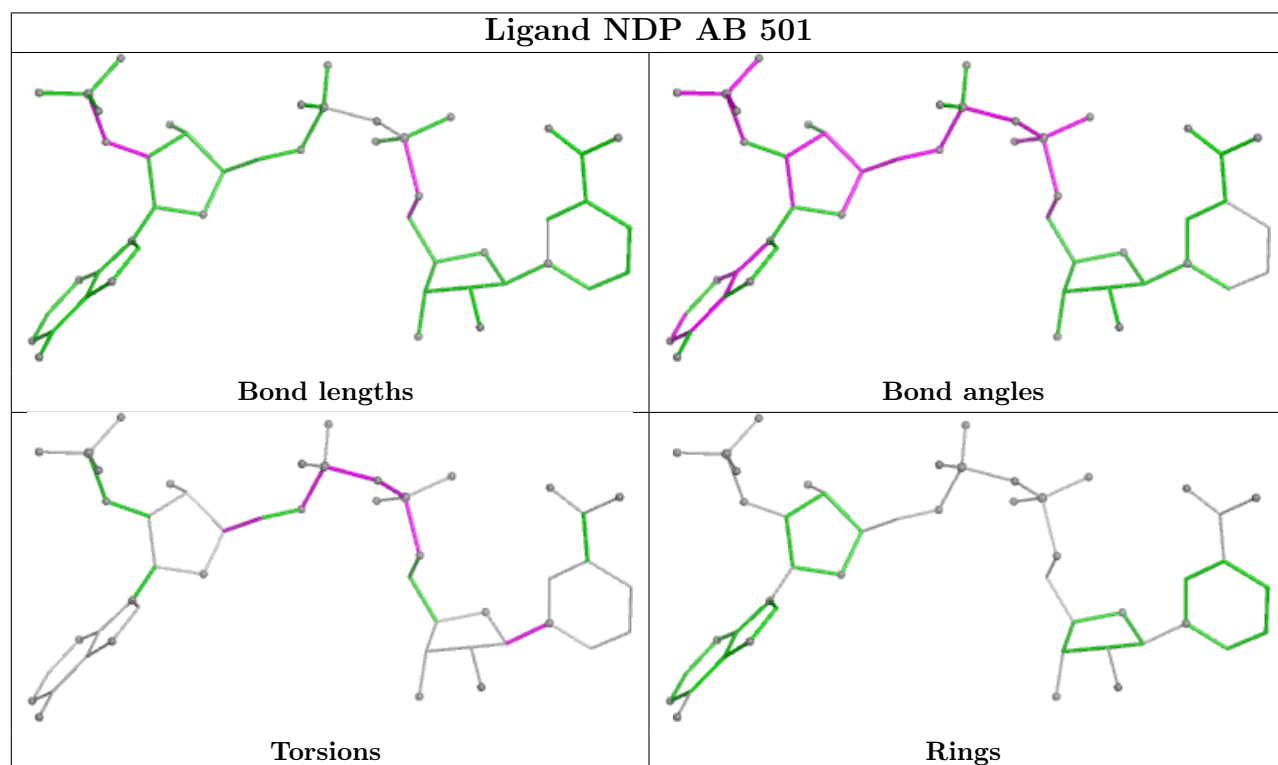


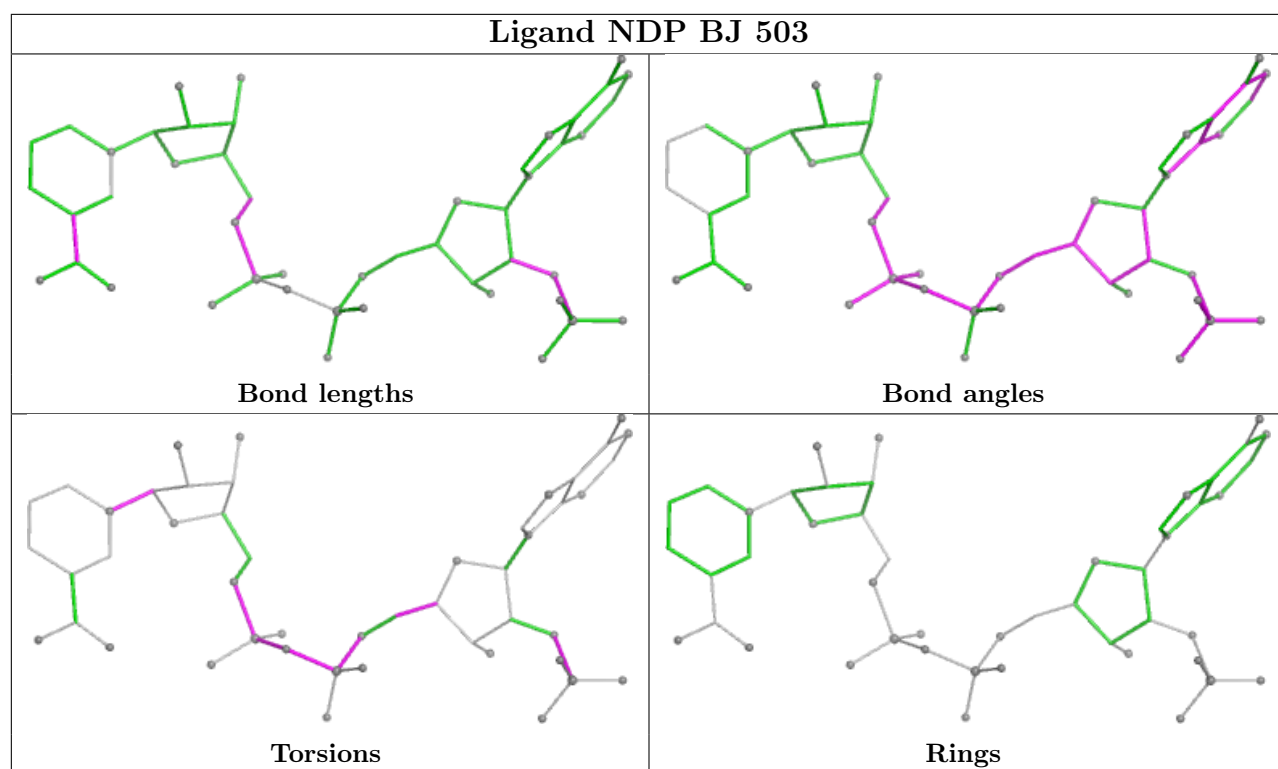


## Ligand LMG BD 501

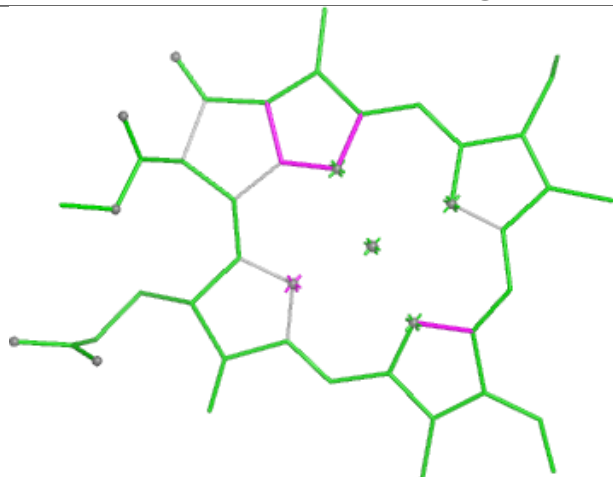


## Ligand NDP AB 501

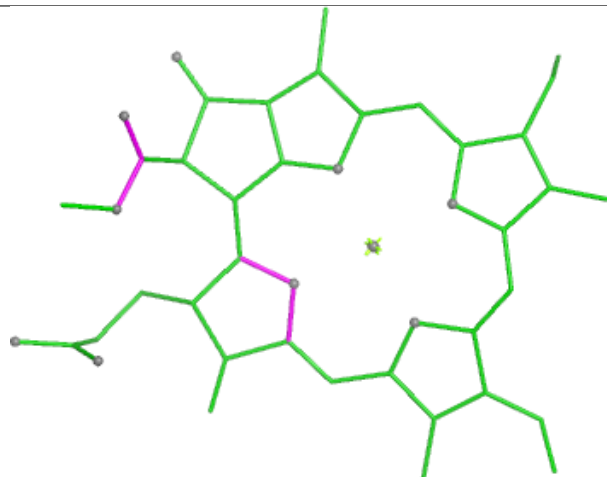




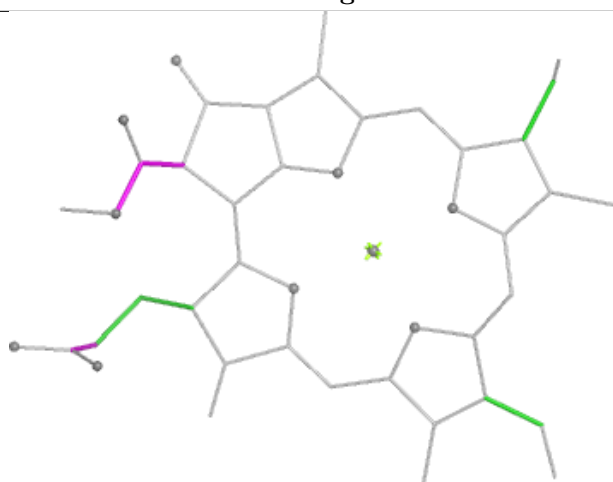
## Ligand A1JWG AL 502



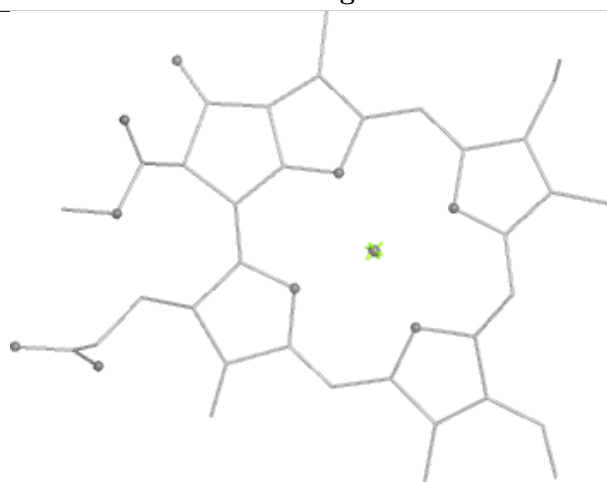
Bond lengths



Bond angles

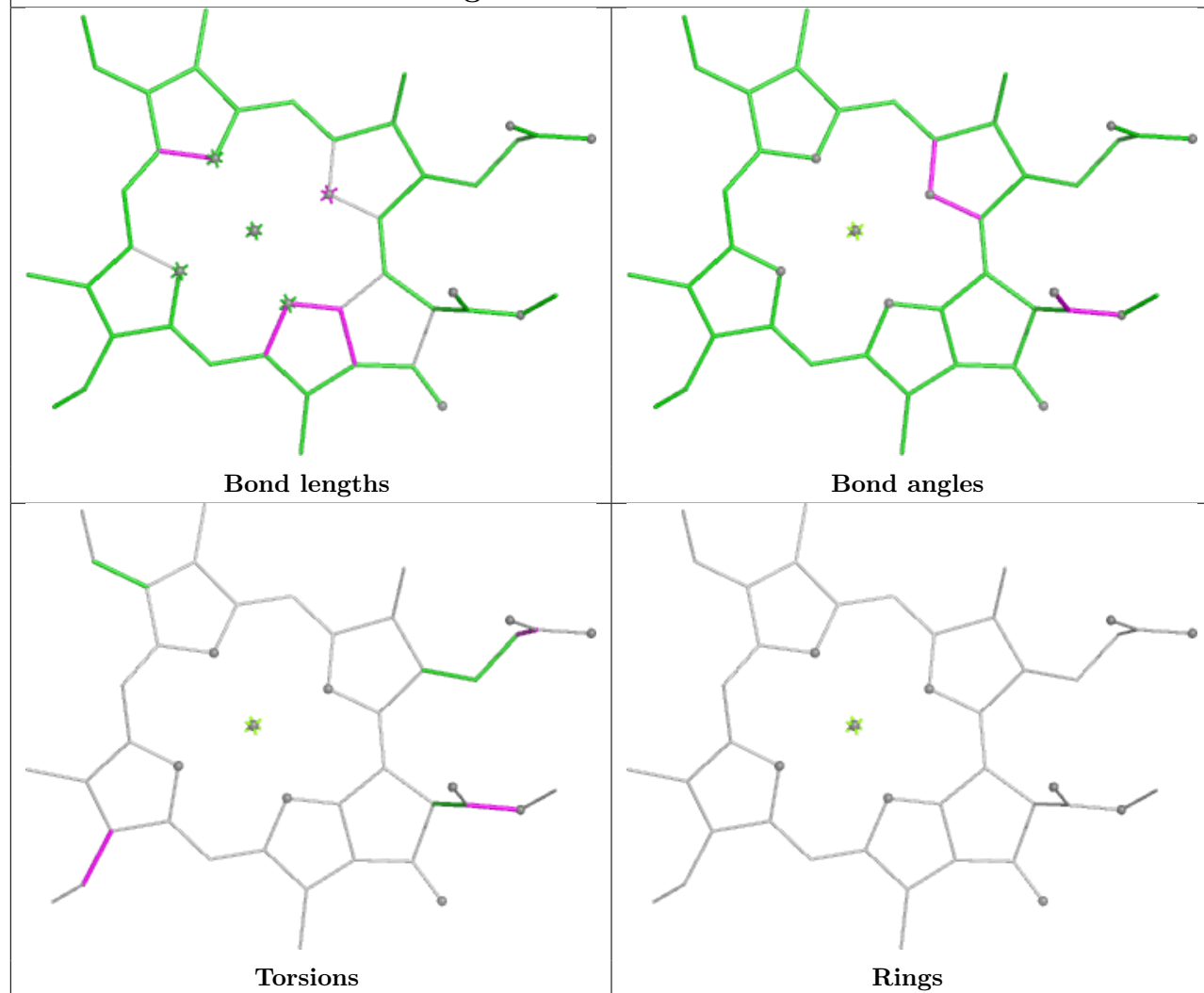


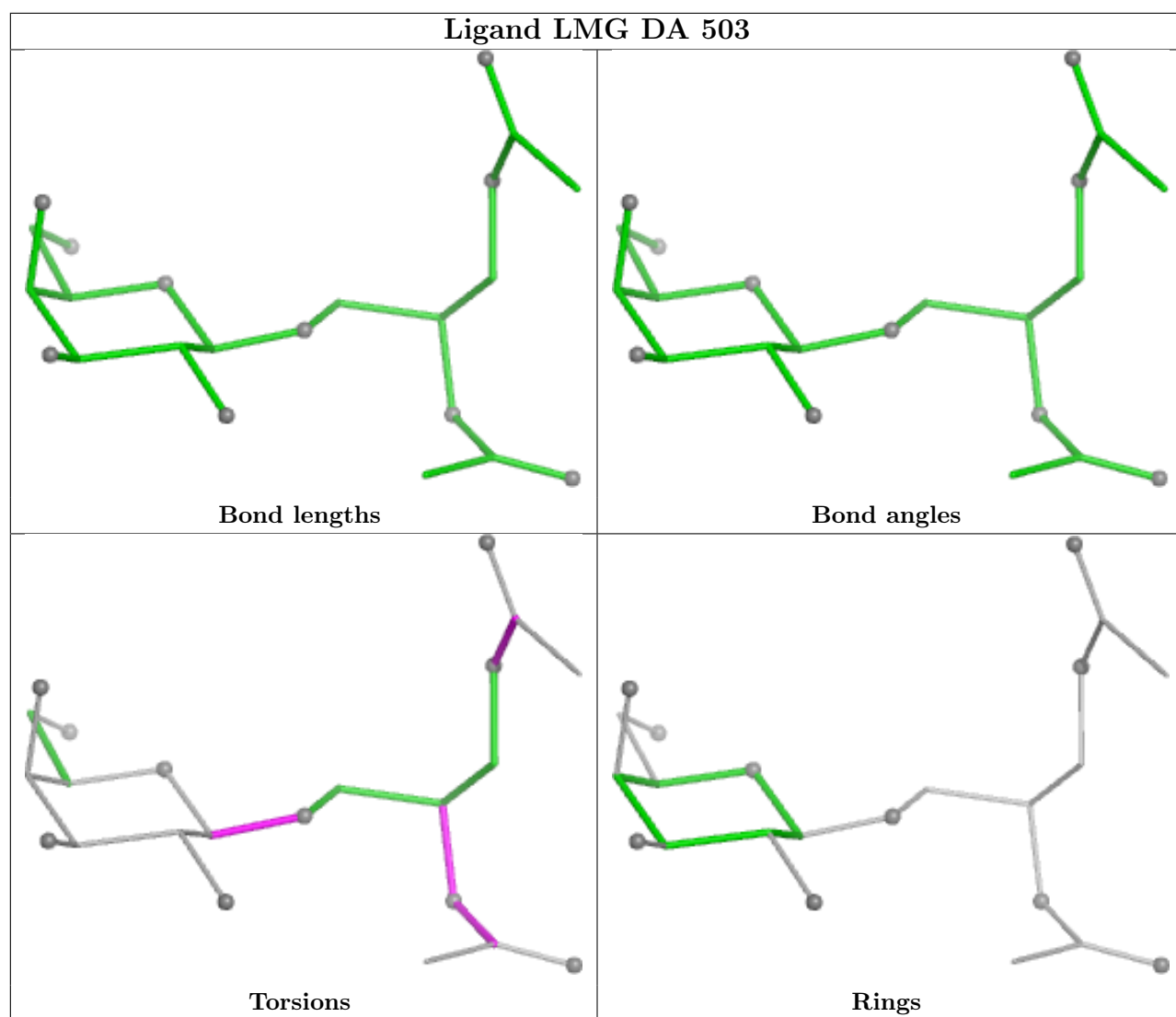
Torsions

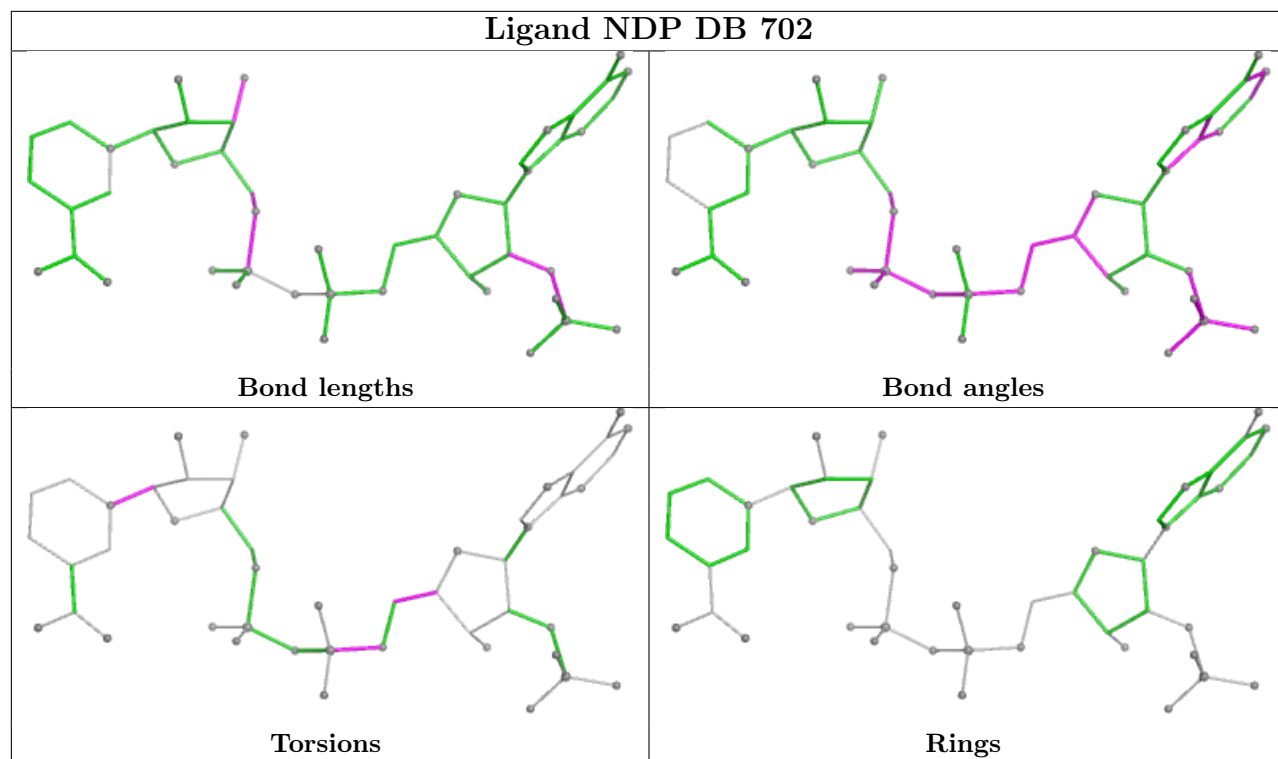


Rings

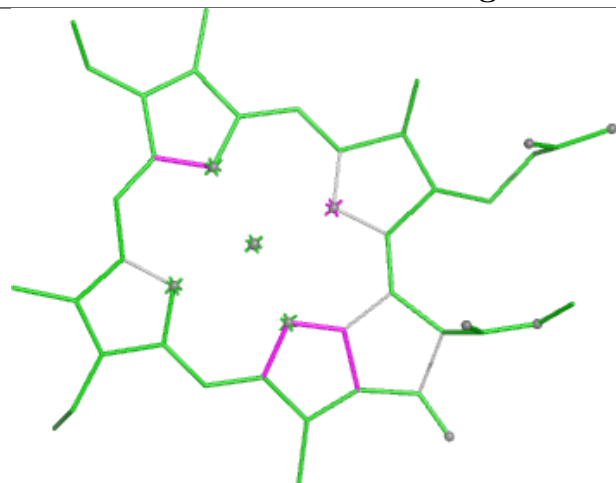
## Ligand A1JWG CC 503



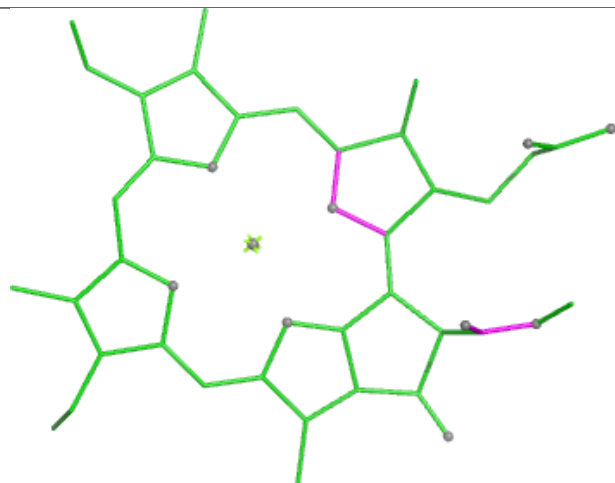




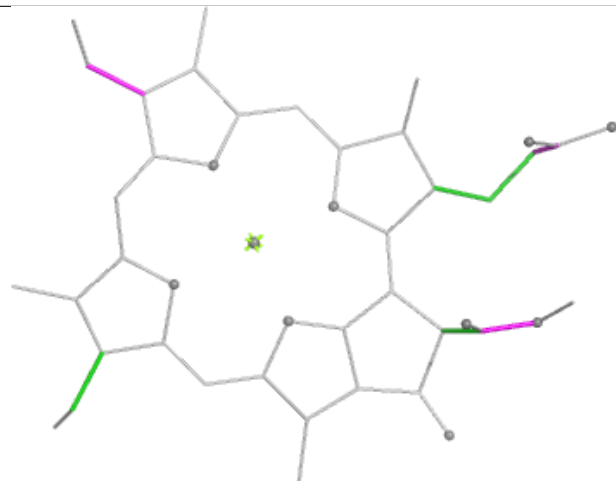
## Ligand A1JWG CL 503



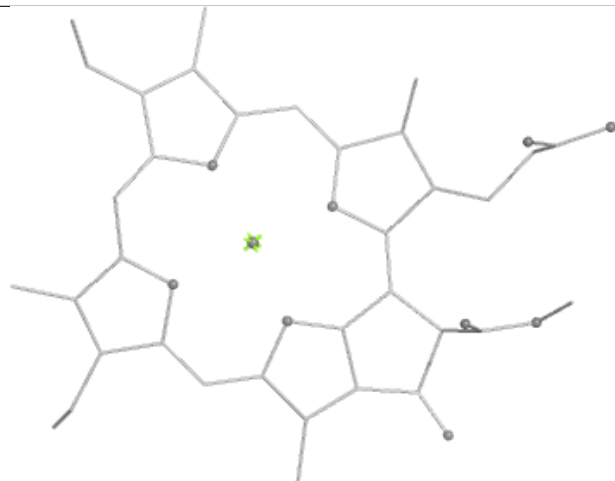
Bond lengths



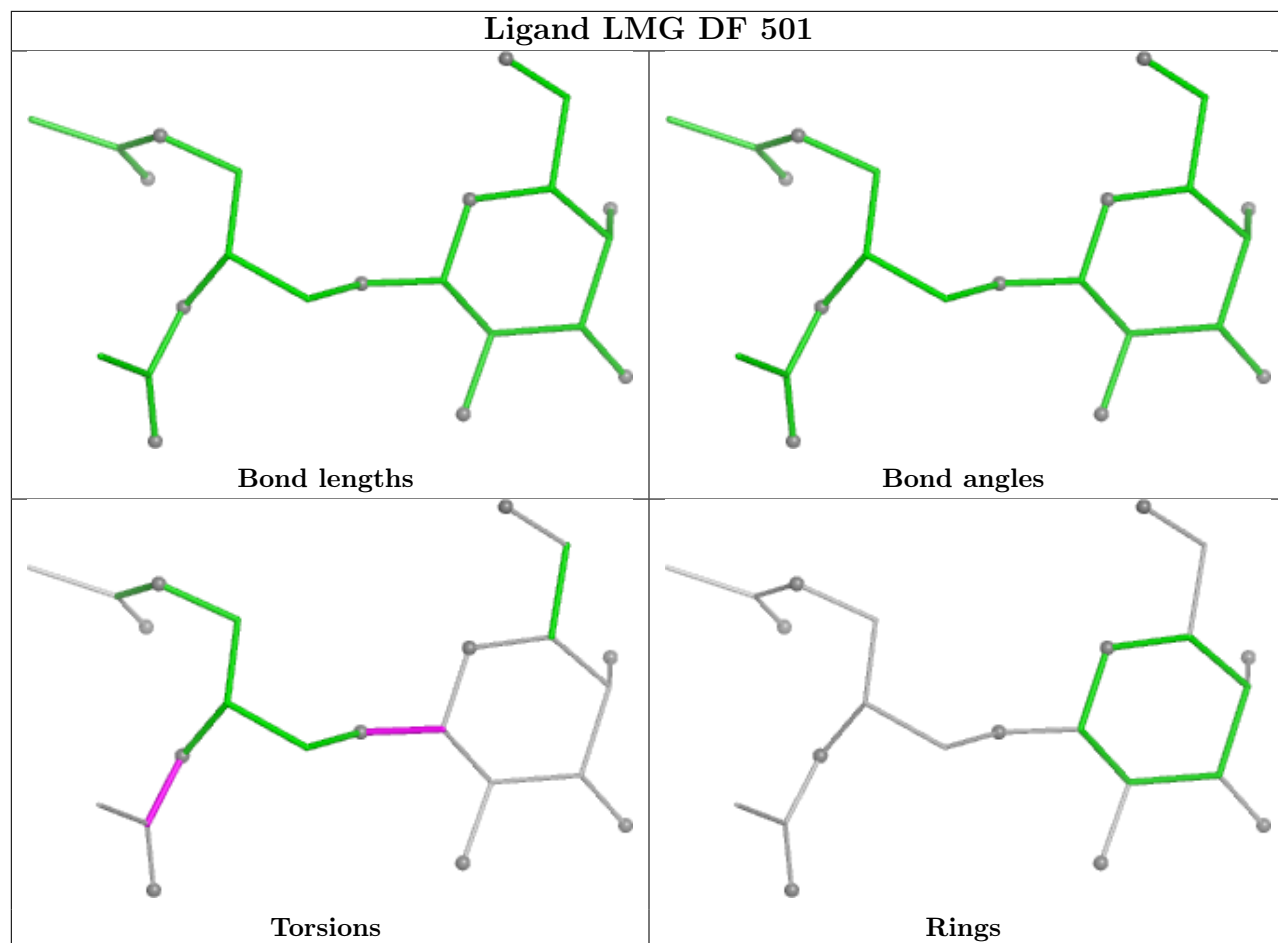
Bond angles



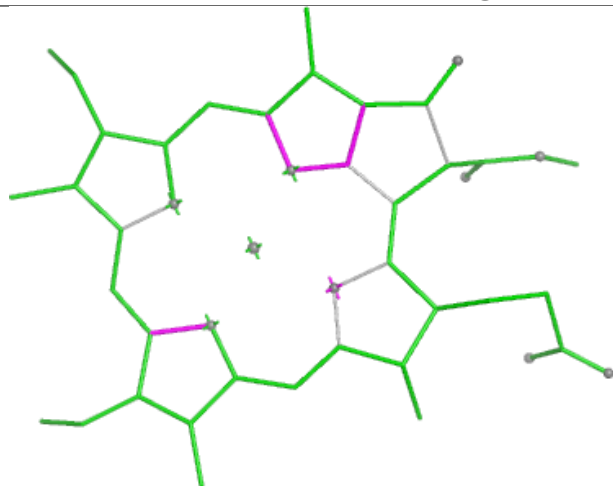
Torsions



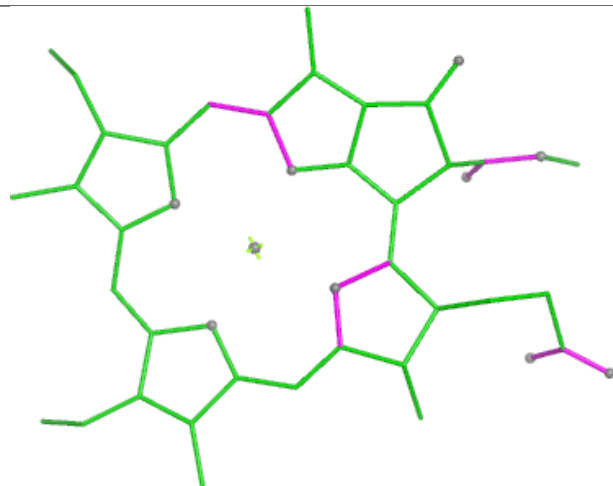
Rings



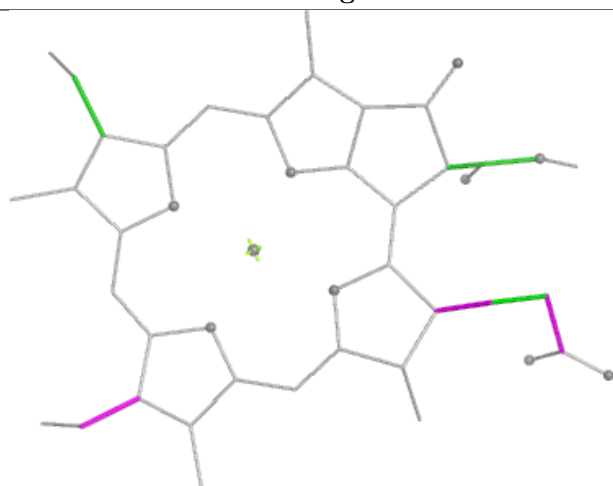
## Ligand A1JWG CF 503



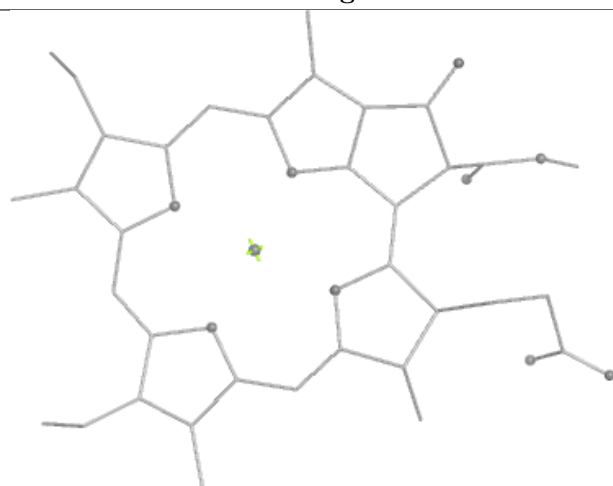
Bond lengths



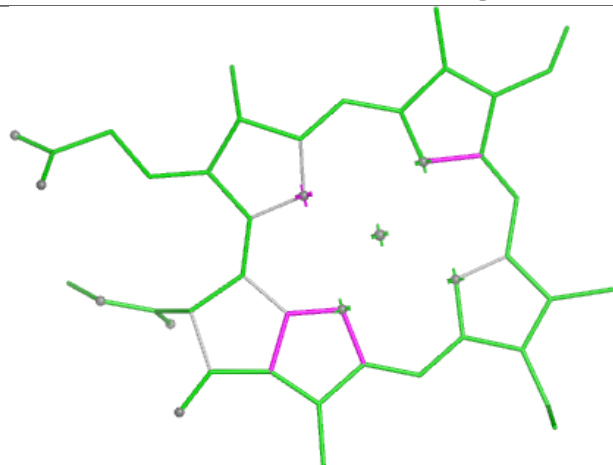
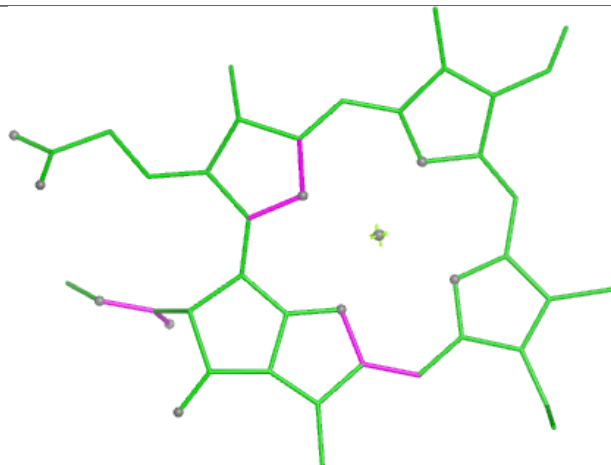
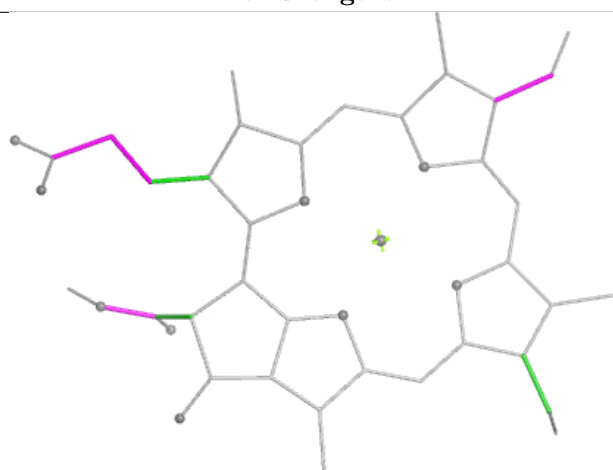
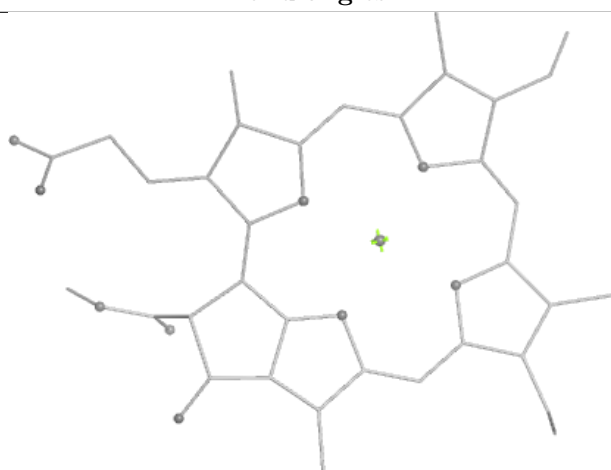
Bond angles

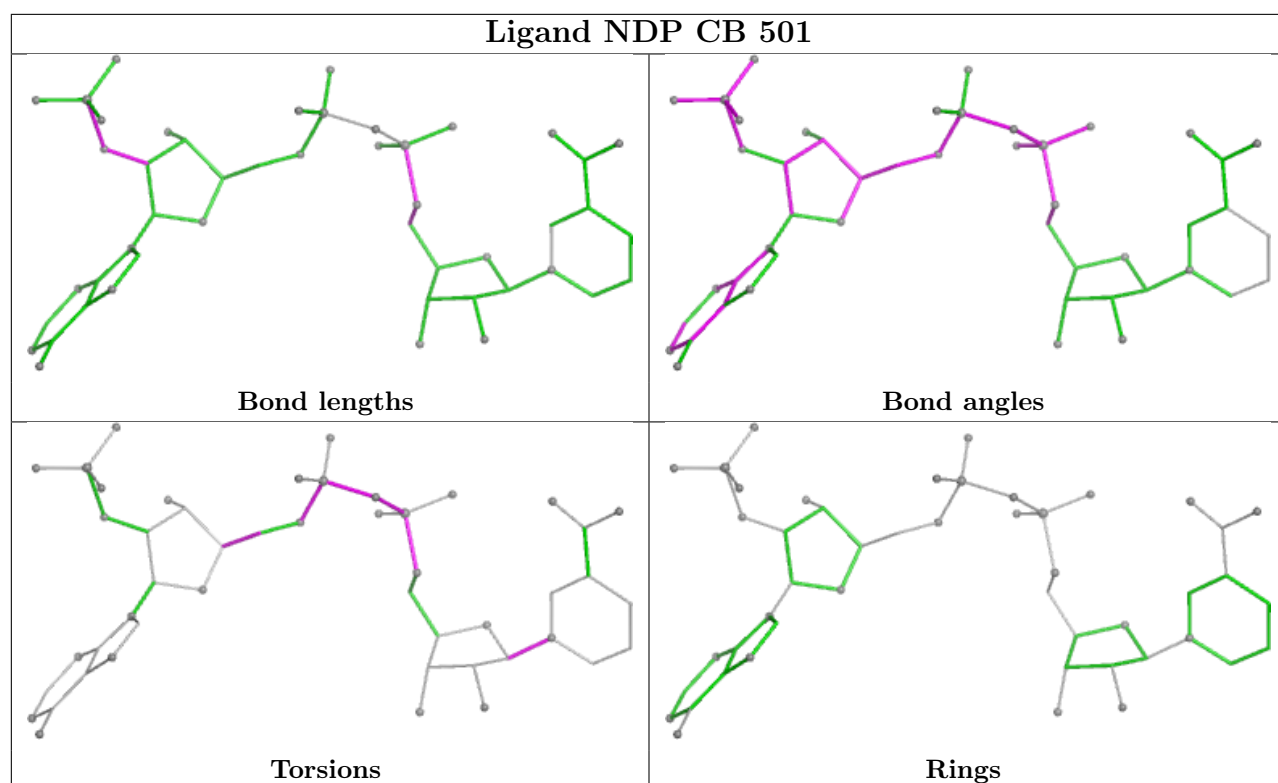


Torsions

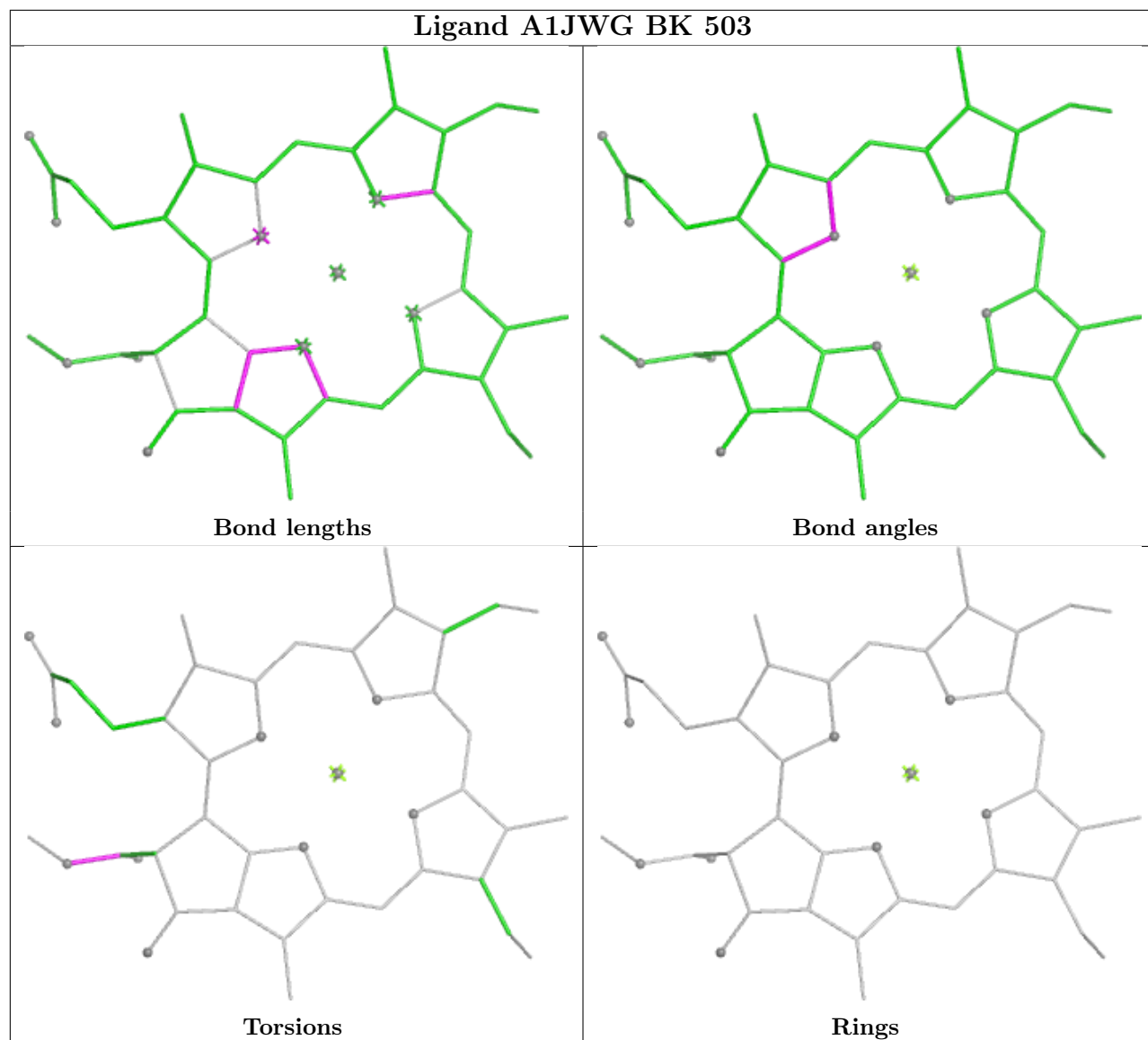


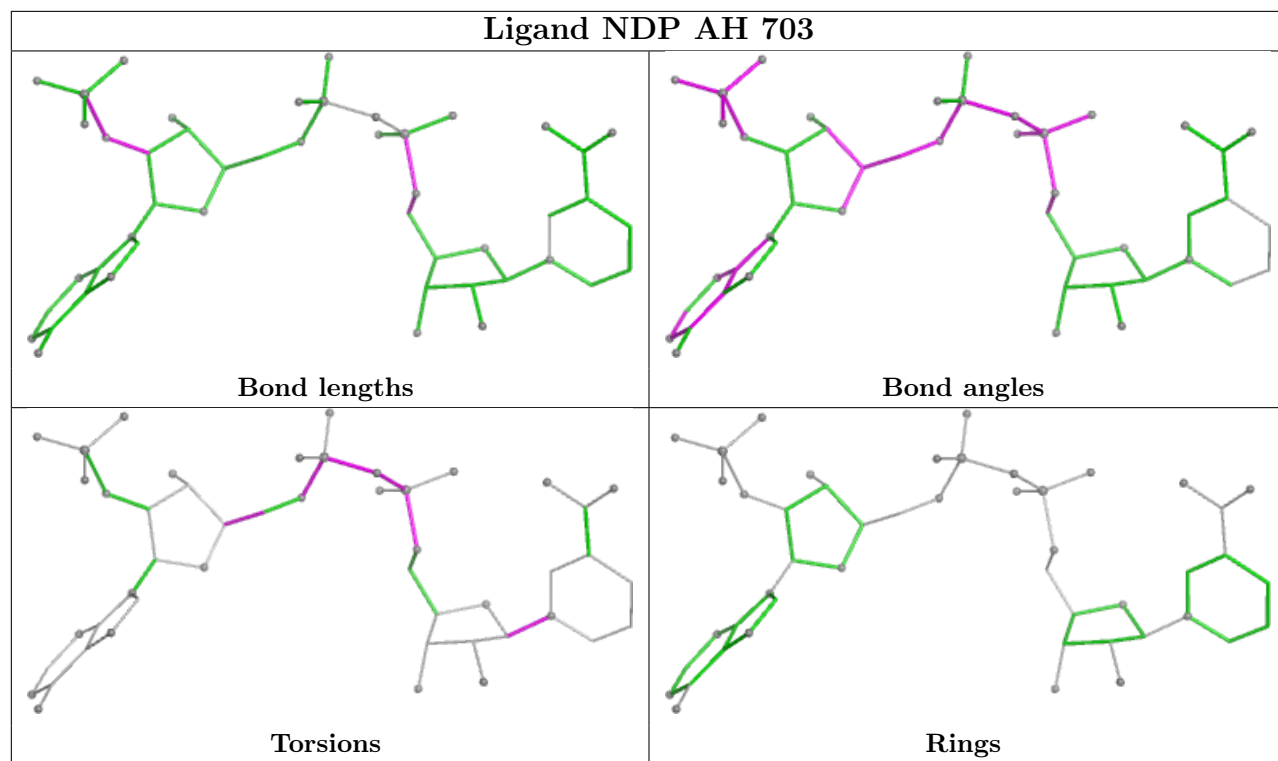
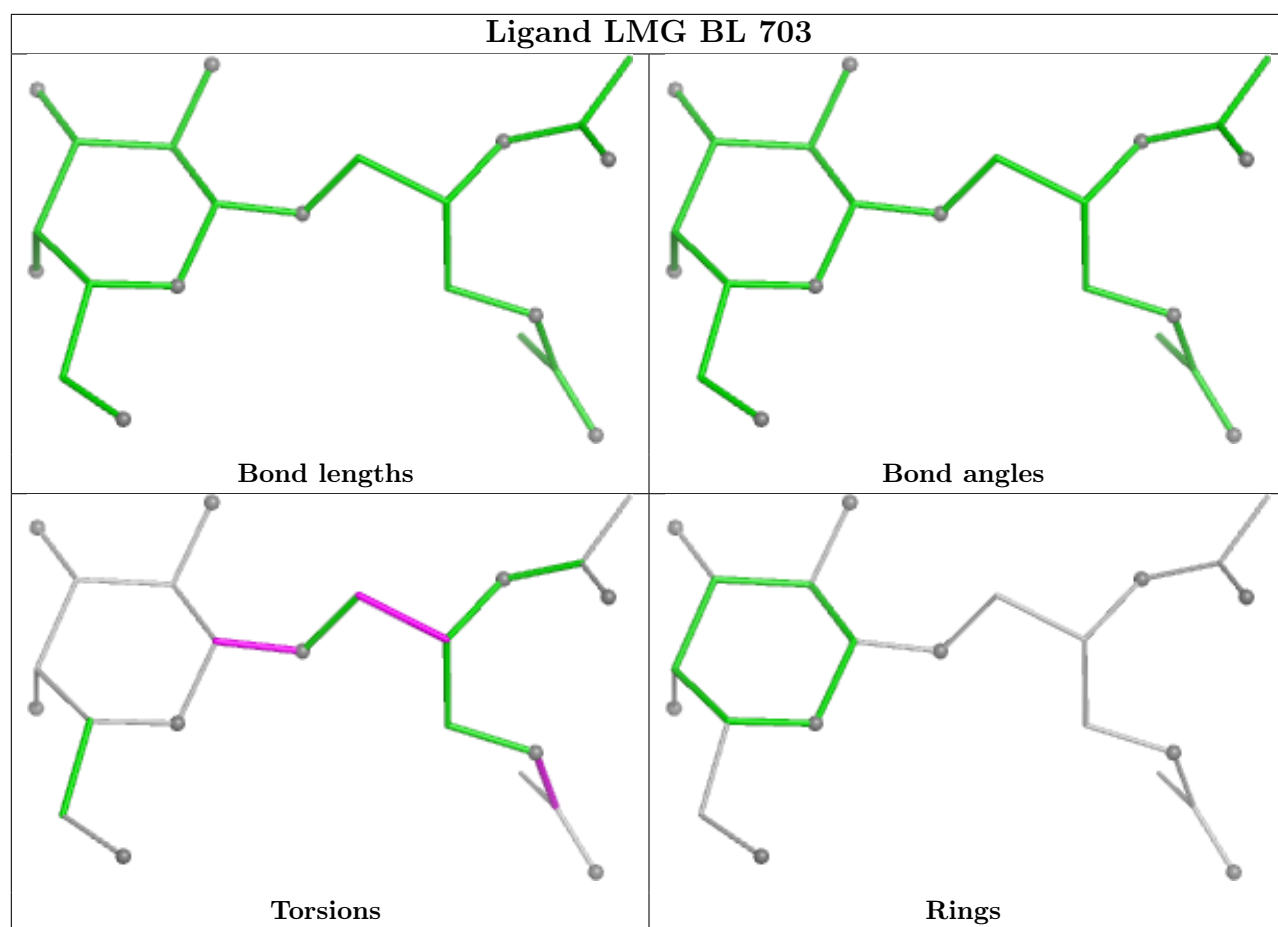
Rings

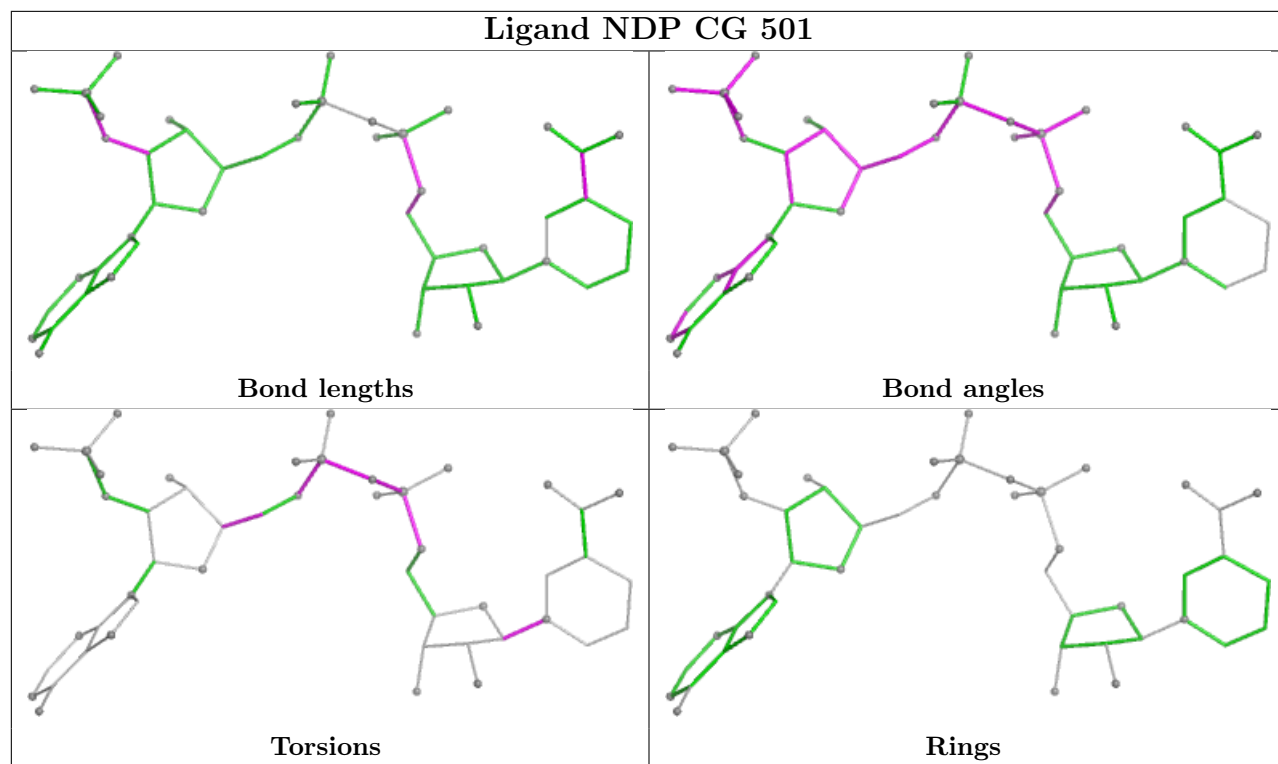
**Ligand A1JWG BD 503****Bond lengths****Bond angles****Torsions****Rings**



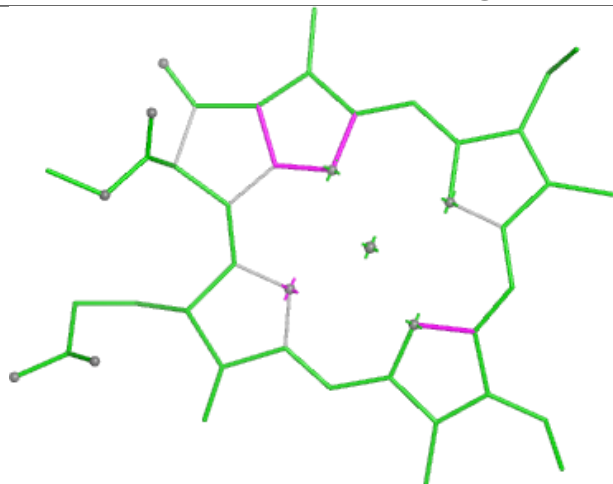
## Ligand A1JWG BK 503



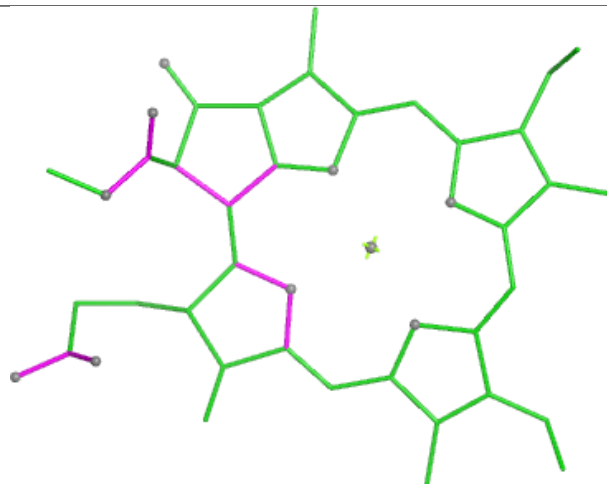




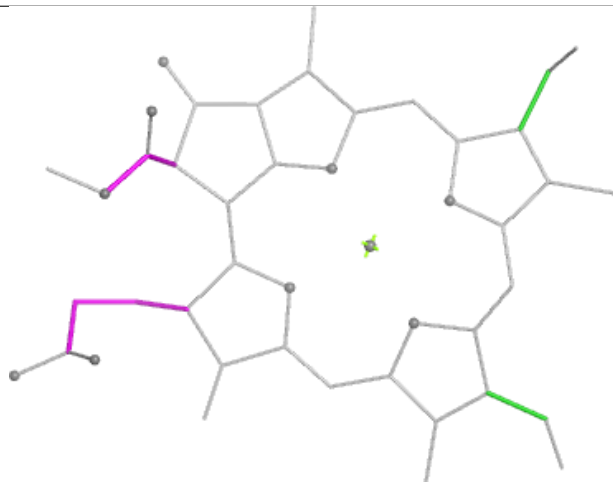
## Ligand A1JWG BE 503



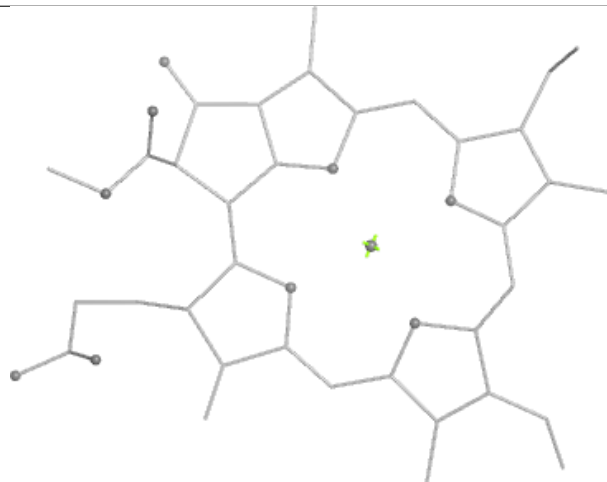
Bond lengths



Bond angles

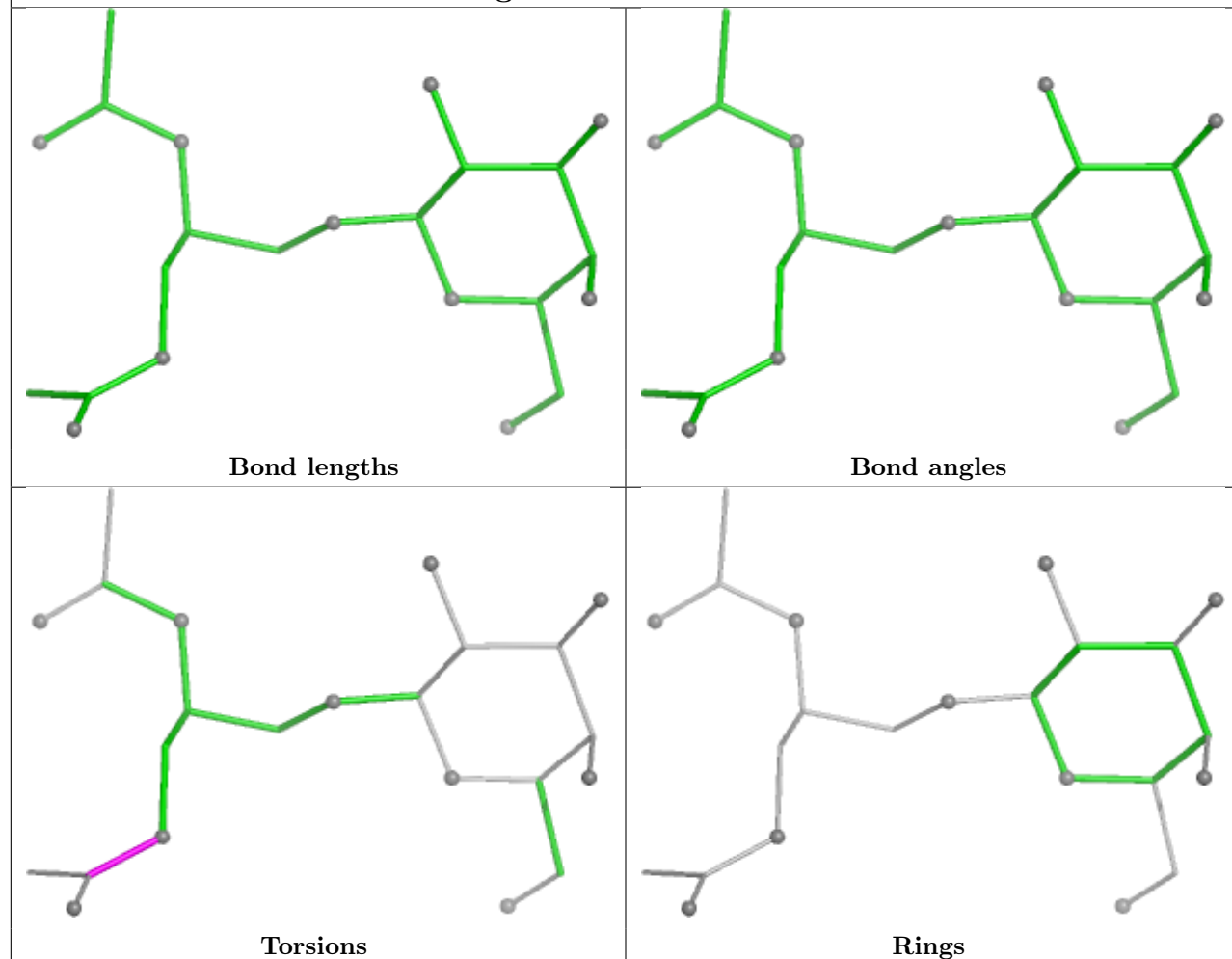


Torsions

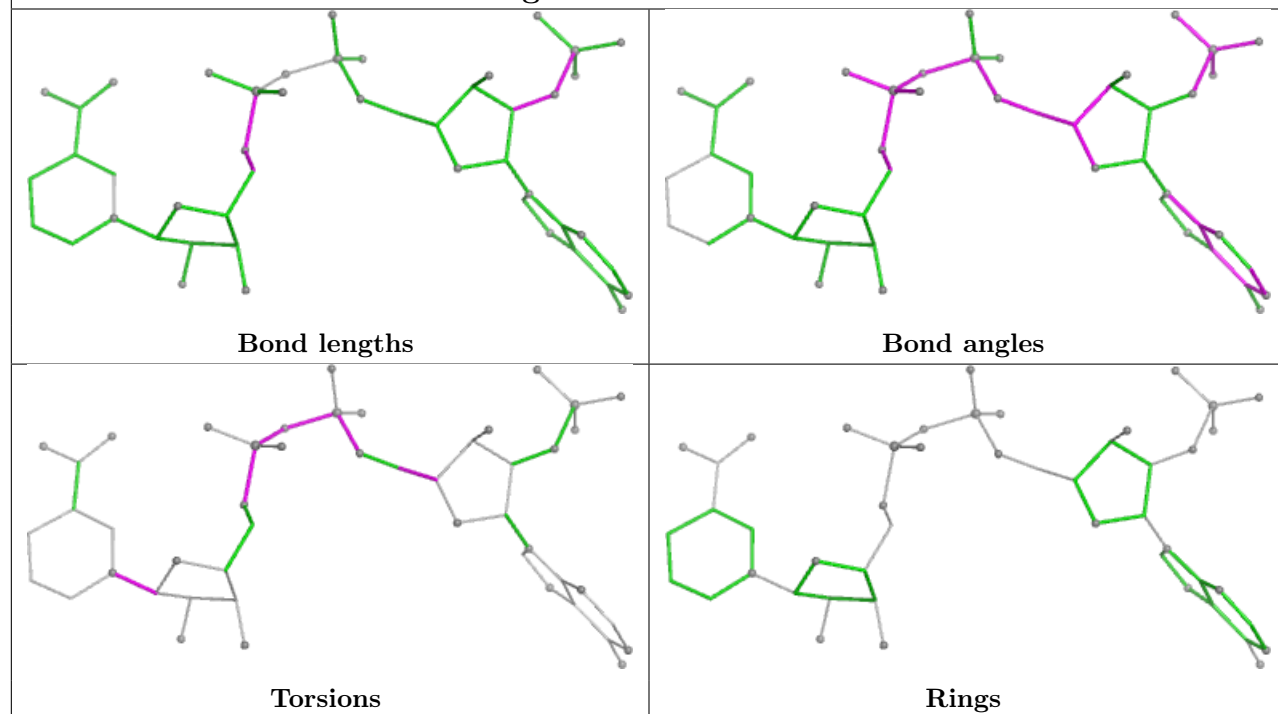


Rings

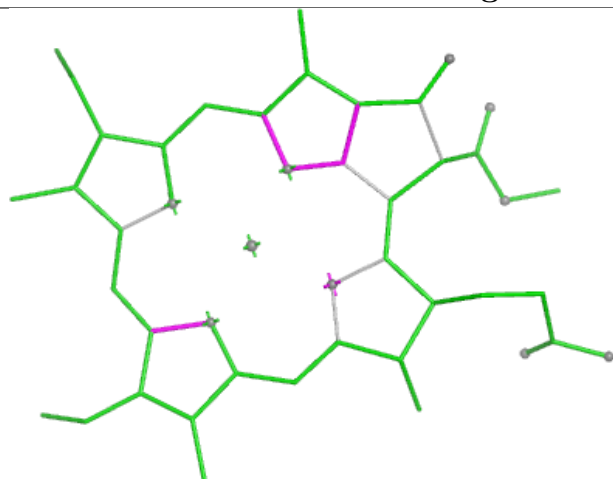
## Ligand LMG CA 702



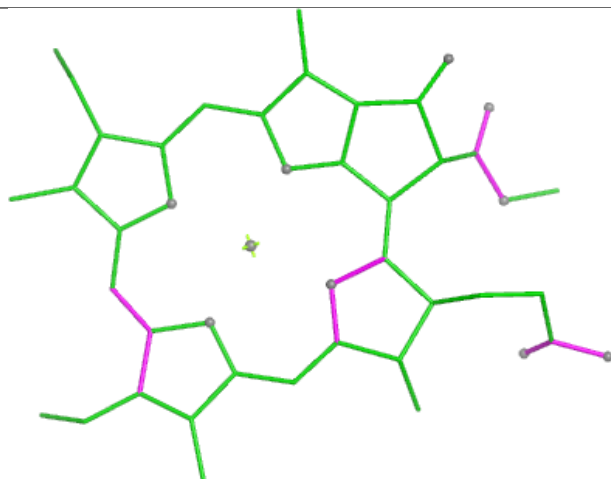
## Ligand NDP AI 501



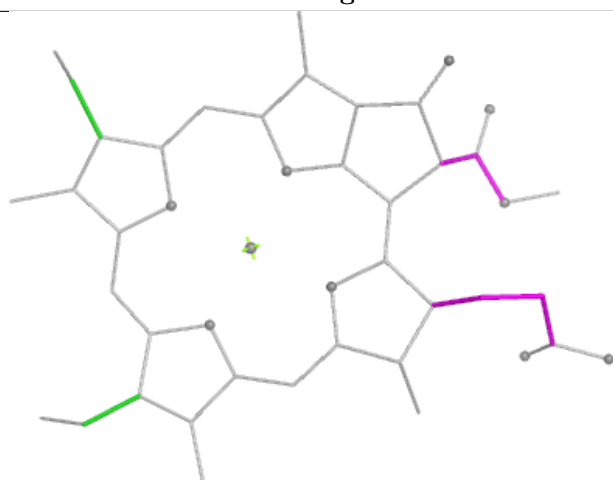
## Ligand A1JWG CI 502



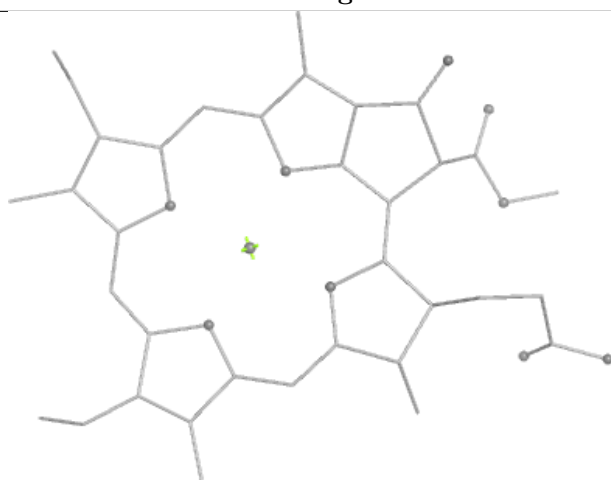
Bond lengths



Bond angles

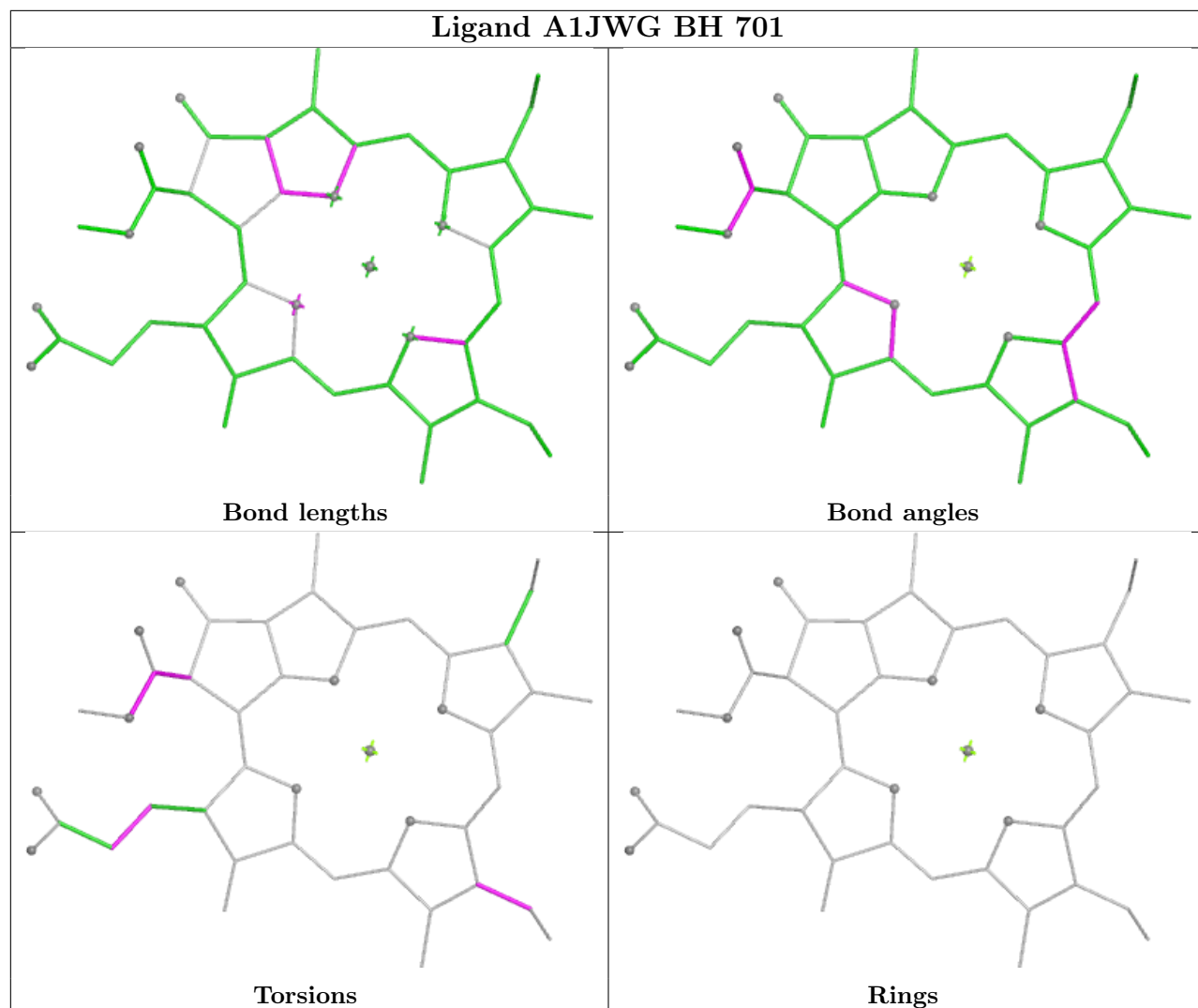


Torsions

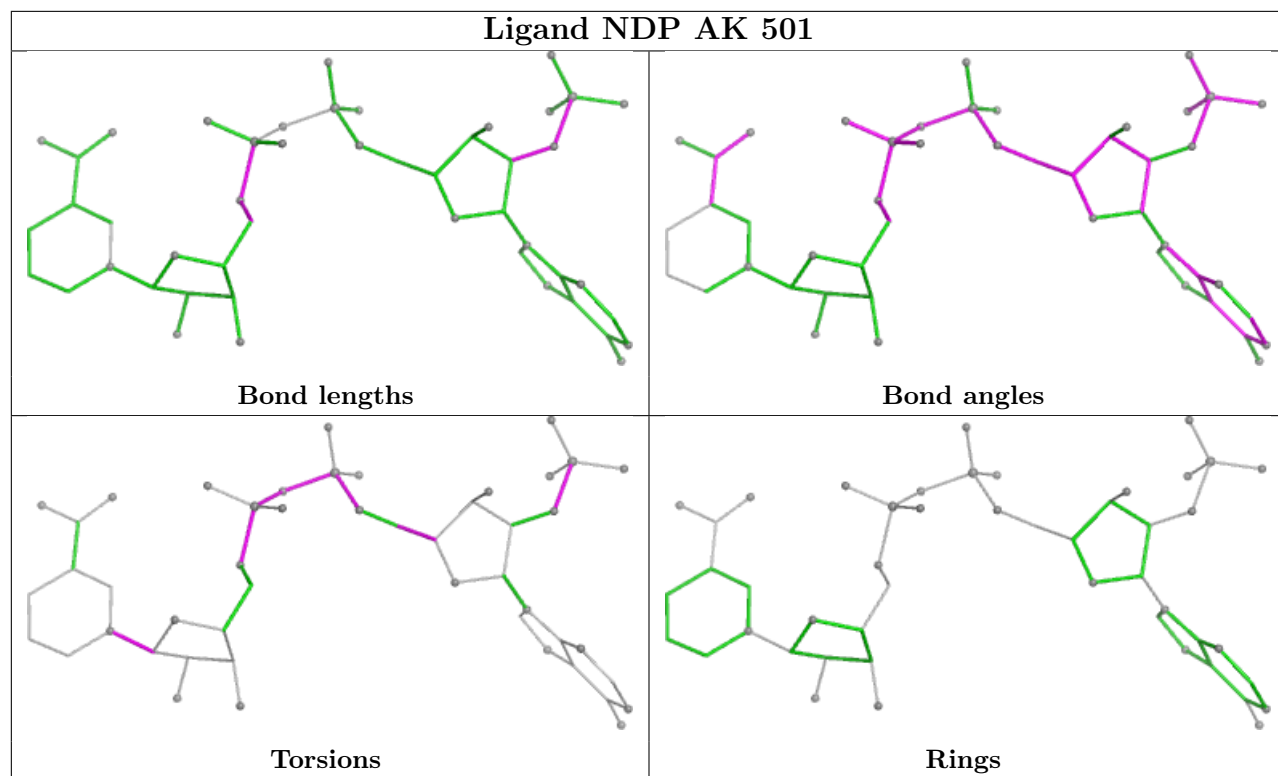


Rings

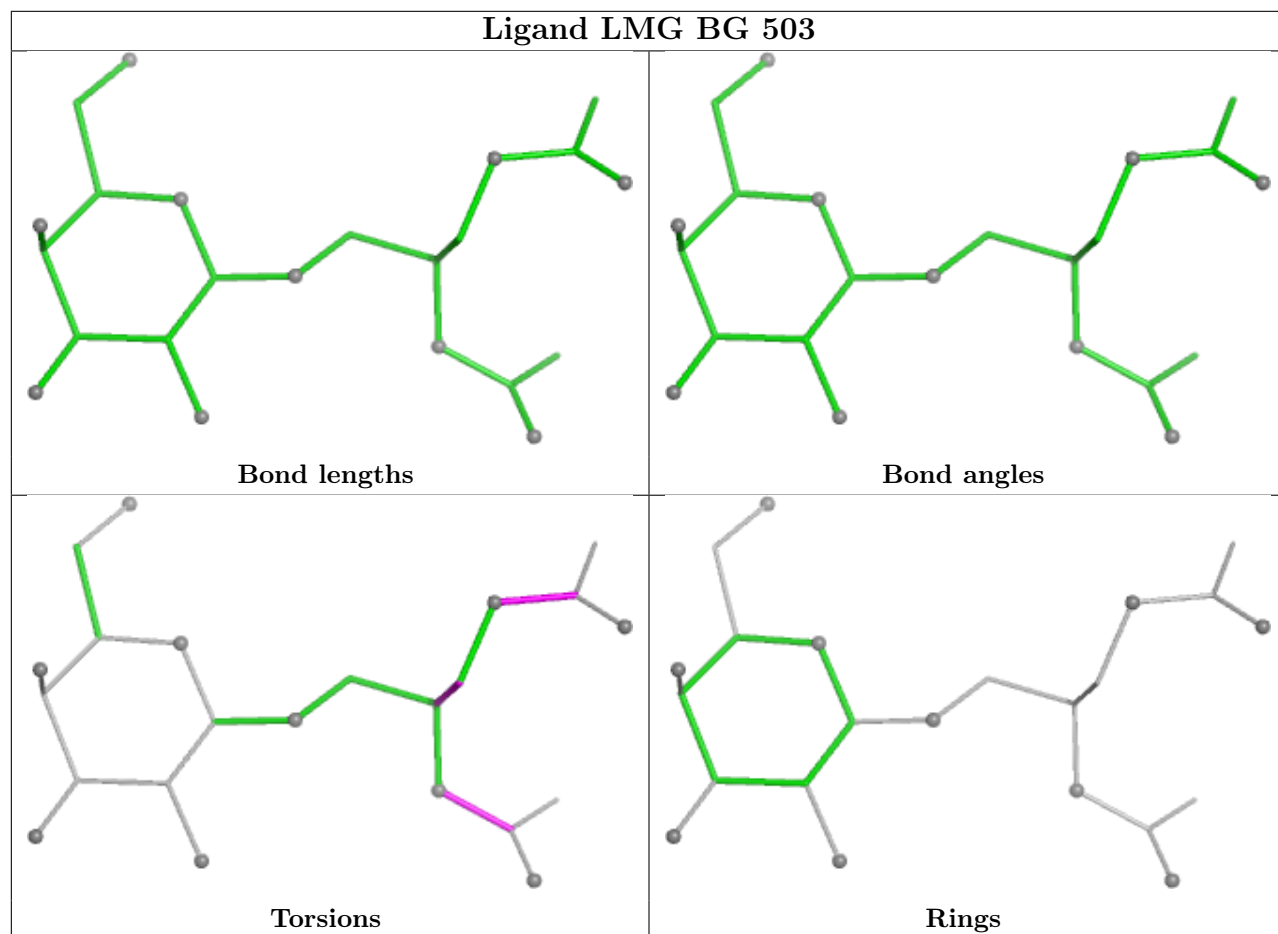
## Ligand A1JWG BH 701

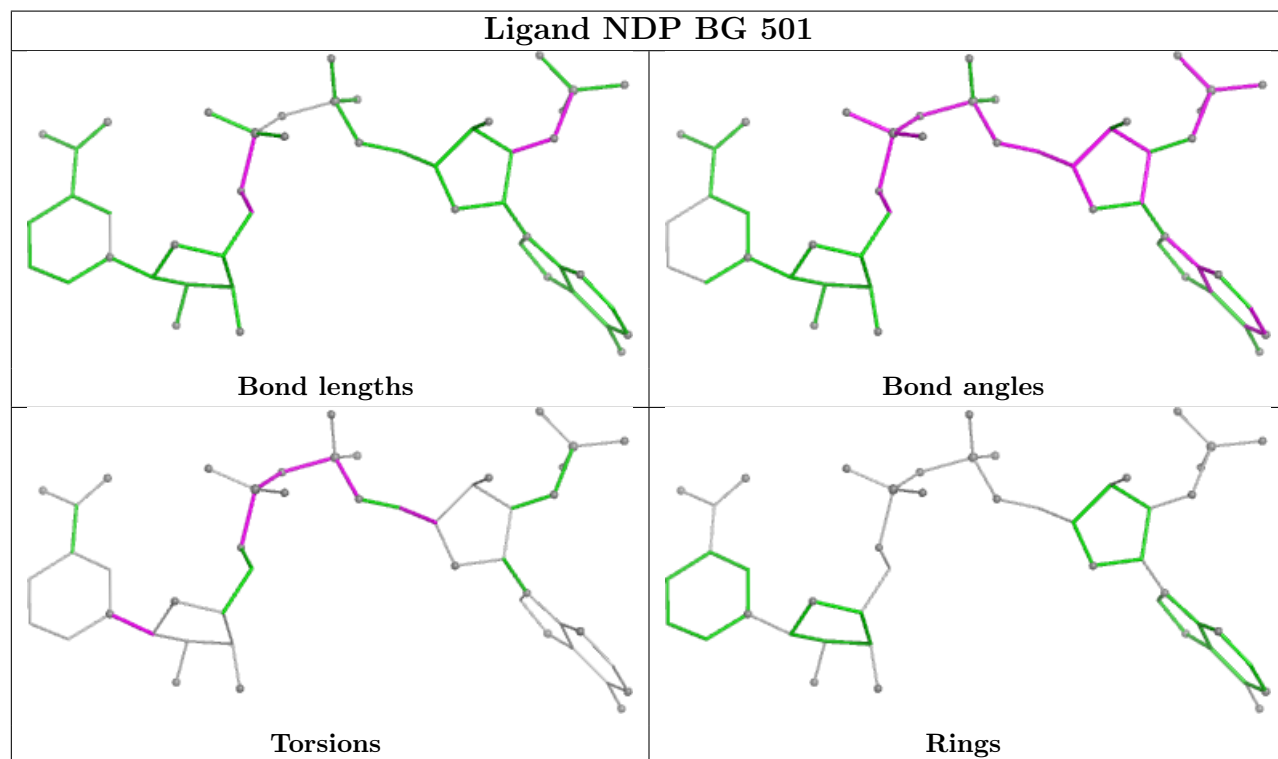
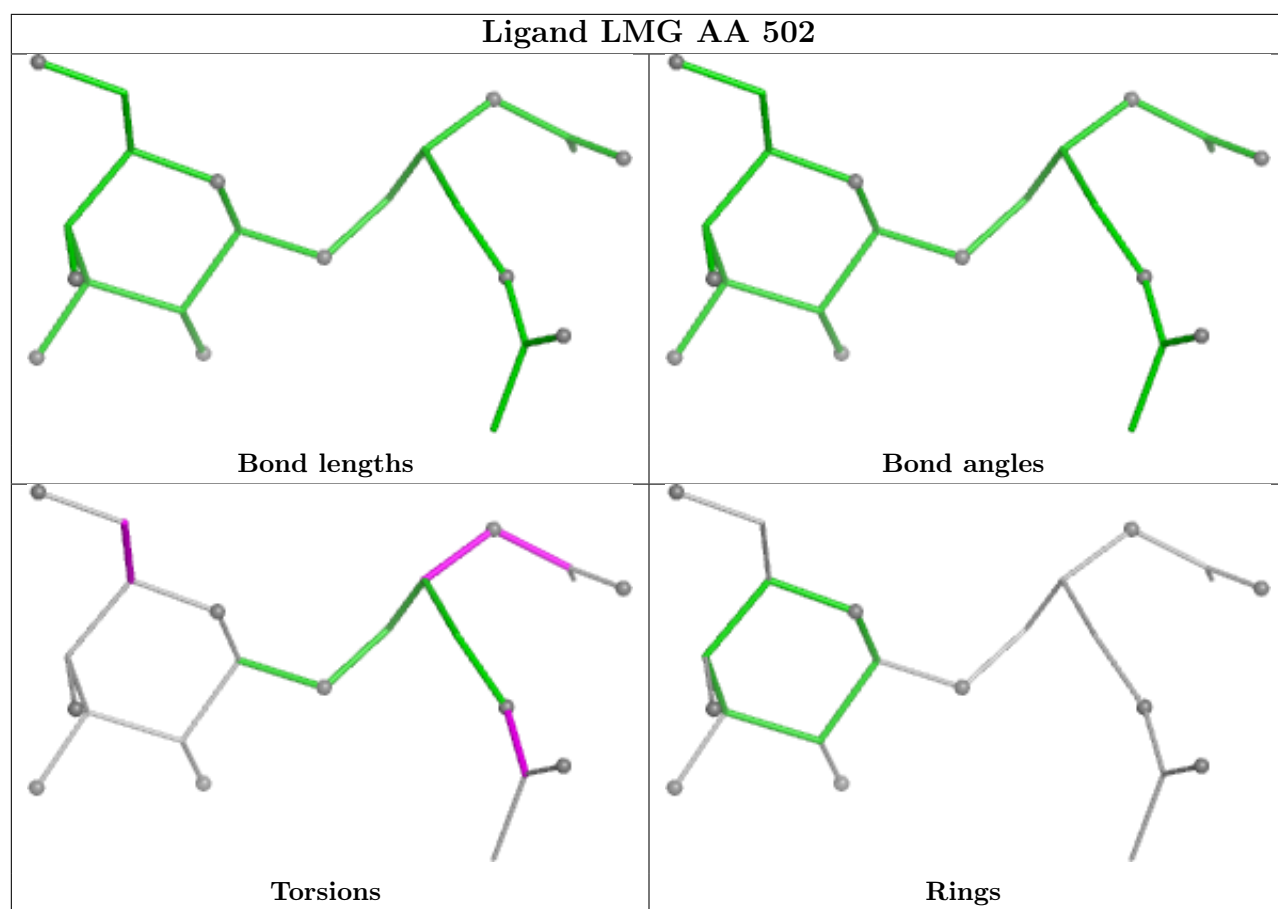


## Ligand NDP AK 501

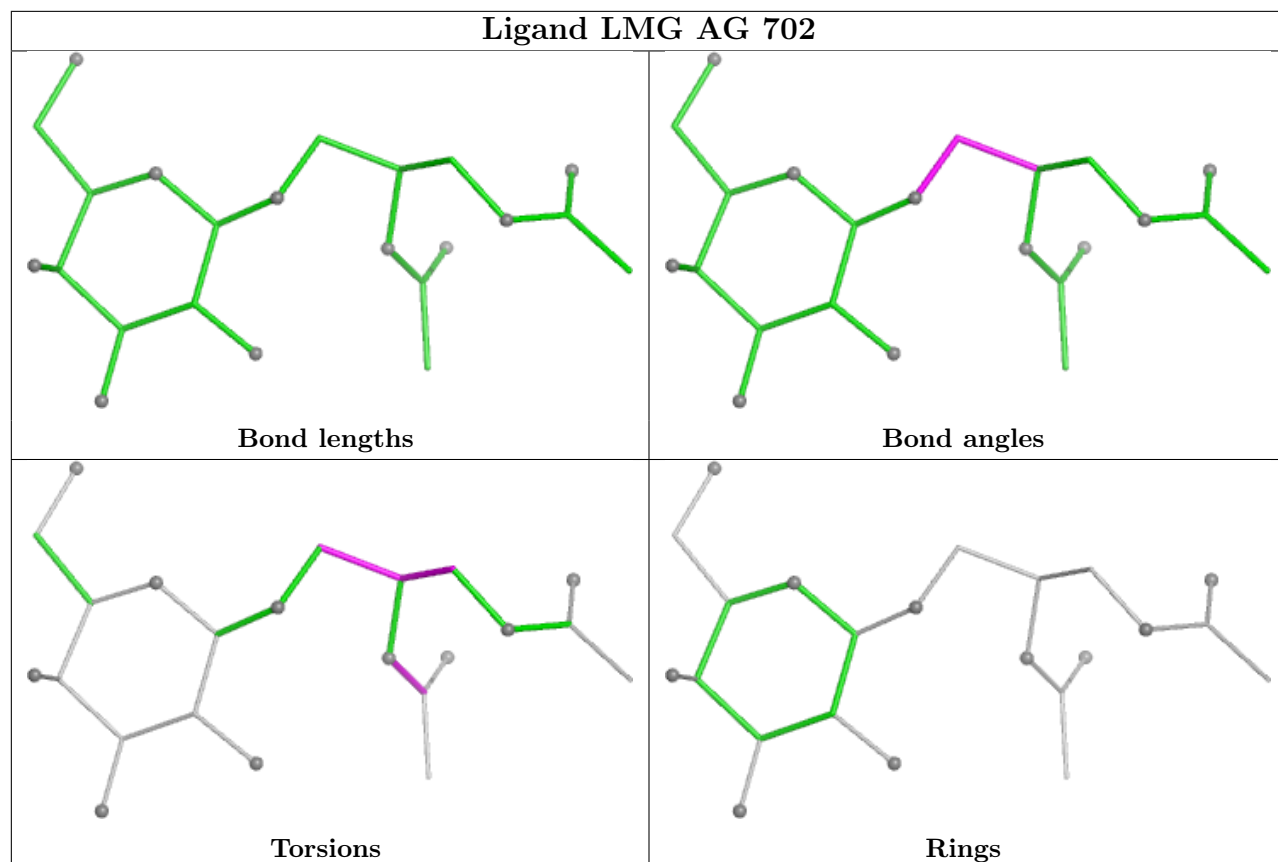


## Ligand LMG BG 503

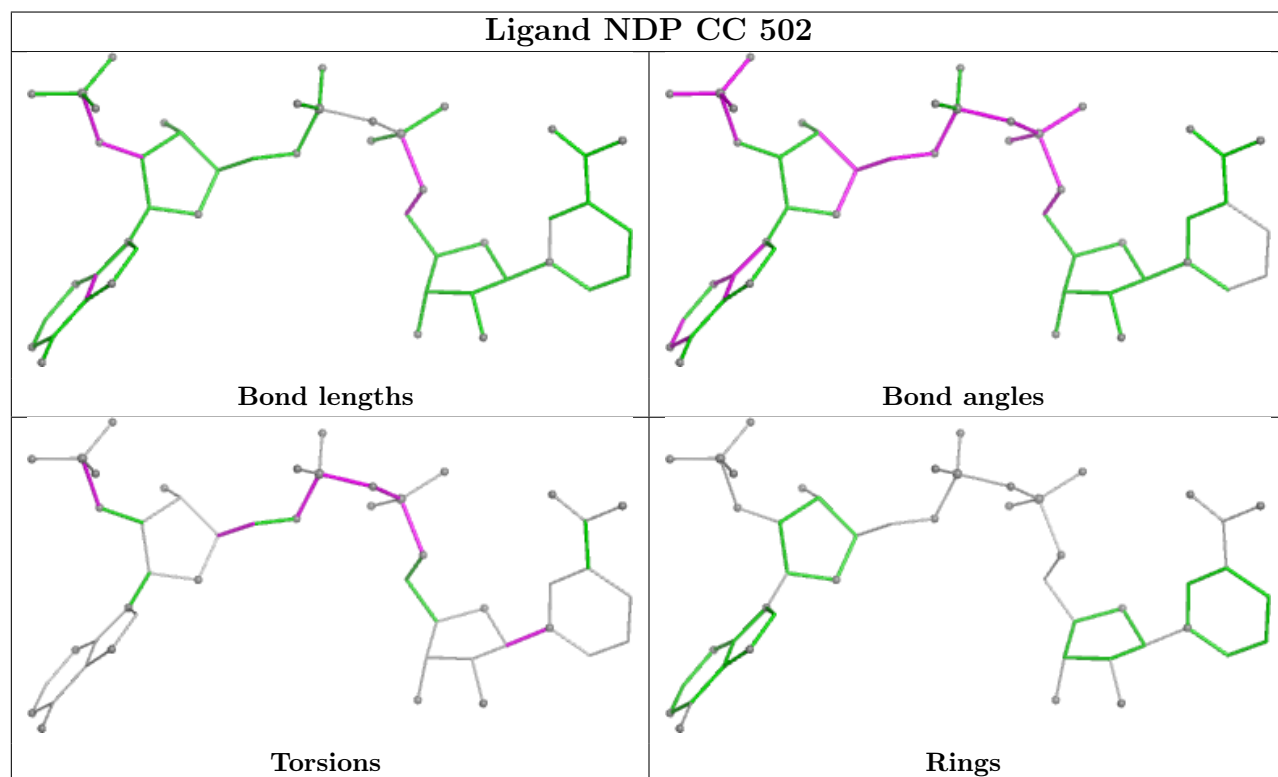




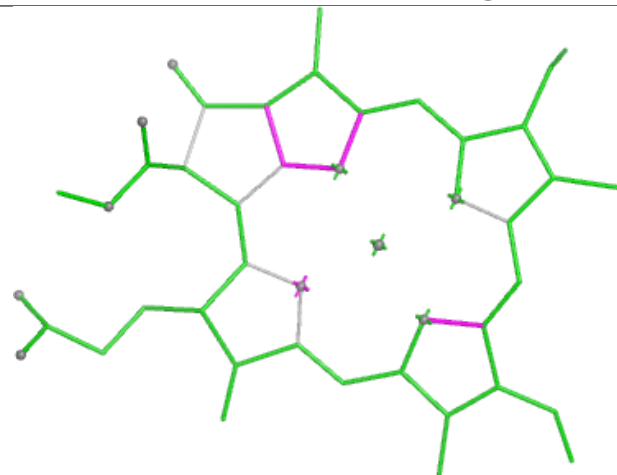
## Ligand LMG AG 702



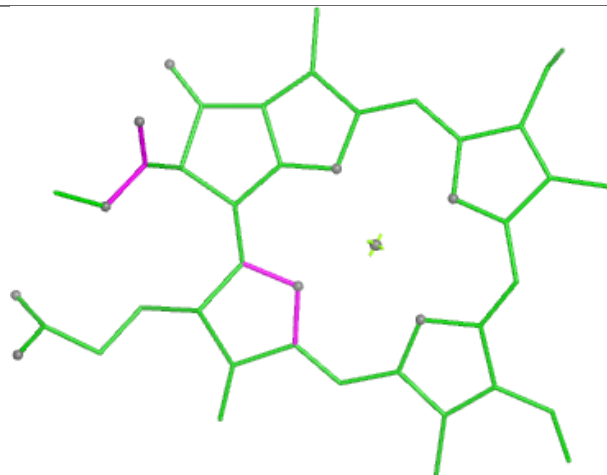
## Ligand NDP CC 502



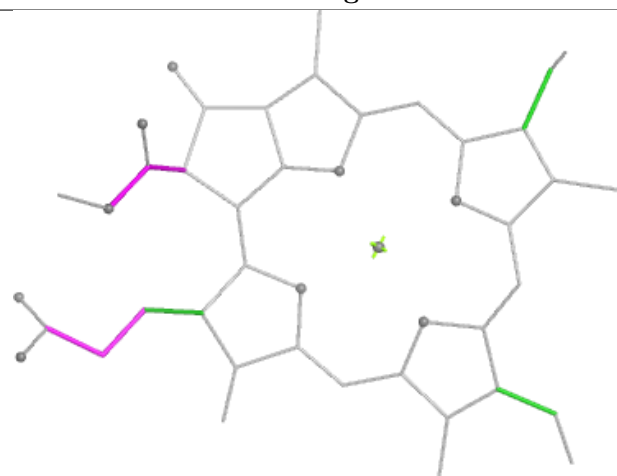
## Ligand A1JWG AE 701



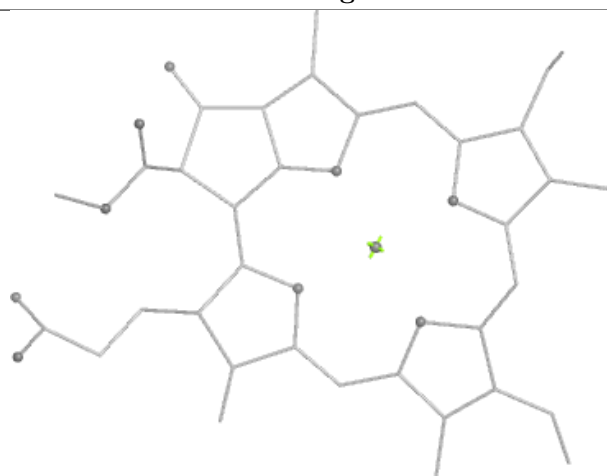
Bond lengths



Bond angles

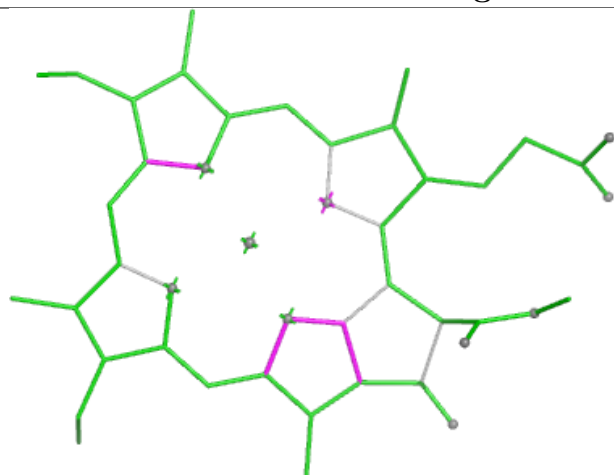


Torsions

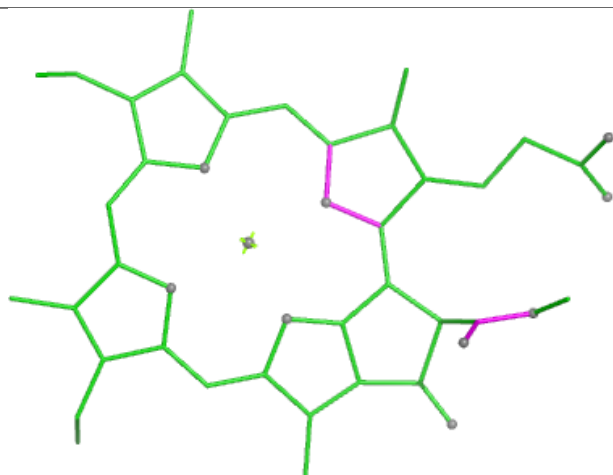


Rings

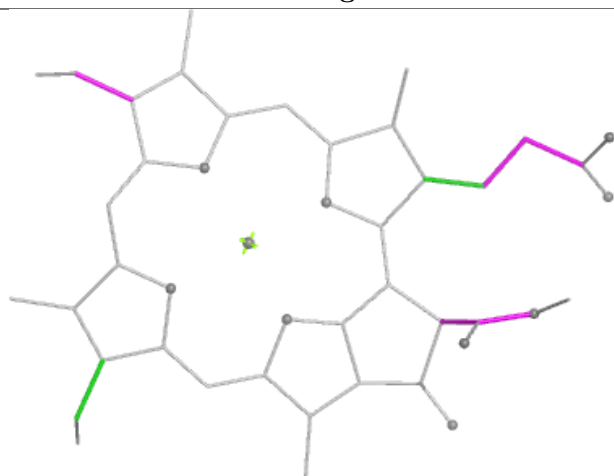
## Ligand A1JWG CH 503



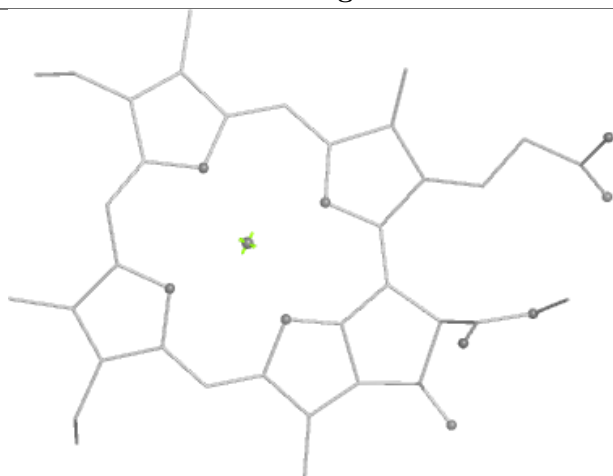
Bond lengths



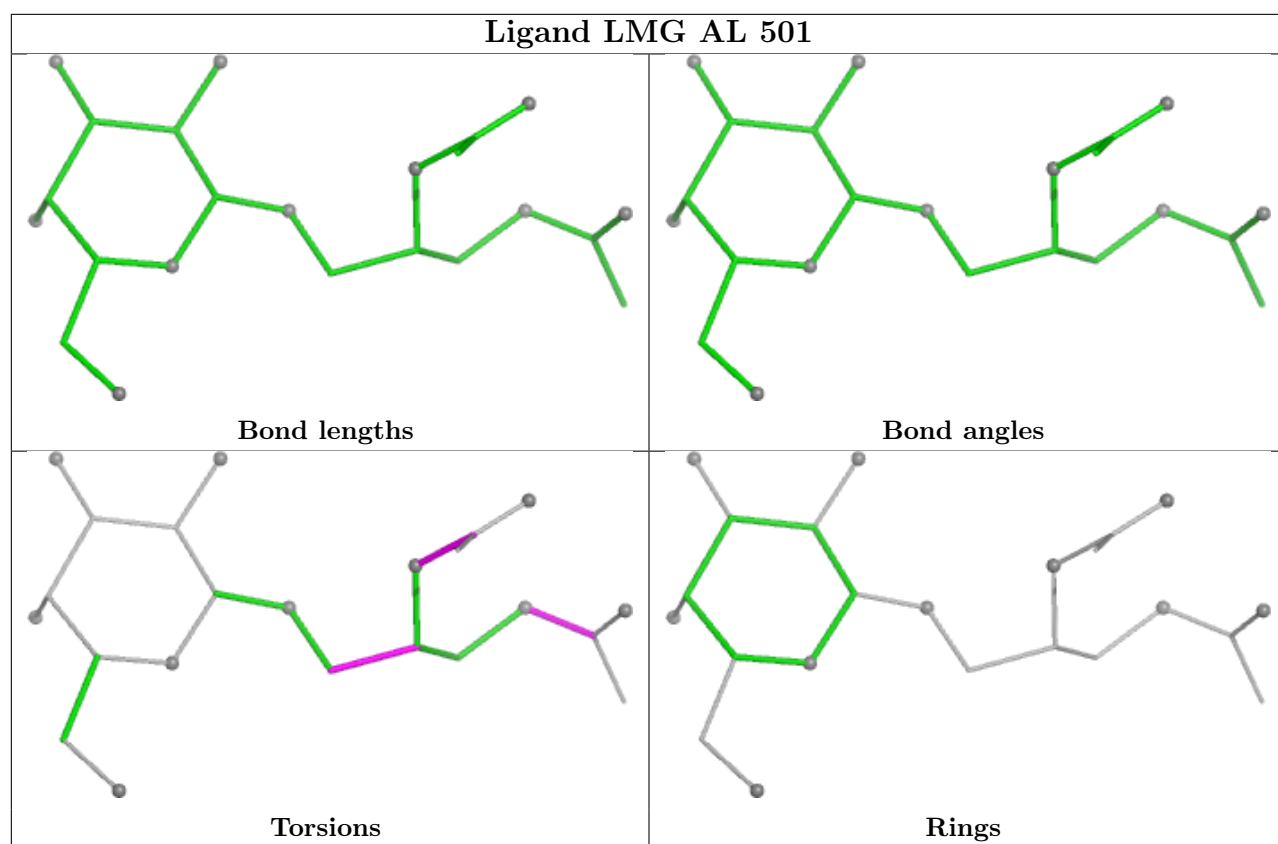
Bond angles



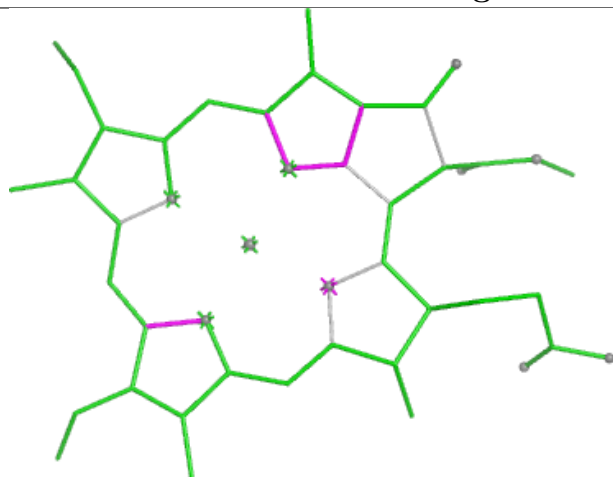
Torsions



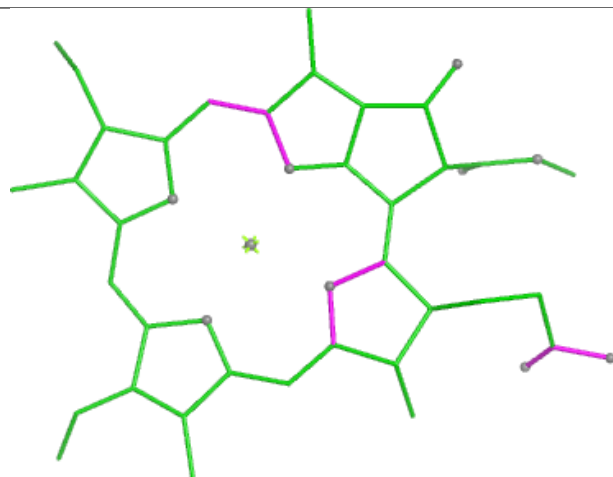
Rings



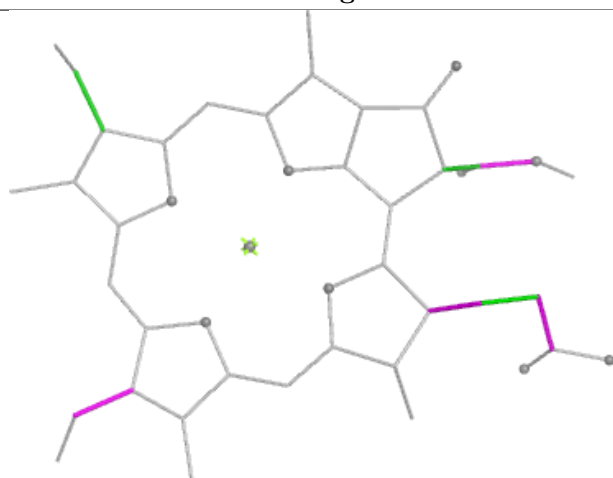
## Ligand A1JWG AK 503



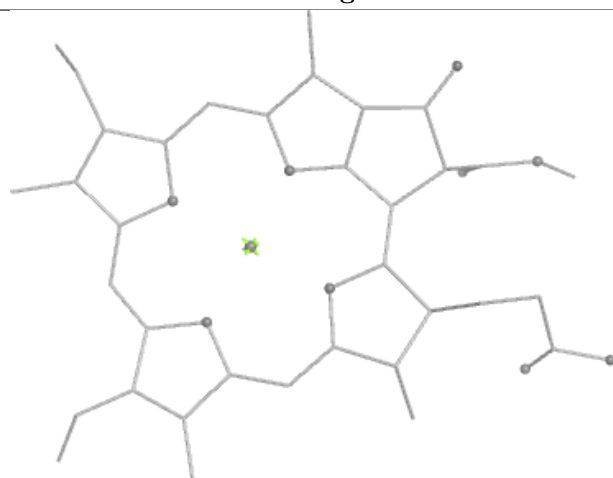
Bond lengths



Bond angles

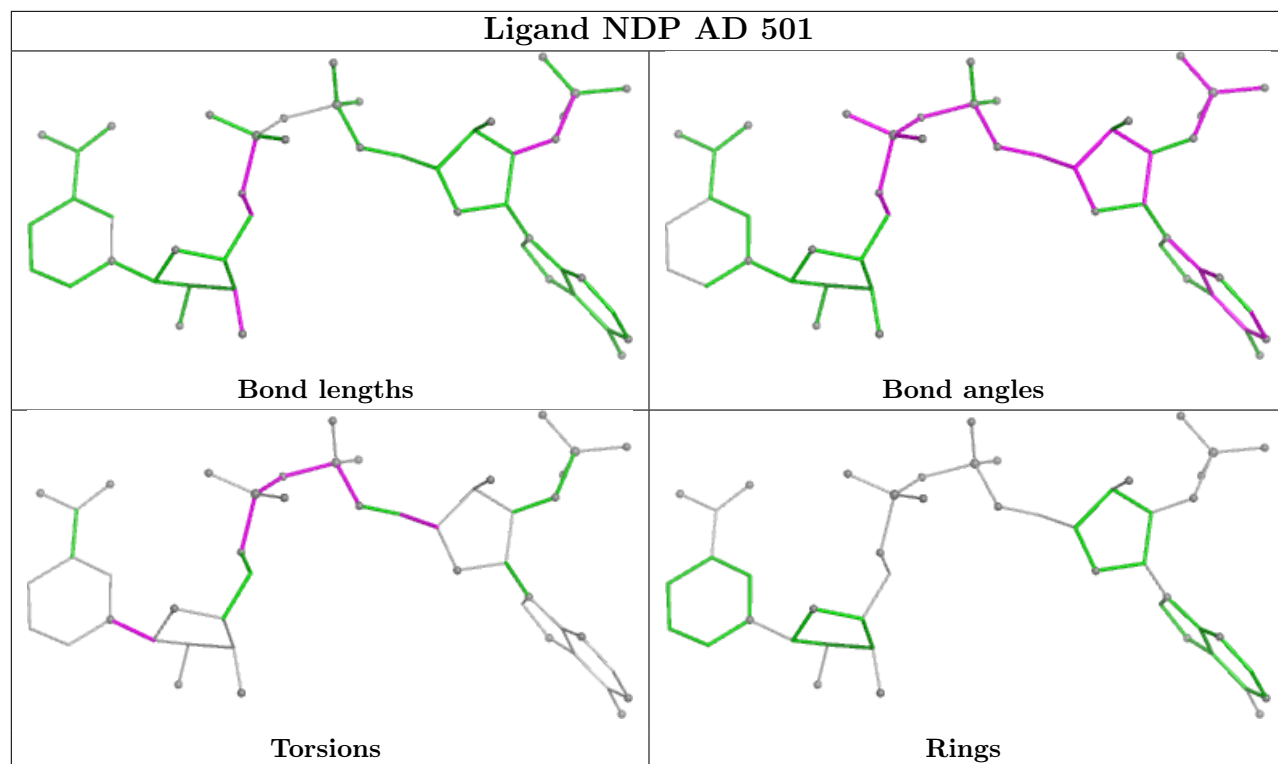


Torsions

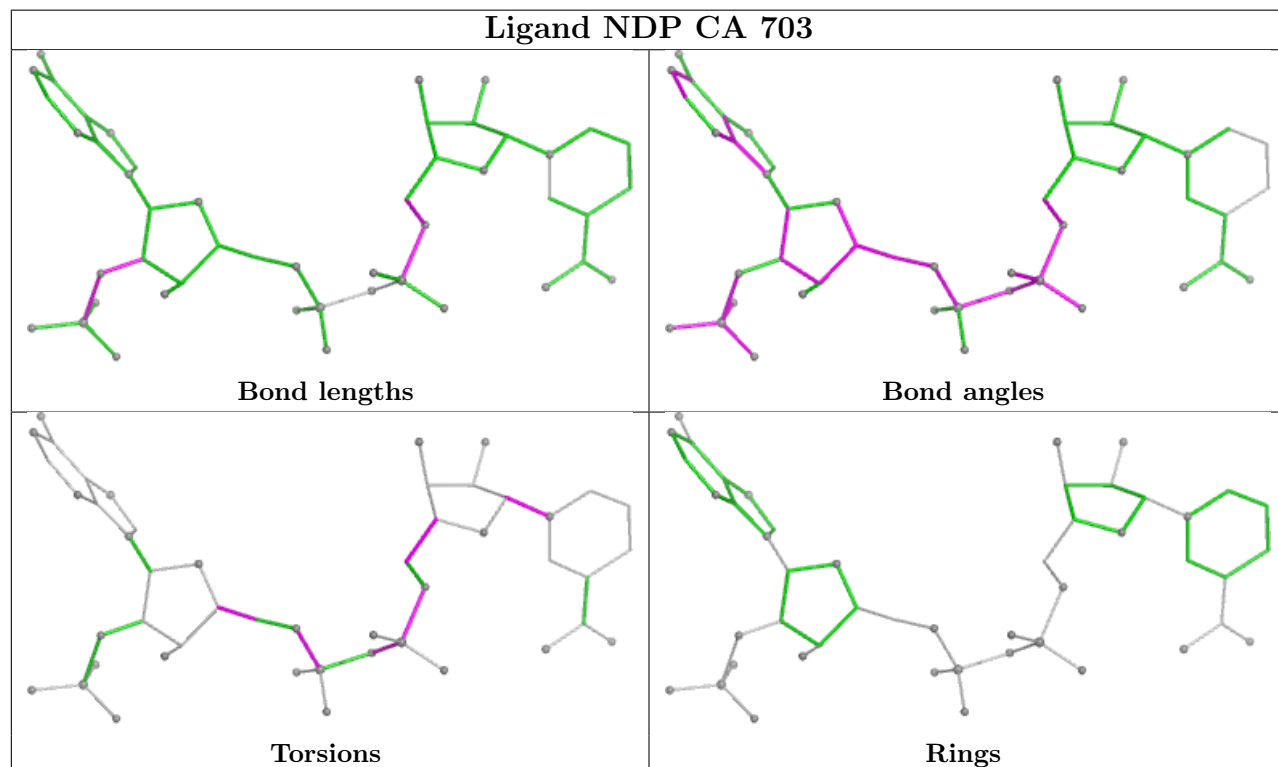


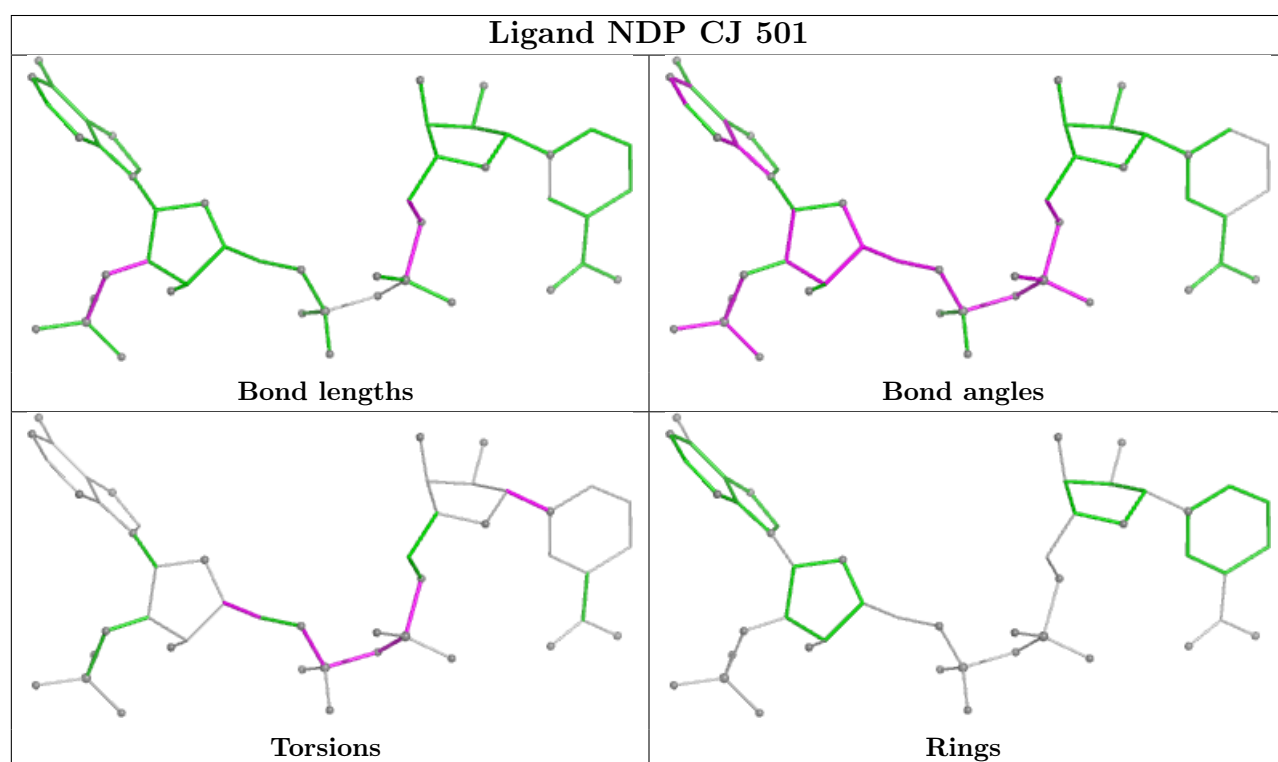
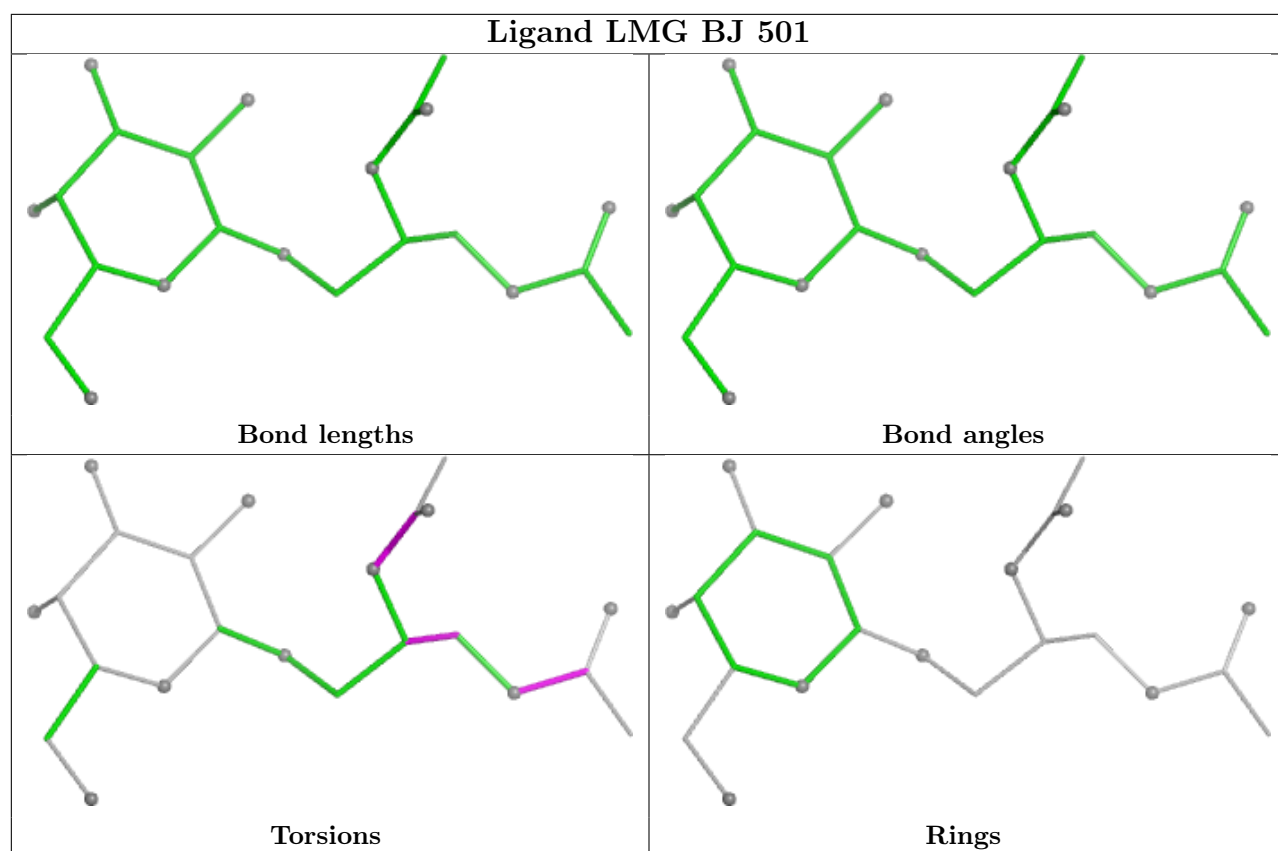
Rings

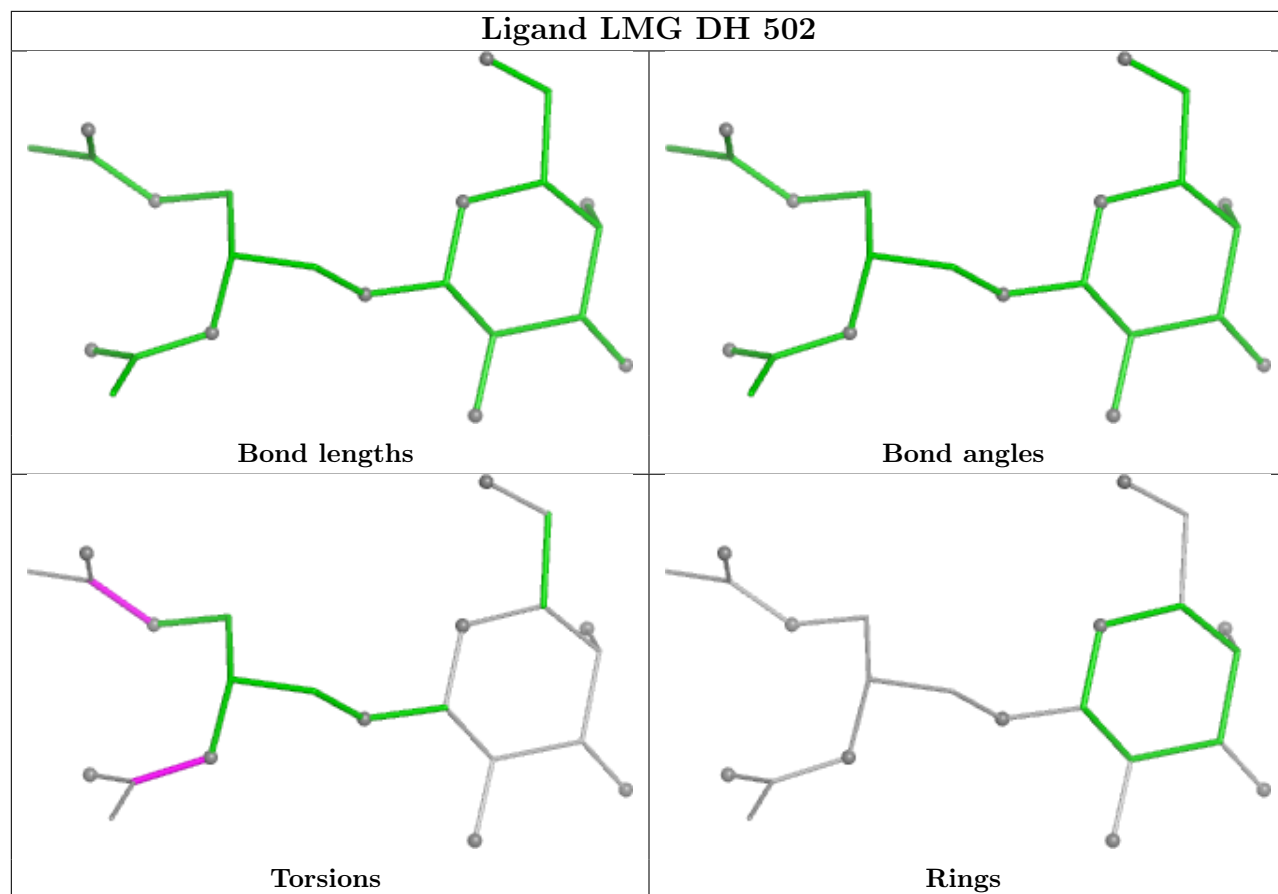
## Ligand NDP AD 501



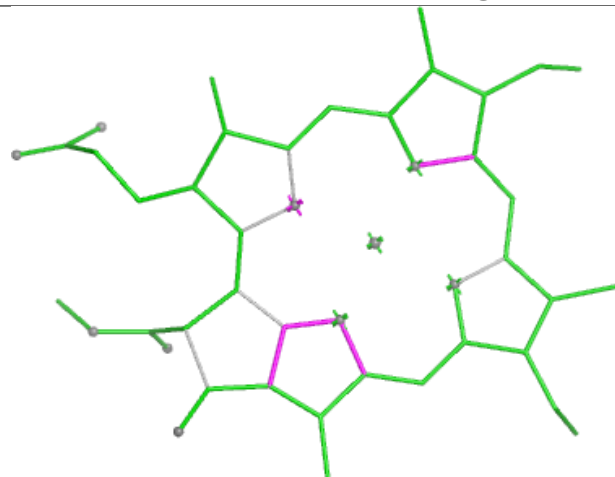
## Ligand NDP CA 703



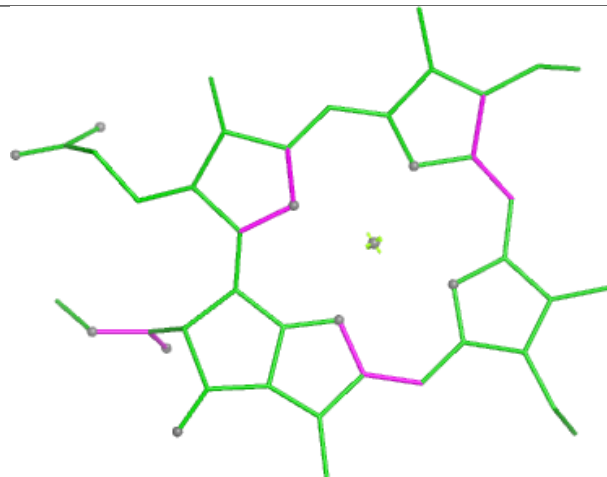




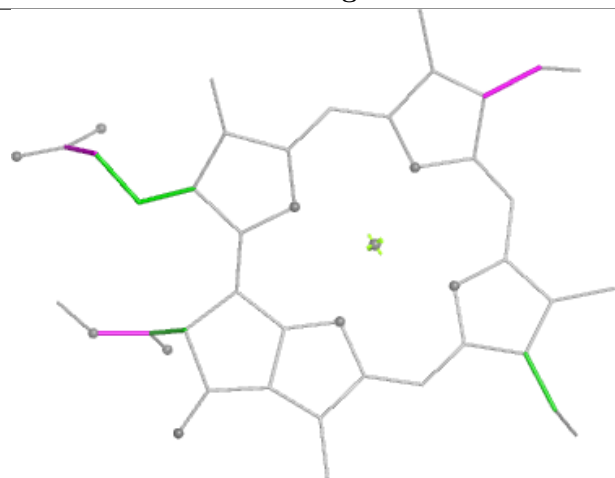
## Ligand A1JWG DG 502



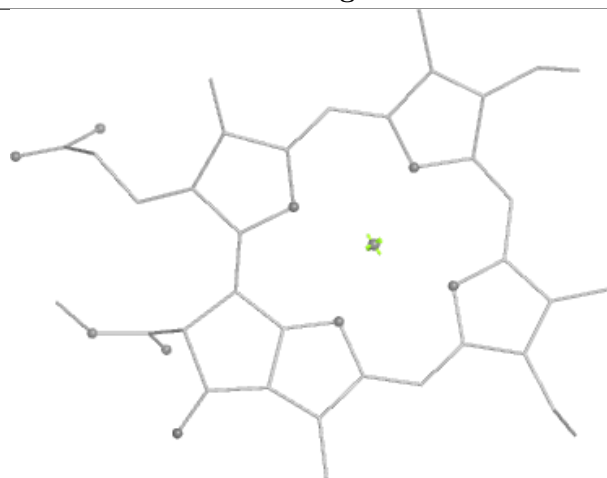
Bond lengths



Bond angles

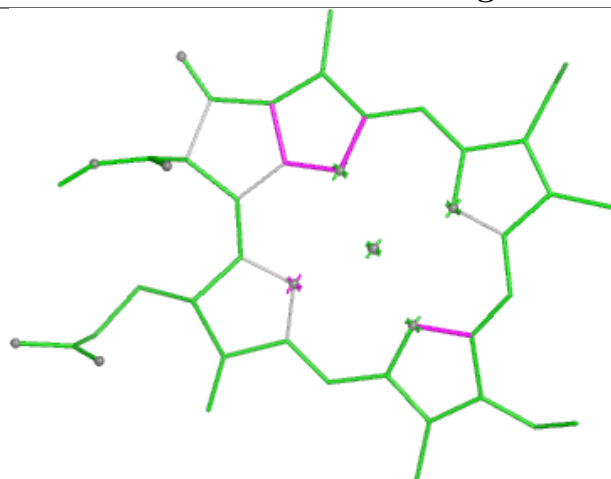


Torsions

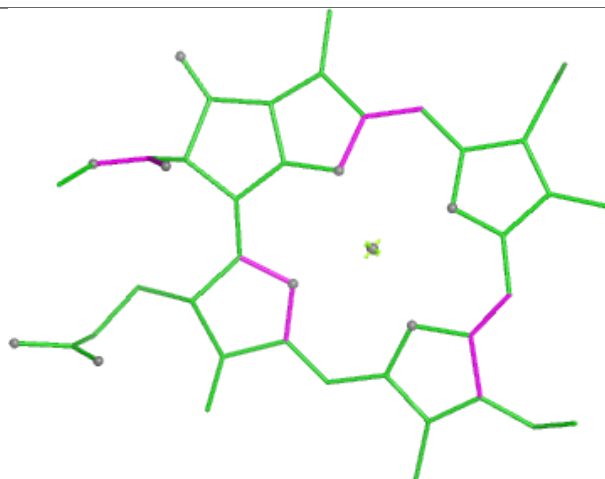


Rings

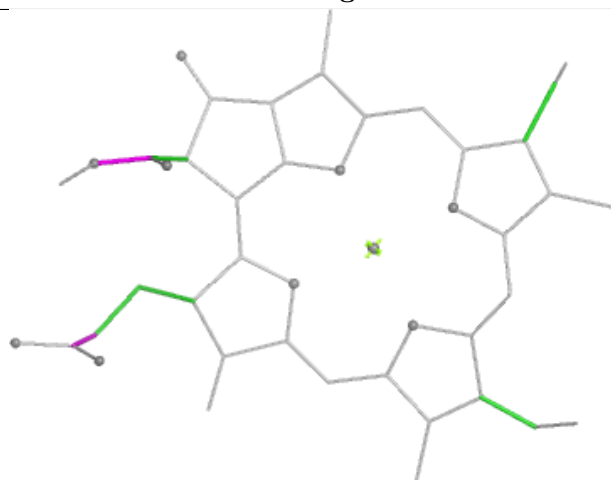
## Ligand A1JWG BL 701



Bond lengths



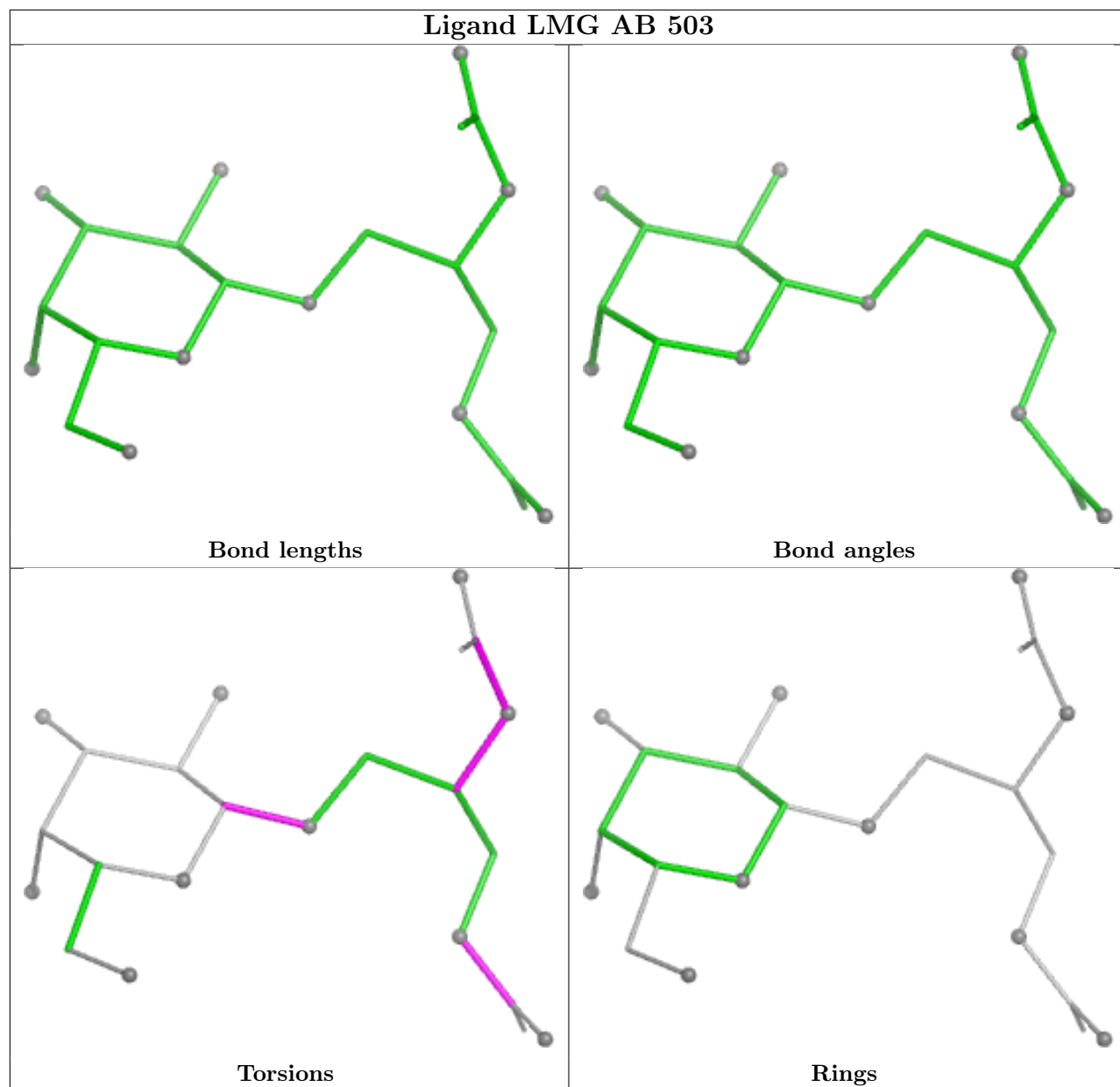
Bond angles

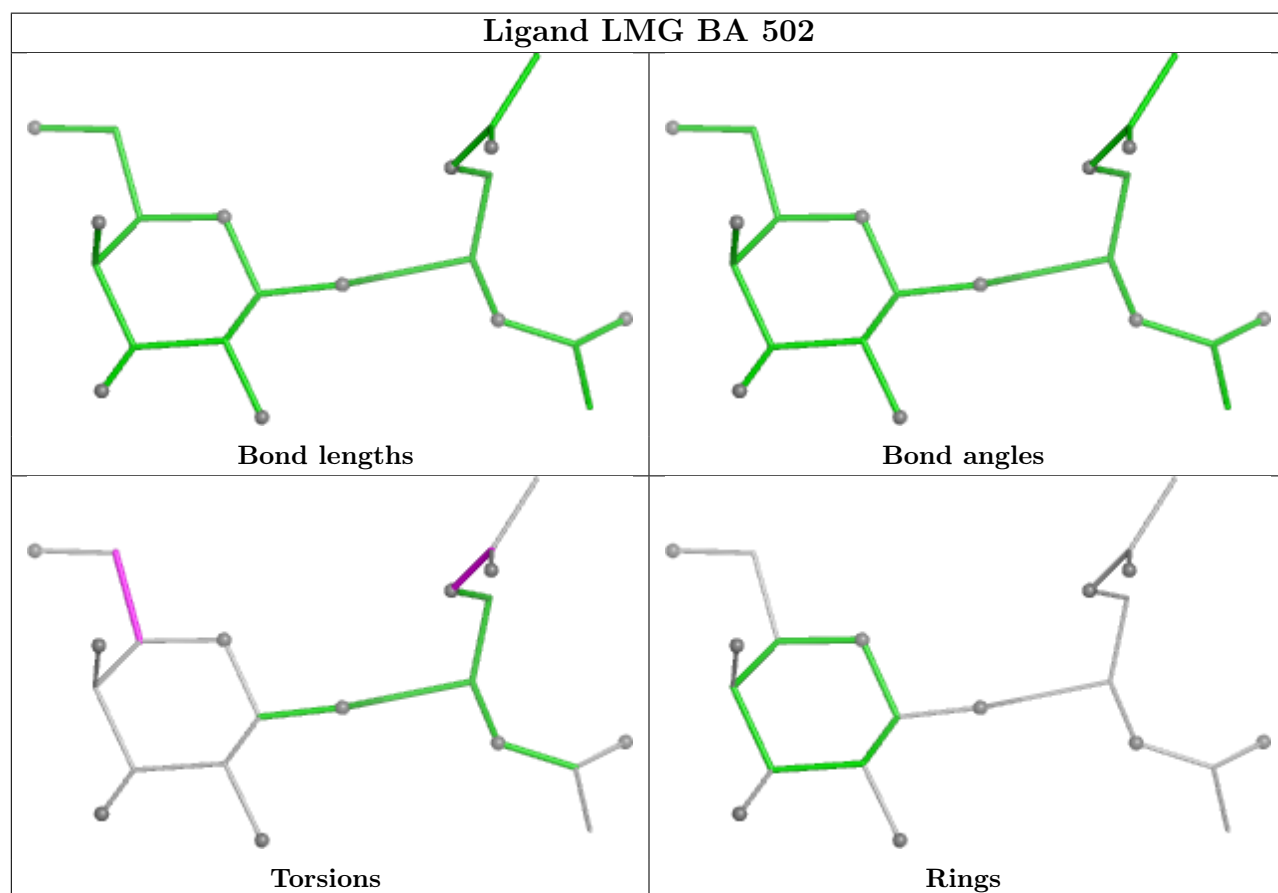
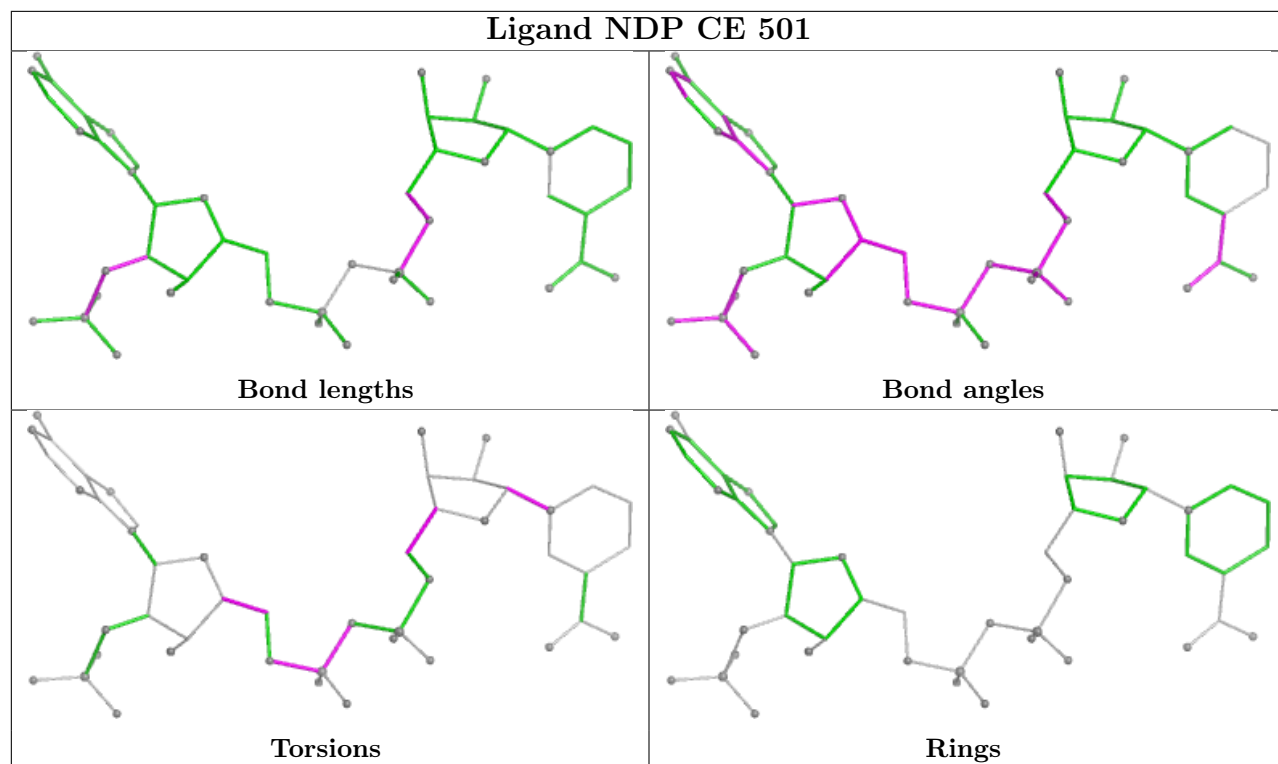


Torsions

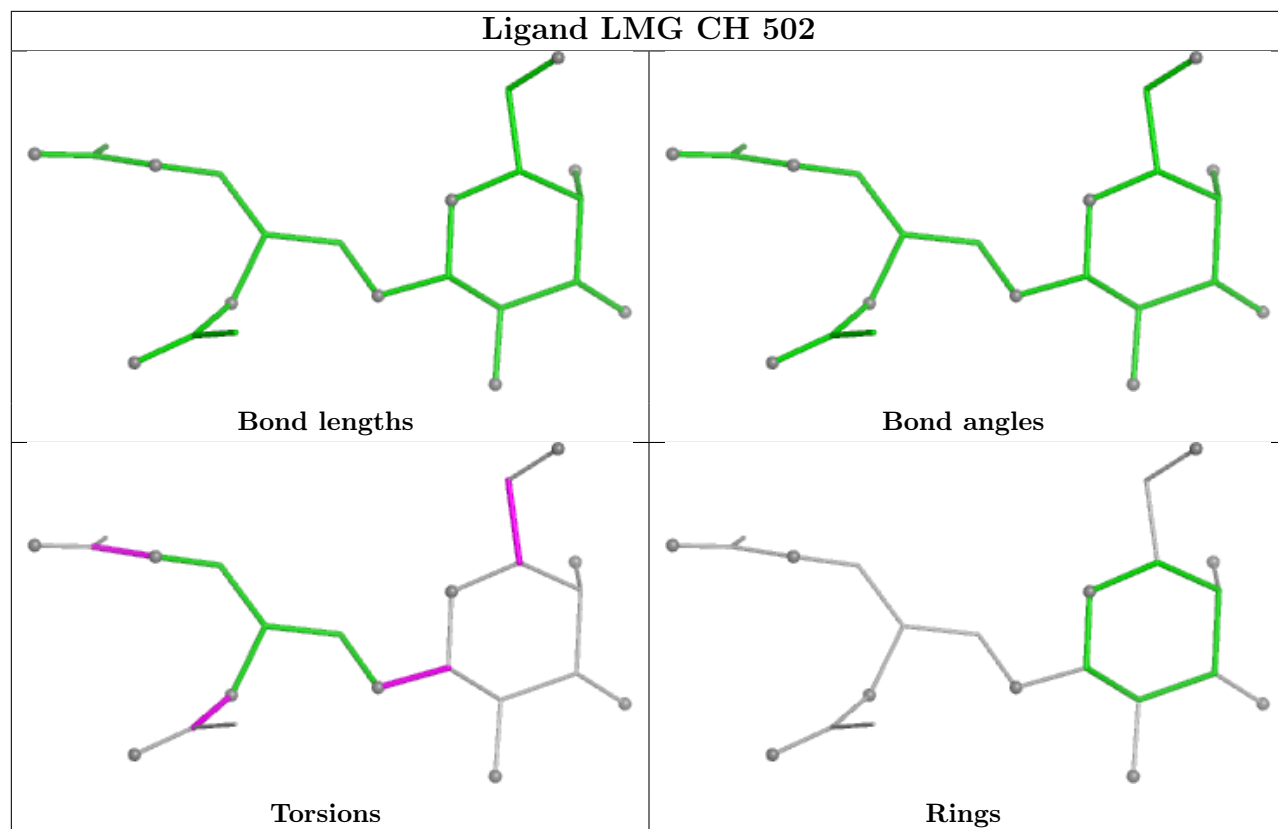


Rings

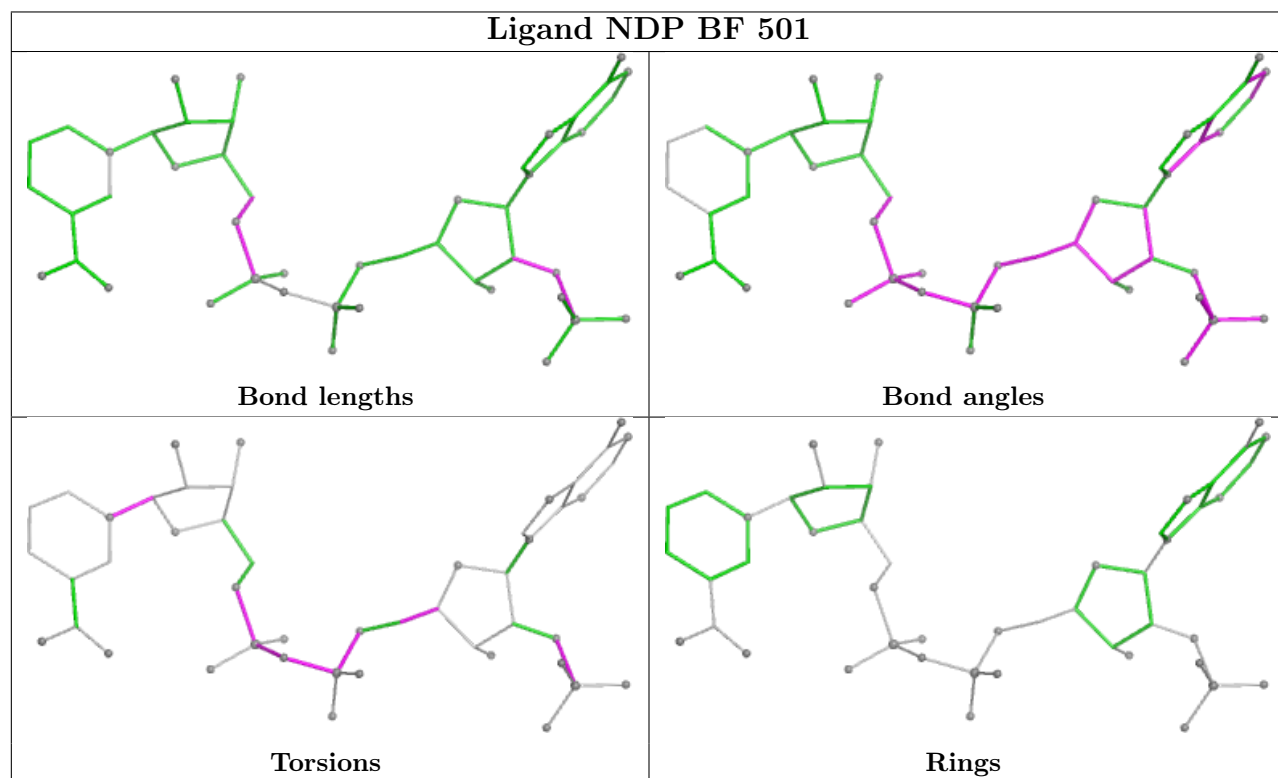




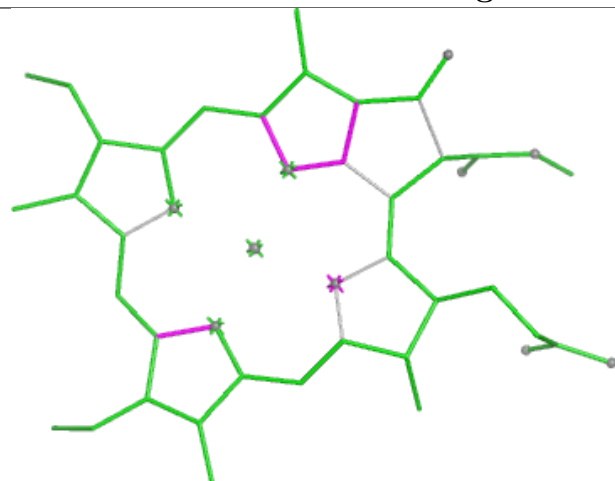
## Ligand LMG CH 502



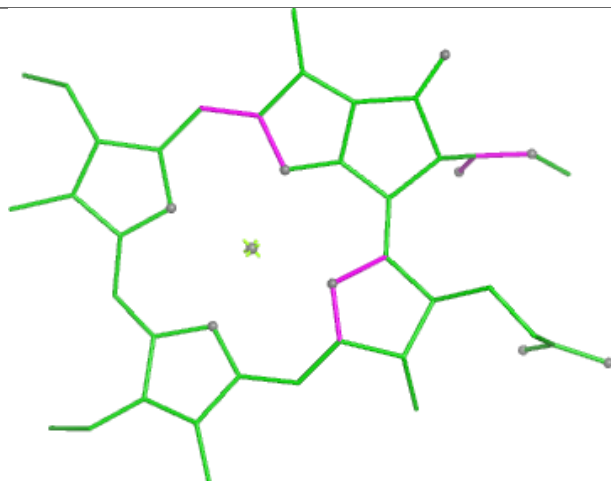
## Ligand NDP BF 501



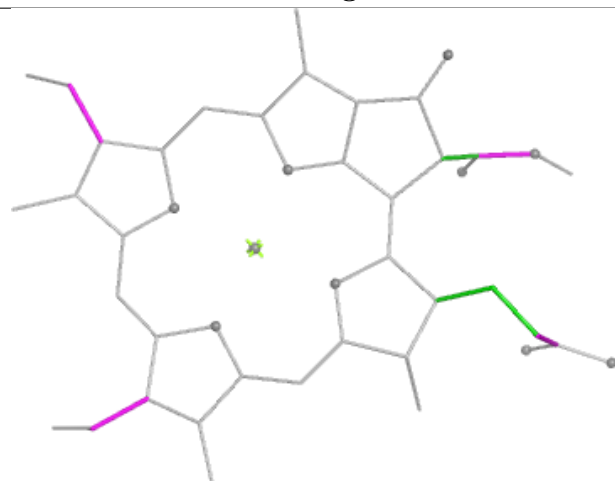
## Ligand A1JWG CA 701



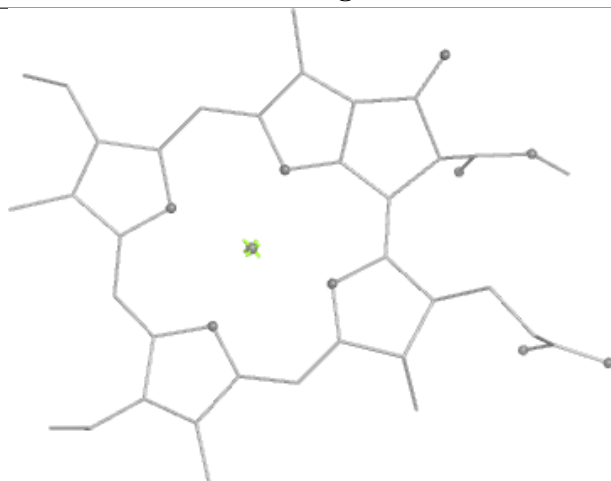
Bond lengths



Bond angles

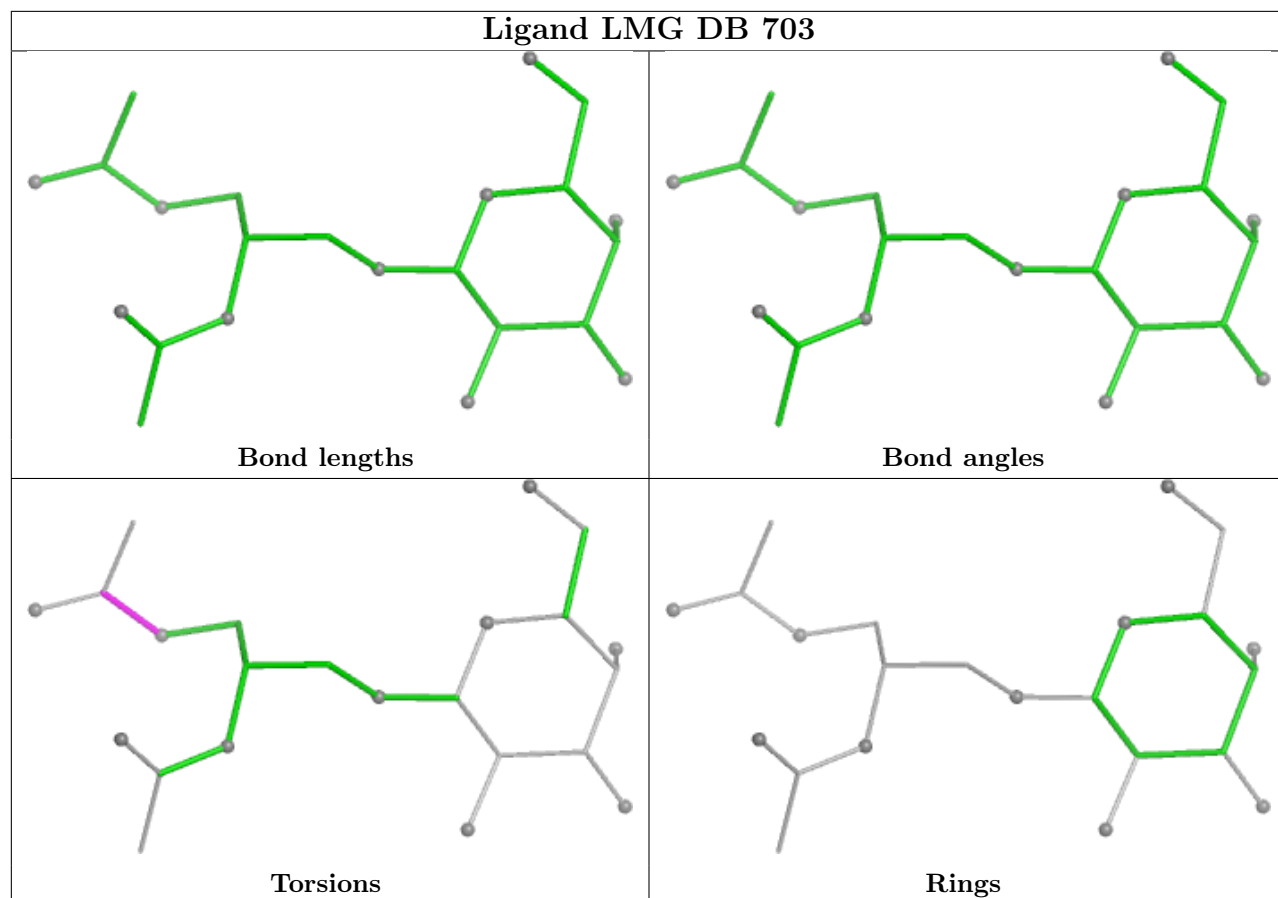


Torsions

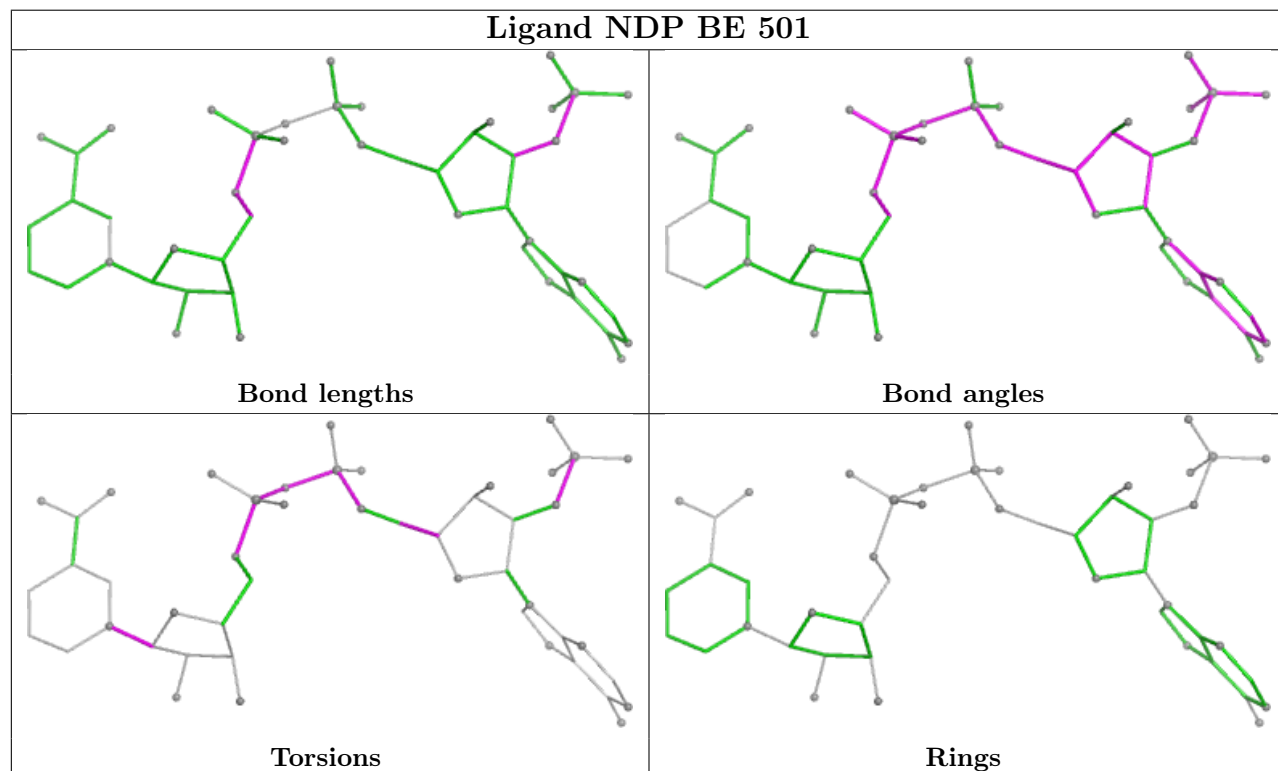


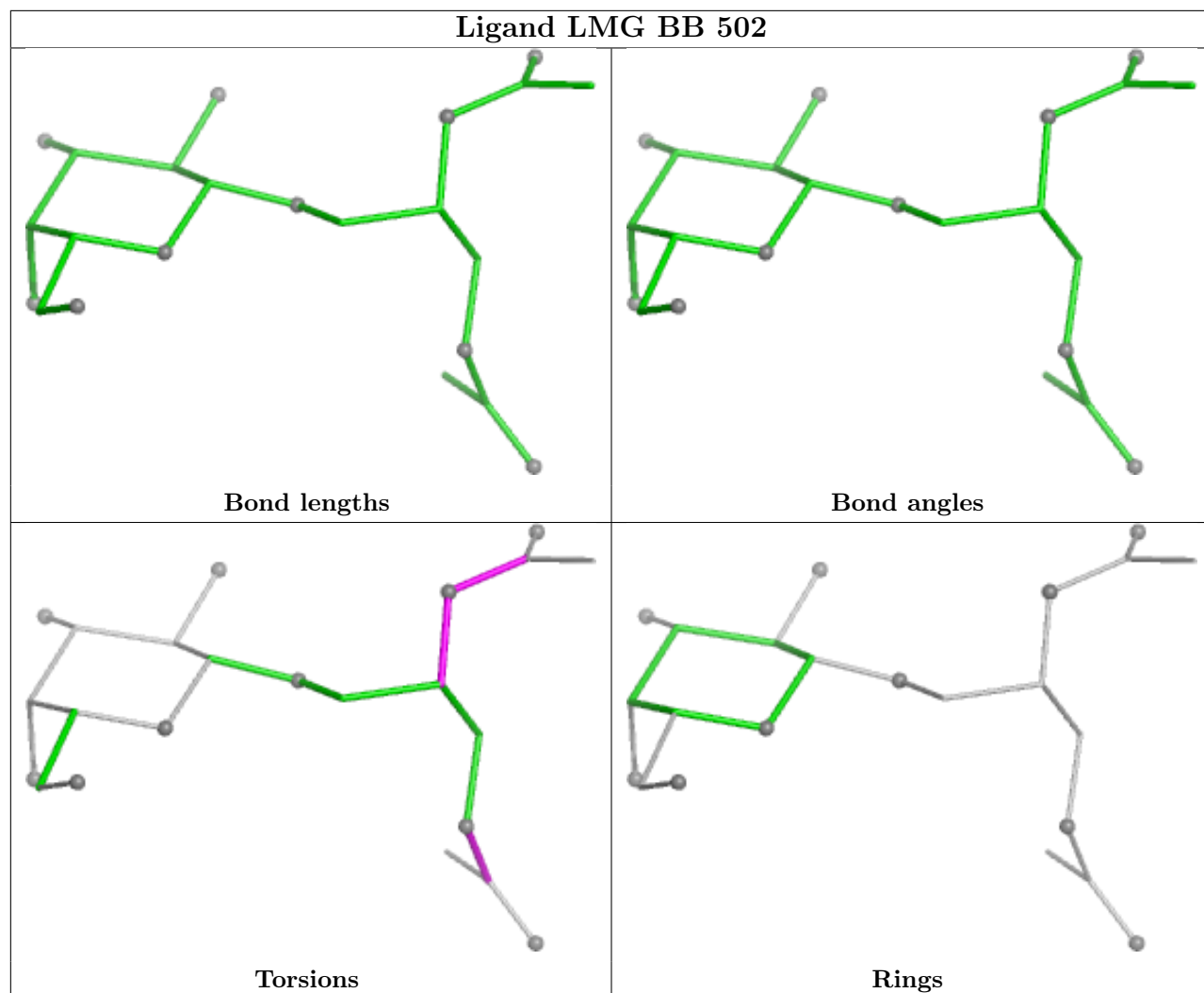
Rings

## Ligand LMG DB 703

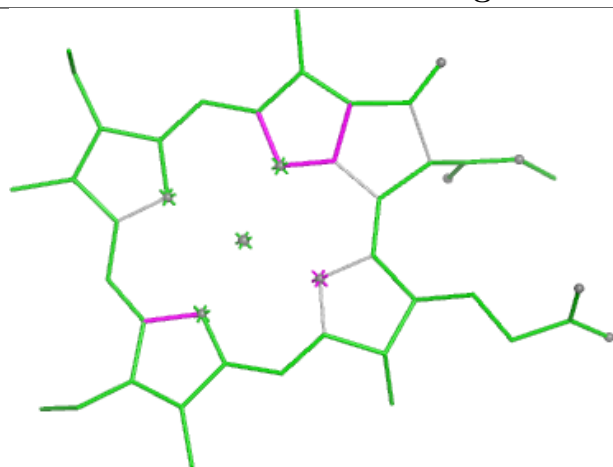


## Ligand NDP BE 501

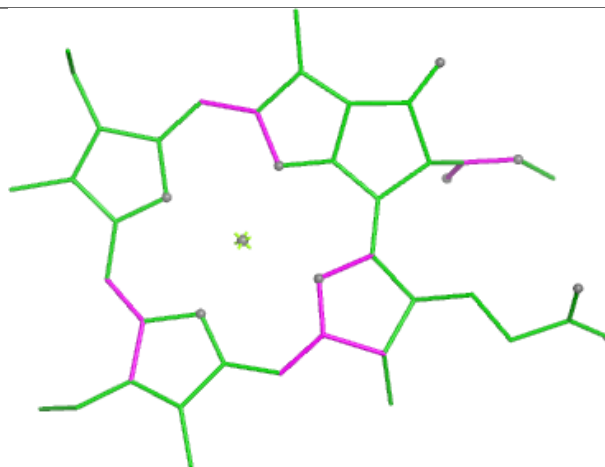




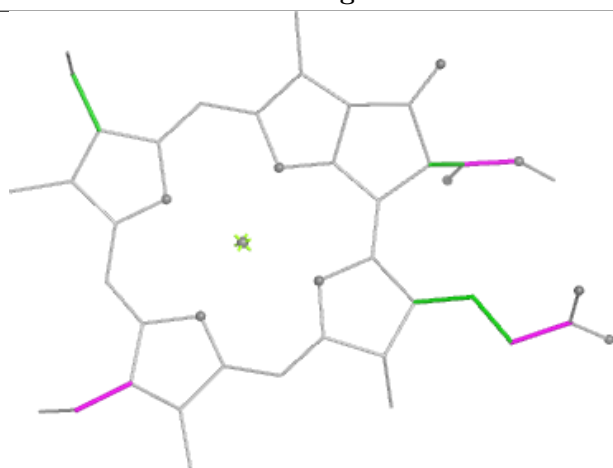
## Ligand A1JWG AA 503



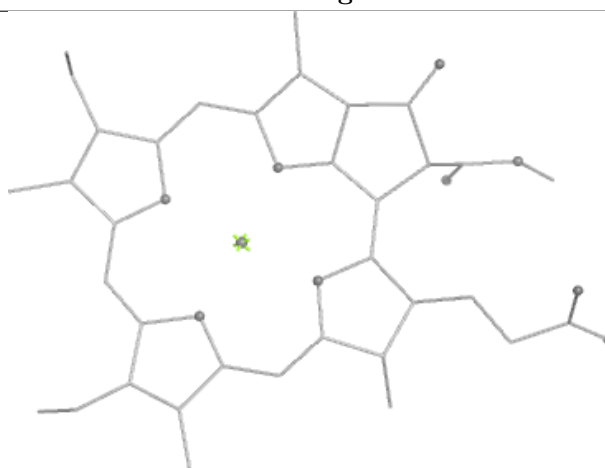
Bond lengths



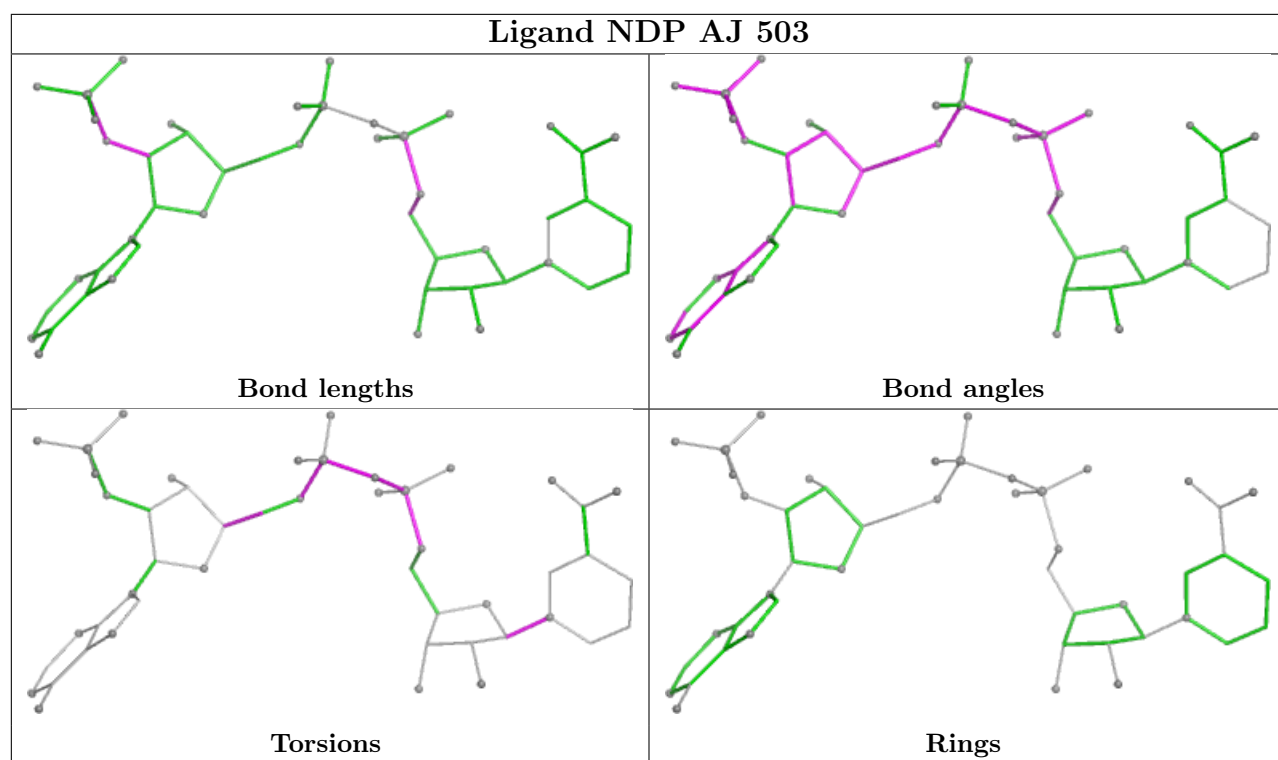
Bond angles



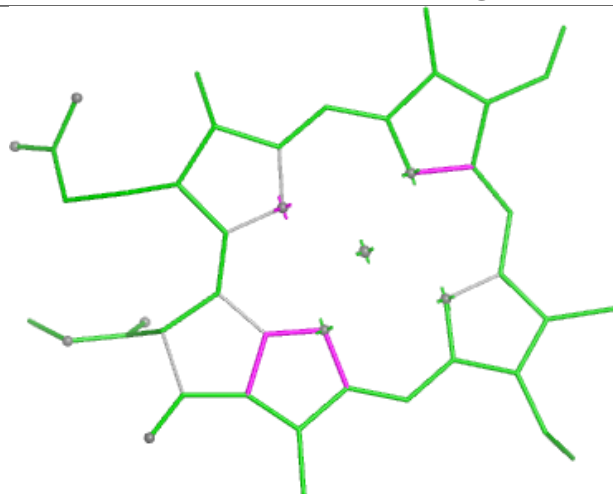
Torsions



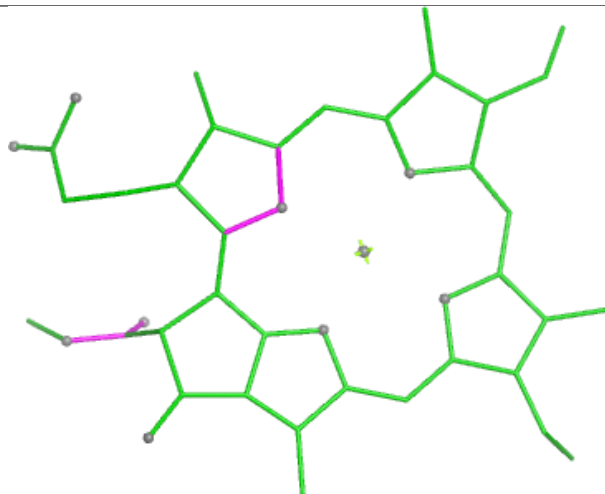
Rings



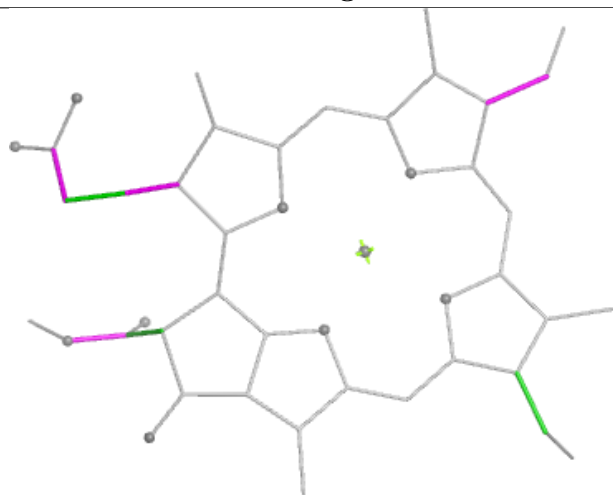
## Ligand A1JWG DD 701



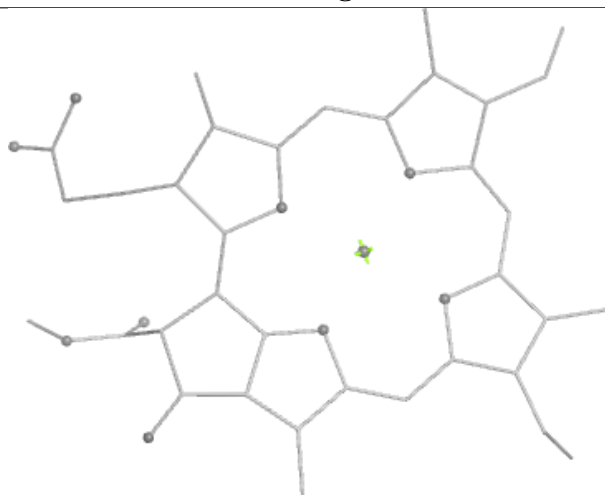
Bond lengths



Bond angles

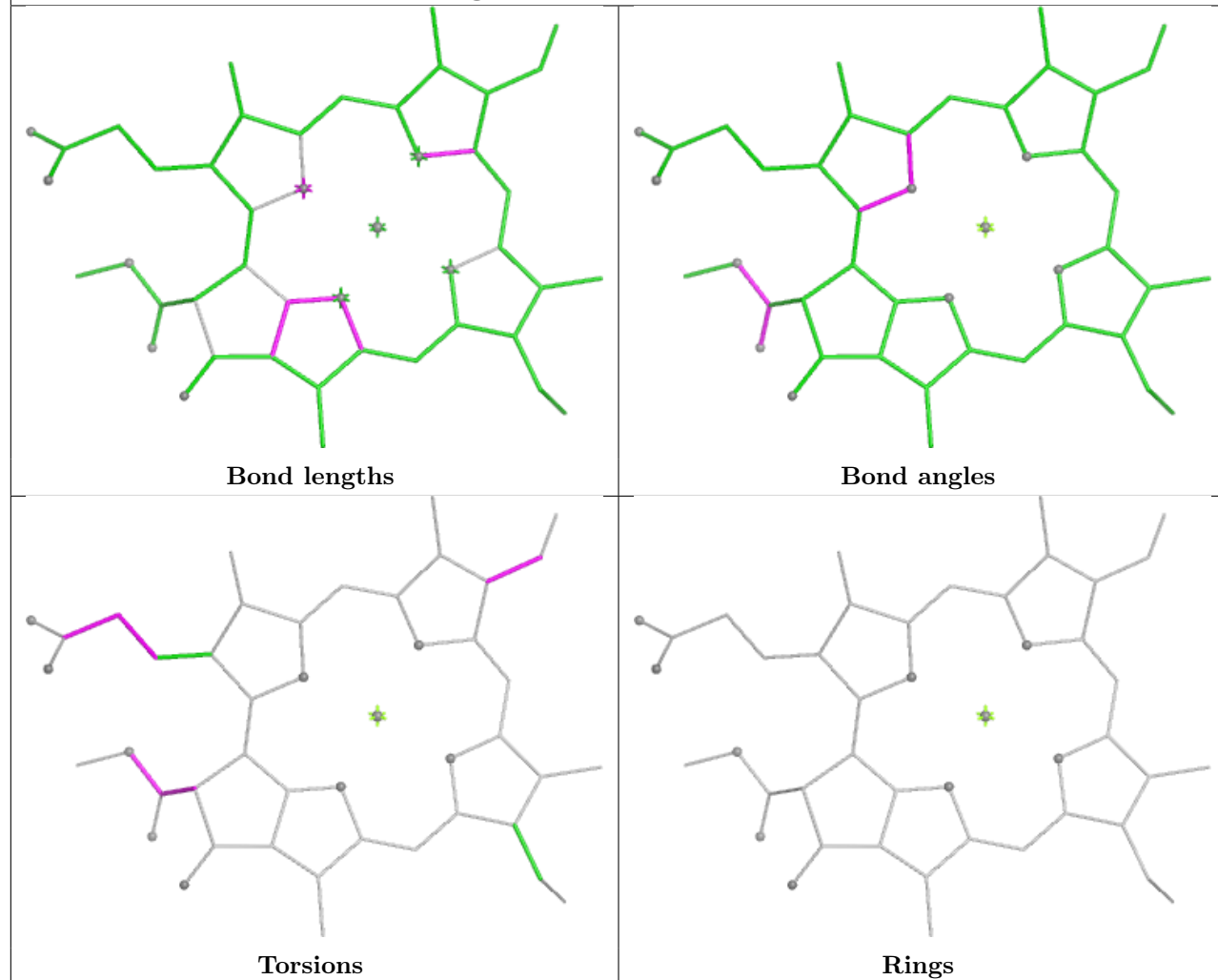


Torsions

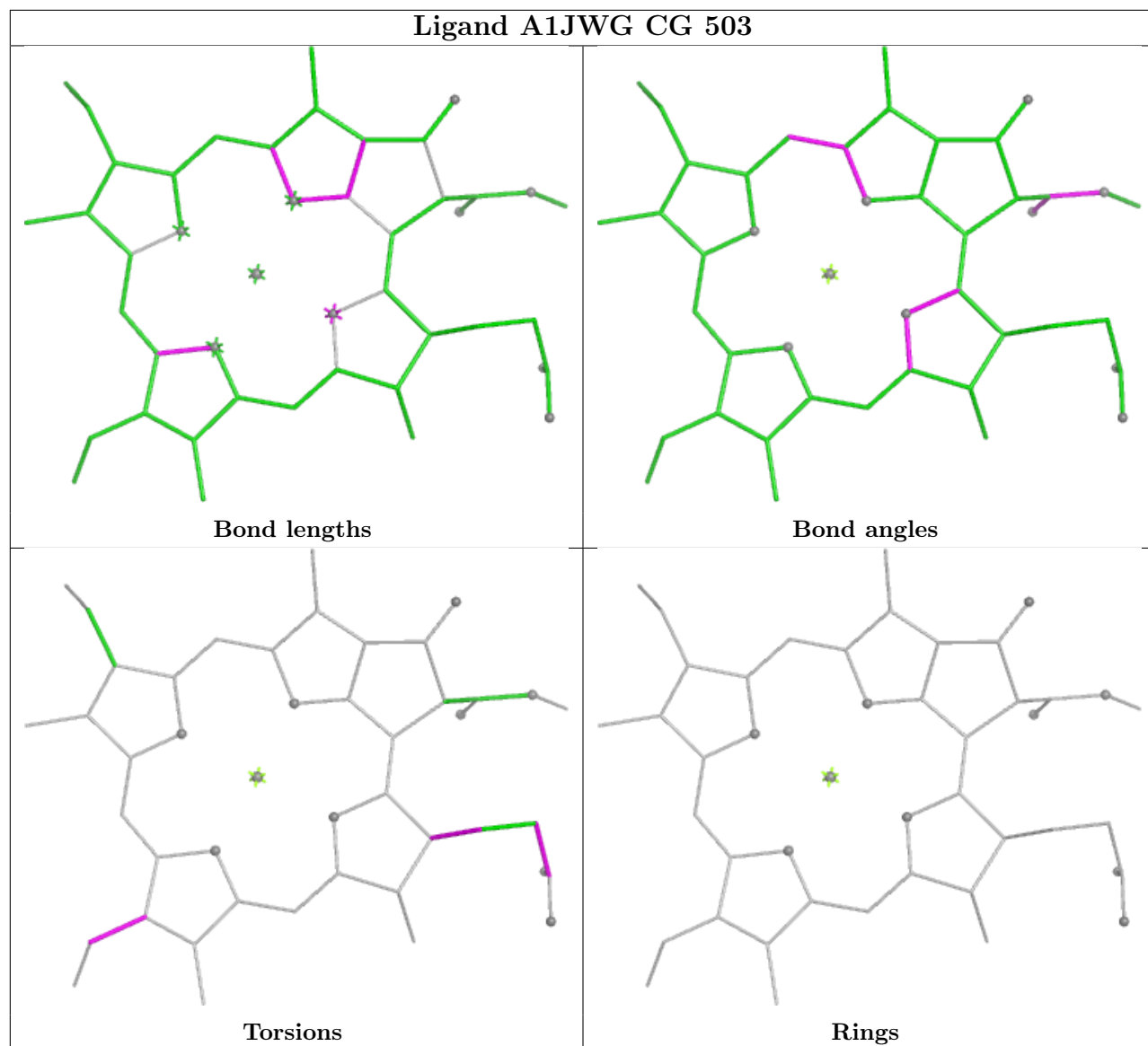


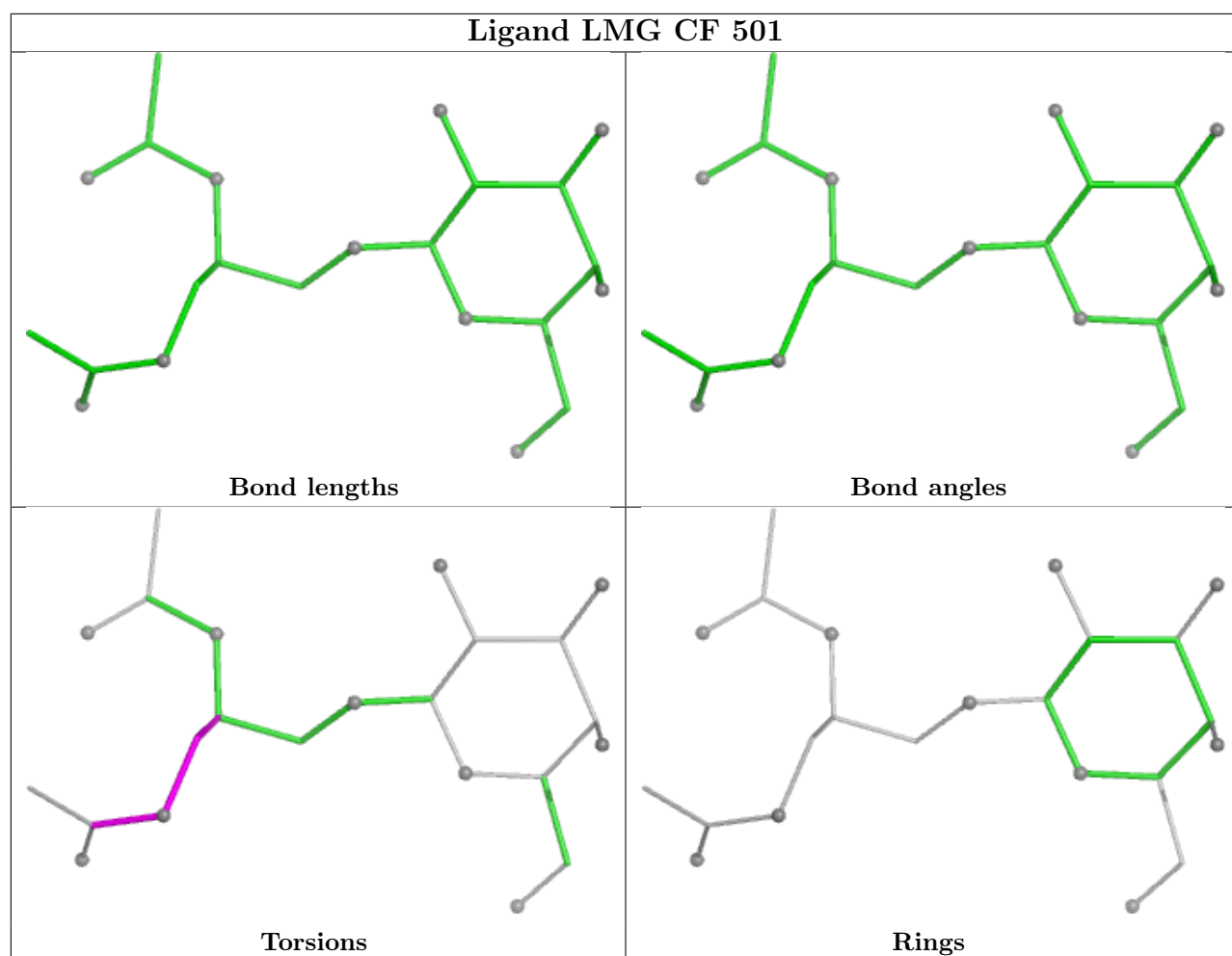
Rings

## Ligand A1JWG BG 502

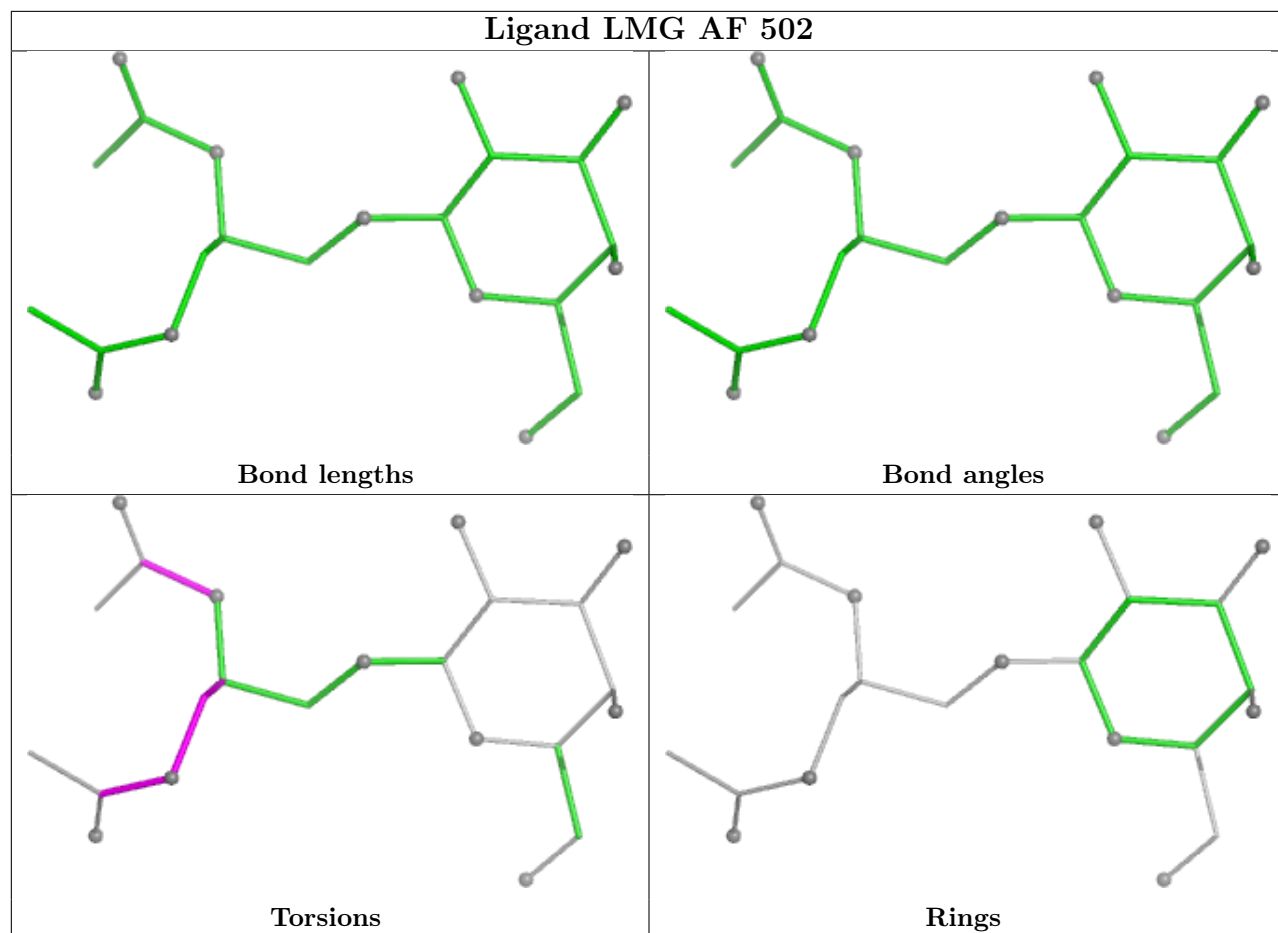


## Ligand A1JWG CG 503

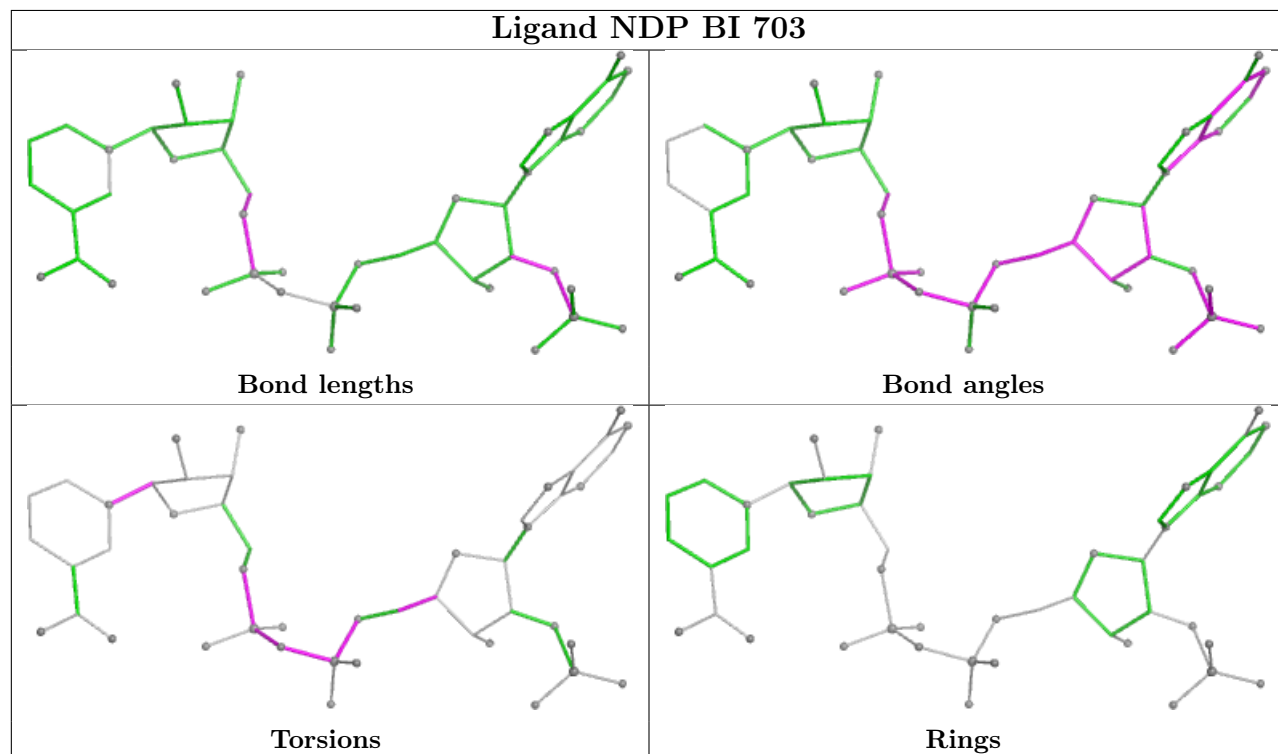


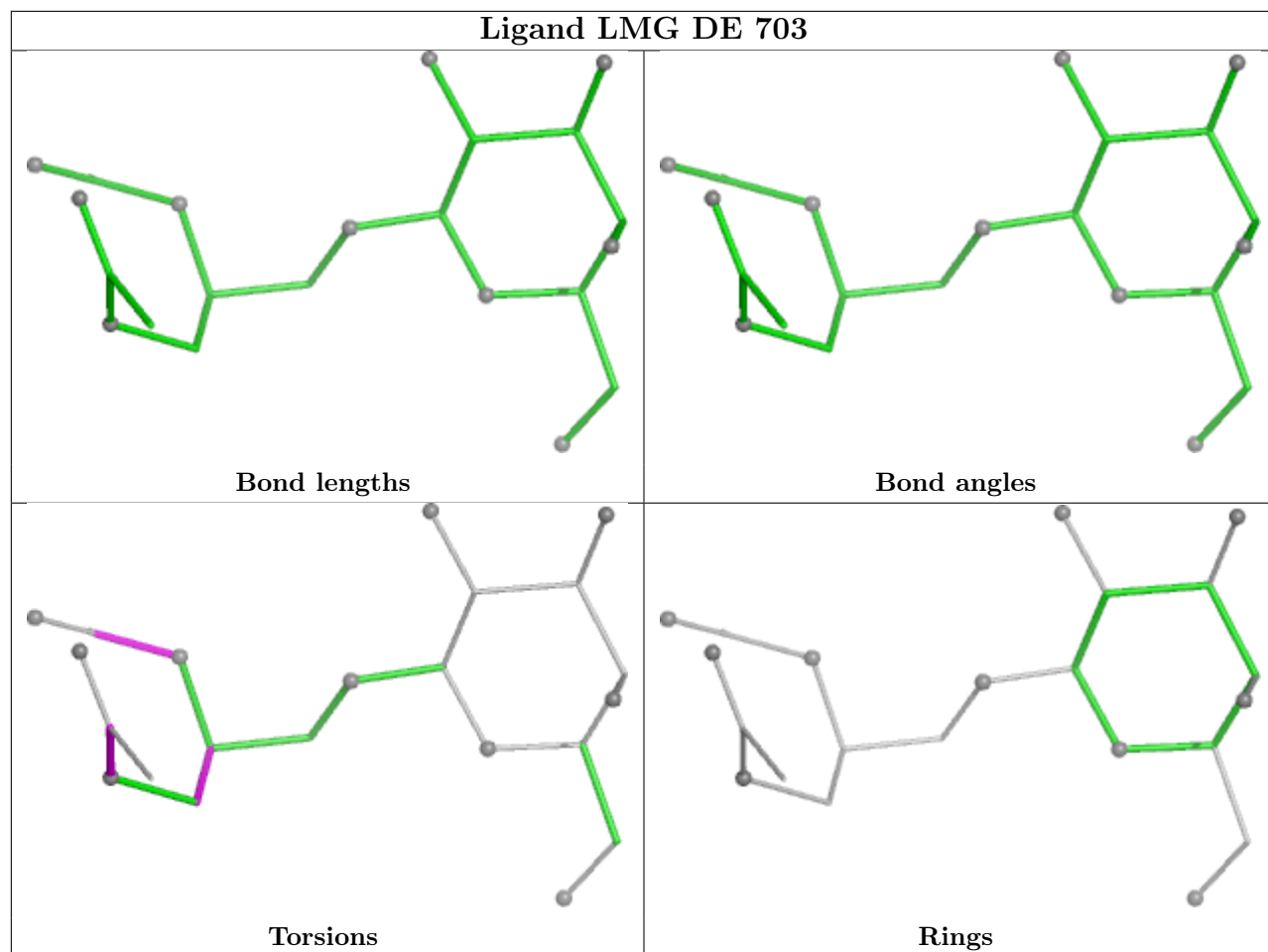


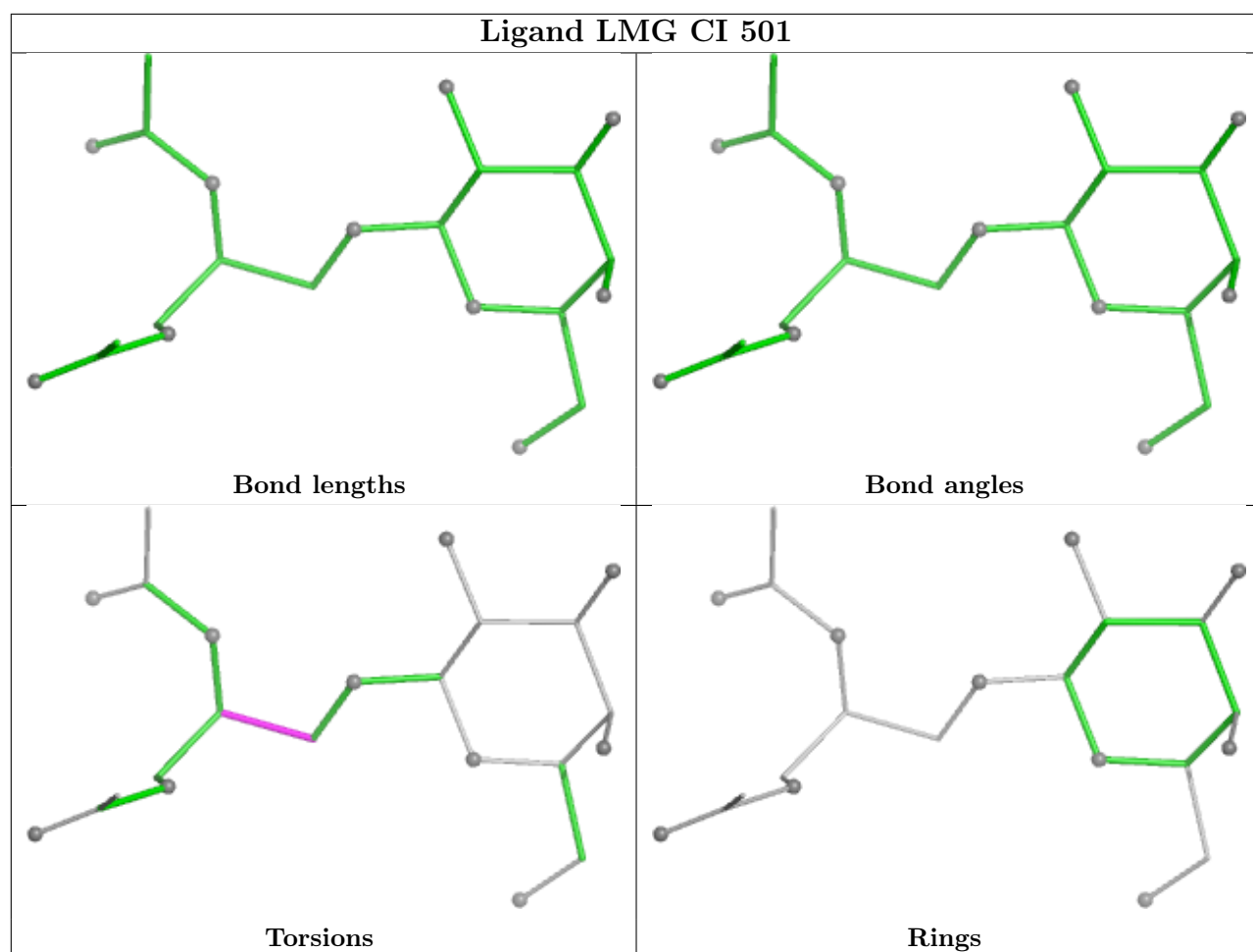
## Ligand LMG AF 502



## Ligand NDP BI 703







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

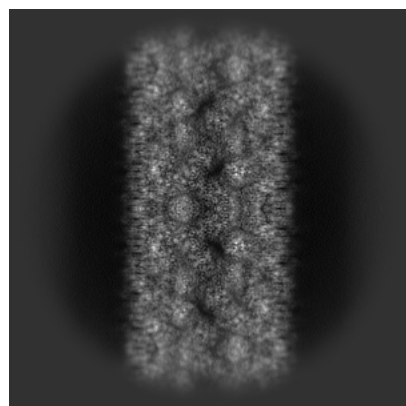
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-56055. These allow visual inspection of the internal detail of the map and identification of artifacts.

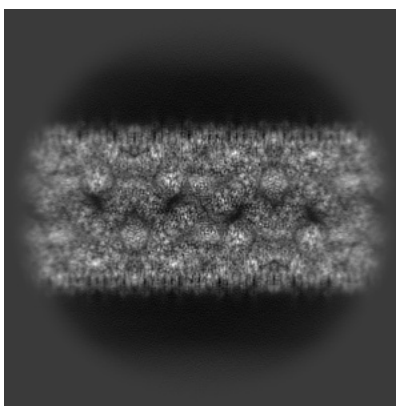
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

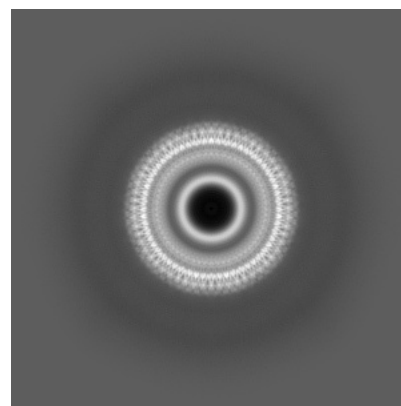
#### 6.1.1 Primary map



X

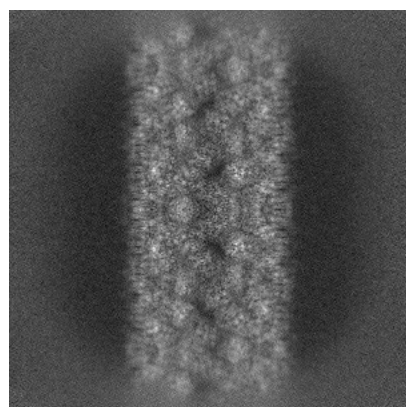


Y

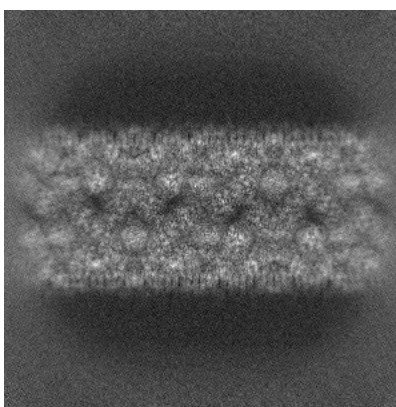


Z

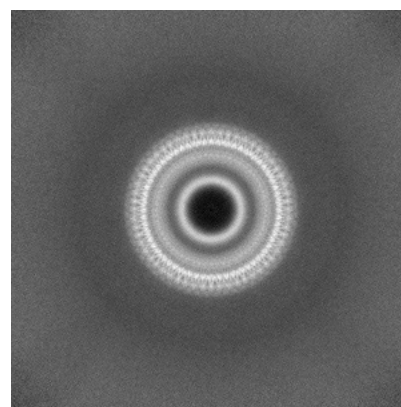
#### 6.1.2 Raw map



X



Y

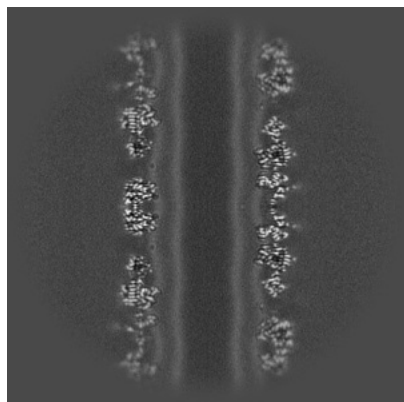


Z

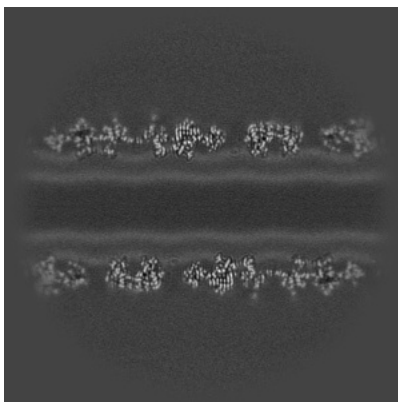
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

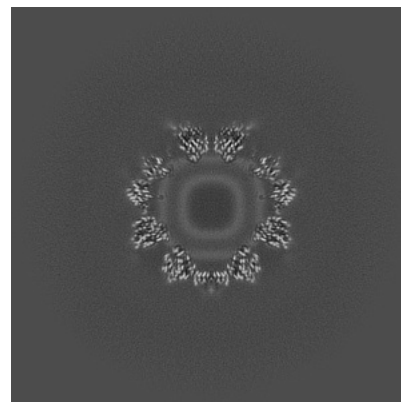
### 6.2.1 Primary map



X Index: 320

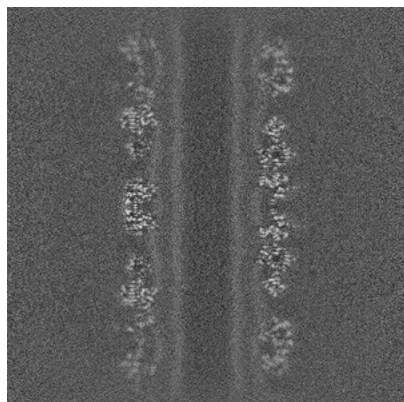


Y Index: 320

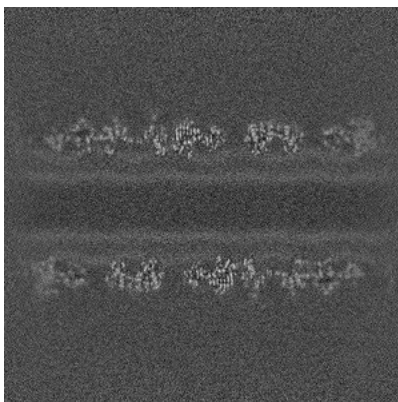


Z Index: 320

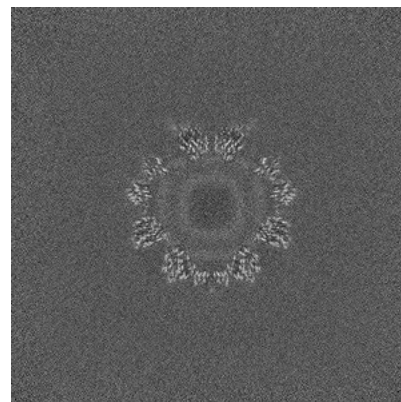
### 6.2.2 Raw map



X Index: 320



Y Index: 320

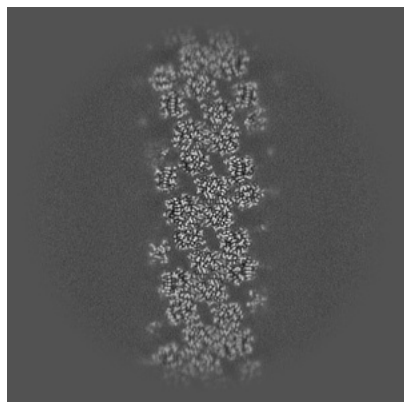


Z Index: 320

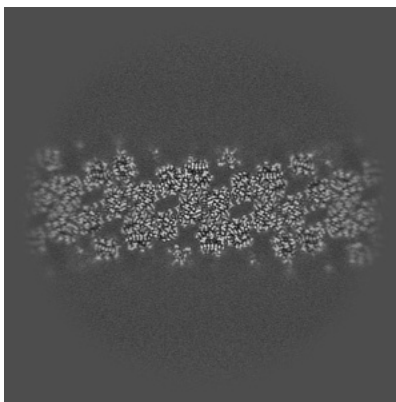
The images above show central slices of the map in three orthogonal directions.

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

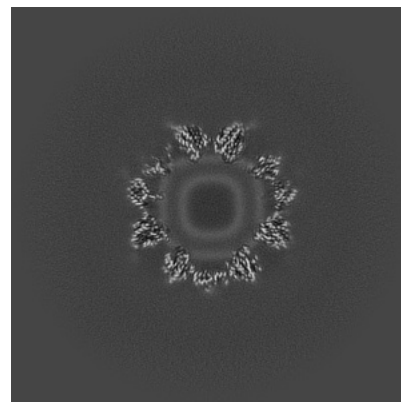
### 6.3.1 Primary map



X Index: 215

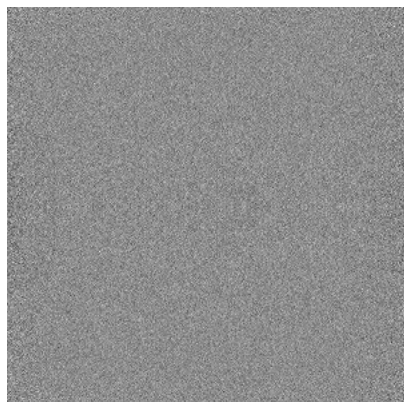


Y Index: 215

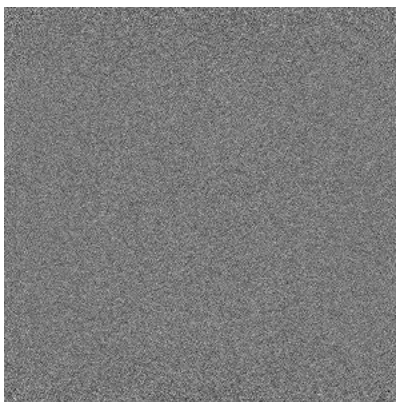


Z Index: 318

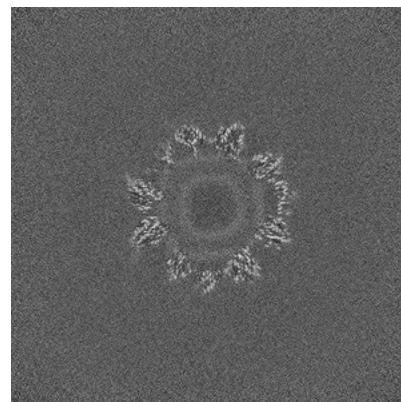
### 6.3.2 Raw map



X Index: 0



Y Index: 0

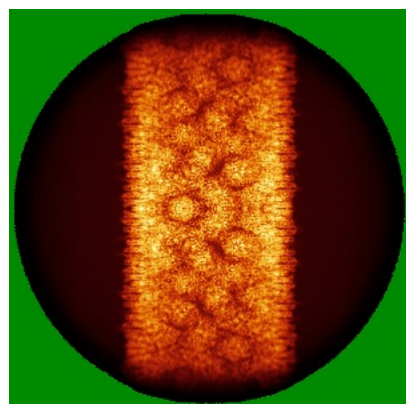


Z Index: 314

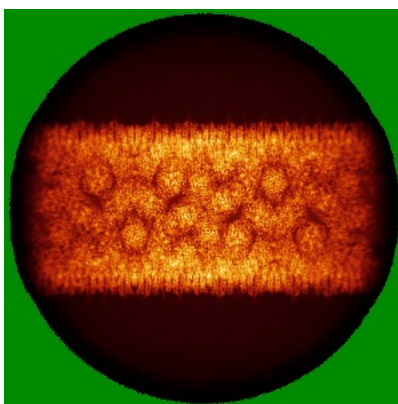
The images above show the largest variance slices of the map in three orthogonal directions.

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

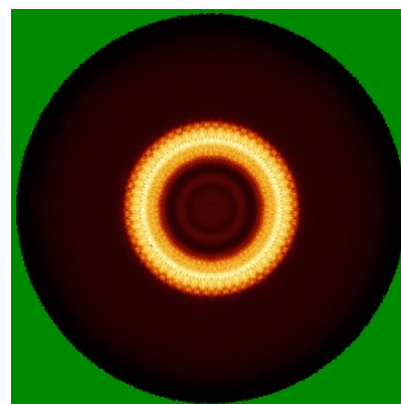
### 6.4.1 Primary map



X

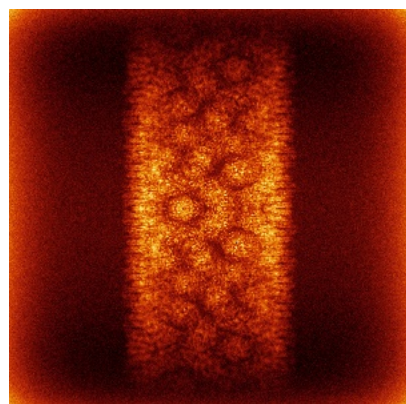


Y

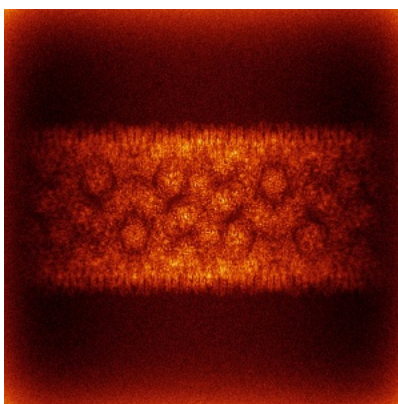


Z

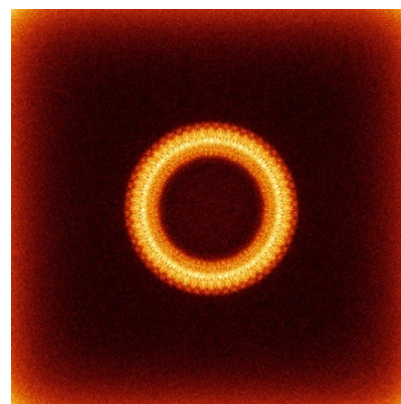
### 6.4.2 Raw map



X



Y

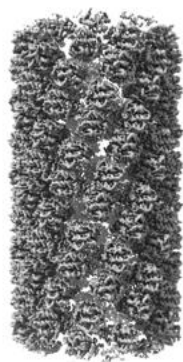


Z

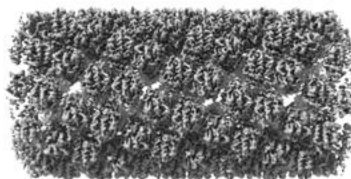
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

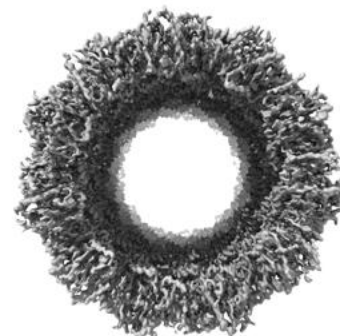
### 6.5.1 Primary map



X



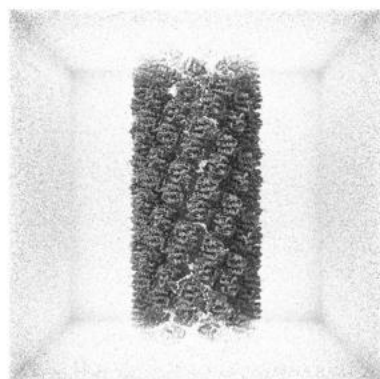
Y



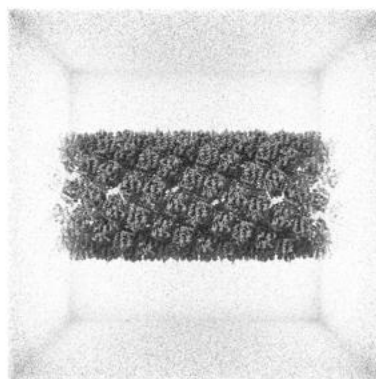
Z

The images above show the 3D surface view of the map at the recommended contour level 0.11. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

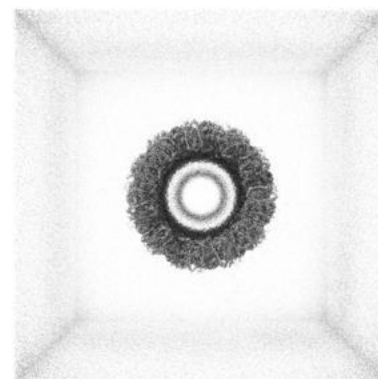
### 6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

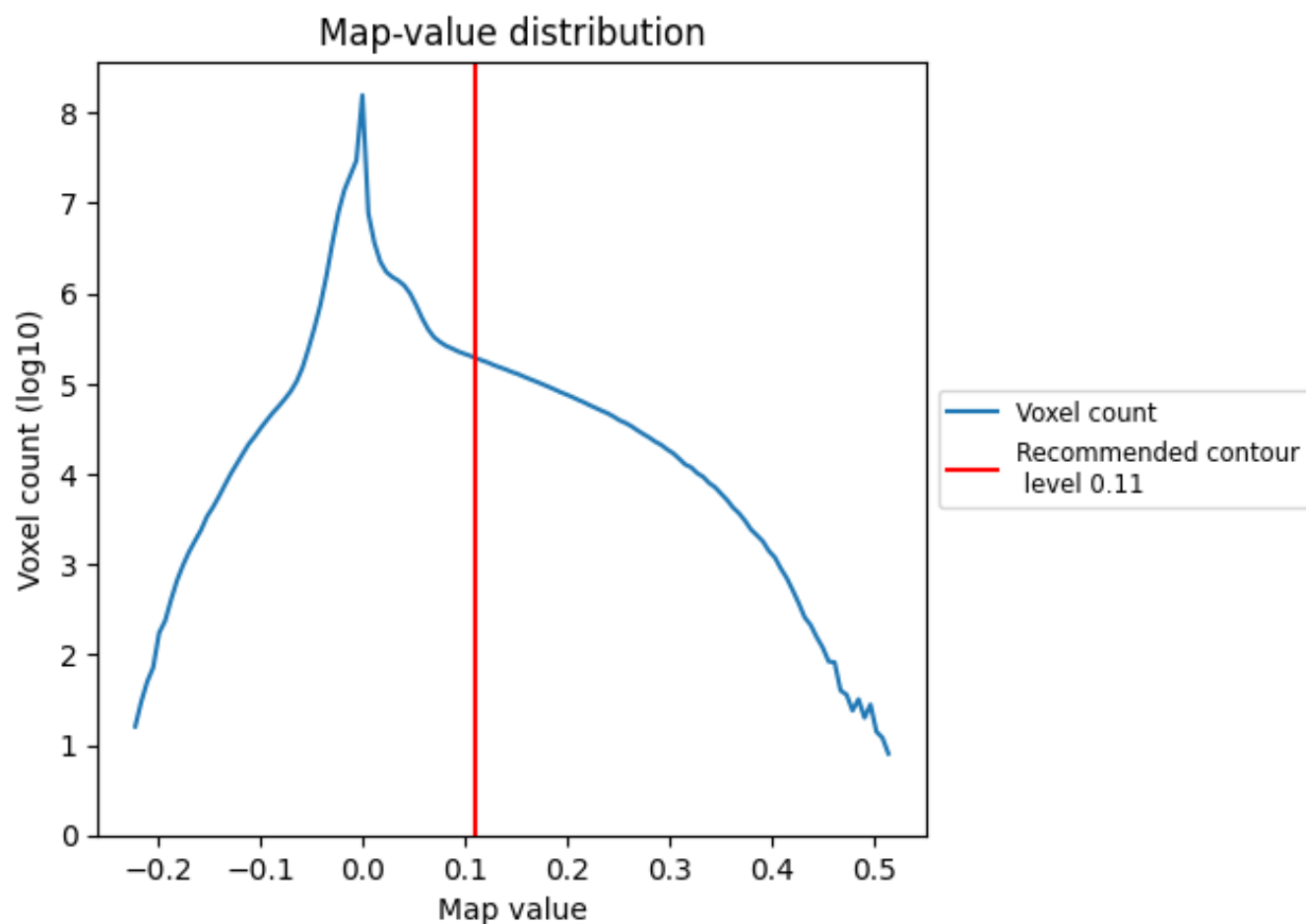
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

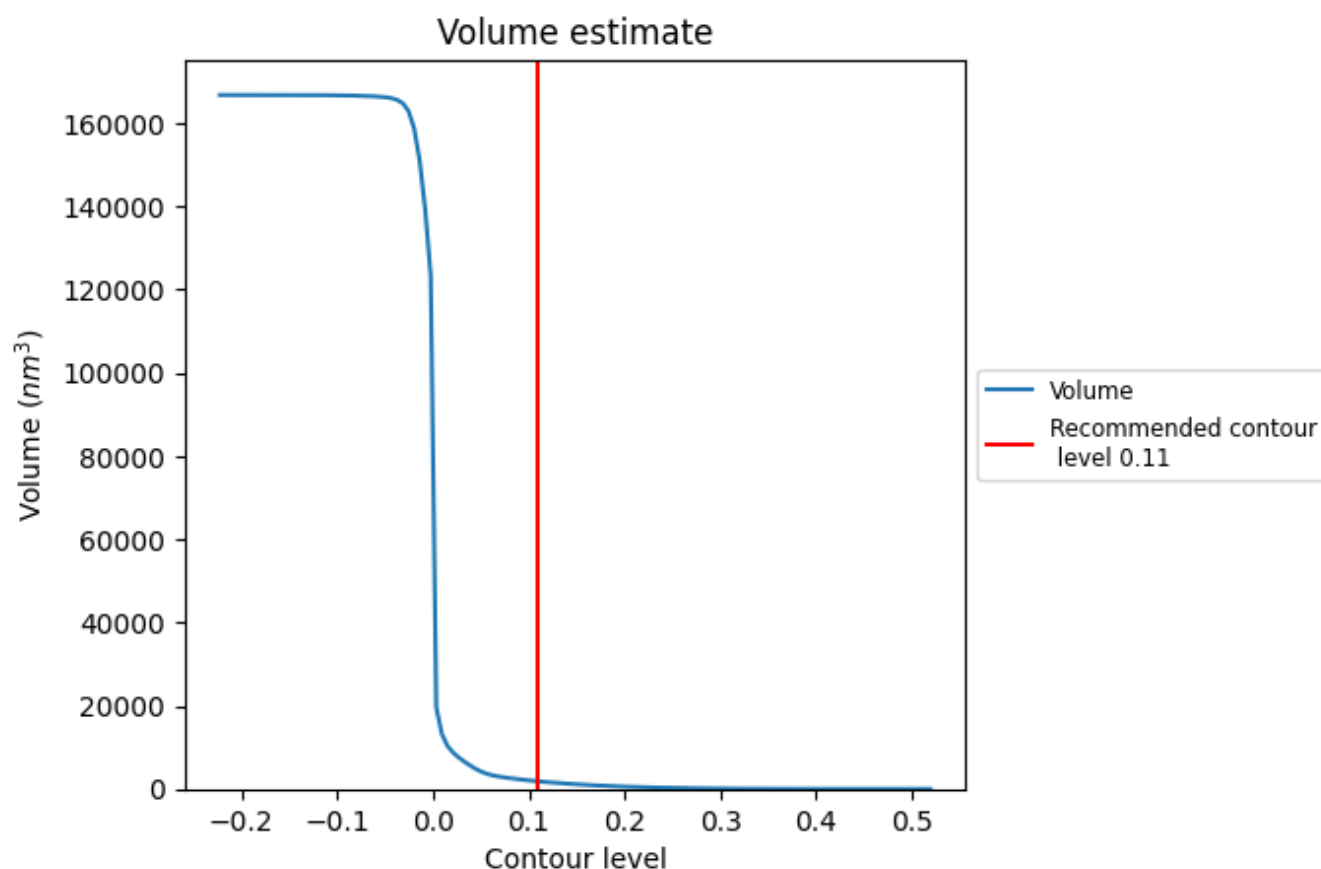
This section contains the results of statistical analysis of the map.

### 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.

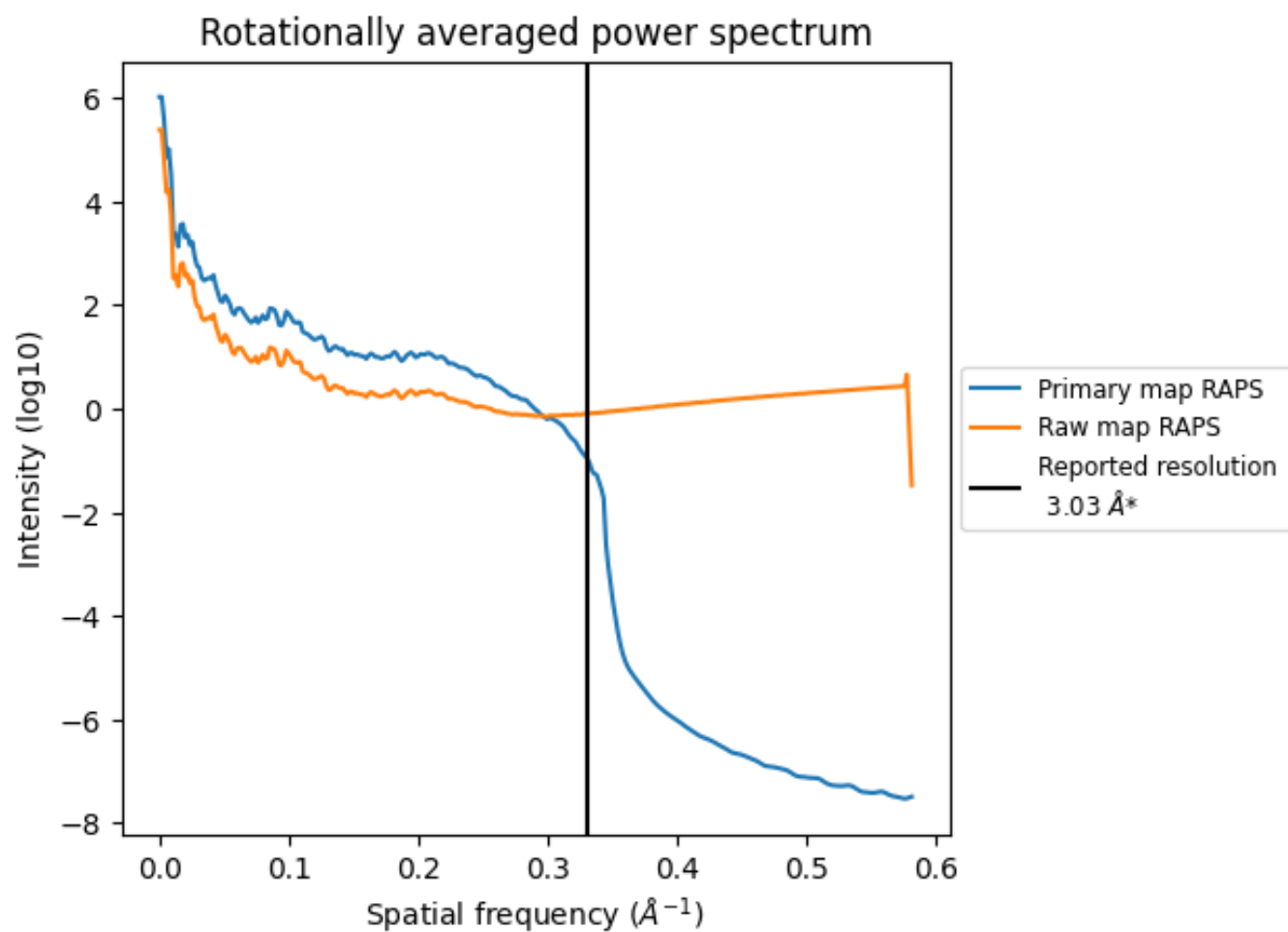
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1833 nm<sup>3</sup>; this corresponds to an approximate mass of 1656 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 ⓘ

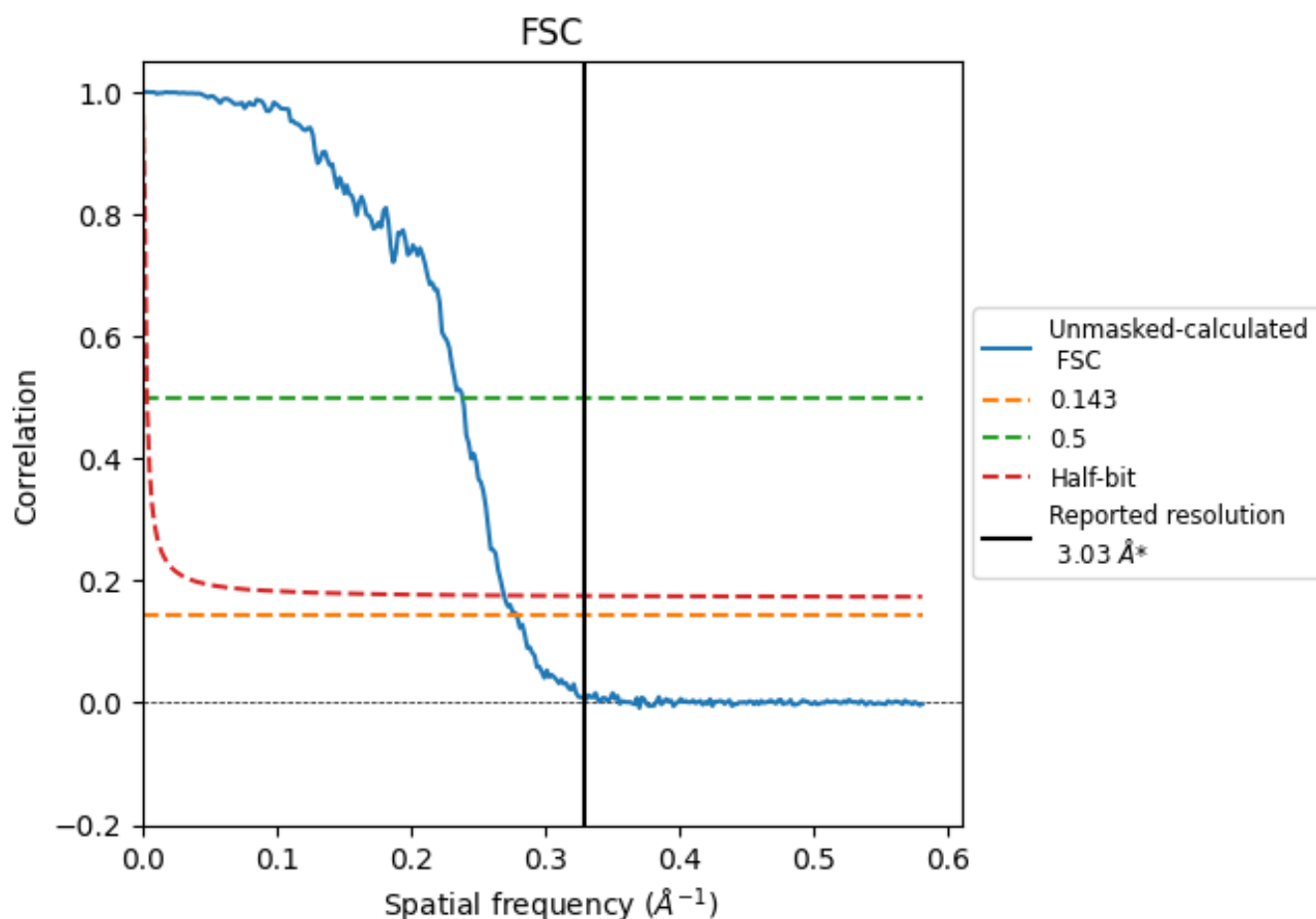


\*Reported resolution corresponds to spatial frequency of 0.330 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.330  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

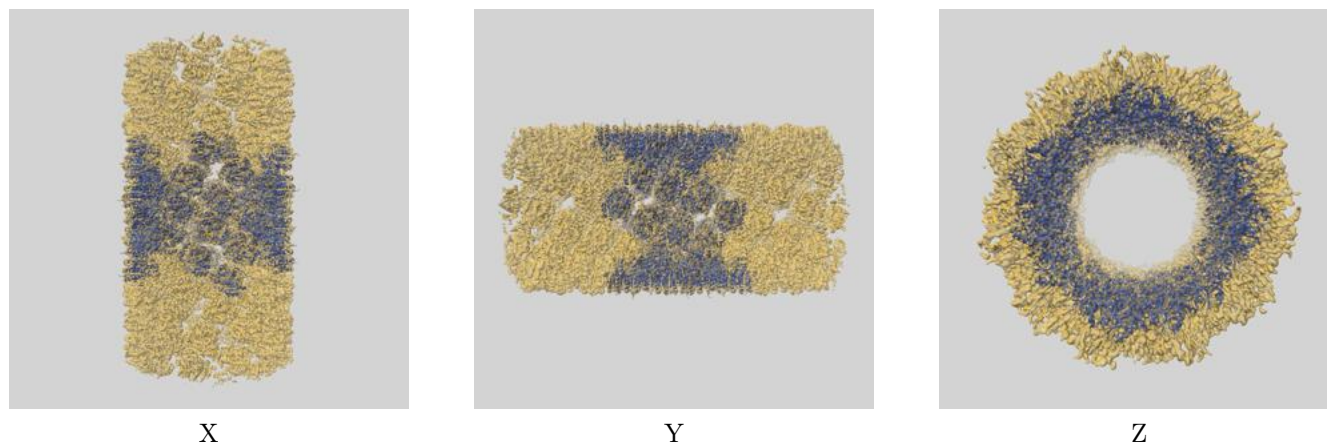
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.03                               | -    | -        |
| Author-provided FSC curve | -                                  | -    | -        |
| Unmasked-calculated*      | 3.59                               | 4.19 | 3.71     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.59 differs from the reported value 3.03 by more than 10 %

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

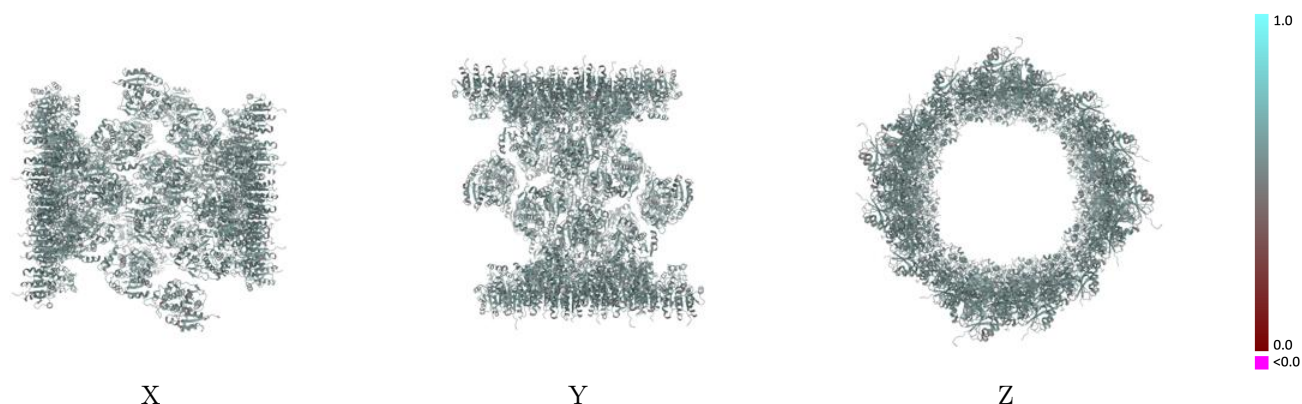
This section contains information regarding the fit between EMDB map EMD-56055 and PDB model 9TLH. Per-residue inclusion information can be found in section 3 on page 36.

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



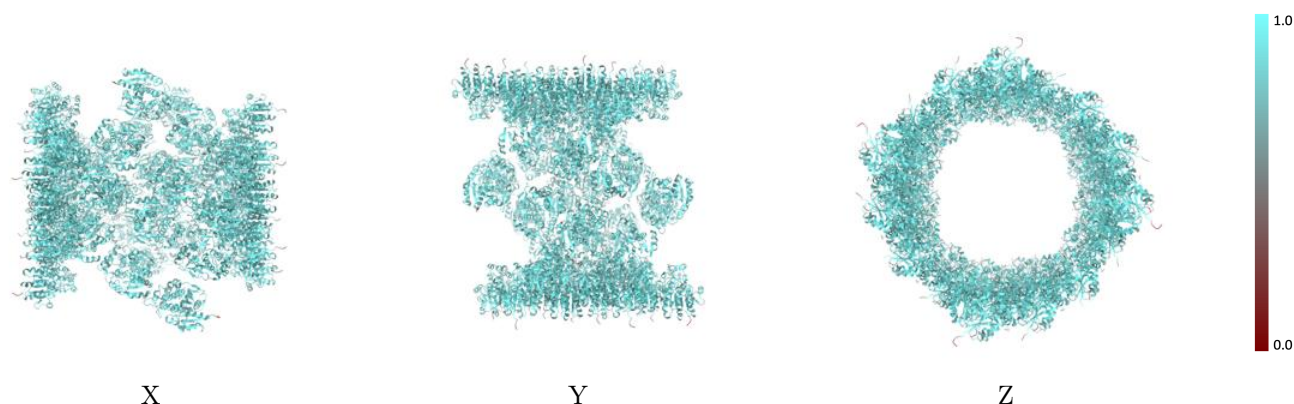
The images above show the 3D surface view of the map at the recommended contour level 0.11 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



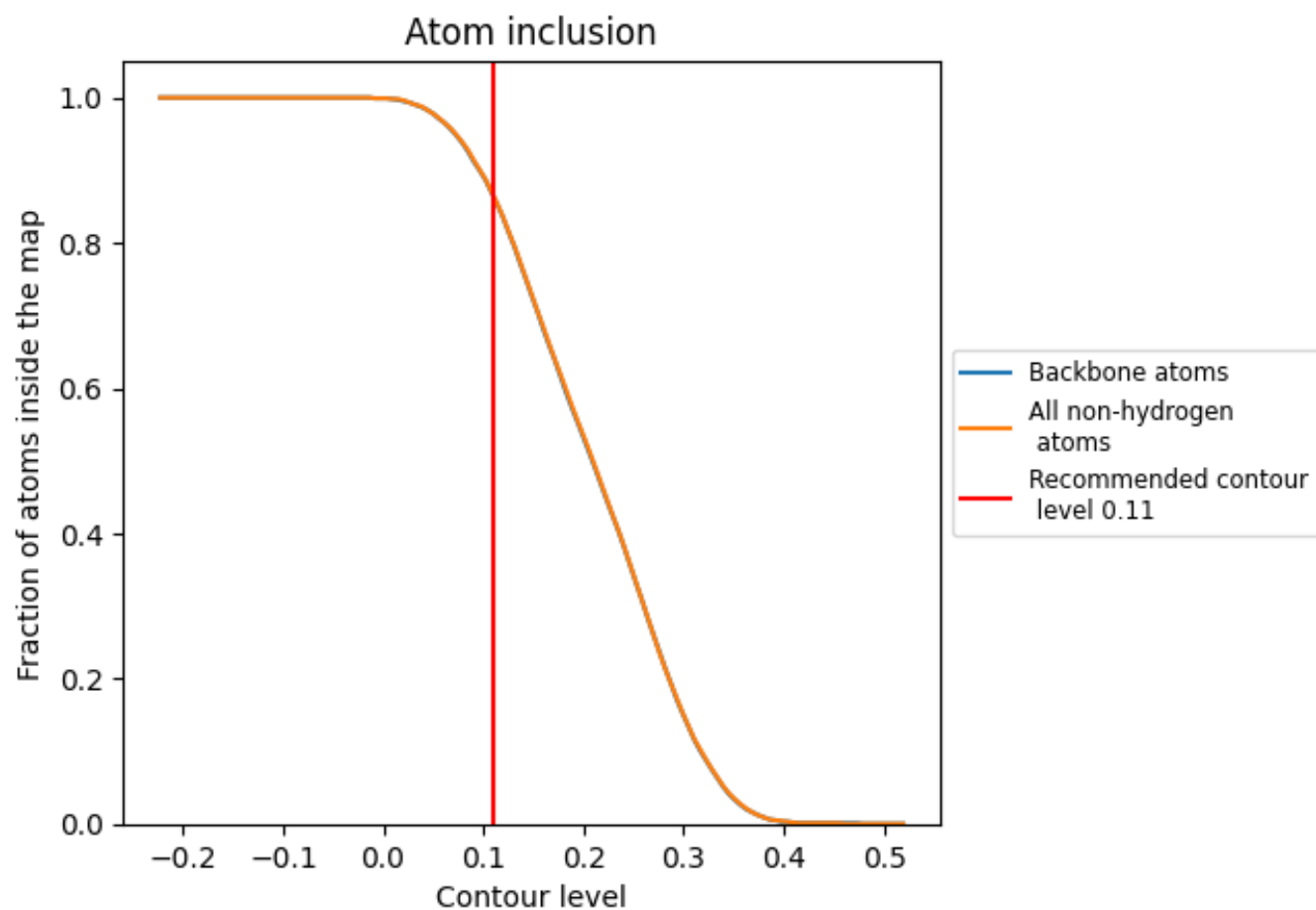
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.11).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 86% 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 (0.11) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8650   |  0.5620   |
| AA    |  0.8340   |  0.5490   |
| AB    |  0.8770   |  0.5650   |
| AC    |  0.8320   |  0.5500   |
| AD    |  0.8840   |  0.5650   |
| AE    |  0.8620   |  0.5610   |
| AF    |  0.8670   |  0.5630   |
| AG    |  0.8830   |  0.5670   |
| AH    |  0.8740   |  0.5630   |
| AI    |  0.8770   |  0.5630   |
| AJ    |  0.8790   |  0.5680   |
| AK    |  0.8850   |  0.5680   |
| AL    |  0.8750   |  0.5670   |
| BA    |  0.8300   |  0.5460   |
| BB    |  0.8740  |  0.5670  |
| BC    |  0.8400 |  0.5510 |
| BD    |  0.8790 |  0.5640 |
| BE    |  0.8640 |  0.5620 |
| BF    |  0.8630 |  0.5590 |
| BG    |  0.8860 |  0.5690 |
| BH    |  0.8670 |  0.5610 |
| BI    |  0.8770 |  0.5640 |
| BJ    |  0.8750 |  0.5660 |
| BK    |  0.8830 |  0.5680 |
| BL    |  0.8760 |  0.5650 |
| CA    |  0.8410 |  0.5530 |
| CB    |  0.8760 |  0.5640 |
| CC    |  0.8250 |  0.5460 |
| CD    |  0.8860 |  0.5650 |
| CE    |  0.8590 |  0.5600 |
| CF    |  0.8690 |  0.5650 |
| CG    |  0.8840 |  0.5690 |
| CH    |  0.8740 |  0.5620 |
| CI    |  0.8730 |  0.5620 |
| CJ    |  0.8830 |  0.5680 |



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*Continued from previous page...*

| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| CK    |  0.8850 |  0.5680 |
| CL    |  0.8790 |  0.5680 |
| DA    |  0.8470 |  0.5520 |
| DB    |  0.8700 |  0.5640 |
| DC    |  0.8490 |  0.5550 |
| DD    |  0.8760 |  0.5650 |
| DE    |  0.8830 |  0.5680 |
| DF    |  0.8690 |  0.5650 |
| DG    |  0.8800 |  0.5660 |
| DH    |  0.8760 |  0.5670 |